Some conjectures on $\mathcal{S}_n$-derived nuclear permutational (or NMR) spin encodings:

On existence of limiting $\mathcal{S}_n$-module decompositional sets for weak $(\lambda \vdash n)$-branching at high n; on Voronoi polyhedral dual as geometric analogues to Cayley's SU2 $\times\, \mathcal{S}_n{\downarrow}\mathcal{G}$ embedding theorem; and on SU$(m \geqslant 3) \times \mathcal{S}_n$ dual group with retention of self-associacy over subduced irrep set, as being the sufficient further condition to ensure the determinacy of SU$(m \geqslant 3) \times \mathcal{S}_n{\downarrow}\mathcal{G}$ embeddings *

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In the context of structures arising from nuclear permutation (NP) or NMR dual-group spin algebras, the first conjecture sets out the high-index n, and thus weak-branching limit (WBL), aspects of $:\lambda:(\mathcal{S}_n)$ module decompositions as giving rise to a set of numerical values for the associated Kostka coefficients which are invariant to further incrementation in the $\mathcal{S}_n$ index; the existence of such combinatorial limit properties, implicit in $\mathrm{sst}^{\lambda'}(\lambda)$ tableaux enumerations, has not been addressed in the mathematics literature to date. Conjectures 2 and 3 are concerned with the questions of geometric and sufficient algebraic realisations of the determinacy of natural finite group embeddings in specific SU$(m) \times \mathcal{S}_n$ permutation groups. In conjecture 2, the Voronoi dual-structures to the regular polyhedra for NP/NMR automorphic SU2 $\times\, \mathcal{S}_n{\downarrow}\mathcal{G}$ embedded spin symmetries hold the key to physical insight. Specifically, they provide a novel combinatorial geometric view of Cayley's theorem; the mid-face intersecting $(i \geqslant 3)$ C_i-axes of the initial NMR automorphic solids become (vertex) body-diagonal axes of the specific-dual Voronoi polyhedra, where a distinctness condition from the spin-sites gives raise to a geometric statement of Cayley's theorem. Conjecture 3 is concerned with SU$(m \geqslant 3) \times \mathcal{S}_n{\downarrow}\mathcal{G}$ embeddings for which the simple Cayley criterion alone is an *insufficient* condition to guarantee determinacy. The $\mathcal{S}_n$ self-associacy property and its retention over the subduced irrep-subset(s) (i.e., comparable to studies of $\mathcal{S}_n$ system-invariants via Yamanouchi–Gel'fand subduction chains) is now seen as indicative of retention of determinacy for such SU$(m \geqslant 3)\times\mathcal{S}_n{\downarrow}\mathcal{G}$ group embeddings through the above sufficiency condition.

* Dedicated to my long-time Manchester friend Joe Lee, on the occasion of his retirement and 67th birthday.

1. Introduction

In recent years, it has become clear that there exists an extensive body of theory [8–10,16,19,36] underlying physical and mathematical modellings which is associated with $\mathcal{S}_n$-encodings and which is of equal pertinence to several disciplines, and over various interdisciplinary areas. At first sight the models might seem unrelated, however, the study of encodings reveal subtle mathematical links. Our original discussions centred on nuclear permutational (NP), or NMR spin, algebras and on the determinacy of the invariants associated with NMR automorphic finite groups ($\mathcal{G}$, i.e., the rotational $\mathcal{D}_3, \ldots, \mathcal{O}, \mathcal{P}$ sub-groups of conventional molecular symmetries), as $\mathcal{S}_n{\downarrow}\mathcal{G}$ embeddings in specific permutation groups [24,27,29]. Balasubramanian's original assertion [2], on role of $\{J_{ij}\}$ intra-cluster coupling hierarchy as the automorphic structure of subduced NMR spin symmetry and its group embeddings, and our subsequent views of the nature of $\mathcal{S}_n{\downarrow}\mathcal{G}$ forms [23,25,28,34], have a wider significance in modelling applications.

This research note is essentially concerned with specific conjectures first utilised in physically-oriented NMR work; these are stated now in explicit forms to allow a better appreciation of their value (as part of discrete mathematical studies), as well as for their importance in wider modelling applications.

Our original interest was in modelling various NMR spin algebras associated with some large isotopomer exocage clusters, e.g., $[\mathrm{CH}]_{20}$ or $[\mathrm{BH}]_{12}^{2-}$; for $\mathrm{H} \equiv {}^1\mathrm{H}$ (^{2}H). It has developed since into a study of $\mathbf{M}^{\lambda} \equiv (:\!\lambda\!:)(\mathcal{S}_n)$ $\mathcal{S}_n$-module (Young rule) decompositions over $[\lambda']$ irreps [24,27–29] of $\{[\lambda']\}$ set, for all λ's preceding ($\trianglerighteq$) $\lambda \vdash n$ (math.) partition, and subsequently has grown into a study of the form and general determinacy [27,29] of automorphic NMR groups into specific $\mathrm{SU}(m) \times \mathcal{S}_n$ groups [24], i.e., *beyond* those $\mathrm{SU2}\times\mathcal{S}_n{\downarrow}\mathcal{G}$ bipartite mappings, for which Cayley's theorem $n(\mathcal{S}_n) = |\mathcal{G}|$, finite group cardinality is a sufficient condition to ensure determinacy of the natural group embedding, as part of a subduction process.

From this vantage point, it was natural to investigate the specific $\mathrm{SU}(m)$-branching of the dual group $\mathrm{SU}(m) \times \mathcal{S}_n({\downarrow}\mathcal{G})$ [27,29] and certain of the regular polyhedral invariants [23–25,28,34] associated with them. These automorphic forms are related to the Sullivan and Siddall III work [21,22] on Casimir invariants of $\mathrm{SU}(m \geqslant 6) \times \mathcal{S}_6{\downarrow}\mathcal{O}$ embedded NMR spin symmetry with its $\lambda \vdash (n = 6)$ partition.

The following conjectures arose in the course of recent discussions [27–29] and represent our views:

(i) On the existence at high $\mathcal{S}_n$ index of a weak-branching limit (WBL) in decomposition processes governed by combinatorial $\mathrm{sst}^{\lambda'}(\lambda)$ rules, i.e., the Kostka co-efficient set $\{\Lambda_{\lambda\lambda'}\}$ (over $\{[\lambda']\}$ set) for high index-n $\mathrm{SU}(m \geqslant 3) \times \mathcal{S}_n$ group dualities, so than all non-WBL decomposition coefficient sets are recognised as distinct subsets of the final invariant WBL set; naturally, applications involving the Littlewood–Richardson rule (LR) would necessarily require use of a much higher n-index for its standard (invariant to further increment in n-index) set of mononial coefficients to appear, than applies to the case of simple YR(III) Young rule decompositions;

(ii) On the *existence and realisation* of geometric analogues of Cayley's theorem, $n = |\mathcal{G}|$, for SU2 $\times\, \mathcal{S}_n{\downarrow}\mathcal{G}$ embedded spin algebras, essentially in terms of Voronoi polyhedra (VP) as dual forms (and where the construction of VP is based on the normals bisecting the edges of the original modelling). The *exclusively combinatorial* form of these spin algebras illuminate the relations between algebraic formalisms and their projective geometry;

(iii) The extension via a further sufficiency condition to Cayley's theorem to yield *general determinacy conditions* for SU(m) $\times\, \mathcal{S}_n{\downarrow}\mathcal{G}$ dual group embeddings, is a more subtle question than either, the form of a Cayley's theorem geometric analogue (i), or the $m \gg n$ branching determinacy of, e.g., six-fold duality problem, set out in [21,22]. However, even here some progress is possible. We evoke a corollory of a self-associate (internal symmetry) irrep property, initially known for hierarchies of Yamanouchi–Gel'fand chain group encodings [20] (see section 3 below), in order to shed some light on the determinacy of naturally-embedded spin algebras at these higher $\lambda \vdash n$ SU(m)-branching. Then our conjecture stated that: "retention of self-associacy over the irrep set derived from a $[\lambda]_{\mathrm{SA}}$ of the SU(m) $\times\, \mathcal{S}_n$ to be embedded constitutes the necessary further *sufficiency* condition to ensure determinacy in the generalised natural embedding."

2. Definitions of the basic notation employed herein

- $\lambda \vdash n$, a mathematical number partition into less than n parts, and λ', a partition occurring in same $\mathcal{S}_n$ algebra, $\trianglerighteq \lambda \vdash n$, higher or equivalent in a sequence ordering, decreasing from n.
- $\mathcal{S}_n{\downarrow}\mathcal{G}$, a natural embedding of a finite group $\mathcal{G}$ in a specific $\mathcal{S}_n$ group, i.e., a single step chain subduction process.
- $:\!\lambda\!:(\mathcal{S}_n)$, model based on a $\mathbf{M}^{\lambda}$ simple $\mathcal{S}_n$-module, a property natural associated with the Young permutational characters $\xi^{:\lambda:}$.
- $\Lambda_{\lambda\lambda'}$, a reduction (or Kostka) coefficient of some form of decomposition process; specifically under Young's rule (third variant), these are Kostka coefficients.
- $[\lambda]$, an irrep of $\mathcal{S}_n$ group of cardinality $|[\lambda]| = \chi^{[\lambda]}_{1^n}$, the principal character.
- $(8,8,3)$, common vertex index of (regular) polyhedra-identifying the set of n-polygons incident thereon.
- $[\lambda]^{(2)(11)}$, the symmetrised (antisymmetrised) identical (inner tensor) product associated with plethysm formation.
- $\widetilde{\mathbf{U}} \times \mathcal{P}(\widetilde{\Gamma})(v)$, the projection operations inherent in mappings under the SU2 $\times\, \mathcal{S}_n$ dual groups where $\widetilde{\mathbf{U}}$ relates to $\mathcal{D}^k(\widetilde{\mathbf{U}})$ rotation aspects of SO(3), from SO(3) vs. SU2 homomorphism, and v is generic for all remaining inner recouplings, or $\mathcal{S}_n$-scalar invariants.

- $\{\ldots\}$ (complete) set of (irreps, or branchings), especially within a hierarchy. SA labelling denotes a self-associate form (irrep) under $\mathcal{S}_n$ – i.e., a form invariant under rotation of Young tableau about its NW/SE diagonal.
- Voronoi structure, a dual (generally regular) figure derived from the intersectrix of bisectors of face-edges of the original (reg.) polyhedron.
- $\rightarrow$ a mapping onto; $\{/\}$ a (complete) set;
- $\mathrm{sst}^{\lambda'}(\lambda)$ refers to tableaux combinatorial enumeration, λ are the contents arranged in standard semi-normal tableaux over the shape(s) λ' as possible, for $\lambda' \trianglerighteq \lambda$ of priority sequence ordering.
- $|\mathcal{G}|$ or $|\mathcal{S}_n{\downarrow}\mathcal{G}|$, the group cardinality (order); $\forall$, for all; $|$, for which.
- YR(III) and LR refer to the third variant of Young's rule and the Littlewood–Richardson rule in combinatorial algorithmic forms, respectively.

3. Brief physical overview: Other aspects of encodings or embeddings for NMR duality

It was Balasubramanian [2] who in the early 1980s recognised that NMR spin symmetries are automorphic forms derived from the inherent structure of the intra-cluster $\{J_{ij}\}$-hierarchy; then, it was seen that such automorphic symmetries for nuclear spin systems were implicit also in the weighting aspects of ro-vibrational spectra [3,14,30,35] and that these constitute important properties of $\mathcal{S}_{n\geqslant 12}{\downarrow}\mathcal{G}$ isotopomeric exocage clusters. For this reason, the question of the *highest* SU(m) level for which *full determinacy* is retained in the associated SU(m) $\times$ $\mathcal{S}_n{\downarrow}\mathcal{G}$ embedded spin algebra represents a topic of much inherent interest, which is central to the weighting spectral-intensity aspects of large exocage clusters.

That dual group algebras represent some form of encoding under $\lambda \vdash n$ is clear from several differing viewpoints. For instance, both the simple $\lambda \vdash n$ partitions themselves, and the corresponding $\mathcal{S}_n$ modules, represent forms of information – encoding, whose determinacy is related to the level of SU(m)-branching [24,28]. Hence in a discrete mathematical sense, the SU(7) $\times$ $\mathcal{S}_6$ branching of [21,22] is a non-attainable partition of $n = 6$. The additional null element of ($\lambda \vdash 7$) immediately implies a degree of indeterminacy, without the need for explicit functional algebraic analysis. The decomposition of $\mathcal{S}_n$-modules [27–29] over bases of $\{[\lambda']\}$ irreps is likewise an encoding within a SU(m)-branching hierarchy. Further aspects of encoding are evident in the way the subsets of Yamanouchi–Gel'fand chain irreps for

$$\mathcal{S}_n \supset \mathcal{S}_{n-1} \supset \cdots \supset \mathcal{S}_3 \supset \mathcal{S}_2,$$

when derived from the $[\lambda_{\mathrm{SA}}]$ self-associate irrep(s) of the (maximal) n-index symmetric group, retain a form of self-associacy *over the resultant set*, as the theoretical chain subduction proceeds over *decreasing indexed* $\mathcal{S}_{n-i}$ subgroups.

Other forms of encoding occur in the $\{\mathrm{D}^k(\widetilde{\mathbf{U}}) \times \widetilde{\Gamma}^{[\lambda]}(v)\}(\mathrm{SU2} \times \mathcal{S}_n)$ irrep set of Liouvillian dual tensors, as seen in their v (generic) inter-group co-operability modes [5] and in the nature of the super-generator derived $\{s_i^2\}$-bosons and their formal ladder algebras. We discussed $\widetilde{\mathbf{U}} \times \mathcal{P}(\widetilde{\Gamma}^{[\lambda]}(v))$ mapping over the related $\widetilde{\mathbb{H}}_v$ carrier subspaces in the context of the retention of SU2 $\times\ \mathcal{S}_n$ simple-reducibility in earlier work [26]. For brevity, the reader is referred to the original work for background on these specific topics concerned with the general substructure of such dual (Liouvillian) tensors [11,12]. Suffice it to say that such direct product aspects provided much of the original motivation for this work.

Conjecture 1. "On the *existence* of a weak-branching high-n index limit (WBL) for the reductive Kostka sets of $\mathcal{S}_n$-module decompositions; the non-WBL Kostka sets being *subsets* of the further n-increment invariant WBL set." For analogous combinatorial processes such the L/R rule, but now at much higher n-index for a WBL, similar invariant sets with a hierarchy of intermediate branching level (varying) subsets apply, as discussed in conjecture 2 below.

Initially, we are concerned with the mappings [19],

$$\left\{:\lambda: \to \otimes_\lambda,\ \Lambda_{\lambda[\lambda']}[\lambda']\right\} \Big| \lambda, \lambda' \vdash n, \tag{1}$$

for the λ-partition spanning $\{[n], \ldots, [\lambda'], \ldots, [\lambda]\}$ basis, i.e., with $\lambda' \trianglerighteq \lambda$ in the ordering sequence. The assertion for high (increasing) index-n permutation groups requires the $\lambda \vdash n$ structures of (incremental) $\mathcal{S}_n$-irreps to be considered over a common (complete) basis for highest feasible branching n index, namely,

$$\begin{aligned}\mathcal{L} \equiv \big\{&[n], [n-1,1], [n-2,2], [n-2,11];\ [n-3,3], [n-3,21], [n-3,1^3];\\ &[n-4,4], [n-4,31], [n-4,22], [n-4,211], [n-4,1111];\\ &[n-5,5], \ldots\big\},\end{aligned} \tag{2}$$

where the marker ';' is used to denote changes in leading $n-\mu$ portion of irrep labels. The logic of assertion (1) comes directly from the Sagan–Young algorithm for standard tableau enumerations [19]. Lower n-indexed $\mathcal{S}_n$ group decompositions are necessarily subsets, both in the sense of certain numeric $\Lambda_{\lambda\lambda'}$s being less than the final limiting value, and also in the sense that, at a lower $\mathcal{S}_n$ n-index, certain initial $[n-\mu, \mu]$ $\lambda \vdash n$ branching of (2) are inaccessible, e.g., the $[-,4]$, $[-,31]$ components preceding $[222](\mathcal{S}_6)$, compared to sequence for higher $\mathcal{S}_n$ algebras.

For *examples* of substructure leading to the weak branching limit at high index $-n$, one may take the $:\lambda: = :n-4, 211:$ 4-part form at $\mathcal{S}_{8,12}$ WBL compared to $\mathcal{S}_6$ subset, where the underlined numeral is an element of the non-WBL subset:

$$:\lambda: (\mathcal{S}_n) \to \{1,3,4,3;\ 3,4,1;\ 1,2,1,1\}\mathcal{L}(\mathcal{S}_n) \quad \forall n \geqslant 8, \tag{3a}$$

$$:\lambda: (\mathcal{S}_6) \to \{1,3,4,3;\ \underline{2},4,1;\ -,-,1,1\}\mathcal{L}, \quad \text{a subset for non-WBL}, \tag{3b}$$

and (unit col.) $\mathcal{L}$ retains full component structure for generality, as in (2) above. As further *examples*, we consider modules $:\lambda: = :6,33:$ and $:4,33:$ both as forms of the deeper branched form of $:n-6,33:$ $\mathcal{S}_n$-module, requiring investigation at high index using the higher $\mathbb{Z}(\mathcal{S}_n)$ characters. For WBL (compared to non-WBL subset), one finds the mappings

$$:n-6,33\colon (\mathcal{S}_{n\geqslant 12}) \to \{1,2,3,1;\ 4,2,-;\ 3,3,1,-,-;\ 2,2,2,0,\ldots;\ 1,1,1,-,1\}\mathcal{L}, \tag{4a}$$

$$:n-6,33\colon (\mathcal{S}_{10}) \to \{1,2,3,1;\ 4,2,-;\ 3,3,1,-,-;\ \underline{1},2,2,0,\ldots;\ -,-,1,-,1\}\mathcal{L}. \tag{4b}$$

Additional checks on these decomposition are possible by evaluating the p-parts of the LHS as a monomial and comparing that result with the sum of $|[\lambda']|$, the principal characters. For further details of other high n-index $\mathcal{S}_n$ modules and their weak branching limits, the reader is referred to discussions and tabulations in refs. [27–29].

It is convenient to discuss the Kostka coefficients sets/subsets, since their derivation via $\mathrm{sst}^{\lambda'}(\lambda)$ enumeration is well understood and documentated in the combinatorial literature. Further in the less-dominant order sector of $\lambda \vdash n$ the Young permutation characters determine the specific Kostka subsets (now well removed from any WBL). Finally the Kostkas associated with $:1^n:$ are defined identically by the (transposed) $\chi^{[\lambda]}_{1^n}$ characters over $\{[\lambda]\}$.

4. Implicit corollory to conjecture 1 for L/R decompositions, given here in terms of $\mathcal{S}_2$-plethysms [4,11,12,15,17]

The analogous (but distinctly more involved) nature of tensor products strongly suggests that their non-SR reductive coefficients be considered in a similar generalised complete form and, in particular, for the first high n-indexed $\mathcal{S}_n$-group(s) which yields a tractable set of results for (say) initial $\{\lambda \vdash n;\ p \leqslant 2,\ \leqslant 3\}$ irreps of $[\lambda] \otimes [\lambda]$ or $[\lambda] \otimes [\lambda']$ inner tensor products (ITPs) [4,11,12,15–17,19]. As an example of a general form of calculation in the weak-branching high-n limit, we give the tensor products in terms of the Schlaflian $[\lambda]^{(2;11)}$ terms [11,12,15,17] – since their direct sum is over sets closer to simple-reducibility than the full ITP and also allows for discrimination between the symmetrised and antisymmetrised $[\lambda]^{(\cdot)}$ forms [4]:

$$[n-2,2] \otimes [n-2,2] \equiv [n-2,2]^{(2)} \otimes [n-2,2]^{(11)}, \tag{5}$$

where the respective mappings for $n \geqslant 8$ become

$$\begin{aligned} [n-2,2]^{(2)} &\equiv \{1,1,2,-;\ 1,1,-;\ 1,-,1\}\mathcal{L}, \\ [n-2,2]^{(11)} &\equiv \{-,-,-,1;\ -,1,1;\ -,1,-\}\mathcal{L}. \end{aligned} \tag{6}$$

The direct sum yields the high n-index WBL-equivalent result given in earlier work [31]:

$$[n-2,2]^{(2)} \oplus [n-2,2]^{(11)} \to \{1,1,2,1;\ 1,2,1;\ 1,1,1\}\mathcal{L}(\mathcal{S}_n) \quad \forall n \geqslant 8. \tag{7}$$

Similarly at high n-index, one finds that the inner tensor product (ITP) $[n-3,3] \otimes [n-3,3]$ now becomes

$$[n-3,3]^{(2)} \oplus [n-3,3]^{(11)} \to \{1,1,2,-;\ 2,1,-;\ 2,1,2,0,0;\ 1,1,1,0,1,-,-;\ 1,-,1\}\mathcal{L} \oplus \{-,-,-,1;\ -,1,1;\ 0,2,0,1,0;\ -,1,1,1,-,-,-;\ -,1,0,0,1\}\mathcal{L}, \quad (8)$$

where the respective subspaces for $\mathcal{S}_{12}(\mathcal{S}_{20})$ are of 11935 and 11781 (450725 vs. 450775) orders. The full ITP mapping becomes

$$[n-3,3] \otimes [n-3,3] \to \{1,1,2,1;\ 2,2,1;\ 2,3,2,1,0;\ 1,2,2,1,1,-;\ (1),(1),1,-,1,-\}\mathcal{L}(\mathcal{S}_n) \quad \forall n \geqslant 12. \quad (9)$$

The discrimination in irrep distribution in (8) corresponds to the recently proposed Carré–Leclerc domino-tableaux rule [4]; a wider discussion with dimensionality checks on a variety of *examples* has been given elsewhere [31]. The earlier work of Esper and Kerber [11,12] on generalised plethysms is especially valuable, despite its restriction to $\mathcal{S}_{10}$-ITPs. Several recent mathematics texts [15,17] provide particularly valuable background to symmetrisation of ITPs via plethysms and to the use of the Lyubarskii formula (10) of ref. [31]. The latter also provided the starting point for Esper's 1975 mathematical computations [11].

As an approach to ITP formation, it is especially useful for higher $\mathcal{S}_n$ groups provided one only requires ITPs derived from bipartite forms. It is necessarily limited in scope for WBL-equivalent limit to (say) maximal $[n-4,4] \otimes [n-4,4]$, where this could well require knowledge of the $\mathbb{Z}(\mathcal{S}_{n\sim16})$ character set.

Conjecture 2. On Distinctive automorphic reg. polyhedra and their Voronoi duals: Cayley's theorem for specific SU2 $\times\ \mathcal{S}_n{\downarrow}\mathcal{G}$ groups now as combinatorial geometry. The form of conjecture 2 reads as follows:

"For SU2 $\times\ \mathcal{S}_n{\downarrow}\mathcal{G}$ finite group embeddings in a specific n-indexed symmetric group obeying Cayley's criterion for n vs. $|\mathcal{G}|$ which correspond to some regular polyhedral model, there exists a Voronoi dual structure whose vertex diagonals correspond to the $\mathcal{C}_i$ axes of the automorphic spin $\mathcal{S}_n{\downarrow}\mathcal{G}$ invariance algebra. The *distinctness* of these from all spin-sites of the original reg. polyhedron ensures the spin invariance properties are *exclusively combinatorial* in form."

These propositions arise from considering the automorphic regular polyhedral forms associated with naturally embedded spin algebras either as geometric solids or alternatively, as their corresponding SO(2) projective tilings [8–10] in the sense of unfolding of the 3-space figure. Both approaches lead to certain Voronoi polyhedral (polygon zonal) constructions. The Cayley-determinable naturally-embedded SU2 spin algebra has certain inherent $\mathcal{C}_i$ axes, $i = 2,3,4,\ldots$, which permit the derivation of invariance properties of the automorphic subduced spin symmetry. While these may be shown to project from mid-face (or mid-edge) of the (automorphic) geometric figure

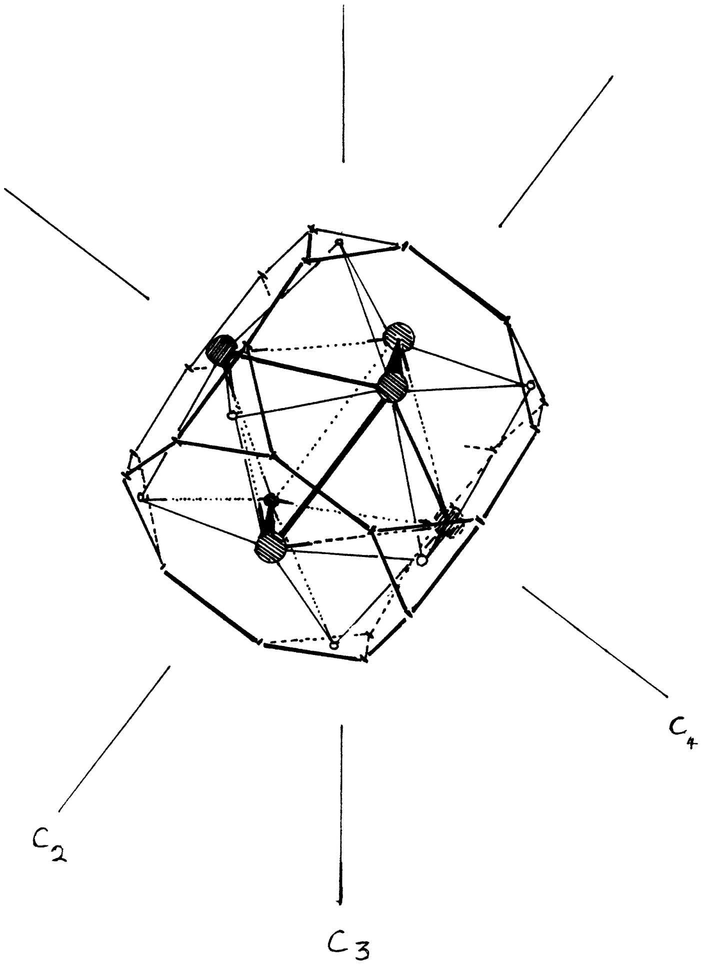

Figure 1. The (outer) original $(8,8,3)$ polyhedral automorphic model of $\mathcal{S}_{24}{\downarrow}\mathcal{O}$ naturally embedded spin symmetry, with its (included) dual the encapped octahedron which constitutes a Voronoi structure based on the (o) (open and (for primary octagon) shaded) circles. The distinctness of the $\mathcal{C}_3, \mathcal{C}_4$ axes, which constitutes the body-diagonals of the Voronoi structure, from the $(8,8,3)$ outer exo-cage vertices provides a geometric and combinatorial statement equivalent to n-index $\equiv |\mathcal{G}|$ property known as Cayley's theorem – see conjectures 2 and 3.

– i.e., as a set of axes totally non-coincident with *any pair* of figure vertices, – for the Voronoi polyhedra the $\mathcal{C}_3$, $\mathcal{C}_4$ axes now constitute the body-diagonal vertex elements of the dual construction to the initial geometric solid. Figure 1 illustrates the points made above, with reference to the $(8,8,3)$ regular polyhedral form of SU2 $\times\, \mathcal{S}_{24}{\downarrow}\mathcal{O}$ natural embedding, as an *example*. As a further *example*, one notes that the $(6,6,4)$ polyhedral form of the same spin algebra, i.e., isomorphic in spin site invariance properties to that of figure 1, exhibits a biprismic-related Voronoi dual, see figure 1 of refs. [6,32].

An analogous discussion of $^{13}C_{60}$ and higher $^{13}C_{60z^2}$ fullerenes [30,35] could be

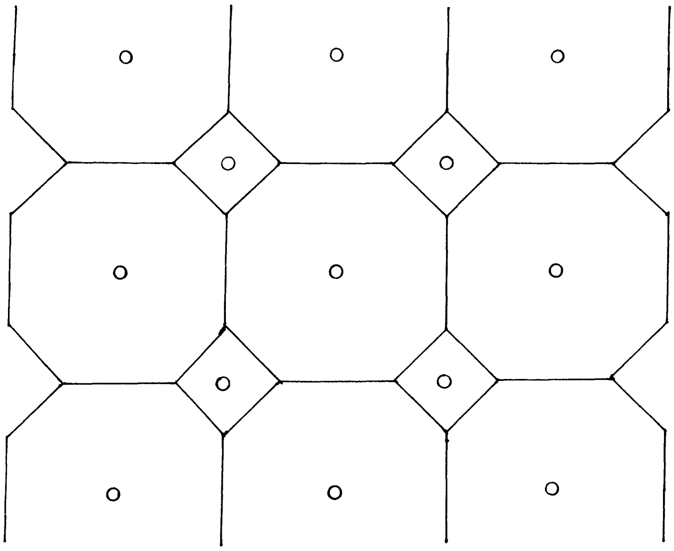

Figure 2. The ‘unfolded’ SO(2)-like projection of $(8, 8, 3)$ reg. polyhedra of figure 1, showing the two distinct types of Voronoi centres (o). Note the absence of recto-linear translation of the new grid to that derived directly from the $(8, 8, 3)$ figure; this stresses the Voronoi construction is non-affine with respect to the original lattice.

made which would serve to confirm the role of the set of Voronoi polyhedra, with one body-diagonal for each distinct ($i \geqslant 3$) $\mathcal{C}_i$ symmetry operator. *Only* for embeddings under the Cayley constraint can the Voronoi polyhedra body-diagonals be associated with the ($i \geqslant 3$) $\mathcal{C}_i$ distinct axes of the spin algebra. Alternatively, on drawing Voronoi figures [8–10,36] to the projective tiling and then inserting the Voronoi centres (o) and zones, one finds that in terms of translation the tiling contains non-(self-)affine substructures, figure 2. From this *example,* it follows that no standard-dissection exists of the SO(2) lattice.

Since it was noted [30,35] that $n = |\mathcal{G}|$ automorphic symmetry polyhedra provide an *exclusively combinatorial* subduced invariance algebra, it is of general interest that the mathematics literature suggests that Voronoi constructions indeed have a wider combinatorial significance [1]. As a result, the form of conjecture given above is a significantly stronger and more general statement that that given previously, in refs. [29,30,35]; it stresses the link between algebraic combinatorics and the fundemental geometric aspects of the physics inherent in such modelling.

Conjecture 3. On ‘set self-associacy’ retention for determinable natural embeddings SU(m) $\times \mathcal{S}_n{\downarrow}\mathcal{G}$, for specific branchings.

From Yamanouchi chain properties of the original self-associate $\mathcal{S}_n$ irreps, it is well-established that progressive subsets over the chain retain an overall total self-associacy (SA) property; table 5 of ref. [27] for $[\lambda]_{\mathrm{SA}}(\mathcal{S}_{12})$ gives some typical *examples.* A further example of determinable subduction chain process retaining overall derived-set self-associacy may be seen on examining the first two step of the Yamanouchi–Gel'fand process applied to $[4321]_{\mathrm{SA}}(\mathcal{S}_{10})$:

$$\begin{aligned}[4321]_{\mathrm{SA}} &\to \{[432]+[4311]+[4221]+[3321]\}_{\mathrm{SA}} \\ &\to \{2[431]+2[422]+2[4211]_{\mathrm{SA}} \\ &\quad + 2[332]_{\mathrm{SA}} + 2[3311] + 2[3221]\}_{\mathrm{SA}}(\mathcal{S}_8).\end{aligned} \tag{10}$$

Hence, it is conjectured here for the single-step subduction that:

"For *natural* embeddings at some SU($m \geqslant 3$) branching level, as implied by the original $\mathcal{S}_n$ group irrep, the subduced symmetry subsets of the irreps derived from a specific $[\lambda_{\mathrm{SA}}]$ must also constitute an overall SA-retaining set, $\{\Gamma(\mathcal{S}_n{\downarrow}\mathcal{G})\}_{\mathrm{SA}}$, in terms now (cf. to Yamanouchi group chain) of the *natural* $(\mathrm{SU}(m) \times \mathcal{S}_n{\downarrow}\mathcal{G})$ embedding for determinacy to be assured."

Conversely, departure from overall SA condition of the subduced spin algebra is to be taken as a reason for presuming that an *indeterminacy* is likely present in the embedded spin algebra at one of the higher SU(m) branching levels surveyed. At the present time, there is no known way to obtain a direct mathematical proof for this assertion; in part, this stems from Cayley's theorem being explicitly concerned only with $\mathrm{SU2} \times \mathcal{S}_n{\downarrow}\mathcal{G}$ natural embedded spin algebras and otherwise, from studies of the invariants for automorphic model regular polyhedral geometric solids still being in an early stage of development [23,24,27–29,34]. What is clear is that under certain subduced natural embedding from specific $\mathrm{SU}(m) \times \mathcal{S}_n$ algebra, one may write generalised algebraic forms of mapping from $[\lambda]_{\mathrm{SA}}$ which meet the criteria given above; as an *example* for $\mathrm{SU}(m) \times \mathcal{S}_8{\downarrow}\mathcal{D}_4$ embeddings [6] from $[4211]_{\mathrm{SA}}$, $[332]_{\mathrm{SA}}$ this implies that for determinacy to be *retained*, the following general form must be adhered to:

$$[\lambda]_{\mathrm{SA}}(\mathcal{S}_8) \to \{\mu(\mathcal{A}_1 + A_2) + \mu'(\mathcal{E}_1 + \mathcal{E}_2)\}_{\mathrm{SA}}(\mathcal{S}_8{\downarrow}\mathcal{D}_4). \tag{11}$$

Table 1
Table of known $\mathrm{SU}(m) \times \mathcal{S}_n{\downarrow}\mathcal{G}$ determinacies examined under the retention of SA properties in mapping from $[\lambda]_{\mathrm{SA}}(\mathrm{SU}(m) \times \mathcal{S}_n) \to \{\Gamma(\mathcal{S}_n{\downarrow}\mathcal{G})\}_{?\mathrm{SA/set}}$.

Finite group	Index of specific $\mathcal{S}_n$ group	SU(m)-branching level	Determinacy[d]
$\mathcal{D}_3$	6[a]	3	Y
$\mathcal{D}_4$	8[b]	4	N
		3	N
$\mathcal{D}_5$	10[c]	5	(Y)
		4	N
$\mathcal{O}$	24	not available	–

[a] From $\mathcal{S}_{12} \supset (\mathcal{S}_6{\downarrow}\mathcal{D}_3) \otimes (\mathcal{S}_6{\downarrow}\mathcal{D}_3)$ discourse in ref. [29]; [b] see [6]; [c] as reported in ref. [33]; [d] Y (N) = yes (no).

Whilst the range of enumerated correlative mapping of the form $\{[\lambda]_{\rm SA} \rightarrow \Gamma(\mathcal{S}_n{\downarrow}\mathcal{G})\}$ has been fairly modest [25,28–30,33,35], the enumerative results found to date all support the validity of this conjecture. Table 1 presents various examples of $\mathcal{G}$-embedding in specific higher dual groups, taken from recent work cited above.

5. Concluding remarks

The above remarks on $\mathcal{S}_n$-module decompositions and their Kostka reduction coefficients serve to summarise much of the tabulated material given in a recent review [28]. In presenting a brief overview of the significance of Voronoi constructions for SU2 $\times\, \mathcal{S}_n{\downarrow}\mathcal{G}$ Cayley theorem-consistent embeddings as dual to the automorphic group geometry, we have set out interesting physical example of the general mathematical contention [1], which demonstrate that Voronoi polyhedra (zones) have a combinatorial significance. Hence, the invariance algebras of all known Cayley-consistent SU2 $\times\, \mathcal{S}_n{\downarrow}\mathcal{G}$ embeddings are seen as *exclusively* combinatorial in nature, as befits our geometric interpretation. Specifically, the automorphic $\mathcal{C}_i$ axes intersect the original geometric solid at mid-face or mid-edge centres and are *wholly distinct* from all spin sites. By contrast, as elements of the Voronoi dual forms the $(i \geqslant 3)$ $\mathcal{C}_i$ axes now constitute the vertix *body-diagonal axes*.

The importance of Voronoi polyhedra (zones) in co-ordination solvation and other physical modelling applications has been noted elsewhere [7,13,18].

Conjecture 3 on the value of studying self-associacy propagation for mapping onto an embedded group symmetry, *here restricted to automorphic NMR symmetries*, such as $\mathcal{O}$, $\mathcal{P}$, $\mathcal{D}_{3-5}$ (as distinct from groups containing inversion-reflection operations) reduces to being *a necessary further sufficiency condition* for the occurrence of determinable correlative mappings and a distinctly interdisciplinary aspects of cluster physics.

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