ELSEVIER

Coordination Chemistry Reviews 143 (1995) 169–218

COORDINATION CHEMISTRY REVIEWS

An overview of higher n-fold exo cage spin clusters, including (t-$\mathscr{I}$) ^{13}C-fullerenes, under $SU(m \leqslant n/2) \times \mathscr{S}_n$ and model $SU(m) \times \mathscr{S}_n{\downarrow}\mathscr{G}$ dual spin symmetries of nuclear magnetic resonance

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Received 5 May 1994; revised 22 July 1994

Contents

SSDI 0010-8545(94)07004-0

Abstract

Certain interesting general properties arise in the higher n $\mathcal{S}_n$ automorphic nuclear magnetic resonance (NMR) spin symmetries associated with 12-, 20-, 60-fold exo cage clusters in the semitopological limit, which implies the absence of any form of NMR "magnetic equivalence". These mapping properties are examined as part of the realization of $\mathcal{S}_n$ dominant $SU(m \leqslant n) \times \mathcal{S}_n$ direct product spin algebra. In addition to their value as complete inventories of dual algebras, the $\lambda \vdash n$ modules with their decompositions over $\{[\lambda']\}(\mathcal{S}_n)$, or as models over the related (automorphic) $\mathcal{S}_n{\downarrow}\mathcal{G}$ hierarchy, provide natural ways of understanding the physics inherent in spin algebras of NMR spin clusters over Hilbert space, and thus of investigating the determinacy of a particular finite group in any specific $\mathcal{S}_n$ group algebra. The question of the limit to Casimir invariants of higher unitary groups discussed by Sullivan and Siddall (J. Math. Phys., 33 (1992) 1964) is closely associated with such matters.

Of particular interest in describing the NMR of icosahedral clusters $[AX]_n$, $n = 12, 20$, and of $[AX]_n$ systems derived from $^{13}C_{60}$-fullerenes is an essentially combinatorial description of the universal (dual) covering group (UCG) invariance aspects of the $[A]_n$ monoclusters. This arises from the recognition of non-coincidence of the spin sites with the model rotational class operator axes used in deriving $\{\chi_i\}(SU(2) \times \mathcal{S}_n{\downarrow}\mathcal{A}_5)$ for (for example) $^{13}C_{60}$-fullerenes, first demonstrated by Temme et al. (Mol. Phys., 79 (1993) 953). Such combinatorial approaches are typical of the NMR of exo cage clusters. Inner tensor products allow the results derived under UCG to be extended, so that the correlative mappings $\{[\lambda](SU(m) \times \mathcal{S}_{60}) \to \Gamma(\mathcal{S}_{60}{\downarrow}\mathcal{A}_5)\}$ become accessible at least in the low branching limit, for $m \ll 5$, despite the absence of detailed knowledge of $\mathbb{Z}(\mathcal{S}_{60})$ characters, beyond the principal component. The review concludes by drawing on our knowledge of the mapping properties of Liouville spin space for multiple quantum NMR and of certain fundamental UCG mappings over its associated carrier subspaces, $\{\tilde{\mathbb{H}}_v\}$ for $v = (k_1 - k_n)\{\mathcal{K}, \ldots\}$. These define the recoupling aspects and permit the retention of simple reducibility under UCG in Liouville space. The wider consequences of these observations are discussed elsewhere (Temme, Physica A, 166 (1990) 676; 202 (1993) 295).

Keywords: ^{13}C-Fullerene NMR; Exo cage cluster NMR; Direct-product spin symmetry; Subgroup embedding in $\mathcal{S}_n$ spin algebras.

1. Prologue

A semitopological view of the $\{J, J', J''\}$ set of spin interactions, associated with each of the identical nuclear magnetic resonance (NMR) nuclei of an exo cage cluster [1], is used to give an overview of NMR cluster symmetry and (t-$\mathcal{I}$) icosahedral fullerene spin symmetry in the higher n-fold exo cage cluster limit [2], in which the non-magnetic equivalence (non-ME) aspects, rather than the restricted ME limit [3], of NMR are dominant [4]. Certain model aspects of combinatorial physics, and of ideas related to $\mathcal{S}_n$ module decompositional mappings, i.e. in the context of permutational aspects of scalar invariants [5] developed by Rota, strongly influence the views expressed here. In particular, the earlier formative ideas of Doubilet et al. [6], concerning scalar invariants of Cayley algebras, and of Biedenharn and Louck [7], on mapping over the carrier space of the direct product cooperative spin algebras of dual groups, dominate our views of both Hilbert and Liouville spin spaces, because of their inherent correspondence to aspects of the universal covering group (UCG), which for spin physics of clusters is clearly $SU(2) \times \mathcal{S}_n$. The correspondence between the $\{J_{ij}\}$ interaction set and the symmetry aspects invoked arises from well-established $\mathcal{S}_n{\downarrow}\mathcal{G}$ automorphisms [1] of NMR, such as (for example) those inherent in Figs. 1–4. The nature of Liouvillian formalisms of modern NMR has been the subject of more extensive theoretical reviews, which will only be drawn on here in respect of their impact on NMR spin cluster problems [8].

The practical question of the existence of limits to the determinacy involved in the natural embedding [9,10] of subgroups $\mathcal{S}_n$ spin algebras is of a more recent origin. It imparts a certain additional motivation to these discussions, in terms of models and spin algebras pertinent to exo cage and high symmetry fullerene spin physics. Certain $\lambda \vdash n$ partitional aspects of permutational modules underlie the physics and the irreducible representation (irrep) branching depth, which is controlled by the associated $SU(m)$ aspects of the dual group spin symmetry. These interrelated questions, themselves derived from the $\{\lambda \vdash n\}(\mathcal{S}_n)$ sets and certain $\Gamma(\mathcal{S}_n{\downarrow}\mathcal{G})$ physical models of finite subgroup embedding in a specific $\mathcal{S}_n$ group, determine the partitioning of the identical-spin problems of NMR [11,12]; they are inherent also in the nuclear spin statistics [13–15] of the rovibrational spectra originating from clusters. In these discussions, the mathematical symbolism $\lambda \vdash n$ denotes "a $\lambda \vdash n$ partition of the number n into p distinct parts" [5].

The topicality of such spin problems arise in part from the recent theoretical work of Sullivan and Siddall [16], who examined (i.e. in terms of explicit algebraic relations) the upper limits to the determinacy of Casimir invariants of $n=6$ $SU(m \leqslant n) \times \mathcal{S}_n{\downarrow}\mathcal{G}$ spin symmetries. Similar questions over more general scalar invariants, such as those associated with various icosahedral $\mathcal{S}_n{\downarrow}\mathcal{A}_5$ spin symmetries for $n = 12, 20, 60, \ldots$ -fold spin clusters, have been raised in subsequent work [17–19]. Both of these areas are conceptually related to aspects of the UCG for spin physics. Naturally, the presentation adopted here, for an inorganic and physical chemical audience, is limited by the need to give an essentially non-mathematical conceptual overview. Hence, the more difficult mathematical questions will only be cited in the present text, rather than discussed explicitly in any detail.

The mathematical treatises on representations of the symmetric groups realized in terms of $\lambda \vdash n$ modules by James and Kerber [20a], and in earlier more traditional form by James [20b], together with recent explicit combinatorial reformulations of these ideas by Sagan [21] are especially important. The strength and pervasive role of these recent extended views of Young's rule are discussed at length in Sagan's mathematical monograph [21], which has implications (via the Littlewood–Richardson (LR) rule) for inner tensor product (ITP) enumerations. The evaluation of the integer Kostka coefficients, on expanding a specific $\lambda \vdash n$ module over the $\{[\lambda']\}(\mathcal{S}_n)$ field, i.e. from $[n]$, $[n-1, 1], \ldots,$ down to the specific $[\lambda]$ form, derives from the study of all possible seminormal contents, defined from λ, which may be fitted into the lattice graph shape associated with each $[\lambda']$ $\mathcal{S}_n$ irrep. The process is referred to as a decomposition of a $\mathcal{S}_n$ module.

The wider physical context of the review will be clear from the relationships between this research area and certain adjoining fields, e.g. those associated with wreath-product spin symmetries of non-rigid clusters in NMR [22,23], or with the extensive NMR area concerned with Liouville spin dynamics [24,25]. Of the other related fields, that concerned with quantum rotational (QR) dynamics and QR tunnelling [26–28] introduces certain interesting additional gauge-dependent questions [29]. The solid state vibrational modes of $^{13}C_{60}$-fullerenes [30–32], e.g. as studied by spin-dependent (incoherent) neutron scattering, or in the context of NMR and spin statistical physics [33], serve to stress the interdisciplinary nature of the physical study of clusters.

The prime focus of our presentation will be on aspects of NMR, or on the analogous rovibrational properties [33–35] of cluster molecules, as treated by Harter and Riemer [33], or Temme et al. [18,36], e.g. under $\mathcal{S}_{60}{\downarrow}\mathcal{A}_5$ models, or by Balasubramanian [34a,b,35], using cycle index (CI) techniques derived from symmetric functions [37]. The importance of understanding the nature of the nuclear spin statistics and their associated subduced symmetry models is stressed throughout. A topical discussion deals with the determinacy of natural embedding of a subgroup in some higher n-fold $\mathcal{S}_n$ group spin algebra. Since these $\mathcal{S}_n$-automorphic properties of spin systems have been largely ignored in the earlier literature, this is an important question. Indeed, the depth to which an $SU(m) \times \mathcal{S}_n{\downarrow}\mathcal{G}$ algebra remains determinable is a totally analogous property to that examined in terms of Casimir invariants by Sullivan and Siddall [16]; however, here the methods used to investigate the question are drawn from $\lambda \vdash n$ dominance order of theoretical physics models appropriate to most "multisite" problems.

2. Initial context of Hilbert space cluster properties: inventorial, mappings and direct product formalisms

Early theoretical work on few-body spin interactions in the context of democratic recoupling [38,39] is of importance in understanding the inherent difficulties of handling high n-fold spin algebras, applicable to the NMR of (bi)clusters, and eventually of realizing the practical transformation coefficient matrices [40]. Even for $n \leqslant 8$ within the well-defined cw quantum formalism involving the zeroth-order hamiltonian [41,42], the real problem is not so much that of factorization under an explicit algebra associated with the dual symmetry as that of the realization of these transformational properties for their fundamental physics. Corio's early NMR text [41] stresses the value of $\Gamma(\mathcal{S}_n \otimes \mathcal{S}_n)$ direct product symmetry formation for *practical bicluster* NMR systems [4,42], as well as the combinatorial simplicity of the total outer M (z projective) states in SU(2) cluster NMR. The writings of Coleman [43] and of Biedenharn and Louck [7] amplify these ideas on the simple reducibility (SR) properties of the carrier space associated with spin 1/2 $SU(2) \times \mathcal{S}_n$ clusters and, as a corollary, of the value of dual projective mapping under this UCG for spin physics; as a consequence of Cayley's theorem, all the common finite groups associated with spectroscopy are subgroups of one of the lower n $\mathscr{S}_n$ groups [41,42b]. The interrelations between these groups and the corresponding general linear groups are set out in Coleman's treatise [43]. Both the hierarchical nature of unitary algebras [2], whose NMR aspects are discussed in Refs. [44–46], and the essential structure of group algebras of interest and practical application in physics and chemistry are set out in Tung's monograph [47], for example.

The treatment of higher identical spin clusters determined by any of these unitary algebras necessarily introduces certain non-SR properties [2] over a spin space. However, the inventorial properties [2,12,48] of $\lambda \vdash n$ partitions [49] for the corresponding "number of distinct parts of n", designated here by p [50,51], such as the $p \leqslant 3$-tuplar forms for SU(3) dual algebras, overcome the counting problem and allow a full description of the $\{|IM(\,)\rangle\}$ spin spaces for all $[\mathrm{A}]^{I^i}(\mathscr{S}_n)$ clusters [2,18,52]. Naturally, the convenience of straightforward boson ladder operators and simple mappings within the projective formalisms [7] are restricted to $\mathrm{SU}(2) \times \mathscr{S}_n$ algebras; these yield the simple mapping

$$U \times \mathscr{P}(\Gamma)\colon \mathbb{H} \to \mathbb{H}\{\mathscr{D}^j(U) \times \Gamma^{[\lambda]} \,|\, U \in \mathrm{SU}(2); \mathscr{P}(\Gamma) \in \mathscr{S}_n\}, \tag{1}$$

over the carrier space $\mathbb{H}$. By contrast, the direct product, or dual group mapping over all $\mathrm{SU}(2) \times \mathscr{S}_n$ Liouville space, is derived from $\tilde{U} \times \mathscr{P}(\tilde{\Gamma}(v))$ superoperators acting over $\tilde{\mathbb{H}} = \Sigma_v \tilde{\mathbb{H}}_v$ subspaces, so that the SR properties are retained. These ideas in Eq. (1) about the nature of the mapping over $\mathbb{H}$ of Hilbert space underlie the ladder operators defining [7] the fundamental Wigner operators within

$$\left\langle \begin{matrix} & 1 & \\ 1 & & 0 \\ & \begin{pmatrix} 1 \\ 0 \end{pmatrix} & \end{matrix} \right\rangle |jm\rangle \equiv [(j \pm m + 1)/(2j+1)]^{1/2} |j + 1/2, m \pm 1/2\rangle$$
$$\left\langle \begin{matrix} & 0 & \\ 1 & & 0 \\ & \begin{pmatrix} 1 \\ 0 \end{pmatrix} & \end{matrix} \right\rangle |jm\rangle \equiv (\mp)[(j \mp m)/(2j+1)]^{1/2} |j - 1/2, m \pm 1/2\rangle \tag{2}$$

which may be related to boson pattern bases on noting the following equivalence:

$$\left| \begin{pmatrix} 2j & & 0 \\ & j+m & \end{pmatrix} \right\rangle \equiv |j, m\rangle \tag{3}$$

a property of $\mathrm{SU}(2) \times \mathscr{S}_n$ algebras. The nature of Gel'fand algebra has been discussed both in earlier general reviews [7] and in the context of NMR clusters [17]. Alternative treatments of Gel'fand formalisms for higher unitary algebras may be found in the work of Moshinsky [53] and in a recent additional review by Biedenharn and Louck [54], which dates from 1992.

The discussions given by Coleman in an early review [55] and in his more specialized monograph [43] on "induced (subduced) representations over $\mathbb{C}$ for the $\mathscr{S}_n$ and $\mathscr{GL}(n)$ groups", as amplified by Sagan's later treatment of similar material in terms of combinatorial algorithms [21], stress the value of combinatorics in deriving $\mathscr{S}_n$ group characters underlying point group tables and allow one a rather fuller insight into the nature of the stepwise processes associated with $\mathscr{S}_n \supset \mathscr{S}_{n-1} \supset \ldots \supset \mathscr{S}_2$ Racah spin symmetry chains of subduction. However, the dominant process of interest in considering NMR spin cluster symmetry is that of natural embedding of a subgroup into a high n $\mathscr{S}_n$ group, denoted by $\mathscr{S}_n{\downarrow}\mathscr{G}$. The Racah stepwise chain of $\mathscr{S}_n$ groups has a contrasting application: in defining the wider aspects of democratic recoupling hierarchies [10,17]. The value of both forms of subduction is extended on introducing the idea of self-associated (SA) $\lambda \vdash n$ partitions or $[\lambda](\mathscr{S}_n)$ irreps, i.e. forms invariant to rotation about a diagonal of the lattice graph, as the choice of an initial $[\lambda]_{SA}$ yields a hierarchy of SA sets in the subduced space, or over the sequence of $\mathscr{S}_n$ chain sysmmetries [9]. While the study of the $\mathscr{S}_n$ symmetric groups in the form of $\mathbb{Z}(\mathscr{S}_n)$ character tables has an extensive history, the explicit $\chi^{[\lambda]}_{(.)}$ characters are only rarely used in physical applications. From theoretical physics, it is known that the ITPs ($\mathscr{S}_n$ ITPs) $[\lambda]\otimes[\lambda']$, derived from the lower 2(3)-tuplar forms, provide insight into the structure of higher unitary algebras [19]. In this context, the presentations given by James and Kerber [20a] and James [20b] for $n \leqslant 10$ $\mathscr{S}_n$ groups and the work of Ziauddin [56] on $\mathscr{S}_{12}$ ($\mathscr{S}_{13}$) groups are invaluable; the more recent work of Liu and Balasubramanian [57] on $\mathbb{Z}(\mathscr{S}_n)$ for $15 \leqslant n \leqslant 18$ is also of value in the context of applications in areas of mathematical and computational chemistry.

An understanding of the analogous combinatorial algorithms [20,21] associated with Young's rule for decomposition of $\lambda \vdash n$ modules over $\{[\lambda']\}$ that defines $\Lambda_{\lambda[\lambda']}$ Kostka coefficients, or with ITP formation [2,19,20], as determined by the analogous LR [21] rule, underlies much of the subsequent presentation. The nature of lexical ordering and dominance in $\mathscr{S}_n$ algebras [21], where the depth of the branching is determined by the SU(m) unitary algebra, is of much practical importance in discussing specific points.

A result from early democratic recoupling studies [38,39] is also of interest. For fixed n sets of ($p \leqslant m$)-tuplar irreps over increasing magnitudes of identical I_i, the outermost total M subspaces are found to take on a common irrep forms, irrespective of yet higher I_i values, a point stressed by Levy-Leblond and Levy-Nahas [38] in discussing analytical scalar invariants under $\mathscr{S}_3$ symmetry. A similar effect over Liouville space has been demonstrated under the $\mathscr{S}_4$ group, as set out in Tables 2–4 of Ref. [58].

3. General higher n SU(m) × $\mathscr{S}_n$ p-tuple modular mappings

Number partitions of n into $p \leqslant m$ distinct parts (p-tuples) give rise to an ordered lexicology, in which each p-tuple has associated with it a monomial form of $(p-1)$-fold product of combinatorial terms which defines the permutational identity, with all the 3 (or 4) -tuples following a general form. Within their intrinsic hierarchical aspects, these $:\lambda: \equiv \lambda \vdash n$ partitional modules represent the scalar invariant forms (over the Rota–Cayley fields) which define the $SU(m) \times \mathcal{S}_n$ algebra. Also they provide the inventorial structure of group dualities over the higher unitary spin spaces [2,12,48].

3.1. *Inventorial hierarchies of $p \leqslant 3$-tuples $\{|IM\rangle\}^M$ of $[^2D]_n(\mathcal{S}_{n \geqslant 12})$ spin clusters*

The corresponding inventorial aspect over the M subspaces for $SU(3) \times \mathcal{S}_{12}$ spin duality is realized in Table 1, in terms of a suitable $\{:\lambda:\}$ $p \leqslant 3$-tuple hierarchy. In addition, the mathematical physics of these p-tuples (modules) encompasses the full set of scalar invariants of Cayley algebra [2,48,58], within which one derives the combinatorial forms over $\{M_1–M_n\}$ inner weight z projection sets of NMR Hilbert space. Much of the following development of the topic rests on this fact and on automorphisms of the $\mathcal{S}_n$ group. The higher outer M aspects of the corresponding spin space for $[^2D]_{20}$ ($\mathcal{S}_{20}$) are set out in Table 4 of Ref. [2b].

3.2. *$\{:\lambda: \to \{[\lambda']\}\}$ $\mathcal{S}_n$ modular mapping in the high n limit*

A further general insight is developed here of these stepwise propagative expansions of $:\lambda: \equiv \lambda \vdash n$ forms for n of $\mathcal{S}_n$ sufficiently large, that the condition $n - r \gg r$ (not equal) holds (for example) for $\lambda \equiv :n-r, r-r', r':$ 3-tuples. However, even for the $n - r \equiv r - r'$ case with its smaller n vs. branching ratio, a subset of the general n non-SR set of irreps is observable with minimal contraction in the $\{:\lambda:(SU(m)) \to \{[\lambda]\}\}(\mathcal{S}_n)$ map for the low branching high n limit.

For completeness, we include the $p \leqslant 2$-tuplar modules, where $r \leqslant n/2$ applies over dominance ordered SR irrep sets [2,21,41], corresponding to the universal covering group for spin algebras, $SU(2) \times \mathcal{S}_n$. The permutational identity, or order $\|:\lambda:\|$, corresponds to a module identity invariance, χ_E. Thus, on introducing the $\binom{n}{r}$ combinatorial term, the maps derived from $p \leqslant 2$ $\lambda \vdash n$ modules become

$$\begin{aligned}
&:n: \to [n]; \ \|:n:\| = 1 \\
&:n-r, r:(\mathcal{S}_n) \to \{[n], [n-1, 1], \ldots, [n-r, r]\}; \ \|:n-r, r:\| = \binom{n}{r}, \quad \forall\, n, r \leqslant n/2
\end{aligned} \tag{4}$$

For 3-tuples, the irrep subset maps onto a subspace which is no longer of a SR form; however, the simple low valued integer $\{0, 1, 2, 3, 4, \ldots\}$ $\Lambda_{[\lambda]}$ terms, or Kostka coefficients, are in principle known quantities, as a consequence of a combinatorial statatement of Young's rule [21]. Thus, they define the mapping from $\lambda \vdash n$ modular forms onto the $\{[\lambda']\}$ set, within (for example)

$$\begin{aligned}
:n-r, r-r', r': \to \{&[n], \Lambda\lambda_{[\lambda']}[n-1, 1], \ldots, \\
&\Lambda\lambda_{[\lambda'']}[n-r, r], \ldots, \Lambda\lambda_{[\lambda]}[n-r, r-r', r']\}
\end{aligned} \tag{5a}$$

for $n/2 > r > r'$ (i.e. with $n - r \gg r$). The specific forms for the Λ may be deduced by using a combinatorial rule and lattice graph shapes. Confirmation of their magnitude comes from modular considerations, involving the sum over $g_i \varepsilon_i^{:\lambda:}$ products yielding

Table 1
The $[A]_{12}^{3/2}$ nuclear magnetic resonance cage spin cluster for the $[^{11}B]_{12}$ framework of the $[BH]_{12}^{2-}$ anion

F_z–l $F_z=18$	$p\leqslant 2$, SU(3)	$p\leqslant 2$, $\underline{SU}(\underline{4})$	$p\leqslant 3$, SU(3)	$p\leqslant 3$, $\underline{SU}(\underline{4})$	$p\leqslant 4$, SU(4)	Dimensionality [b]below line, dimensionality given refers to *new* Su(4) form.
$l=0$	:12:					1
$l=1$	:11, 1:					$\binom{12}{1}$
$l=2$	:10, 2:, :11, –, 1:					$\binom{12}{1}+\binom{12}{2}$
$l=3$	:9, 3:	:11–,–1:	:10, 11:			$\binom{12}{1}+\binom{12}{3}+\binom{12}{2}\binom{2}{1}$
$l=4$	:8, 4:, :10, –, 2:		:9, 21:	:10, 1, –, 1:		$\binom{12}{8}+\binom{12}{2}+\binom{12}{3}\binom{3}{1}+\binom{12}{2}\binom{2}{1}$
$l=5$	:7, 5:		:8, 31:, :9, 12:	:10, –11:, :92, –, 1:		$\binom{12}{5}+\binom{12}{4}\binom{4}{1}+\binom{12}{2}\binom{2}{1}+2\binom{12}{3}\binom{3}{1}$
$l=6$	:6, 6:, :9, –, 3:	:10–,–2:	:7, 41:, :8, 22:	:83–1:	:9111:	$\binom{12}{6}+\binom{12}{3}+\binom{12}{2}\binom{12}{5}\binom{5}{1}+$ $\binom{12}{4}\binom{4}{2}+\binom{12}{4}\binom{4}{1}+\binom{12}{3}\binom{3}{2}\binom{2}{1}$
$l=7$	:5, 7:		:6, 51:, :7, 32:, :8, 13:	:74–1:, :91–2:	:8211:	[b]$\binom{12}{4}\binom{4}{2}\binom{2}{1}$
$l=8$	:4, 8:, :8, –, 4:		:6, 42:, :723:, :561:	:82–2:, :65–1:	:7311:, 8121:	$\binom{12}{5}\binom{5}{2}\binom{2}{1}+\ldots$
$l=9$	:3, 9:	:9–,–3:	:6, 33:, :7, 14:, :552:	:7, 3–2:	:6411:, :7221:, :8112:	$\binom{12}{6}\binom{6}{2}\binom{2}{1}+\binom{12}{5}\binom{5}{3}\binom{3}{1}+\ldots$

$l=10$[a]	:2, 10:, :7, –, 5:		:624:	:8–22:	:5511:, :6321:, :7131:, :7212:	$\binom{12}{7}\binom{7}{2}\binom{2}{1}+\binom{12}{6}\binom{6}{3}\binom{3}{1}+\cdots$
$l=11$	:1, 11:		:6, 15:		:5421:, :6231:, :7122:, :6231:	$\binom{12}{7}\binom{7}{3}\binom{3}{1}+$
$l=12$	:–, 12:, :6, –, 6:	:8—4:		:63–3:	:5331:, :5412:, :7113:, :6212:	$\binom{12}{6}\binom{6}{1}\binom{6}{3}+\cdots$

The outer M subspaces of the 12-fold identical spin 3/2 problem for $[^{11}B]_{12}$ are shown. This is realized in terms of $p \leqslant 4$ $\lambda \vdash n$ modular models, as an inventory including re-ordering, discussed in the text.

[a] For $l \geqslant 10$, the table focuses on the 4-tuple partitional contributions; over $-18 \leqslant M \leqslant 18$, $\{\chi_i\} = \{4^{12}, 4^6, 4^3, 4^3, 4^3\}$, with a total cardinality of $4^{12} =$ 16 777 216.

[c] Underlined SU(m) refers to a fieldwidth within which a p<m form occurs.

the group order, or from the property that the general weighted sum over the $\chi^{[\lambda']}_{(1^n)}$ principal characters of the resultant $[\lambda']$ irreps must be identical to the numeric (combinatorially derived) modular identity, which is a specific characteristic of each such p-tuplar form, as in

$$\|{:}\lambda{:}\| \equiv \binom{n}{r}\binom{r}{r'}, \quad \forall\, \lambda \equiv {:}n-r, r-r', r'{:} \text{ of } p=3 \text{ parts} \tag{5b}$$

The specific non-SR maps for ordered 3-tuples form a hierarchy within

$$\begin{aligned} &{:}n-2, 11{:}(\mathscr{S}_n) \rightarrow \{[n], 2[n-1,1], [n-2,2], [n-2,11]\} \\ &{:}n-3, 21{:} \rightarrow \{[n], 2[n-1,1], 2[n-2,2], [n-2,11], [n-3,3], \\ &\qquad [n-3,21]\}, \end{aligned} \tag{6}$$

where the principal characters of the $\mathscr{S}_n$ group irreps are defined by the standard hook length formula [21,55,59] for all $\mathscr{S}_n$ groups. The uniqueness of these characters for many higher $\mathscr{S}_n$ groups also provides help with initial determinations of the set of $\{A_{\lambda[\lambda']}\}$ irrep coefficients within the non-SR map, i.e. prior to invoking Young's rule. Further, the combinatorial properties of p-tuples over the branching hierarchy allow a stepwise enumerative process to be used. Examination of the outermost irrep components indicates that the concluding $\{[n-r, r], [n-r, r-1, 1], [n-r, r-2, 2]\}$ subsets are frequently an SR aspect of a more general non-SR map, as in

$$\begin{aligned} {:}n-4, 2, 2{:}(\mathscr{S}_n) \rightarrow \{&[n], 2[n-1,1], 3[n-2,2], \\ &[n-2,11], 2[n-3,3], 2[n-3,21], \\ &\{[n-4,4], [n-4,31], [n-4,22]\}\}, \quad \forall\, n \geqslant 8 \end{aligned} \tag{7a}$$

where the general ${:}n-r, r-r', r'{:}$ modular identity follows directly from

$$\|{:}n-r, r-2, 2{:}\| \equiv \binom{n}{r} \times \binom{r}{2} \tag{7b}$$

On taking the unit column vector $\mathfrak{L}(\mathscr{S}_{n\leqslant 8})$ of $p \leqslant 3$ irreps in lexical order (where * denotes the (future) position of an additional 4-tuplar irreps in modular expansions over higher (p) sets),

$$\begin{aligned} \mathfrak{L}^{\dagger} = \{&[n], [n-1], [n-2], [n-2,11], [n-3,3], [n-3,21], *, \\ &[n-4,4], [n-4,31], [n-4,22], *, \ldots\} \end{aligned}$$

one readily obtains the further mappings

$$\begin{aligned} &{:}n-5, 3, 2{:} \rightarrow \{1,2,3,1;\ 3,2,-;\ 2,2,1;\ 1,1,1\}\mathfrak{L} \\ &{:}n-6, 4, 2{:} \rightarrow \{1,2,3,1;\ 3,2,-;\ 3,2,1;\ 2,2,1;\ 1,1,1\}\mathfrak{L}(\mathscr{S}_n) \\ &{:}n-7, 5, 2{:} \rightarrow \{1,2,3,1;\ 3,2,-;\ 3,2,1;\ 3,2,1;\ 1,2,1,\ldots;\ 1,1,1\}\mathfrak{L}, \end{aligned} \tag{8}$$

in agreement with relation (5b). The more highly branched form $:n-6,3,3:(\mathscr{S}_{12})$ gives rise to the specific $\mathscr{S}_{12}$ subset map

$$:6,3,3:\rightarrow\{1,2,4,1;\ 3,3,-;\ 3,3,1;\ 3,3,1;\ 1,1,1,1\}\mathfrak{L}(\mathscr{S}_{12}) \tag{9a}$$

within the constraints imposed by the modular identity

$$\|:n-6,3,3:\| \equiv 20\times\binom{n}{6} \tag{9b}$$

As an alternative to explicit use of Young's rule, the detailed $n\geqslant 12$ symmetric group characters, with their wider span of $\{[\lambda']\}$ field and higher value of n, may resolve the form of the general mapping in the low branching limit [12]. The rapid (two-fold) enhancement of the dimensionality of the p-tuplar identities restricts this approach to $p\leqslant 4$ modules. A couple of general forms are readily accessible for $n\leqslant 12$ $\mathscr{S}_n$ algebras, using these arguments. Hence, one obtains

$$:n-3,111:\rightarrow\{1,3,3,3;\ 1,2,1\}\mathfrak{L}(\mathscr{S}_n) \tag{10a}$$

from the modular identity

$$\|:n-3,111:\| \equiv 6\times\binom{n}{3} \tag{10b}$$

while the mapping relationship

$$:n-4,211:\rightarrow\{1,3,4,3;\ 3,4,1:\ 1,2,1,1)\mathfrak{L}(\mathscr{S}_n) \tag{11a}$$

extends the form of the $:2211:(\mathscr{S}_6)$ tuple, derived below. The specific 4-tuplar identity is given by

$$\|:n-4,211:\| \equiv 2\binom{n}{4}\times\binom{4}{2}=12\times\binom{n}{4} \tag{11b}$$

A further property of Kostka $\Lambda_{\lambda[\lambda]}$ coefficients is worth noting, namely that the coefficients associated with the $[n]$ and the specific "named" $[\lambda]$ irrep of the set, i.e. identical in branching structure to the module $\lambda\vdash n$ form, are always unity.

Since the $\{\Lambda_{\lambda[\lambda']}\}$ coefficients effectively define the overall $\Gamma(\mathscr{S}_n)$ irrep associated with a module, the corresponding set of permutational invariances $\{\varepsilon_i^{:\lambda:}\}(\mathscr{S}_6)$ in the context of $\mathbb{Z}(\mathscr{S}_6)$ may be utilized in enumeration within [49a,60] (Table 2)

$$\Gamma\text{, specific for }:\lambda:=(1/n!)\textstyle\sum_{[\lambda']}\sum_i g_i\varepsilon_i^{:\lambda:}\chi_i^{[\lambda']} \tag{12}$$

For the segment $:\lambda:=:2211:$ to $:1^6:$, this relationship yields the low n subset of Kostka coefficients. Over adjacent unitary algebras these are seen to differ only by one (or a couple) of entries from the high n general result, e.g. of Eq. (11a), compared with the :2211: expansion. This is a useful point to bear in mind in understanding SU(m) branching of different $\mathscr{S}_n$ algebras, or under intermediate branching regimes.

Table 2
The $\varepsilon_i^{:\lambda:}(\mathscr{S}_6)$ permutational invariance properties of the complete set of p-tuplar modules over the full $\mathscr{S}_6$ group cycle algebra [49]

$\mathscr{S}_6$	(111111) 1	(11112) 15	(1122) 45	(222) 15	(1113) 40	(123) 120	(33) 40	(114) 90	(24) 90	(15) 144	(6) 120
:6:	1	1	1	1	1	1	1	1	1	1	1
:51:	6	4	2	0	3	1	0	2	0	1	0
:42:	15	7	3	3	3	1	0	1	1	0	
:4, 11:	30	12	2	0	6	0	0	2	0		
:3, 3:	20	8	4	0	2	2	2	0			
:321:	60	16	4	0	3	1	0				
:3, 111:	120	24	0	0	6	0					
:2, 22:	90	18	6	6	0						
:2, 211:	180	24	4	0							
:2, 1111:	360	24	0								
:111111:	6! = 720	0	0	0	0	0	0	0	0	0	0

As derived from self-consistency relationships and unit components of $:\lambda:$ maps for $[n]$ and $[\lambda]$ (last or name entry) in $:\lambda: \to \{[n], [n-1, 1], \ldots, \ldots, [\lambda], 0, \ldots, 0\}$; the generality of simple reducibility of SU(2) duality serves to define the properties of all the 2-tuples over their invariance hierarchy, as implied in Ref. [41].

4. Highly branched $\mathscr{S}_n$ module subsets for $(n-r \gtrless r-r')$ compared with the generalized maps

As examples of the low n $\mathscr{S}_n$ subset variations compared with the generality of the $n > n-r$ condition given in the last section, we present the 3(4)-tuples of $\mathscr{S}_n$, $4 \leqslant n \leqslant 8$, in a compact form listing the coefficients over $\{[\lambda']\}$-ordered lexical field $\mathfrak{L}$; here the isolated variations within the subset are shown as underlined integers. Certain terms from amongst these are naturally omitted from the ordered lexicology for a specific value of p and need not detain us further. Hence, we find that

$$:211{:}(\mathscr{S}_4) \to \{1, 2, 1, 1;\ -\}\mathfrak{L},\ \text{for}\ \mathfrak{L}(\mathscr{S}_4)^{\dagger} = \{[4], [31], [22], [211];\ [1111]\}$$
$$:1111{:} \to \{1, 3, \underline{2}, 3;\ 1)\mathfrak{L} \tag{13}$$

where the latter set corresponds to the principal character set of the symmetric group $\mathscr{S}_4$. Hence, the origin of the $:1^4:$-tuple properties under the $\mathscr{S}_4$ group, or by isomorphism under the physical finite group $\mathscr{S}_4{}^{\downarrow}T_d$, is clear [58].

Further, on treating the full $SU(m=n) \times \mathscr{S}_6$ group the augmented lexicology (in natural $\trianglerighteq$ dominance order) now spans the irrep set

$$\mathfrak{L}(\mathscr{S}_6)^{\dagger} = \{[6], [51], [42], [411];\ [33], [321], [3111];$$
$$[222], [2, 211], [2, 1111], [1^6]\}$$

thus the mappings for $p \geqslant 3$-tuplar modules, as elements of $SU(m) \subset SU(6)$, take the form [49]

$$
\begin{aligned}
&:411:(\mathcal{S}_6)\rightarrow\{1,2,1,1;\ -\}\mathfrak{L},\\
&:321:\rightarrow\{1,2,2,1;\ 1,1,-;\ -\}\mathfrak{L}(\mathcal{S}_6)
\end{aligned}
\tag{14}
$$

$$
\begin{aligned}
&:3111:\rightarrow\{1,3,3,3;\ 1,2,1;\ -\}\mathfrak{L},\\
&:222:\rightarrow\{1,2,3,1;\ \underline{1},2,-;\ (-,-)\ 1\}\mathfrak{L}\\
&:2211:\rightarrow\{1,3,4,3;\ \underline{2},4,1;\ (-,-)\ 1,1\}\mathfrak{L}
\end{aligned}
\tag{15}
$$

$$
\begin{aligned}
&:21111:\rightarrow\{1,4,6,6;\ 3,8,4;\ (-,-)\ 2,3,1;\ -\}\mathfrak{L}\\
&:111111:\rightarrow\{1,5,9,10;\ 5,16,10;\ (-,-)\ 5,9,5;\ 1\}\mathfrak{L}
\end{aligned}
\tag{16}
$$

Once again, the higher (3, 6)-tuplar forms of the final component irreps, $[2^3]-[1^6]$, and the generality of $:1^n$: n-tuple come directly from aspects of the abstract n-fold symmetric group and its corresponding modular invariance properties [21], arising as from Burnside's lemma.

For the branched $\mathcal{S}_8$ modules over $p\leqslant 4$ fields of irreps, the lexicology spans

$$
\begin{aligned}
\mathfrak{L}(\mathcal{S}_8)^{\dagger}=\{&[8],[71],[62],[611];\ [53],[521],[5111];\\
&[44],[431],[422],[4211];[332],[3311],[3221],*;\\
&[2222],[22211],\ldots\}
\end{aligned}
$$

and the requisite $:\lambda:(\mathcal{S}_8)$ mappings [60] take the form

$$
\begin{aligned}
&:422:\rightarrow\{1,2,3,1;\ 2,2,-;\ 1,1,1\}\mathfrak{L}\\
&:4211:\rightarrow\{1,3,4,3;\ 3,4,2;\ 1,2,1,1\}\mathfrak{L}(\mathcal{S}_8)
\end{aligned}
\tag{17}
$$

$$
\begin{aligned}
&:332:\rightarrow\{1,2,3,1;\ 3,2,-;\ \underline{1},2,1,0;\ 1\}\mathfrak{L}\\
&:3311:\rightarrow\{1,3,4,3;\ 4,6,1;\ 2,4,1,1,-;\ 1,1\}\mathfrak{L}\\
&:3221:\rightarrow\{1,3,5,3;\ 5,6,1;\ 2,5,3,2,-;\ 2,1,1\}\mathfrak{L}\\
&\ \vdots
\end{aligned}
\tag{18}
$$

$$
\begin{aligned}
&:2222:\rightarrow\{1,3,6,3;\ 6,8,1;\ 3,7,6,3-;\ 3,2,3,-,-;\ 1\}\mathfrak{L}\\
&:2221^2:\rightarrow\{1,4,8,6;\ 9,14,4;\ 4,13,9,9,1;\ 6,5,6,2,-;\ 1,1\}\mathfrak{L}(\mathcal{S}_8)
\end{aligned}
\tag{19}
$$

$$
\begin{aligned}
&:221^4:\rightarrow\{1,5,11,10;\ 13,24,10;\ 6,23,16,21,5;\ 11,12,13;8,1;\ 2,3,1\}\mathfrak{L}\\
&:21^6:\rightarrow\{1,6,15,15;\ 19,24,20;\ 9,40,30,45,15;\ 21,26,30,24,6;\ 5,9,5,1\}\mathfrak{L}\\
&:1^8:\rightarrow\{1,7,20,21;\ 28,64,35;\ 14,70,56,90,35;\ 42,56,70,64,21;\\
&\qquad 14,28,20,7,1\}\mathfrak{L}.
\end{aligned}
\tag{20}
$$

The consistency of these results for $n=(6,8)$, 12, 20, 24, 36 even n $\mathcal{S}_n$ groups, and for $n = 7, 9, 11, 15$ for odd n $\mathcal{S}_n$ groups, is demonstrated in the tables and subsequent discussion. For the higher $\mathcal{S}_n$ groups, it is the mapping involving the SA modules which presents the most difficult aspect of Kostka enumerations as applied to NMR spin clusters.

As specific comparisons of subset–full set $\mathcal{S}_n$ module expansions [49a], the following offer direct insight into the relationship imposed by the combinatorial counting rule for seminormal contents in the general and limiting cases, where omitted "–" coefficients refer to non-existent irreps under the specific lexical module; hence,

$$\begin{pmatrix} :1^4: \\ :31^3: \end{pmatrix} \to \begin{pmatrix} \{1, 3, \underline{2}, 3;\ -, -, 1\} \\ \{1, 3, 3, 3;\ 1, 2, 1\} \end{pmatrix} \mathfrak{L}(\mathcal{S}_n) \tag{21}$$

where the underlined integers refer to components of smaller magnitude in the subset, compared with their counterparts in the full high n weak branching set or modules, and

$$\begin{pmatrix} :222: \\ :422: \end{pmatrix} \to \begin{pmatrix} \{1, 2, 3, 1;\ \underline{1}, 2, -;\ -, -, 1\} \\ \{1, 2, 3, 1;\ 2, 2, -;\ 1, 1, 1\} \end{pmatrix} \mathfrak{L} \tag{22}$$

or

$$\begin{pmatrix} :2211: \\ :4211: \end{pmatrix} \to \begin{pmatrix} \{1, 3, 4, 3;\ \underline{2}, 4, \underline{1};\ -, -, 1, 1\} \\ \{1, 3, 4, 3;\ 3, 4, 2;\ 1, 2, 1, 1\} \end{pmatrix} \mathfrak{L} \tag{23}$$

for the lower unitary algebras, whereas for a pair of modular $\lambda \vdash n$ drawn from higher unitary algebras the correspondence is less obvious, for example as in

$$\begin{pmatrix} :1^6: \\ :31^5: \end{pmatrix} \to \begin{pmatrix} \{1, 5, \underline{9}, 10;\ \underline{5}, \underline{16}, 10;\ -, \ldots, 5;\ -, -, -, -, 1\} \\ \{1, 5, 10, 10;\ 10, 20, 10;\ 4, (\ldots)\, 5;\ 5, 6, 6, 4, 1\} \end{pmatrix} \mathfrak{L} \tag{24}$$

where we restrict consideration to the initial and finite irreps in the expansion sequence.

5. A wider demonstration of *p*-tuplar module properties over $\{[\lambda']\}(\mathcal{S}_n)$

While the $\mathbb{Z}(\mathcal{S}_n)$ tabulations of the full $\mathcal{S}_n$ characters are known [20,56] up to $n \leqslant 13$ $\mathcal{S}_n$ may be computed up to $n \leqslant 16, 18$, as indicated in Ref. [57]. The principal characters $\chi^{[\lambda]}_{(1^n)}$ follow directly from the hook length graphs [55,59] and Table 15. These properties are now invoked in demonstrating the consistency of the $\|{:}\lambda{:}\| = \Sigma A_{\lambda[\lambda']} \times \|[\lambda']\|$ product relationship for 3(4)-tuple modular mappings derived earlier. This is examined in Eq. (25) (in Table 3) for SU(3(4)) $\times\ \mathcal{S}_n$, for $n = 12$, 20, 24, and 36, as in the right-hand column vectors.

The validity of a set *p*-tuple maps now for odd-valued *n*-fold spin clusters is

Table 3

The matrix equation defining $\mathscr{S}_n$ modules' $:\lambda: \rightarrow \{\Lambda_{\lambda[\lambda']}[\lambda'](\mathscr{S}_{n\geqslant 12})\}$ decompositional mapping properties, within the appropriate dimensionality constraints

$\{:\lambda:\}$		$\{\Lambda_{\lambda[\lambda']}\}$	$\{[\lambda']\}$	$\lVert:\lambda:\rVert(\mathscr{S}_{12})$	$\mathscr{S}_{20}$	$\mathscr{S}_{24}$	$\mathscr{S}_{36}$	
			$[n]$	1	1	1	1	
$:n-2,1,1:$		1, 2, 1, 1	$[n-1,1]$	132	380	552	1260	
$:n-3,2,1:$		1, 2, 2, 1; 1, 1 0	$[n-2,2]$	660	3420	6072	21420	
$:–,1,1,1:$		1, 3, 3, 3; 1, 2, 1	$[–,11]$	1320	6840	12148	42840	
$:n-4,3,1:$		1, 2, 2, 1; 2, 1, –; 1, 1	$[n-3,3]$	1980	19380	42504	235620	
$:–,2,2:$		1, 2, 3, 1; 2, 2, 0; 1, 1, 1	$[–,21]$	2970	29070	63756	353430	
$:–,2,1,1:$		1, 3, 4, 3; 3, 4, 1; 1, 2, 1, 1	$[–,111]$	5940	58140	127512	706860	
$:n-5,4,1:$		1, 2, 2, 1; 2, 1, –; 2, 1, –, –; 1, 1	$[n-4,4]$	3960	77520	212520	1884960	
$:–,3,2:$		1, 2, 3, 1; 3, 2, –; 2, 2, 1, –; 1, 1, 1	$[–,31]$	7920	155040	425040	3769920	
$:–,3,11:$		1, 3, 4, 3; 4, 4, 1; 3, 4, 1, 1; 1, 2, 1, 1	$[–,22]$	15840	310080	850050		
$:–,2,21:$	≡	1, 3, 5, 3; 5, 6, 1; 3, 5, 3, 2; 1, 2, 2, 1, 1	$[–,211]$	23760	465120	1275120		(25)
$:n-6,5,1:$		1, 2, 2, 1; 2, 1, –; 2, 1, –, –; 2, 1, –; 1, 1	$[n-5,5]$	5544	232560	807576	11686752	
$:–,4,2:$		1, 2, 3, 1; 3, 2, –; 3, 2, 1, –; 2, 2, 1; 1, 1, 1	$[–,41]$	13860	581400	2018940	29216880	
$:–,4,11:$		1, 3, 4, 3; 4, 4, 1; 4, 4, 1, 1; 3, 4, 1, 1; 1, 2, 1, 1	$[–,32]$	27720	1162800			
$:–,3,3:$		1, 2, 4, 1; 3, 3, –; 3, 3, 1, –; 3, 3, 1, ; 1, 1, 1, –, 1	$[n-6,6]$	18480	775200	2691920	38955840	
$:–,3,21:$		1, 3, 5, 3; 6, 6, 1; 5, 7, 3, 2; 3, 5, 4, 2, 1; 1, 2, 2, 1, 1, 1	$[–,5,1]$	55440	2325600			
$:n-7,5,2:$		1, 2, 3, 1; 3, 2, ; 3, 2, 1, –; 3, 2, 1, –; 1, 2, 1, –; 1	$[–,4,2]$	16632	1627920	7268184	17530128	
$:–,5,1,1:$		1, 3, 4, 3; 4, 4, 1; 4, 4, 1, 1; 4, 4, 1, 1; 2, 4, 1, 1; 1, 1	$[–,4,11]$	33264	3255840			
$:–,4,3:$		1, 2, 3, 1; 4, 2, –; 4, 3, 1, –; 3, 3, 2, –; 1, 2, 2, –, 1; 1, –, 1	$[–,3,3]$	27720	2713200	12113640		
$:n-8,4,4:$		1, 2, 3, 1; 4, 2, –; 5, 3, 1, –; 3, 4, 2, –; 1, 2, 3, –, 1; 1, –, 2, –; 1	$[n-7,5,2]$	34650	8817900	51482970		

The final four columns give the p-tuple dimensionalities under the $\mathscr{S}_n$ groups indicated. The $\Lambda_{\lambda[\lambda']}$ are called Kostka coefficients.

Questions of uniqueness and determinacy in terms of independence of invariance expression for subduction groups become more difficult to establish as the branching increases towards the SA group irreps, especially so for the $p \geqslant 4$-tuples. The permutation group modules for $p \geqslant 4$ parts also require progressively higher n $\mathscr{S}_n$ *properties to establish the most general form of the decompositional mapping properties, within the appropriate dimensionality constraints.*

considered, for $\mathscr{S}_n$ with $n = 7$, 9, 11 and 15; within these odd n sets one obtains

$$\{:\lambda:\} \qquad \{\Lambda'_{\lambda[\lambda']}\} \qquad \{[\lambda']\}$$

$$\begin{pmatrix} :n-2,11: \\ :n-3,21: \\ :n-3,111: \\ :n-4,31: \\ :n-4,22: \\ :n-4,211: \end{pmatrix} \equiv \begin{pmatrix} 1,2,1,1 & & & 0 \\ 1,2,2,1; & 1,1 & & \\ 1,3,3,3; & 1,2,1 & & \\ 1,2,2,1; & 2,1,-; & 1,1 & \\ 1,2,3,1; & 2,2,-; & 1,1,1 & \\ 1,3,4,3; & 3,4,1; & 1,2,1,1 & \end{pmatrix} \begin{pmatrix} [n] \\ [n-1,1] \\ (n-2,2] \\ [n-2,11] \\ [n-3,3] \\ [n-3,21] \\ [n-3,111] \\ [n-4,4] \\ [n-4,31] \\ [n-4,22] \\ [n-4,211] \end{pmatrix};$$

$$\| :\lambda: \| (\mathscr{S}_7) - (\mathscr{S}_9) - (\mathscr{S}_{11}) - (\mathscr{S}_{15})$$

$$\times \begin{pmatrix} 42 \\ 105 \\ 210 \\ 140 \\ 210 \\ 420 \end{pmatrix} \begin{pmatrix} 72 \\ 252 \\ 504 \\ 504 \\ 756 \\ 1512 \end{pmatrix} \begin{pmatrix} 110 \\ 495 \\ 990 \\ 1320 \\ 1980 \\ 3960 \end{pmatrix} \begin{pmatrix} 210 \\ 1365 \\ 2730 \\ 5470 \\ 8190 \\ 16\,380 \end{pmatrix} \tag{26}$$

For $\mathscr{S}_7$, $[n-4, 4]$ is naturally excluded by the lexicology. Using the principal characters of Table 3 the sum of $\Sigma_{[\lambda']} \Lambda_{\lambda[\lambda']} \times \| [\lambda'] \|$ terms again is identical to the combinatorial dimensionality of the 3(4)-tuples surveyed down to $:n-4, r-r', r'$: 3-tuple forms (for $n \leqslant 15$), or to $:n-6, r-r', r'$: forms, for the $\mathscr{S}_{12}$ or $\mathscr{S}_{20}$ groups, as set out in Ref. [12] and Ref. [2] respectively.

For proof of the existence of this $n-r \gg r$ limit in $:n-r, r-r', r'$:, or similar permutational modular expansions, one merely has to look at the exigencies associated with the combinatorial counting rule in this high n limit, compared with more general enumerations. The existence of a non-incremental limit for the Λ, once a certain value of $n-r$ to r is reached, follows directly. More comprehensive tables of Kostka coefficients and the $\{\varepsilon_i^{:\lambda:}\}(\mathscr{S}_n)$ permutational invariance sets are set out in Table 2 and Tables 4–7; a modular property [21] in this context is one associated with $\Sigma_i g_i \varepsilon_i^{:\lambda:}$, for which all $\lambda \vdash n$ partitions generate the cardinality number $\| \mathscr{S}_n \| = n!$; here, g_i is simply the order of the ith cycle (class) operators $\mathbb{Z}(\mathscr{S}_n)$, as given by Cauchy's relationship [20, 21].

Table 4
$:\lambda: \equiv \lambda \vdash n$ vs. $\varepsilon^{:\lambda:}_{(..)}(\mathscr{S}_7)$ over the full $\mathscr{S}_7$ cycle algebra with $\|\mathscr{S}_7\| = 5040$

$\lambda \vdash n$	X_1	X_2	X_3	X_4	X_5	X_6	X_7	X_8	X_9	X_{10}	X_{11}	X_{12}	X_{13}	X_{14}	X_{15}	
	1	21	105	105	70	420	210	280	210	630	420	504	504	840	720	$\|X_i\|$
:7:	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	
:61:	7	5	3	1	4	2	0	1	3	1	0	2	0	1	0	
:52:	21	11	5	3	6	2	2	0	3	1	0	1	1	0		
:511:	42	20	6	0	12	2	0	0	6	0	0	2	0			
:43:	35	15	7	3	5	3	1	2	1	1	1	0				
:421:	105	35	9	3	12	2	0	0	3	1	0					
#:4111:	210	60	6	0	24	0	0	0	6	0						
:331:	140	40	12	0	8	4	0	0	0							
:322:	210	50	22	6	6	10	2	0								
:3211:	420	80	12	−4	12	2	0									
$:31^4:$	840	120	0	0	24	0										
:2221:	630	90	18	6	0											
$:2^21^3:$	1260	120	12	0												
$:21^5:$	2520	120	0													
$:1^7:$	5040	0														

The skew-triangular matrix of $\varepsilon^{:\lambda:}_{(...)}$ permutational invariances of the $\lambda \vdash n$ p-tuples associated with $SU(m \leqslant n) \times \mathscr{S}_{n=7}$ duality over cycle structure of the $\mathscr{S}_7$ group is shown, the lower skew-triangular space being a null space aspect of the algebra.

6. Significance of mapping for models under higher $SU(m \geqslant n/2) \times \mathscr{S}_n(^{\downarrow}\mathscr{G})$ dualities

The p-tuples modules are also invaluable in discussing the subductive mapping under group duality in either Hilbert or Liouville spin spaces [2,11], because of the way they focus attention on the SU(p) depth from the $p \leqslant m$ (m^2) distinct -tuplar structures respectively. Surprisingly, the use of mathematical subduced space modelling with p-tuples becomes more tractable for the higher p forms; many of the invariance aspects are directly realizable from suitably labelled solid geometric (quasi-combinatorial) models of the p-tuplar modules. Hence, the distinct $\{\Gamma(\mathscr{S}_n{}^{\downarrow}\mathscr{G})\}$ irrep sets for all 3-tuples of form $:n-r, r-r', r':$ and those for higher-order $\lambda \vdash n$ partitions follow directly. On combining these results with findings from the initial $\{:\lambda: \rightarrow \{[\lambda]\}\}$ mappings of Eqs. (25) and (26), which address the non-SR problem of defining the values of specific $\Lambda_{\lambda[\lambda']} > 1$ Kostka coefficients, a difference mapping of specific physical interest comes to light. Hence the $\{:\lambda:(\mathscr{S}_n) \rightarrow \Gamma(\mathscr{S}_n{}^{\downarrow}\mathscr{G})\}$ initial mapping associated with subduction may be extended in its scope so that the corresponding $\{[\lambda](\mathscr{S}_n) \rightarrow \Gamma(\mathscr{S}_n{}^{\downarrow}\mathscr{G})\}$ mapping associated with natural subgroups embedded in a high n $\mathscr{S}_n$ groups is derivable in a direct manner. However, such a conceptual result also demonstrates the existence of an NMR spin symmetry chain under group dualities derived from highest $m = n, \ldots, n/2, \ldots$ unitary aspects and the corresponding sequence of modules.

Perhaps it is useful to remind ourselves that these distinctive properties of specific symmetry chains are a consequence of the origin of spin algebras in theories of $\mathscr{S}_n$

Table 5
$:\lambda: \rightarrow \{[\lambda']\}(\mathscr{S}_7)$: $\Lambda_{\lambda[\lambda']}$ Kostka coefficients inherent in the non-simply-reducible homomorphic mapping

$\lambda \vdash n$	[7]	[61]	[52]	[511]	[43]	[421]	[4111]	[331]	[322]	[3211]	[31111]	[2221]	[221^3]	[21^5]	[1^7]
Section A															
:511:	1	2	1	1											
:421:	1	2	2	1	1	1									
:4111:	1	3	3	3	1	2	1								
:331:	1	2	2	1	2	1	—	1							
:322:	1	2	3	1	2	2	—	1	1						
Section B															
:3211:	1	3	4	3	3	4	1	2	1	1					
:31111:	1	4	6	6	4	8	4	3	2	3	1				
:2221:	1	3	5	3	4	6	1	3	3	2	—	1			
:22111:	1	4	7	6	6	11	4	6	5	6	1	2	1		
:21^5:	1	5	10	10	9	20	10	11	10	15	5	5	4	1	
:1^7:	1	6	14	15	14	35	20	21	21	35	15	14	14	6	1

The $\Lambda_{\lambda[\lambda']}$ coefficients of the non-SR expansion of $:\lambda: \equiv \lambda \vdash n$ partitions corresponding to $SU(m \leqslant n) \times \mathscr{S}_{n=7}$ dualities are shown. The subsections refer to the direct combinatorial λ shape and a contrasting $(\varepsilon_i^{:\lambda:})$ module invariance method of enumeration for the Kostka coefficients [49]. The Λ also serve to define the mapping properties inherent in the various aspects of a dual group Racah symmetry chain.

Table 6
$:\lambda: \equiv \lambda \vdash n(\mathrm{SU}(p \leqslant 8) \times \mathcal{S}_8)$ vs. $\{\varepsilon^{\lambda:}_{(\ldots)}\}(\mathcal{S}_8)$ over the cycle algebra

$\lambda \vdash n$	X_1 1	X_2 28	X_3 210	X_4 420	X_5 105	X_6 112	X_7 1120	X_8 1680	X_9 1120	X_{10} 1120	X_{11} 420	X_{12} 2520	X_{13} 1260	X_{14} 3360	X_{20} 3360	X_{21} 5760	X_{22} 5040	$\Vert X_i \Vert$
:431:	280	85	28	6	0	25	9	1	4	0	4	2	0	0	0			
:422:	420	120	32	12	12	30	6	2	0	2	6	2	2	0				
#:4211:	840	210	36	6	0	60	6	0	0	0	12	2	0					
:41111:	1680	356	24	−4	2	124	2	10	−3	0	24	0						
#:332:	560	140	40	12	0	20	8	4	2	2	0							
:3311:	1120	240	48	0	0	40	12	0	4	0								
:3221:	1680	300	56	12	0	30	6	2	0									
:32111:	3360	480	48	0	0	60	6	0										
$:31^5:$	6720	720	0	0	0	120	0											
:2222:	2520	360	72	24	24	0												
:22211:	5040	540	72	12	0													
$:221^4:$	10080	720	48	0														
$:21^6:$	20160	720	0															
$:1^8:$	40320	0																

The upper skew-triangular permutational module characters of the $\mathrm{SU}(m \leqslant 8) \times \mathcal{S}_8$ algebra over the full cycle algebra are shown; the middle portions below the SA λ_{SA} prove to be the most difficult aspect of any enumeration. Even though available in principle for the higher dualities, this may be inherently indeterminate in practical terms.

Table 7
$:\lambda: \rightarrow \{[\lambda']\}(\mathscr{S}_8)$; $\Lambda_{\lambda[\lambda']}$ Kostka coefficients

$\lambda \vdash n$	[8]	[71]	[62]	[611]	[53]	[521]	[5111]	[44]	[431]	[422]	[4211]	[41^4]	[332]	[3311]	[3221]	[321^3]	[31^5]	[2^4]	[2^31]	[2^21^4]	[21^6]	[1^8]
Section A																						
:521:	1	2	2	1	1	1																
:5111:	1	3	3	3	1	2	1															
:431:	1	2	2	1	2	1	—	1	1													
:422:	1	2	3	1	2	2	—	1	1	1												
:4211:	1	3	4	3	3	4	1	1	2	1	1											
:41^4:	1	4	6	6	4	8	4	1	3	1	3	1										
:332:	1	2	3	1	3	2	—	1	2	1	—	—	1									
Section B																						
:3311:	1	3	4	3	4	6	1	2	4	1	1	—	1	1								
:3221:	1	3	5	3	5	6	1	2	5	3	2	—	2	1	1							
:32111:	1	4	7	6	7	11	4	3	9	5	6	1	3	3	2	1						
:31^5:	1	5	10	10	10	20	10	4	15	10	15	5	5	6	5	4	1					
:2222:	1	3	6	3	6	8	1	3	7	6	3	—	3	2	3	—	—	1				
:22211:	1	4	8	6	9	14	4	4	13	9	9	1	6	5	6	2	—	1	1	—		
:221^4:	1	5	11	10	13	24	10	6	23	16	21	5	11	12	13	8	1	2	3	1		
:21^6:	1	6	15	15	19	24	20	9	40	30	45	15	21	26	30	24	6	5	9	5	1	
:1^8:	1	7	20	21	28	64	35	14	70	56	90	35	42	56	70	64	21	14	28	20	7	1

A summary of the $\Lambda_{\lambda[\lambda']}$ expansion coefficients of the λ module mapping associated with the dual symmetry of 8-fold NMR spin clusters, with subsections for the two modes of calculation [9,10], discussed in Ref. [49].

automorphisms [1,4,11,12] for NMR spin cluster problems, from the associated $\{J_{ij}: J'_{i'j'}\}$ intracluster interaction hierarchies (under $\mathscr{S}_n$ automorphisms) of Figs. 1–4. The use of these ionic 3-space models is itself a reflection of group automorphism, since there is no direct physical single-group 3-space involvement (i.e. without an $\mathscr{S}_n$ group aspect) in NMR. Finally, it is noted that the wider ITP algebras for these $\mathscr{S}_n$ and $\mathscr{S}_n{\downarrow}\mathscr{G}$ group spaces allow one to extend the initial results, derived from $SU(2) \times \mathscr{S}_n$ and $SU(2) \times \mathscr{S}_n{\downarrow}\mathscr{G}$ symmetries, into calculations associated with the higher unitary dual groups [2,18,19].

The use of semitopological schemata for $4 \leqslant n \leqslant 20, 60, \ldots$ $\mathscr{S}_n$ spin symmetries is a topic which allows extensions to the CI views of Balasubramanian [13–15], as well as to other viewpoints [33]. Earlier interest in spin algebras in the contexts of SU(m) dualities [44] largely neglected the value of $\mathscr{S}_n$ automorphisms [1]. Similarly, any restriction of discussions to SU(m) monoclusters over Hilbert space causes the value of group duality with its cooperative v recoupling aspects [61], inherent in $D^k(\tilde{U}) \times \tilde{\Gamma}^{[\lambda]}(v)$ dual irreps of Liouville space, to be overlooked. (A mathematical work by Kummer and McLean [62] on Bell's theorem for hidden variables does not apply to (v).) Thus, the existence of a distinct duality symmetry chain for NMR spin cluster algebras under $SU(m) \times \mathscr{S}_n$ was not considered in pre-1990 work, to our

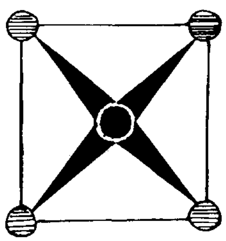

Fig. 1. The $\mathscr{S}_6{\downarrow}\mathcal{O}$ automorphism associated with a $\{4J, J'\}$ interaction set.

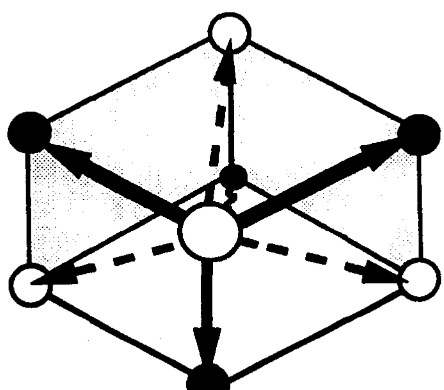

Fig. 2. The $\mathscr{S}_8{\downarrow}\mathcal{O}$ automorphism associated with a $\{3J, 3J', 3J''\}$ interaction set. Reproduced with permission from Ref.[9].

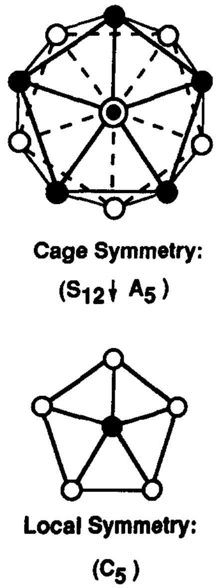

Fig. 3. The $\mathscr{S}_{12}\downarrow\mathscr{I}$ automorphism associated with a $\{5J, 5J', 5J''\}$ interaction set. A projected view about a specific nuclear spin site, with a subdiagram of the local symmetry. Reproduced with permission from Ref[12a]. (○ and ● for BH are for perspective only)

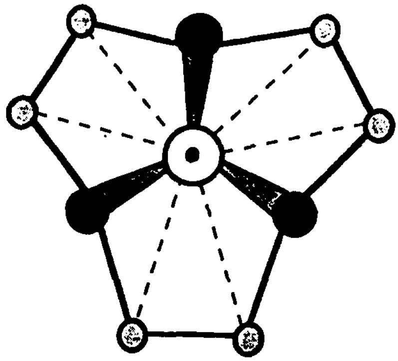

Fig. 4. The $\mathscr{S}_{20}\downarrow\mathscr{I}$ automorphism associated with a $\{3J, 6J', (3J'', 6J'''), J''''\}$ interaction set, in a contracted view of $\mathscr{S}_{20}\downarrow\mathscr{A}_5$ spin symmetry subduced further to C_3 at the spin site chosen. The subset components in parentheses are omitted for clarity.

knowledge, as it is a consequence of the above Liouville space mapping considerations [61]. These are discussed in more detail in a later section. An indication of the need to include a distinct dual symmetry chain may also be seen in the hierarchical structure of SU(m) $\times$ $\mathscr{S}_n$ modular $\lambda \vdash n$ sets [49,60].

The enumerative aspects of mapping onto the related finite subduced symmetries involve additional models which are subject to the general limitations of class (cycle) algebras with regard to the ability of the finite subgroup to lift any degeneracies associated with (identity) invariances under the subduced symmetry. While it is evident that these combinatorial models from the theory of $\lambda = 1^n$ partitions and the forms of projective geometry are analogous to traditional formalisms [4,41,42,63] for higher I_i spin clusters for $n \geqslant 12, 20, 60$ symmetric groups, the use of the latter would be somewhat lengthy and tedious in such cases. An inspection of Ziauddin's $\mathbb{Z}(\mathscr{S}_{12})$ characters [56] should convince the reader on this point. Some recent computational work [57] which reports the enumeration of $\mathscr{S}_n$ characters using the Schur function [37] approach for $14 \leqslant n \leqslant 18$ serves to confirm this point and to put some practical logistical limit to the use of explicit $\mathscr{S}_n$ algebras.

Further, by considering (permutational) invariance properties successively in both abstract mathematical and physical spaces, one obtains details of the full dual symmetry chain; the p-tuplar modules closest to the total branched λ:1^n: limit, for which a specific form exists, i.e.

$$\Lambda_{\lambda[\lambda']} \equiv \chi_{1^n}^{[\lambda']}, \quad \forall\, [\lambda'] \tag{27}$$

from the Burnside lemma, become scalar invariants of the higher unitary dualities. These are of value in discussing the highest I_i SU(m) spin clusters, within projective geometries associated with the specialized $\mathscr{S}_n$ groups for $n = 6, 8, 12, 20$, whose $\chi_{1^n}^{[\lambda]}$ characters have been given already in Table 2.

7. High unitary aspects and explicit SU(6) × $\mathscr{S}_6 \supset \mathscr{S}_6 \supset$ SU(m) × $\mathscr{S}_6{\downarrow}\mathcal{O}$ nuclear magnetic resonance spin dual group symmetry chains

By drawing on the $p \leqslant m$-tuples specifying the SU(m) algebra, we are in a position to describe the SU(4) × $\mathscr{S}_6 \supset \mathscr{S}_6 \supset$ SU(4) × $\mathscr{S}_6{\downarrow}\mathcal{O}$ dual group symmetry chain as an enlargement of a p-tuple, $\{:\lambda: \to \{[\lambda']\}(\mathscr{S}_n{\downarrow}\mathscr{G})\}$ mapping problem [2,12]. The full details of the six-fold dual symmetry chain are shown in Table 8, where retention of many of the original dual group properties follow from the v recoupling term; this derives from v being an explicit aspect of the Liouville space dual SU2 mapping. The completeness possible here arises from our previous examination of the SU(m) × $\mathscr{S}_6$ dual group algebra [49] and a conjecture on the nature of the maximal n-tuple expansions [21].

The $\mathscr{S}_6{\downarrow}\mathcal{O}$ view of ME NMR clusters presented in Ref. [16] is a formal view for a theoretical monocluster; it does not reflect a practical NMR need, either for a formalism within which the MQ NMR spin dynamics of a cage system are amenable to treatment or as a model for general $[AX]_n$ (SU(m) × $\mathscr{S}_n$) bicluster systems; however, it does remain an interesting insight. A comparable analogy would be to Ramachrandran and Murthy's view [65] of alternative density matrix formalisms for treatment of $\eta = 0$ NQR problems. In particular, the Sullivan and Siddall approach [16], since it is not combinatorial in origin and does not utilize the symmetric group properties of spin algebras, takes no account of the high n limiting behaviour of such dualities, as demonstrated in terms of $\mathscr{S}_n{\downarrow}\mathscr{G}$ semitopological theory [1], or of an implicit role for ($\mathscr{S}_n$ democratic) recoupling [38,39] under duality.

Table 8
Towards a demonstration of an explicit Racah symmetry chain, SU6 × $\mathscr{S}_6 \supset$ SU(4) × $\mathscr{S}_6 \supset \mathscr{S}_6 \supset \mathscr{S}_6 \downarrow \mathcal{O}$ (after Ref. [49])

M	$A_{ij}(:.,..,.: = :\lambda_i:)$(SU4)										$A'_{ij}([\lambda_i])(\mathscr{S}_6)$										$\Gamma(\mathscr{S}_6 \downarrow \mathcal{O})$				
9	1	0									1										1	.	.	.	.
8	0	1	0								1	1									1	—	1	1	—
7	0	1	1	0							2	2	1								3	—	3	2	2
6	0	1	0	1	1						3	4	2	1	1						5	3	6	7	5
5	0	0	2	1	0	1					4	6	5	2	1	1					9	4	13	13	15
4	0	1	0	1	0	3	0			$\mathfrak{W} \equiv$	5	9	7	4	3	3				$\mathfrak{L} \equiv$	12	10	22	26	24 $F^\dagger$
3	1	0	1	1	1	1	1	1			7	11	11	6	4	5	1	1			21	14	32	38	41
2	0	1	0	1	0	4	0	0	1		7	14	12	9	6	7	2	1	1		23	21	44	55	53
1	0	1	2	0	0	2	1	1	1		8	15	15	10	6	7	3	2	1		30	24	52	63	67
0	0	0	0	2	2	2	0	0	2		8	16	14	12	8	10	4	2	2		30	28	54	70	68
Σ	4	12	12	12	6	24	4	4	6		84	140	120	56	50	56	16	10	6		240	176	400	480	480

$\mathfrak{W}$, $\mathfrak{L}$ are column vectors of $\{:\lambda:\}$, $\{[\lambda]\}$ with λ in ($\trianglerighteq$) dominance order: $\{\lambda\} \equiv \{6;\ 5,1;\ 4,2;\ 4,11;\ 3,3;\ 3,21;\ 3,111;\ 2,22;\ 2,211\}$.
$F^\dagger \equiv \{A_1, A_2, E, T_1, T_2\}(\mathscr{S}_6 \downarrow \mathcal{O})$.
For earlier CI work (in part on $^{33}SF_6$), which has been brought to my attention only recently, see Ref. [64].

For the higher $n = m$ group dualities over spin algebras, the difficulty arises from the $n!$ dimensionalities, which are implicit in the $SU(m = n) \times \mathscr{S}_n{\downarrow}\mathscr{A}_5$ ($n = 20, 60$) NMR spin cluster algebras. The self-consistency implicit in the module and modular permutational approach implies that further progress is only limited by the extensive form of calculations involved in deriving $\mathbb{Z}(\mathscr{S}_n)$ or Kostka integers, or the incompatibility of the physically related subgroup with the primary spin algebra, as found for $n = 8$-fold group duality [9], whose accidental degeneracies render the SA irreps inaccessible.

8. Specific model aspects of exo cage $SU(m \leqslant n/2) \times \mathscr{S}_n{\downarrow}\mathscr{G}$ spin symmetries

8.1. $\{:\lambda: \to \Gamma(\mathscr{S}_n{\downarrow}\mathscr{G})\}$ mappings for physical models

In addition to the $SU2 \times \mathscr{S}_{12}$ $p \leqslant 2$-tuples [41], whose invariances under $\mathscr{S}_{12}{\downarrow}\mathscr{A}_5$ are well established [12b], it is possible to model the 3(4)-tuples under the subduced icosahedral symmetry to obtain insight into the structure of the more branched irreps contained within them. In part the approach comes from the structure of ITP algebras [19,20]; these provide some additional confirmation of the consistency of these p-tuplar module expansions. We restrict the present discussion to examples of $\{\chi_i\}$ invariance sets under $\mathscr{S}_{12}{\downarrow}\mathscr{A}_5$ subduced symmetry [12], over the $\mathfrak{C}^\dagger = \{\mathscr{C}_i\} \equiv \{E, C_2, C_3, C_5, C_5'\}$ cycle (class) operator set for the (automorphic 3-space) model [12],

$$\begin{aligned} &\{\chi_i\}(:10, 1, 1:) \equiv \{132, 0, 0, 2, 2\}\mathfrak{C}, \\ &\{\chi_i\}(:9, 2, 1:) \equiv \{660, 0, 0, 0, 0\}\mathfrak{C}, \end{aligned} \tag{28}$$

together with

$$\begin{aligned} &\{\chi_i\}(:8, 3, 1:) \equiv \{1980, 0, 0, 0, 0\}\mathfrak{C}, \\ &\{\chi_i\}(:8, 2, 2:) \equiv \{2970, 30, 0, 0, 0\}\mathfrak{C}, \end{aligned} \tag{29}$$

which leads for $F^\dagger \equiv \{A, G, H, T_1, T_3\}$ [66] to the realizations

$$\begin{aligned} &:10, 1, 1: \to \{\{3, 8, 11, 7, 7\}F \mid \chi_{C_2} = 2\} \\ &:8, 2, 2: \to \{\{57, 198, 255, 141, 141\}F \mid \chi_{C_2} = 30\} \end{aligned} \tag{30}$$

$$\begin{aligned} &:6, 4, 2: \to \{\{246, 924, 1170, 678, 678\}F \mid \chi_{C_2} = 60\} \\ &:6, 3, 3: \to \{\{312, 1236, 1536, 924, 924\}F \mid \chi_{C_3} = 12\} \end{aligned} \tag{31}$$

$$\begin{aligned} &:5, 5, 2: \to \{\{278, 1108, 1386, 832, 832\}F \mid \chi_{C_5, C_5'} = 2\} \\ &:4, 4, 4: \to \{\{60, 2310, 2910, 1710, 1710\}F \mid \chi_{C_2} = 90\} \end{aligned} \tag{32}$$

where the result of the rotational operation itself is derived from a combinatorial formalism, or monomial-like product of such terms. From the $SU4 \times \mathscr{S}_{12}$ 4-tuples, one obtains (for example) the following mappings:

$$:9, 1, 1, 1: \rightarrow \{22, 88, 110, 66, 66\}F$$
$$:8, 2, 1, 1: \rightarrow \{99, 396, 495, 297, 297\}F \quad (33)$$

$$:7, 3, 1, 1: \rightarrow \{264, 1056, 1320, 792, 792\}F$$
$$:7, 2, 2, 1: \rightarrow \{396, 1584, 1980, 1188, 1188\}F \quad (34)$$

$$:6, 3, 2, 1: \rightarrow \{924, 3696, 4620, 2772, 2772\}F$$
$$:6, 2, 2, 2: \rightarrow \{\{1416, 5544, 6960, 4124, 4128\}F | \chi_{C_2} = 120\} \quad (35)$$

$$:5, 5, 1, 1: \rightarrow \{\{556, 2216, 2772, 1664, 1664\}F | \chi_{C_5, C_5'} = 4\}$$
$$:3, 3, 3, 3: \rightarrow \{\{6168, 24648, 30792, 18480, 18480\}F | \chi_{C_3} = 24\} \quad (36)$$

8.2. Specific higher invariants over subduced spin symmetries

It is of interest to compare Casimir invariants associated with even-rank tensorial properties and Rota invariants over a field, of for example $(M_1, \ldots, M_n)$ in Hilbert space or $(k_1, \ldots, k_n)$ (with $\Sigma k_i = k$) over Liouville space, associated with individual spin inner set z projection. The use of projective geometric views allowing for the existence of higher regular solids, other than those invoked in Ref. [16], for which $\{\chi_i\}$, $:1^6: \equiv \{720, 0, 0, 0, 0\}(\mathscr{S}_6 \downarrow \mathscr{O})$. The regular icosahedron and dodecahedron 3-spatial structures provide additional insight into the properties of the various maximally branched p-tuples from, for example, $:2^6:$ under the duality $SU(6) \times \mathscr{S}_{12}$, or of $:3^6 11:$ under $SU(8) \times \mathscr{S}_{20}$ of Fig. 5, both of which contribute to their corresponding $M = 0$ subspaces.

Here, we note that there are six distinct C_2 pairs of spin sites under simple icosahedral symmetry and a similar number of sets of equivalent C_3 sites for the 20-fold dodecahedral subduced symmetry, as shown in Fig. 5, i.e. within a simple

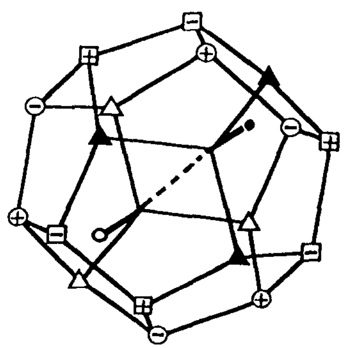

Fig. 5. A mathematical model for $\{\chi_i\}$ of the module and scalar invariant $:3^6 11:$ $(SU8 \times \mathscr{S}_{20} \downarrow \mathscr{A}_5)$ as a determinable invariance set. One further analogous projective geometry derived from a higher regular solid is known [49]. Reproduced with permission from Ref.[49a].

mathematical labelling. Inclusion of the specific "on"-C_3 axis labels introduces an extra factor of 2; simple combinatorial logic allows one to deduce the following invariance and irreps sets associated with the two p-tuples:

$$\begin{aligned}&\{\chi_i\}, :2^6:(\mathrm{SU6} \times \mathscr{S}_{12}{\downarrow}\mathscr{A}_5) = \{7\,484\,400, 6!, 0, 0, 0\}\mathfrak{C}\\&\Gamma(\mathscr{S}_{12}{\downarrow}\mathscr{A}_5) = \{124\,920A, 498\,960G, 623\,712H, 727\,640(T_1 + T_3)\}\end{aligned} \tag{37}$$

or

$$\begin{aligned}&\{\chi_i\}, :3^6 11:(\mathrm{SU8} \times \mathscr{S}_{20}{\downarrow}\mathscr{A}_5) = \{52\,145\,533\,440\,000, 0, 2 \times 6!, 0, 0\}\mathfrak{C}\\&\Gamma(\mathscr{S}_{20}{\downarrow}\mathscr{A}_5) = \{869\,092\,224\,480A, 3\,476\,368\,896\,240G, 4\,345\,461\,119\,760H,\\&\qquad 2\,607\,276\,672\,000(T_1 + T_3)\}\end{aligned} \tag{38}$$

where the identity is simply

$$6! \equiv \binom{6}{5}\binom{5}{4}\binom{4}{3}\binom{3}{2}\binom{2}{1}.$$

Clearly, the use of these higher projective geometries for multisite problems allows one to deduce many aspects of the dual symmetry chain $\mathrm{SU}(m = n) \times \mathscr{S}_n \supset \mathrm{SU}(m = n/2) \times \mathscr{S}_n \supset \mathscr{S}_n \supset \mathscr{S}_n{\downarrow}\mathscr{A}_5$ and its associated properties.

Invariants of these higher dualities are especially pertinent to the NMR of cage boranes and exo cage clusters, as well as for $\mathrm{t} - \mathscr{I}$ fullerenes discussed in the next section. For all these $n \gg 6$ spin cluster problems, adoption of the non-ME condition is a necessity. Indeed, the ME constraint [16] is an unphysical restriction in the high n-fold cluster limit. An additional step in the symmetry subduction chain may be included where the spectra are deceptive–simple. This would apply to NMR spectra derived from strictly localized $\{J_{ij}\}$ cluster interactions.

8.3. Specific $\{[\lambda] \rightarrow \Gamma(\mathscr{S}_n{\downarrow}\mathscr{G})\}$ subductive mappings

A comparison of the two earlier mappings allows one to derive the $\{p \leqslant 4, \ldots,$ irrep to $\Gamma(\mathscr{S}_{12}{\downarrow}\mathscr{A}_5)\}$ subductive mappings, such as $\{[\lambda](\mathscr{S}_6) \rightarrow \Gamma(\mathscr{S}_6{\downarrow}\mathscr{O})\}$, presented in Ref. [49].

In contrast, the corresponding subductive mappings [12] for $\mathrm{SU}(m) \times \mathscr{S}_{12}$ take the forms

$$\begin{pmatrix}[11, 1]\\ [10, 2]\\ [10, 1, 1]\end{pmatrix} \rightarrow \begin{pmatrix}(-, -, 1, 1, 1)\\ (2, 4, 6, 1, 1)\\ (-, 4, 3, 4, 4)\end{pmatrix} \Gamma(\mathscr{S}_{12}{\downarrow}\mathscr{A}_5 \equiv \mathscr{I}) \tag{39}$$

$$\begin{pmatrix}[9, 3]\\ [9, 2, 1]\\ [9, 111]\end{pmatrix} \rightarrow \begin{pmatrix}(2, 12, 10, 9, 9)\\ (4, 20, 28, 16, 16)\\ (5, 12, 14, 7, 7)\end{pmatrix} \Gamma \tag{40}$$

Table 9
Correlation and mapping of $[\lambda](\mathcal{S}_{12})$ irreps onto $\mathcal{S}_{12}\downarrow\mathcal{A}_5$ under a natural group embedding, after Ref.[12a]

	P. character	X_2	X_3	X_4	X_5	X_6	X_7	X_8	X_9	$A(\mathcal{S}_{12}\downarrow\mathcal{A}_5)$	G	H	T_1+T_3
[12]	1	1	1	1	1	1	1	1	1	1	—	—	—
[11, 1]	11	9	8	7	7	6	6	5	5	—	—	1	1
[10, 2]	54	36	27	20	22	15	14	9	10	2	4	6	1
[10, 11]	55	35	28	21	19	14	15	10	9	—	4	3	4
[9, 3]	154	84	49	28	42	21	14	5	10	2	12	10	9
[9, 21]	320	160	104	64	64	34	35	16	16	4	20	28	16
[9, 111]	165	75	57	35	21	15	20	10	5	5	12	14	7
[8, 4]	275	125	50	15	55	20	0	−5	5	7	17	28	10
[8, 31]	891	351	162	69	111	36	21	0	9	13	59	72	47
[8, 22]	616	224	112	56	56	14	21	5	4	18	42	56	25
[8, 211]	945	315	189	91	49	21	35	9	1	12	63	75	51
[8, 1111]	330	90	78	34	−6	6	15	5	−6	7	21	31	14
[7, 5]	297	117	27	−7	49	15	−13	−9	1	2	19	21	19
[7, 41]	1408	448	112	0	128	28	−22	−16	0	24	96	116	70
[7, 32]	1925	525	140	35	105	0	0	−5	−5	27	127	158	100
[7311]	2376	576	216	56	56	6	1	−9	−4	46	158	204	113
[7221]	2079	441	189	77	7	−21	14	0	−5	32	139	171	106
[72111][a]	1728	288	216	64	−64	−6	13	0	−16				
$[7, 1^5]$[a]	462	42	84	14	−42	0	7	1	−14				
[6, 6]	132	48	6	−8	20	6	−8	−4	0	10	10	14	2
[6, 51]	1155	315	21	−49	91	21	−35	−11	−1	16	75	97	59
[6, 42]	2673	567	0	−63	117	0	−27	0	−9	55	179	234	122
[6, 411]	3080	560	56	−56	56	14	−35	−9	4	42	206	246	164
[6, 33]	1650	300	−15	−20	50	−15	0	5	−10	21	114	123	93
[6, 321]	5632	768	64	0	0	−48	−8	0	0	95	374	475	279
[6, 222]	1925	175	35	35	−35	−35	0	0	5	43	131	166	88
[6, 2211][a]	3564	216	162	48	−132	−36	−6	0	0				
$[6, 21^4]$[a,b]	2100	0	210	0	−140	0	0	0	−20				
$[6, 1^6]$	462									$[1^{12}]\otimes[71^5]$			
[5, 52]	1320	240	−48	−56	56	6	−15	5	−4	14	90	98	76

[5, 511]	1485	225	−27	−55	29	15	−20	0	5	36	99	135	63
[543]	2112	288	−120	−64	64	−6	7	16	−16	35	136	183	103
$[5321^2]$[b]	7700	0	−70	0	−140	0	0	0	20				
[444]	462	42	14	−14	14	0	7	5	−6	17	34	39	19
[4422][a,b]	2640	0	−168	0	16	0	20	0	0				
[3333]	462										$[1^{12}]\otimes[444]$		

For completeness the initial aspects of the character algebra under the $\mathscr{S}_{12}$ group and its associated (X_i) cycle–class algebra are given. The absence of modular model degeneracies prior to the first SA λ partition underlies the validity and determinacy of these mappings onto $\mathscr{S}_{12}{\downarrow}\mathscr{A}_5 \equiv \mathscr{I}$ for a natural group embedding into $\mathscr{S}_{12}$.

The character of $\mathscr{S}_{12}$ are from the work of Ziauddin [56]; [a]further details of the correlative aspects may be found in Ref. [12].

[b] SA irreps.

$$\begin{pmatrix}[8,4]\\ [8,3,1]\\ [8,2,2]\end{pmatrix} \rightarrow \begin{pmatrix}(7,17,28,10,10)\\ (13,59,72,47,47)\\ (18,42,56,25,25)\end{pmatrix} F \tag{41}$$

$$\begin{pmatrix}[8,211]\\ [8,1^4]\end{pmatrix} \rightarrow \begin{pmatrix}(7,12,63,51,51)\\ (7,21,31,14,14)\end{pmatrix} F \tag{42}$$

Higher $\mathrm{SU}(m \leqslant n/2) \times \mathscr{S}_n$ irreps may be determined in principle, where the unit vector F spans the set given in the context of relation (30). Table 9 provides a summary of some additional aspects of $\{[\lambda] \rightarrow \Gamma(\mathscr{S}_{12}{\downarrow}\mathscr{A}_5)\}$ subductions.

9. General combinatorial physics approach to SU2 × $\mathscr{S}_n{\downarrow}\mathscr{G}$ spin systems for exo cage models

For higher n-fold spin systems, the essential focus is on the non-ME semitopological limit [1], where the dominant symmetric group is linked to SU(m) by group duality. In this limit and for $n \geqslant 12, 20, 60$ $\mathscr{S}_n{\downarrow}\mathscr{A}_5 \equiv \mathscr{I}$ cage clusters, geometric considerations imply that the NMR spin sites are seen as being in apicial configurations, with respect to the specific axes associated with the edge-centred C_2, or face-centred C_3, rotational class operators of the $\mathscr{S}_{60_z 2}{\downarrow}\mathscr{A}_5 \equiv \mathscr{I}$ NMR spin symmetry group [12,18]. This realization allows a fuller exploitation of the purely combinatorial basis of NMR spin invariance of value to the enumeration of the $[^{13}C]_{60}$ and $[^{13}CF]_{60}$ fullerene spin systems.

In contrast to both the specialized subduced tensorial techniques, e.g. as discussed by Harter and Reimer [33] under the full molecular symmetry group, and the CI symmetric function approaches [13–15] (as utilized in the enumeration both of rovibrational statistics and of structural isomerism), the present focus is on group duality aspects of spin algebras, which essentially retain their permutation symmetry within the subduction chain for (group) duality. For these, the t-dodecahedrally-related dualities provide a $\mathscr{S}_n$ automorphic and totally combinatorial approach to spin invariance problems [18,36]. Further, such forms of subduction may be contrasted with the typical unit-operator-dominated (single group) Racah symmetry chain, i.e. that leads to the 3-space icosahedral group [66] for conventional non-spin molecular symmetries.

Additional material arises from consideration of group duality within the projective geometry of $\mathscr{S}_n{\downarrow}\mathscr{A}_5$ icosahedral spin symmetry [12], or from the viewpoint of "contracted" tensors [67] over the SO(3) group or physical finite groups, e.g. the $\mathscr{I}_h$ icosahedral group [66]. Conceptual use of the invariants of higher dualities, recently considered by Sullivan and Siddall [16] in the context of mapping onto the 3-space defined by Casimir invariants, together with the technique of $\mathscr{S}_n$ ITP formation, imparts further breadth to our understanding of group duality in the semitopological (non-ME) NMR spin cluster limit. The motivation for these ideas lies in their power to demonstrate the generality of the integer z properties of $\mathrm{SU}(m) \times \mathscr{S}_{60_z 2}$

dualities, beyond the case of $^{13}C_{60}$-fullerene, whose C_2, C_3, and C_5 central axis views are shown in Fig. 6, and in the equivalence between the algebraic view and a proof for integer z and the geometric construction of a subsequent figure (Fig. 7). Some contrasts between the latter $z \geqslant 1$ cases and the (highest) regular borane, $[BH]_{12}^{2-}$, and dodecahedrane, as spin cluster systems with $z = 1/5, 1/3$ values, are set out in Tables 10 and 11; however, these $z < 1$ cases only allow specific partial combinatorial invariance analyses.

10. Specific role of combinatorics over SU2 × $\mathscr{S}_{60z^2}{\downarrow}\mathscr{A}_5$ spin invariance, $z \leq 1$ cases

Utilizing the Balasubramanian viewpoint [1] and some of our earlier presentations [2,12,18] on invariance under SU(m) × $\mathscr{S}_n$ duality for $n = (6), 12, 20, 60$, one may derive a totally combinatorial form for the $\{\chi_l\}^M$, over $l \leqslant 5$, inherent in higher t-dodecahedral symmetries, since for $z \geqslant 1$ integer C_{60z^2} there is no coincidence between the spin site locations and the edge- (or face-) centred configurations of the rotational axes under class (cycle) operators of the invariance algebra over the cage spin symmetry.

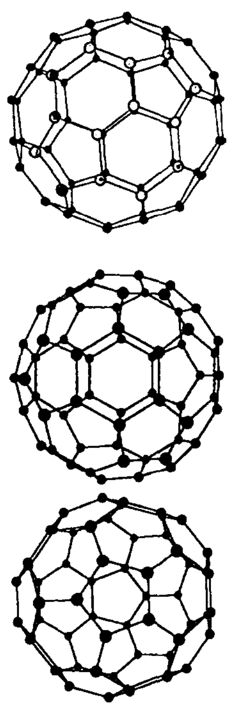

Fig. 6. Diagram showing the $\mathscr{I}_h$ structure of C_{60} fullerene as viewed along the C_2, C_3 and C_5 axes; note the separation between the 5-membered ring components of the structure. The symmetry axes are centred about mid-edge or face centre of the cage solid. (From Ref. [18] with permission.)

Table 10
The non-coincidence of spin site to rotational axes C_2, C_3, C_5 C_5' for the simple and higher (t-) dodecahedral symmetries of various fullerene structures leading to supermolecular fullerene $[^{13}C]_n$ spin clusters $n = 240, 250, 960, \ldots$ of the $n = 60z^2$ series for general integer z, discussed in the text

n	z, of $60z^2$	C_2	C_3	C_5, C_5'
	$z<1$			
12	$(1/5)^{1/2}$	0	0	1
20	$(1/3)^{1/2}$	0	1	0
	$z \geqslant 1$ [a]			
60	1	0	0	0
240	2	0	0	0
540, 960, ..., 2160	3, 4, ..., (6)	0	0	0

The utility of the analysis lies in its application to analogous bicluster spin systems, or to endohedral cluster problems.
(a) Edge-centred class operation; (b) face centred for all hexagonal–dodecahedral supermolecular models; (c) face centred via pentagonal "corners" of supermolecular forms.
[a] Focus here is on $z > 1$ aspects and proof of generality of these properties for integer z.

On utilizing //…// for the integer part of the quotient, the combinatorial generalizations become clear. For pure combinatorial aspects arising from non-coincidence of C_l axis and spin apicial site, these are based on odd–even parity under C_2 and $//i/2// = \mu$, or under the $\{+, -, 0\}$ set of triples in the sequence $\{//(i/3)// = \mu'$ (integer), $i/3 = \mu' + 1/3$ or $\mu' + 2/3\}$ under C_3, or over the quintuple set $\{+, -, 0, 0, 0,\}$ similarly associated with $i/5$ under $C_{5'}$ (C_5') rotational operators. Hence using the notation $\Delta\{\{\chi_l\}(\mathscr{S}_n)\}^{M-i}$ for $\{\chi_l\}^{M-i} - \{\chi_l\}^{M-(i-1)}$, as the subduced group class invariance is equivalent to a specific $[\lambda](\mathscr{S}_n)$ ($\equiv (\chi_l)$, $[\lambda]$ of Ref. [18]), within the structure of the UCG [41] SU(2) $\times\, \mathscr{S}_n$, one obtains the general combinatorial relationships. These first apply as partial descriptions for icosahedral, dodecahedral spin cluster invariance properties underlying the $(z<1)$ spin symmetries within decreasing $M-i$ weight sequence, with μ, μ', μ'' being incremental integer functions of i, in recursive derivation from $\{\chi_i\}^M = \{1, 1, 1, 1, 1\}$ (itself equivalent to $[n]$ for $n = 12, 20, 60, \ldots$), of

$$[\lambda] \equiv [n-i, i](\mathscr{S}_n) \equiv \Delta\{\{\chi_l\}\mathfrak{C}(\mathscr{S}_n \downarrow \mathscr{A}_5)\}^{M-i} \tag{43}$$

with

$$\Delta\{\{\chi_l\}\mathfrak{C}(\mathscr{S}_{12} \downarrow \mathscr{A}_5)\}^{M-i} = \left\{\binom{12}{i} - \binom{12}{i-1};\ \pm\binom{6}{\mu};\ \left\{\pm\binom{4}{\mu'}, 0\right\};\right.$$
$$\left\{+\binom{2}{\mu''}, +\binom{2}{\mu''}, -\binom{2}{\mu''}, 0, 0\right\},$$
$$\left.\left\{+\binom{2}{\mu''}, +\binom{2}{\mu''}, -\binom{2}{\mu''}, 0, 0\right\}\right\}\mathfrak{C}, \quad (M \geqslant)\ i \geqslant 1 \tag{44}$$

Table 11

$\{[n-m, m] \ldots \rightarrow \Gamma(\mathcal{S}_{n=60z^2} \downarrow \mathcal{A}_5 \equiv \mathcal{I})\}$: coefficients over $\{A, G, H, T_1 + T_3\}$ components

$[\lambda]$	$\mathcal{S}_{12}$ $z < 1$	$\mathcal{S}_{20}$	$\mathcal{S}_{60}$ $z = 1$	$\mathcal{S}_{240}$ (subset of $(\mathcal{S}_{60z^2})$) $(z > 1)$
$[n-1, 1]$	–, 1, 1, 1	–, 2, 1, 1	–, 4, 5, 3	3, 16, 20, 12
$[n-2, 2]$	2, 4, 6, 1	5, 11, 17, 6	36, 114, 150, 78	504, 1896, 2400, 1392
$[n-2, 11]$	–, 4, 3, 4	1, 11, 12, 11	22, 114, 135, 93	445, 1896, 2340, 1452
$[n-3, 3]$	2, 12, 10, 9	15, 65, 75, 50	540, 2170, 2690, 1630	37440, 149800, 187160, 112360
$[n-3, 21]$	4, 20, 28, 16	30, 126, 162, 96	1076, 4324, 5420, 3248	74864, 299536, 374480, 224672
$[n-3, 1^3]$	5, 12, 14, 7	20, 67, 81, 46	55, 2174, 2710, 1618	37503, 149816, 187240, 112312
$[n-4, 4]$	7, 17, 28, 10	75, 249, 318, 174	7659, 30221, 37900, 22562	2210676, 8835644, 11046400, 6624968
$[n-4, 31]$	13, 59, 72, 47	180, 754, 933, 574	22599, 90801, 113400, 68202	6625476, 26508924, 33134400, 19883448
$[n-4, 22]$	18, 42, 56, 25	145, 505, 655, 360	15360, 60580, 75920, 45220	—[a]
$[n-4, 211]$	12, 63, 75, 51	178, 762, 949, 584	22640, 90895, 113595, 68255	—[a]
$[n-5, 5]$	2, 19, 21, 19	166, 707, 879, 545	82794, 331587, 414381, 248805	103802196, 415215828, 519018024, 311413680
$[n-5, 41]$	24, 96, 116, 70	728, 2909, 3648, 2188	332164, 1328660, 1660804, 996484	415253752, 1661015096, 2076268840, 1245761296
$[n-5, 32]$	27, 127, 158, 100	915, 3705, 4620, 2790	415575, 1662515, 2078050, 1247000	—[a]
$[n-6, 6]$	10, 10, 14, 2	419, 1555, 1965, 1132	744446, 2973558, 3717814, 2229100	4047676808, 16190423328, 20238096976, 12142746472
$[n-10, 10]$	—	352, 1124, 1456, 778	—[a]	
$[n/2, n/2]$			$\chi_E = 3814987 \times 10^9$ $n = 60$	7512693×10^{62}; 4557960×10^{152}; 52160.5×10^{280} $n = 240$; $n = 540$; $n = 960$

Summary of mappings of various $\mathcal{S}_n$, $\mathcal{S}_{60z^2}$ groups onto their $\Gamma(\mathcal{S}_{60z^2} \downarrow \mathcal{A}_5)$ ($\equiv \mathcal{I}$, icosahedral group) irreps, contrasting the $z < 1$ clusters with the $z \geqslant 1, 2, \ldots, 5$ (integer) t-dodecahedral supermolecular clusters, which are relevant to the generality of the properties of integer z $60z^2$ clusters.

[a] Further $\mathcal{S}_n$ irrep correlative entries are omitted on account of their magnitudes.

$$\Delta\{\{\chi_l\}\mathfrak{C}(\mathscr{S}_{12}{\downarrow}\mathscr{A}_5)\}^{M-i}=\left\{\binom{20}{i}-\binom{20}{i-1};\ \pm\binom{10}{\mu};\ \left\{+\Delta',\binom{6}{\mu'},-\binom{6}{\mu'}\right\};\right.$$
$$\left.\left\{\pm\binom{4}{\mu''},0,0,0\right\},\left\{\pm\binom{4}{\mu''},0,,0,0\right\}\right\}\mathfrak{C},$$
$$\text{for } (M\geqslant)\ i\geqslant i,\ \Delta'=\binom{6}{\mu'}-\binom{6}{\mu'_{\text{prior}}} \tag{45}$$

and subsequently as a completely combinatorical form for fullerene under SU2 × $\mathscr{S}_{60}$

$$\Delta\{\{\chi_l\}\mathfrak{C}(\mathscr{S}_{60}{\downarrow}\mathscr{A}_5)\}^{M-i}=\left\{\binom{60}{i}-\binom{60}{i-1};\ \pm\binom{30}{\mu};\ \left\{\pm\binom{20}{\mu'},0\right\};\right.$$
$$\left\{\pm\binom{12}{\mu''},0,0,0\right\},$$
$$\left.\left\{\pm\binom{12}{\mu''},0,0,0\right\}\right\}\mathfrak{C}\quad (M\geqslant)\ i\geqslant 1 \tag{46}$$

where $\{\chi_l\}^M=\{1,1,1,1,1\}$ for the M maximal outer projective quantum number under SO2, l is over the $\mathfrak{C}$ class operator set and $0\leqslant M-i$ is a decreasing integer; in addition, $\mu=//i/2//$, $\mu'=//i/3//$, and $\mu''=//i/5//$ arise in the course of these recursive calculations. Due allowance has been made for the only non-combinatorial aspects implicit in the simple $\mathscr{S}_n{\downarrow}\mathscr{A}_5$ icosahedral or in the initial dodecahedral cluster symmetry, as a subset of the $n=60z^2$ series, for which z is clearly non-integer, i.e. 1/5 or 1/3, rather than integer as in the C_{60} case or in the higher $n\geqslant 240$ fullerenes with their $z\geqslant 2$ values. (A similar totally combinatorial analysis of $[^{13}C]_{24}(SU(2)\times\mathscr{S}_{24}{\downarrow}\mathscr{O})$ is possible [52], but no series of higher $\mathscr{O}$-fullerenes are envisaged.)

11. SU2 × $\mathscr{S}_{60z^2}{\downarrow}\mathscr{A}_5\equiv\mathscr{I}$, $z\geqslant 2$ integer, higher t-icosahedral spin dualities

From further consideration of the nuclear spin configurations, within respect to the structure of the supermolecular cage and the implied C_2, C_3, C_5 axes, one deduces the existence of continuity over $z=1,2,\ldots,5$, of the edge- or face-centred disposition of such axes within a set of extended t-dodecahedron structures, whose faces derive [68] from the generalized hexagonal forms of Fig. 7. For the $n=60z^2$ integer z series of fullerenes, this depicts the observed non-coincidence of the "spin site to C_j rotational axes" for $j=2,3,5$ which under SU(2) yield further generalized combinatorial relationships; for $^{13}C_{240}$ as the $z=2$ member this becomes

$$\Delta\{\chi_l\}^{M-i}=\left\{\left\{\binom{240}{i}-\binom{240}{i-1}\right\},\pm\binom{120}{\mu};\ \left\{\pm\binom{80}{\mu'},0\right\};\right.$$
$$\left.\left\{\pm\binom{48}{\mu''},0,0,0\right\};\ \left\{\pm\binom{48}{\mu''},0,0,0\right\}\right\}\mathfrak{C}\quad M\geqslant i\geqslant 1 \tag{47}$$

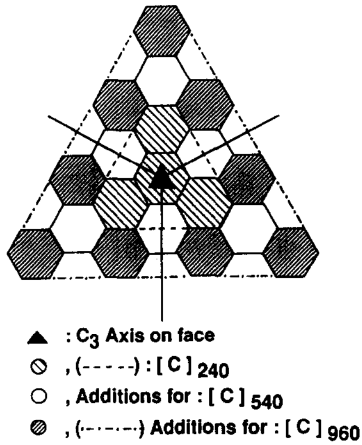

Fig. 7. A generalized hexagonally derived face for the z integer $n = 60z^2$ series of augmented t-dodecahedral supermolecular fullerenes: the specific diagram draws on the discussions given by McKay et al. [68]. Reproduced with permission from Ref.[36].

In general, the truncated-dodecahedral $t = 60z^2$, $z \geqslant 1$ fullerene spin invariance corresponds to

$$\Delta\{\chi_i\}^{M-i} = \left\{\left\{\binom{t}{i} - \binom{t}{i-1}\right\}, \pm\binom{t/2}{\mu};\ \left\{\pm\binom{t/3}{\mu'}, 0\right\};\right.$$
$$\left.\left\{\pm\binom{t/5}{\mu''}, 0, 0, 0\right\};\ \left\{\pm\binom{t/5}{\mu''}, 0, 0, 0\right\}\right\}\mathfrak{C}, \quad M \geqslant i \geqslant 1 \qquad (48)$$

In consequence these $\{\chi_i\}$ properties, i.e. both directly and from a consideration of the invariance products inherent in ITP algebras, allow the subduction from $\mathscr{S}_{60z^2}$ $(\mathscr{S}_{240}, \ldots)$ to $\mathscr{S}_{60z^2}{\downarrow}\mathscr{A}_5$ $(\mathscr{S}_{240}{\downarrow}\mathscr{A}_5$ etc), to be derived as shown in the last columns of Table 11.

Such tabulations also serve to contrast the simple icosahedral, dodecahedral $[A]_n$, $n = 12, 20$ clusters with the (augmented) fullerene spin clusters, $n = 60, 240$ etc. Examples of the outermost $p \leqslant 3, 4$ irreps for $[^2D]_n$ of $[^2D^{13}C]_n$, and for $[X(SU4)]_n$, $n = 60z^2$, are given for completeness. Such higher p-tuplar irreps are of special interest because of their role in Liouville formalisms of spin dynamics, for which $SU(m) \times \mathscr{S}_n$ dualities are over $p \leqslant m^2$, or 4, (9, 16), -tuplar structured irrep set. Presentation of the extreme members of the series, such as $SU(4) \times \mathscr{S}_{2160}$, or $SU(9) \times \mathscr{S}_n$, is restricted by the magnitude of their digital fields or, in the latter case, by the number of irreps in the lexicology represented by $p \leqslant 9$ (or 81) in the respective $\mathbb{H}$ (or $\tilde{\mathbb{H}}_v$) carrier spaces.

The use of conventional methods of determining invariance properties would prove tedious in the extreme if utilized for supermolecular or fullerene spin clusters. A fuller comparison between $z < 1$ and $z \geqslant 1$ dodeca- (t-) icosahedral spin systems is given in Ref. [36].

12. Higher invariants and the determinacy of natural embeddings, $\mathscr{S}_n{\downarrow}\mathscr{G}$: $n \geqslant (8, 12), 20$

From a consideration of the compatibility of a finite subgroup with an $\mathscr{S}_n$ group in which it is to be embedded, one naturally faces the question of the determinacy of the resultant $\mathscr{S}_n{\downarrow}\mathscr{G}$ spin algebras, as an extension of the determinacy [16] of higher $SU(m) \times \mathscr{S}_n$ Casimir invariants. A recent revised overview [9] of the $\mathscr{S}_8{\downarrow}\mathscr{O}$ ^{13}C-cubane problem [13b] serves to point out how the presence of degeneracy in the subduced invariance sets associated with $p \leqslant 5$-tuple modular models renders the subduced $\mathscr{S}_n{\downarrow}\mathscr{G}$ model indeterminate under this natural embedding. Subsequently, two criteria have been suggested on which the occurrence of determinate natural embeddings may be based [10]. The first of these is the need for a lack of any degeneracy in the model invariance sets associated with $SU(m \leqslant n/2) \times \mathscr{S}_n{\downarrow}\mathscr{G}$ modular models. The other criterion constitutes a reliable proof of the absence of indeterminacy; it utilizes the fact that under the multistep chain of $\mathscr{S}_n$-induced symmetry the subduced irrep sets, derived from the SA irrep of the original $\mathscr{S}_n$ group, $\lambda_{SA}(\mathscr{S}_n)$, retain the overall property of self-association over all $\mathscr{S}_n$ subgroups. In Ref. [10], we postulated that retention of this property for single-step subduction under natural embedding does not admit of the presence of either indeterminacy or significant degeneracy, i.e. in the λ dominance sector prior to the λ_{SA}. The difficulty with applying this criteria is that the λ_{SA} are located in the module region associated with $SU(m \sim n/2) \times \mathscr{S}_n$. An examination [12] of the modular models derived from $\mathscr{S}_{12}{\downarrow}\mathscr{A}_5 \equiv \mathscr{I}$ under these criteria supports the view that the (automorphic) icosahedral group lifts the prospect for any significant degeneracy; an indication of the multistep subduction process, from combinatorially derived induced symmetry irreps sets, over the $\mathscr{S}_{12} \supset \mathscr{S}_{11} \supset \ldots \supset \mathscr{S}_6 \supset \mathscr{S}_5$ subduction chain is given in Table 12, where $\mathscr{A}_5$ is a proper subgroup to $\mathscr{S}_5$. In the lower dominance sector of $\lambda_{SA} \trianglerighteq \lambda$ modules, the p-tuple models merely reflect the non-SR properties of these high unitary dual spin algebras, without giving rise to any indeterminacy in the model systems, in the present sense.

13. A brief introduction to some group theoretical aspects of Liouville space

The structure of Liouville space under group duality is determined by zeroth bilinear $\hat{\hat{L}} = [\hat{H}_0,]_-$ properties and its related $\tilde{\chi} = \chi^2 = \mathrm{tr}\,\mathscr{X}_c$ invariance terms over $\mathfrak{C}(\mathscr{S}_n)$, as in Refs. [11,25c], within the class superoperators $\mathscr{X}_c$ defined by

$$\mathrm{tr}\,\mathscr{X}_c \equiv X_c|kq\,v = (k_1 - k_n)\{\ldots\} >> X_c^\dagger \tag{49}$$

and where the spin cluster basis arises from the standard tensorial properties [25],

$$\hat{\mathscr{I}}^2|kqv>> \equiv \hat{\mathscr{I}}.\hat{\mathscr{I}}|kqv>> \equiv [\hat{I}\cdot[\hat{I}, |kqv>>]_-]_-$$
$$= k(k+1)|kqv>> \tag{50}$$

$$\hat{\mathscr{I}}_0|kqv>> = [I_0, |kqv>>]_- = q|kqv>> \tag{51}$$

Table 12
The induced-symmetry derived properties of the self-associated (#) $\mathscr{S}_{12}$ partitions for the alternative completely stepwise Racah chain group embedding of $\mathscr{I} \equiv \mathscr{A}_5$ in $\mathscr{S}_{12}$

$[\lambda_{SA}](\mathscr{S}_{12}) \supset \ldots$	$\supset \{[\lambda]\}(\mathscr{S}_9) \supset \ldots$	$\supset \{[\lambda]\}(\mathscr{S}_7) \supset \ldots$	$\supset \{[\lambda]\}(\mathscr{S}_5) \supset$	$\Gamma(\mathscr{S}_{12}{\downarrow}\mathscr{A}_5)$
		5 [6, 1]		
	[6, 21]	5 [5, 2]	35 [5]	70 A
	3 [6, 111]	20 [5, 11]	105 [4, 1]	210 G
	3 [5, 211]	10 [4, 21]	35 [3, 2]	70 H
$[6, 21^4]$#	6 $[5, 1^4]$#	30 [4, 111]#	140 [3, 11]#	140 $(T_1 + T_3)$
	3 $[4, 21^3]$	10 [3, 211]	35 [2, 21]	
	3 $[4, 1^5]$	20 $[3, 1^4]$	105 [2, 111]	
	$[3, 21^4]$	5 $[2, 21^3]$	35 $[1^5]$	
		5 $[2, 1^5]$		
		15 [5, 2]		
	3 [5, 31]	20 [5, 11]	35 [5]	70 A
	3 [5, 22]	15 [4, 3]	245 [4, 1]	490 G
	6 [5, 211]	60 [4, 21]	255 [3, 2]	510 H
[5, 3211]#	2 $[5, 1^4]$#	40 [4, 111]#	420 [3, 11]#	420 $(T_1 + T_3)$
	3 [4, 32]	30 [3, 31]	255 [2, 21]	
	6 [4, 311]	30 [3, 22]	245 [2, 111]	
	6 [4, 221]	60 [3, 211]	35 $[1^5]$	
	6 $[4, 21^3]$	20 $[3, 1^4]$		
	3 [3, 321]	15 [2, 221]		
	3 $[3, 31^3]$	15 $[2, 21^3]$		
	3 [3, 2211]			
	2 [4, 41]	10 [4, 3]		
	3 [4, 32]	20 [4, 21]	56 [4, 1]	112 G
	3 [4, 311]		140 [3, 2]	280 H
[4, 422]#	3 [4, 221]#	6 [4, 111]#	132 [3, 11]#	132 $(T_1 + T_3)$
	3 [3, 321]	20 [3, 31]	140 [2, 21]	
	2 [3, 222]	20 [3, 22]	56 [2, 111]	
		20 [3, 211]		
		10 [2, 221]		

An induced $\mathscr{S}_n$ symmetry approach leads to a group embedding under a Racah symmetry chain which is distinct from the natural embedding of $\mathscr{A}_5$ in $\mathscr{S}_{12}$.

for a single spin, and similarly for multispin problems using $\hat{\mathscr{F}}^2$, $\hat{\mathscr{F}}_0$ of $\mathscr{F} = \Sigma_i I_i$. The form of Eq. (51) implies that Liouville space of $\{|kqv>>\}$ is a direct product space. Hence,

$$\tilde{n}_\mu = \mathrm{tr}\, \mathscr{P}_\mu = (1/G) \sum g_i \chi_i^\mu\, \mathrm{tr}\, \{\mathscr{X}_\mu |kqv>>\} \quad (52)$$

applies, with G and g_i being the group and class orders respectively. Alternatively, one may use aspects of the $\mathscr{X}_i$ class superoperator, associated with projectors over Liouville space, directly in simple cases [25c], in the sense

$$\mathscr{X}_2 T^{kq}(11) = T^{kq}(11), \quad k \text{ even} \quad (53)$$

$$\mathscr{X}_2 T^{kq}(11) = -T^{kq}(11), \quad k \text{ odd} \quad (54)$$

for $\mathscr{X}_2$ a Liouville space permutational superoperator under $\mathscr{S}_2$, and finally

$$\mathscr{P}_{[\tilde{2}]/[\tilde{1}^2]} T^{kq}(11) = \delta_{[\tilde{2}],k:\mathrm{even}/[\tilde{1}^2],k:\mathrm{odd}}\, T^{kq}(11)$$
$$\mathscr{P}_{[\tilde{2}]/[\tilde{1}^2]} T^{0}(00) = \delta_{[\tilde{2}],k=0}\, T^{0}(00), \quad \text{where } \delta_{[\tilde{2}],k=1},\ \delta_{[\tilde{1}^2],k:\mathrm{even}} \text{ vanish}$$
$$\mathscr{P}_{[\tilde{2}]/[\tilde{1}^2]}(T^{1q}(10) \pm T^{1q}(01))/2^{1/2} = \delta(T^{1q}(10) \pm T^{1q}(01))/2^{1/2} \tag{55}$$

for

$$1 = \delta_{[\tilde{2}],+} = \delta_{[\tilde{1}^2],-}, \quad \text{or else } \delta_{\mu\pm} \text{ vanishes}$$

[8a], [25c]: here we have written out the Liouville basis as explicit tensors, whose matrix representation may be realized as shown in Table 13.

A more general technique exists where the invariance properties over the Hilbert space are already known; this uses a Latin square construction to derive $\tilde{n}_{[\tilde{\lambda}]} \equiv \mathrm{tr}\, \mathscr{P}_{[\tilde{\lambda}]}$. An example taken under $\mathscr{S}_4$ is shown in Table 14. Since this process implies that a progressive direct product is being formed, it follows that (for example) both the $[^2D^{13}C]_n$ biclusters and the Liouvillian direct product basis sets of spin dynamics are derivable from ITP considerations [2,19,20,58]. Further, this viewpoint means the $\mathscr{S}_n$ irreps over Liouville space will span the square of the number of Hilbert space components, while the form of $[\hat{\lambda}](\mathrm{SU}(m) \times \mathscr{S}_n)$ may be seen as spanning the full $p \leqslant m^2$-tuplar set in place of the $p \leqslant m$ structure of Hilbert space.

14. Mapping over distinct Liouvillian carrier subspaces $\{\tilde{\mathbb{H}}_v\}$

In addition, simple ITP arguments yield the $\mathrm{SU}(2) \times \mathscr{S}_n$ spin cluster irreps over Liouville space, which spans a ($p \leqslant 2^2$-tuplar) irrep spin space, in contrast to $p \leqslant 2$ irreps of Hilbert space; this is rendered SR on introducing the explicitly labelled $\tilde{\mathbb{H}}_v$ "superboson" carrier space [17,61] derived from the formal augmented mappings

$$\tilde{\mathbf{U}} \times \tilde{\mathscr{P}}(\tilde{\Gamma}): \tilde{\mathbb{H}} \to \tilde{\mathbb{H}}\{D^k(\tilde{\mathbf{U}}) \times \tilde{\Gamma}^{[\lambda]}(v) \mid \tilde{\mathbf{U}} \in \mathrm{SU}(2); \tilde{\mathscr{P}}(\tilde{\Gamma}) \in \mathscr{S}_n\} \tag{56}$$

where the SU2 recoupling term

$$v \equiv (k_1 - k_n)\{\tilde{\mathscr{K}}, \tilde{\mathscr{K}}', \ldots\}$$

defines the carrier space $\tilde{\mathbb{H}} \equiv \Sigma_v \tilde{\mathbb{H}}_v$. This comprises a set of distinct subspaces labelled by the ($\mathscr{S}_n$ democratic) recouplings v; these terms are now explicit aspects of the dual irrep hierarchy in the latter context, as well as affording a link between the two distinct component groups constituting the duality. Fig. 8 demonstrates the propagative aspects of Liouville space underlying relation (56).

In addition to the difficulties inherent in wider enumeration of ITPs of $n \geqslant 20$ $\mathscr{S}_n$ group irreps [2], there are more subtle problems concerning transformational aspects of higher dualities over the field of (bi)clusters within NMR spin dynamics, in that the v recoupling terms (as derived from a $\mathbf{Z}_{\alpha\beta}$ diagram, or other scheme) are now implicitly within the scope of $\mathscr{S}_n$-induced symmetry and democratic recoupling, topics contributing to the theoretical physics of many-body problems.

Table 13

Representations of the two spin 1/2 $\mathscr{S}_2$-adapted coupled multiple operators $T^{00}(11)$, $T^{2q}(11)$, $T^{1q}(\mathscr{A}/\mathscr{B}) = 2^{-1/2}[T^{1q}(10) \pm T^{1q}(01)]$ and $T^{1q}(11)$, in terms of $\mathscr{S}_2$-adapted Hilbert space components $\alpha\alpha$, $(\alpha\beta \pm \beta\alpha)/\sqrt{2}^{1/2}$, $\beta\beta$

$$\begin{array}{cccc} & (\alpha\beta+\beta\alpha)/\sqrt{2} & & (\alpha\beta-\beta\alpha)/\sqrt{2} \\ \alpha\alpha & \downarrow & \beta\beta & \downarrow \end{array}$$

$$T^{00}(11) = \frac{1}{\sqrt{12}} \left(\begin{array}{ccc|c} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & -3 \end{array}\right) \qquad T^{20}(11) = \frac{1}{\sqrt{6}} \left(\begin{array}{ccc|c} -1 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ \hline 0 & 0 & 0 & 0 \end{array}\right)$$

$$T^{10}(\mathscr{A}) = \frac{i}{\sqrt{2}} \left(\begin{array}{ccc|c} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ \hline 0 & 0 & 0 & 0 \end{array}\right) \qquad T^{11}(\mathscr{A}) = -i \left(\begin{array}{ccc|c} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 \end{array}\right)$$

$$T^{10}(\mathscr{B}) = \mathbf{0} \qquad T^{11}(\beta) = -i \left(\begin{array}{ccc|c} 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ \hline 0 & 0 & 0 & 0 \end{array}\right)$$

$$T^{10}(11) = \frac{1}{\sqrt{2}} \left(\begin{array}{ccc|c} 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right) \qquad T^{11}(11) = \frac{1}{\sqrt{2}} \left(\begin{array}{ccc|c} 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ \hline 0 & 0 & 0 & 0 \end{array}\right)$$

$$T^{21}(11) = \frac{1}{\sqrt{2}} \left(\begin{array}{ccc|c} 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 \end{array}\right) \qquad T^{22}(11) = \frac{1}{\sqrt{2}} \left(\begin{array}{ccc|c} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 \end{array}\right)$$

Note that the traces of the matrix representations vanish and that the $T^{kq}(\mathscr{A})$ exhibit no off-diagonal elements linking the subspaces of Hilbert space. The contrasting analogous representations in terms of primitive $\alpha\alpha$, $\alpha\beta$, $\beta\alpha$, $\beta\beta$ Hilbert components are summarized in Table A1 of Ref. [58]. After Table 5 of Ref. [58].

Table 14
The invariance hierarchy associated with the $[A]_4^{(l_i=1)}$ spin cluster under $\mathscr{S}_4 \Leftrightarrow T_d$ based on the relationship $\mathscr{P}_\mu(\mathscr{S}_4) \equiv \mathbf{P}(\otimes) : \mathscr{S}_4[x](\mathscr{S}_4)^\dagger$

$[A]_4^{(l=1)}: \|kqv>>$ $\{\tilde{\chi}_i\}^q(\mathscr{S}_4)$:	$q \to 8$ $\to \{1, 1, 1, 1, 1\}$	7 $\{8, 2, 0, 0, 4\}$	6 $\{36, 3, 4, 0, 12\}$	5 $\{112, 4, 0, 0, 24\}$	4 $\{266, 5, 10, 2, 42\}$
M $\downarrow$	4	3	2	1	0
	$\{\chi_i\}^M \to$				
−4	{1, 1, 1, 1, 1}	{4, 1, 0, 0, 2}	{10, 1, 2, 0, 4}	{16, 1, 0, 0, 4}	{19, 1, 2, 1, 5}
−3	{4, 1, 0, 0, 2}	{16, 1, 0, 0, 4}	{40, 1, 0, 0, 8}	{64, 1, 0, 0, 8}	
−2	{10, 1, 2, 0, 4}	{40, 1, 0, 0, 8}	{100, 1, 4, 0, 16}		
−1	{16, 1, 0, 0, 4}	{64, 1, 0, 0, 8}			
0	{19, 1, 2, 1, 5} etc.				

The $\{\tilde{\chi}_i\}^q$ and $\{\chi_i\}^M$ sets refer to Liouville and state space respectively. After Ref. [58].

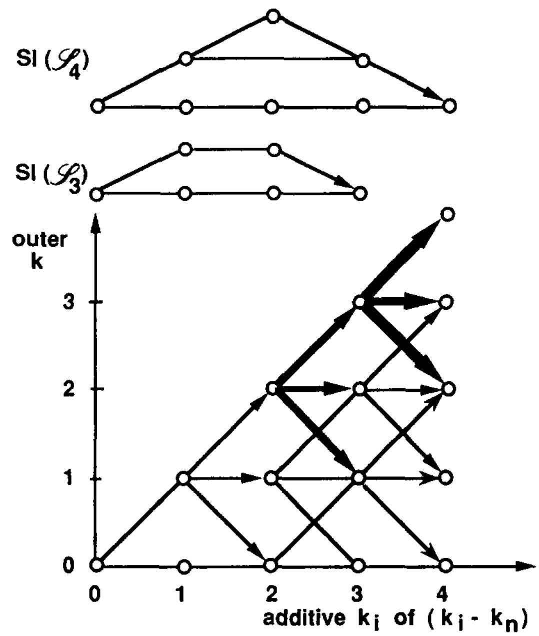

Fig. 8. Propagative $k_i - k_n$ recoupling over Liouville space of the $2 \leqslant n \leqslant 4, \ldots$ -fold spin 1/2 cluster. The diagram, after Ref. [69a], gives the pictorial forms for two scalar invariants. In addition, it incorporates a small correction to the original version.

As a consequence of the dominance of the Heisenberg-like term and its associated permutational properties, the case of NMR spin algebras for high n is quite distinct from that associated with, for example, the typical [53,54] electronic, nuclear structure, or conventional molecular physics problems [47], in that the invariance properties of higher n cluster NMR (originating from bilinearity of the dominant Heisenberg term) ensure the importance of the permutational and $\mathscr{S}_n$ automorphic viewpoint [1,2]. Indeed within the carrier subspaces there remain sets of subduced dualities which retain aspects of the universal covering dual group $SU(2) \times \mathscr{S}_n$ in regard to these v terms.

14.1. The role of induced symmetry in many-body democratic recoupling

The structure of Liouville space under group duality for higher n essentially is determined by zeroth bilinear $\hat{L} = [\hat{H}_0, \,]_-$ and related invariance terms. The permutational properties give a more explicit indication of the role of democratic recoupling under induced symmetry [17,55] which defines Liouville mapping formalisms [61]. Hence, analysis of the abstract augmented Heisenberg algebra for Liouville operators in such terms yields the ladder-like structure of Liouville space [61,69] and the v recoupling, as an explicit aspect of irrep structure inherent in mapping over the related carrier (sub)spaces. Indeed, the concepts derived from theoretical studies of spin monoclusters yield a better understanding of the nature of NMR coherent transfer [70] from the structure of coherent superpositional bases [8b] for homonuclear AGM ... X n-fold distinct (non-cluster) spin systems.

The recognition of $\tilde{\mathbb{H}}_v$ as distinct carrier subspaces of Liouville space has revived interest in the role of the $\mathscr{S}_n$ group with its implied generalized democratic recoupling for the v terms [17]. Hence these SU(2)–$\mathscr{S}_n$ cooperative relationships for v serve to link the various distinct literature contributions to the field of cluster spin dynamics. For instance, within $v \equiv (k_1 - k_n)\{\tilde{\mathscr{K}}, \ldots\}$ there are $n-2$ $\tilde{\mathscr{K}}$-type inner recoupling components; it would appear to be no accident that there are also precisely $n-2$ scalar invariants over a spin algebra and similarly $n-2$ component irreps within the multistep $\mathscr{S}_{n-1} \supset \mathscr{S}_{n-2} \supset \ldots \supset \mathscr{S}_3 \supset \mathscr{S}_2$ induced symmetry sequence describing the Racah chain. One is forced to the conclusion that many-body democratic recoupling, as an extension of the 1965–1972 work of Levy-Leblond and Levy-Nahas [38] and of Galbraith [39], may be equally well described by either scalar invariants or a set of irrep labels associated with the $\{\tilde{\mathscr{K}} \ldots\}$ aspects under induced symmetry. This well-founded comment does not appear to have been recognized prior to 1990 and the publication of Ref. [61] on Liouvillian mapping over the distinct carrier subspaces $\{\tilde{\mathbb{H}}_v\}$ whose propagative properties are given below; the induced stepwise build-up of distinct subspatial v labelling to $\mathscr{S}_4$ is exemplified by the v subspaces of Fig. 9, after Ref. [69a]. While under the dual UCG over Liouville space the dimensional order of the $\tilde{\mathbb{H}}_v$ subspaces for $v = (k_1 - k_n)\{\tilde{\mathscr{K}}, \ldots\}$, $k_i \leqslant 1$, arises naturally in a combinatorial form,

$$\|\tilde{\mathbb{H}}_v\| = \binom{n}{r} \prod_{i=1}^{r} (2k+1), \quad \text{for } v \sim (111_r 0_{r+1} 00_n) \tag{57}$$

for all higher dual algebras over Liouville space, no closed expression is known for the cardinality, $\|\tilde{\mathbb{H}}_v\|$. This difficulty arises from the non-SR nature of SU(m>2) spaces.

14.2. A few brief comments on practical multiple quantum (MQ) NMR aspects of spin clusters

Since the mid-1980s, applications concerning the Liouville NMR formalisms [25,70,71] over (high) q quantal subspaces of MQ NMR benefit from the realization that much of the information content of practical (bi)cluster MQ NMR systems is contained in a number of the outer weight q subspaces [72], without the need to examine the scalar invariants of all the lower q aspects. Indeed, similar interest in scalar invariants as replicative subspectra over Hilbert space was typical of the cw NMR era [4,42]. In addition to "rigid" exo cage, endohedral and similar ^{13}C met. car(b) clusters [9,73] (where Ref. [73] extends Ref. [13b]), or pure molecular dynamic wreath-product spin clusters, there exist interesting solid state plastic crystal-like clusters in which the distinction between intracluster, external lattice mode motions and even more general structural deformations may not be made.

A recent single-crystal publication from the Heidelberg NMR group [74] on bullvalene, $[^{13}CH]_{10}$, is typical of such cluster-like spin systems.

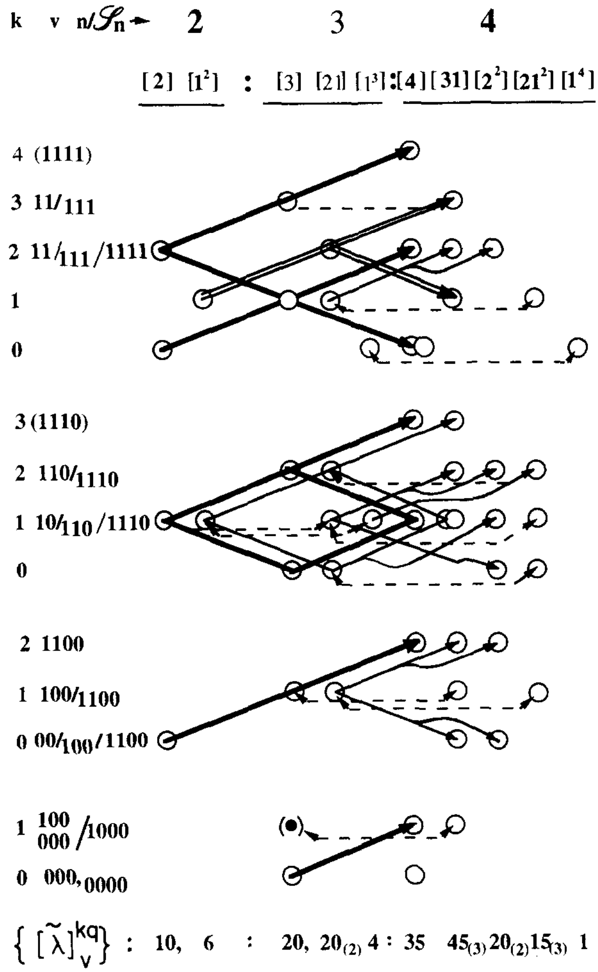

Fig. 9. A view of propagation and branching over specific $\hat{\mathbb{H}}_v$ carrier subspatial sets associated with SU2 × $\mathcal{S}_n$ Liouville spin space of $[A]_n$ clusters, from Ref. [69a] with permission; here v arises form recoupling which under democratic recoupling becomes associated with $\mathcal{S}_n$-induced symmetry.

15. Summary

The viewpoint adopted in the present work is based on the inherent structure [17–21] of group duality, with certain associated mappings over Liouville space [10,20], where the inner recoupling v term remains as a link between the distinct unitary $\mathcal{S}_n$ and $\mathcal{S}_n \downarrow \mathcal{G}$ groups [2,17,61].

Further background to these views will be found in recent discussions of democratic recoupling [17] within $\mathcal{S}_n$-induced symmetry [61], with its augmented space boson algebra [17], whereas Rota–Cayley algebra over $\{M_1 \ldots M_n\}^M$ sets, or $(\{k_1 \ldots k_n\})$ aspects of Liouvillian recoupling v terms, may be associated with p-tuples $(\mathcal{S}_n)$. These

"p parts of integer n" over the Hilbert space $\{M_i\}^M$ sets act both as SU(m) lexical inventories for $\{|IM(\ )>\}$ and as a way of characterizing the scalar invariants under the specialized direct product group SU($m \leqslant n$) $\times \mathscr{S}_n$. This review gives an overview of spin cluster NMR studies for $6 \leqslant n \leqslant 12, (20), 60, \ldots$ n-fold clusters for various SU(m) related identical spins. Since the Liouville aspects are related to certain ITPs [19] and technical aspects of NMR [70], we have considered Hilbert space aspects in more detail here to bring out the spin cluster aspects of NMR and of the modelling associated with these larger exo cage spin systems. Fuller details on applications of the CI symmetric function techniques may be found in the work of Balasubramanian [35,64,75–77]. Analogous NMR problems involving dynamical exchange processes between sites of high 3-space symmetry have been reviewed by Szymanski and Binsch [78] and subsequently developed further by Szymanski [79]. For reasons of brevity, no discussion of the fundamental wreath-product symmetries [22,77] is presented here; the latter extensive authoritative works of Balasubramanian should be consulted for their group theoretical insight into this aspect of NMR.

A summary of the $\chi^{[\lambda]}_{1^n}(\mathscr{S}_n)$ principal characters under groups associated with icosahedral or dodecahedral spin symmetries is given in Table 15, for its value in understanding the "structure" of spin cluster NMR. The range of p-tuple forms, for a specific $\mathscr{S}_n$ group of interest in the study of spin clusters, naturally suggests that a table of the $f(p, n)$ frequency factors for $\lambda \vdash n$ partitions (Table 16), should be included for reference purposes, where higher $f(p, n)$ factors may be found using the MAPLE computer package [80].

The physical insight gained from mapping and from the dominance order of $\lambda \vdash n$ partitions could not have been obtained directly by any other possible methods; the discerning reader will have noted that a couple of additional problems remain in fully incorporating high n clusters into Liouville formalisms [25]. Hence, the full $[AX]_n$ bicluster spin dynamics and relaxation problem has yet to be treated in that manner. In contrast, the value of the corresponding coherent superpositional Liouville bases (i.e. equivalent to bases for $\mathscr{S}_n$ monoclusters) in understanding coherence transfer phenomena has been stressed by Listerud et al. [70]. As a brief

Table 15
Some $\chi^{[\lambda]}_{1^n}$ principal characters of the higher fullerene-related symmetric groups as realized by the enumerative combinatorics associated with the idea of hook lengths [9,10,21,55][a]

n	$\|[n-1,1]\|$	$\|[n-2,2]\|$	$\|[n-2,11]\|$	$\|[n-3,3]\|$	$\|[n-3,21]\|$	$\|[n-3,111]\|$	$\|[n-4,4]\|$
12	11	54	55	154	320	165	275
20	19	170	171	950	1920	969	3705
60	59	1710	1711	32450	64960	32509	453415
240	239	28440	28441	2246600	4493440	...	132535060
540	539	144990	144991	25952850	51906240	...	3477609135
960	959	459360	459361	146535200	293071360	...	35021682640
1500	1499	1122750	1122751	560251250	1120540000	...	209533405375

[a] In accord with the combinatorial hook length techniques [59] discussed in earlier monographs and reviews [22,55].

Table 16
The $f(p:n)$ frequencies for λ partitions of $n = 12, 20, (28), 36, 60$ subdivided into p distinct parts, of $p \leqslant 16$

n	$p=2$	3	4	5	6	7	8	9	10	11	12	13	14	15	16		$P(n)$
8	4	5	5	3	2	1	1										22
12	6	12	15	13	11	7	5	3	2	1	1						77
20	10	33	64	84	90	82	70	54	42	30	22	15	11	7	5	3	627
28	14	65	169	291	391	436	434	393	340	278	224	174	135	101	77	56	3718
36	18	108	351	748	1206	1579	1801	1845	1761	1586	1380	1158	957	602	488		17977
60	30	300	1575	5260	12736												966467

postscript to this review, we mention a few 3-space symmetry aspects which have acquired significance [30–32,66,81–86] as a result of work on $\mathcal{S}_n$ cluster molecules.

The strongly interdisciplinary nature of the body of the review precludes any attempt at completeness in the references; selection has been governed solely by the need to give representative examples of the subtopics presented.

Acknowledgements

The author is indebted to Professor H.W. Kroto (University of Sussex, UK) for several brief general comments, reprints and for his enthusiasm for the field of fullerenes, to Professor K. Balasubramanian (University of Arizona, Tempe) and to Professor R.B. King (University of Georgia, Athens) for a couple of useful brief comments on applications of combinatorics and on practical aspects of the higher symmetric groups; also, I am indebted to K.B. for a number of useful additional references. In addition, an anonymous *Journal of Mathematical Physics* reviewer is especially thanked for his insightful brief comments, in particular those on permutational modules of the $\mathcal{S}_n$ group. The author is appreciative of continuing contact with a number of Canadian theoretical chemical physicists and with his long-time European neutron scattering colleagues. Finally, the Natural Science and Engineering Research Council (NSERC) of Canada is thanked for their support of the original molecular physics work of the author in this area. The permission extended to us by North-Holland, Springer-Verlag and Taylor and Francis to reproduce figures subject to their copyright is greatfully acknowledged.

Notation

$\mathcal{A}_n$, an Alternate Group.
$\mathcal{P}$, $\mathcal{P}_{[\tilde{\lambda}]}$, Projection operators in distinct spaces.
$\mathcal{S}_n$, a Symmetric Group.
$T^{kq}(11..) \equiv T^{kq}(v)$, a recoupled tensor.
$[\lambda']$, an irrep of $\mathcal{S}_n$ group.
k, k_i, outer (inner) tensorial ranks.
$:\lambda:$, a model p-tuple, or $\mathcal{S}_n$ module.
$\mathbb{Z}(\mathcal{S}_n)$, Character table for $\mathcal{S}_n$.
q, z-projection or weight (Liouville space).
$\mathbb{H}$, $\tilde{\mathbb{H}}_v$, Hilbert (Liouville) carrier spaces.
M, z-projection or weight (Hilbert space).
$\lambda|$-n, a partition of n.
$\tilde{\mathcal{K}}$, a recoupling term from k_is.
$\otimes$, direct product in group theory.
v, a generic all-embracing recoupling term.
$\downarrow$, Group Subduction.
|, 'for which' (in context of mapping).

$\supset$, 'contains' as defining a symmetry chain.
X_i, a cycle operator of $\mathcal{S}_n$ algebra.
$\trianglerighteq$, Dominance order, of $\{[\lambda']\}$.
$\Lambda_{\lambda[\lambda']}$, a Kostka coefficient of module decomposition.
$\|..\|$, cardinality, or order.
$//i/5//$, integer part of quotient.
$\binom{n}{r}$, combinatorial term.
$p \leq m$, the number of parts of $\lambda|$-n in $SU(m)$ branching.
$\longrightarrow >$, a mapping (onto).
λ_{SA}, $\lambda(\#)$, self-associate irreps of $\mathcal{S}_n$.
g_i, class, or cycle, order.
$\in$, 'element of'.
$\varepsilon_i^{:\lambda:}$, permutational invariance of $:\lambda:$ over cycle algebra, X_i.
$\{\chi_i\}$, χ_{C_i}, invariance under group: (a) as a set over classes; (b) for specific cyclic class.
$\chi_{1^n}^{[\lambda]}(\mathcal{S}_n)$, principal characters of $\mathcal{S}_n$.
$\mathfrak{C}$, unit (col.) vector over cycles, or classes.
$\mathfrak{L}$, unit (col.) vector over irrep set, $\{[\lambda']\}$.
F, unit (col.) vector over irrep set of finite group.
Γ, a representation of a finite group.
$\mathcal{G}$, $\mathcal{O}$, $\mathcal{I}$, general and specific finite groups.
$\{/\}$, a set of.

Appendix A: Some 3-space symmetry-related aspects of C_{60} fullerene

As a more general physical science addendum to the review, we draw attention to several 1994 reviews and reports of work in 3-space symmetry-related areas of pertinence of C_{60} fullerenes and $\mathcal{I}$ ($\mathcal{I}_h$) symmetry. The nature of $SO(3) \rightarrow \mathcal{I}_h$ correlations has been given by Fowler and Woolrich [81] and by Weekes and Harter [66b]; interest in the molecular dynamics of C_{60} has been considerable with fundamental papers by Ceulemans and co-workers [31] and others on breathing modes of shell-like cages and extensive inelastic incoherent neutron investigations [32] utilizing the spin-dependent cross-section to overcome the symmetry-forbidden nature of specific modes in other conventional spectroscopic techniques. Axe et al. [82] have presented an exhaustive review of these aspects of the molecular physics of C_{60} fullerene, while the phonon density of states work from coherent neutron scattering and studies of the electronic structures of alkali metal fullerides have been surveyed by Picketts [83]. The development of icosahedral (spherical) harmonic formalism by Weekes and Harter [66a,b] deserved to be mentioned. Theoretical spectroscopic work of $M@C_{60}$ with M = He, Li by a Canadian group [84] and calculations [85] of the polarizability of C_{240} (a cluster discussed in the main text) are notable contributions with a high symmetry content; finally, work on NMR spin rotational relaxation of C_{60} by Walton et al. [86] is particularly pertinent to aspects of the above discussion concerned with Liouville formalisms for NMR spin dynamics [25].

References

[1] K. Balasubramanian, Chem. Rev., 85 (1985) 599; J. Chem. Phys., 78 (1983) 6358; 73 (1980) 3321.
[2] F.P. Temme, Chem. Phys. Lett., 200 (1992) 534.
F.P. Temme and J.P. Colpa, Z. Phys. D, 25 (1992) 275.
[3] D.R. Whitman, J. Mol. Spectrosc., 10 (1962) 1372.
[4] R.G. Jones and S.M. Walker, Mol. Phys., 10 (1965) 349.
R.M. Lynden-Bell, Mol. Phys., 15 (1968) 529.
[5] G.-C. Rota, Finite Operator Algebra, Academic Press, New York, 1976.
[6] P. Doubilet, G.-C. Rota and J. Stein, Stud. Appl. Math., 53 (1974) 185.
[7] L.C. Biedenharn and J.D. Louck, Theory of Angular Momenta, Theory and Applications, Vol. 8, Wigner–Racah Algebra, Vol. 9, Cambridge University Press, Cambridge, 1982, 1985; The Permutation Group in Physics and Chemistry, Springer, Berlin, 1979.
[8] (a) F.P. Temme, J. Magn. Reson., 83 (1989) 383.
(b) J.P. Colpa and F.P. Temme, Mol. Phys., 74 (1992) 953.
[9] J.P. Colpa and F.P. Temme, Physica A, 209 (1994), 140.
[10] F.P. Temme, Chem. Phys. Lett., (1995), to be published.
[11] F.P. Temme, Chem. Phys., 132 (1989) 9.
[12] (a) F.P. Temme, Mol. Phys., (1995), in press.
(b) J.P. Colpa and F.P. Temme, in M. Mehring (ed.), Proc. Colloq. AMPERE XXV, Stuttgart, 1990, Springer, Berlin, 1990, p. 1691.
[13] (a) K. Balasubramanian, Chem. Phys. Lett., 183 (1992) 292.
(b) K. Balasubramanian, K.S. Pitzer and H.L. Strauss, J. Mol. Spectrosc., 93 (1982) 447.
[14] K. Balasubramanian, Chem. Phys. Lett., 200 (1992) 649; 210 (1993) 153.
[15] K. Balasubramanian, J. Mol. Spectrosc., 157 (1993) 254.
[16] J.J. Sullivan and T.H. Siddall III, J. Math. Phys., 33 (1992) 1964; J. Phys. Chem., 96 (1992) 5789, and references cited therein.
[17] F.P. Temme, Z. Phys. B, (1995); Physica A, 198 (1993) 245.
[18] F.P. Temme, C.E.J. Mitchell and M.S. Krishnan, Mol. Phys., 79 (1993) 953.
[19] F.P. Temme, J. Math. Chem., 13 (1992) 153.
[20] (a) G.D. James and A. Kerber, Representations of $\mathcal{S}_n$ Groups, Vol. 16, Cambridge University Press, Cambridge, 1985.
(b) G.D. James, Symmetric Group Representations, Notes in Mathematics 682, Springer, Berlin, 1976.
[21] B.E. Sagan, The Symmetric Group, its Representation, Combinatorial Algorithms, Functions and Wadworth-Cole, Pacific Grove, CA, 1991.
[22] K. Balasubramanian, J. Chem. Phys., 95 (1991) 8273, and references cited therein; Theor. Chim. Acta, 59 (1981) 237.
[23] H.C. Longuet-Higgins, Mol. Phys., 6 (1963) 445.
[24] D. Dubbers, Z. Phys. A, 276 (1976) 245.
[25] (a) B.S. Sanctuary and T.K. Halstead, Adv. Opt. Magn. Reson., 15 (1991) 97.
(b) I. Furo, B. Halle and T.C. Wong, J. Chem. Phys., 89 (1988) 5282.
(c) B.C. Sanctuary and F.P. Temme, Mol. Phys., 55 (1985) 1049; 58 (1986) 659.
[26] A. Heidemann, in T. Springer, R. Richter, A. Magerl and A. Heidemann (eds.), Quantum Aspects of Molecular Motions in Solids, Springer, Berlin, 1987, p. 44.
[27] W. Press, Single Particle Rotations in Molecular Crystals, Springer, Berlin, 1982.
[28] H. Blank and G.R. Kearley, Quantum Rotational Motions Conf., Rottach-Ergen, Bavaria, April 1991.
[29] S. Clough, Phys. Rev. A, (1995), to be published.
S. Clough, A.J. Horswell and M. Johnson, Chem. Phys. Lett., 208 (1993) 143; Mol. Phys., 78 (1993) 781.
[30] J.W. White, G. Liddell, L. Pang, D. Sivia and J. Tomlinson, Chem. Phys. Lett., 191 (1992) 92.
[31] A. Ceulemans, P.W. Fowler and I. Voss, J. Chem. Phys., 100 (1994) 5491.
F. Negri, G. Orlandi and F. Zerbi, Chem. Phys. Lett., 196 (1992) 303.

[32] R.L. Cappelletti, J.R. Copley, W. Kamitakahara, L. Fang, J.S. Lannin and D. Ramage, Phys. Rev. Lett., 66 (1991) 3261.
C. Coulombeau, H. Jobic, P. Bernier, C. Fabre, D. Schutz and A. Rasset, J. Phys. Chem., 96 (1992) 22.
K.P. Prassides, T. Dennis, J.P. Hare, J. Tompkinson, H.W. Kroto, R. Taylor and D.R. Walton, Chem. Phys. Lett., 187 (1991) 455.
[33] W.G. Harter and T.C. Reimer, Chem. Phys. Lett., 198 (1992) 429.
[34] (a) K. Balasubramanian, Chem. Phys. Lett., 197 (1992) 55; J. Mol. Spectrosc., 157 (1993) 254.
(b) A.A. Bliznizyk, M. Shen and H.F. Schaefer, Chem. Phys. Lett., 198 (1992) 249.
[35] K. Balasubramanian, Chem. Phys. Lett., 202 (1993) 217.
[36] F.P. Temme, Physica A, (1995) in press.
[37] V. Krishnamurthy, Combinatorics, its Theory and Application, Ellis Horwood, Chichester, 1988.
[38] J.M. Levy-Leblond and N. Levy-Nahas, J. Math. Phys., 6 (1965) 1372.
[39] H.W. Galbraith, J. Math. Phys., 12 (1972) 782.
[40] N.C. Pyper, Mol. Phys., 21 (1971) 1; 22 (1971) 433.
[41] P.L. Corio, Structure of High-resolution NMR Spectra, Academic Press, New York, 1966.
[42] (a) R.J. Jones, R.C. Hirst and H.J. Bernstein, Can. J. Chem., 43 (1965) 683.
(b) R.J. Jones, Principles Prog. NMR, 1 (1967) 1.
[43] A.J. Coleman, Induced Representations on $\mathbb{C}$ for $\mathcal{S}_n, \mathcal{GL}_n$ Groups, Vol. 4, Queen's Mathematics Publications, Kingston, 1964.
[44] R.L. Flurry and T.H. Siddall III, Phys. Rev. B, 31 (1985) 4513.
R.D. Kent, M. Schlessinger, P. Ponnapoulis, Phys. Rev. B, 31 (1985) 1253.
[45] T.H. Siddall III, J. Phys. Chem., 86 (1982) 91.
[46] Q. Zhang and X. Li, J. Phys. A, 20 (1989) 6185.
[47] K.-W. Tung, Group Theory in Physics, World Scientific Publishers, Singapore, 1988.
[48] F.P. Temme, Physica A, 166 (1990) 685.
[49] (a) F.P. Temme, Physica A, 202 (1994) 595.
(b) J.P. Colpa and F.P. Temme, Chem. Phys., 154 (1991) 97.
[50] G.E. Andrews, Theory of Partitions, Addison Wesley, Reading, MA, 1976.
[51] A.Z. Mekjian and S.J. Lee, Phys. Rev. A, 44 (1992) 6294.
[52] F.P. Temme, Chem. Phys. Lett., (1995) in press.
[53] M. Moshinsky, Many-body Problem, Gordon and Breach, New York, 1964.
[54] L.C. Biedenharn and J.D. Louck, Adv. Quantum Chem., 23 (1993) 120.
[55] A.J. Coleman, Adv. Quantum Chem., 4 (1968) 81.
[56] M. Ziauddin, Proc. London Math. Soc., 42 (1936) 340.
[57] X. Liu and K. Balasubramanian, J. Comput. Chem., 10 (1989) 417.
[58] F.P. Temme, Mol. Phys., 66 (1989) 1075.
[59] J.S. Frame, G. de B. Robinson and R.M. Thrall, Can. J. Math., 6 (1954) 316.
[60] F.P. Temme, Physica A, 210 (1994) 435.
[61] F.P. Temme, Physica A, 166 (1990) 676.
[62] H. Kummer and R.G. McLean, Found. Phys., 24 (1994) 739.
[63] R.M. Lynden-Bell, unpublished work, 1968 (quoted by R.K. Harris and R.M. Lynden-Bell).
[64] K. Balasubramanian, J. Chem. Phys., 74 (1981) 6824.
[65] G. Ramachandran and M.V. Murthy, Nucl. Phys. A, 337 (1980) 629.
[66] (a) W.G. Harter and D.E. Weekes, J. Chem. Phys., 90 (1989) 4727.
(b) D.E. Weekes and W.G. Harter, Chem. Phys. Lett., 144 (1988) 366.
(c) F. Negri, G. Orlando and F. Zerbetto, Chem. Phys. Lett., 144 (1988) 31.
[67] J.A.R. Coope and R.F. Snider, J. Math. Phys., 11 (1970) 1103.
J.A.R. Coope, J. Math. Phys., 11 (1970) 1591.
[68] K. McKay, H.W. Kroto and D.J. Wales, J. Chem. Soc., Faraday Trans., 88 (1992) 2815.
[69] F.P. Temme, Z. Phys. B, 88 (1992) 83; J. Math. Phys., 32 (1991) 1638.
[70] J. Listerud, S.J. Glaser and G.P. Drobny, Mol. Phys., 78 (1993) 629.
S.J. Glaser and G.P. Drobny, Chem. Phys. Lett., 184 (1991) 553.

[71] M. Munowitz, Adv. Chem. Phys., 66 (1986) 1.
M. Munowitz and M. Mehring, J. Chem. Phys., 86 (1987) 3172.
[72] A. Pines, in B. Maravaglia (ed.), Proc. 100th E. Fermi Physics Institute, North-Holland, Amsterdam, 1988.
[73] F.P. Temme, Mol. Phys., 78 (1992) 747.
[74] A. Muller, U. Haeberlin, H. Zimmerman, R. Poupko and Z. Luz, Mol. Phys., 81 (1994) 1239.
[75] K. Balasubramanian, Mol. Phys., 80 (1993) 655.
[76] K. Balasubramanian, J. Phys. Chem., 97 (1993) 4647, 8736.
[77] K. Balasubramanian, J. Chem. Phys., 72 (1980) 665.
[78] S. Szymanski and G. Binsch, Annu. Rep. NMR Spectrosc., 23 (1991) 210.
[79] S. Szymanski, J. Magn. Reson. A, 108 (1994) 151.
S. Szymanski, Mol. Phys., 55 (1985) 763; 58 (1986) 439.
[80] S. Geddes (ed.), Handbook to "MAPLE" Symbolic Computing, Waterloo University Computer Science Publications.
[81] P.W. Fowler and J. Woolrich, Chem. Phys. Lett., 127 (1986) 78.
[82] J.D. Axe, S.C. Moss and D.A. Neumann, Solid State Phys., 48 (1994) 149.
[83] W.E. Picketts, Solid State Phys., 48 (1994) 225.
[84] C.S. Joslin, C. Gray, S. Goldman, J.D. Goddard and J.D. Poll, Chem. Phys. Lett., 213 (1993) 377.
C.G. Joslin, G.C. Gray, S. Goldman, J. Yang and J.D. Poll, Chem. Phys. Lett., 215 (1993) 144.
P.R. Birkett, H.W. Kroto, R. Taylor, D.R. Walton, R. Grose, P.J. Hendra and P.W. Fowler, Chem. Phys. Lett., 205 (1993) 399.
[85] B. Shanker and J. Applequist, J. Phys. Chem., 94 (1994) 6486.
[86] J.A. Walton, A. Kamese-Quashie, J.M. Joers and T. Gullion, J. Chem. Phys., 203 (1993) 237.