Group-embeddings for NMR spin dual symmetries, to $\lambda_{SA} \vdash n$: Determinate $[{}^{10}BH]_{12}^{2-}$ (SU(m ≤ 12) $\times S_{12} \downarrow \mathcal{I}$) natural subduction via symbolic S_n combinatorial generators: Complete sets of bijective maps, CNP-weights

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Abstract. Modelling of the properties of high-spin isotopomers, as polyhedra- on-lattice-points which yield various symbolic-computational S_n -encodings of nuclear permutation (upto some specific SU(m) branching level), is important in deriving the spin-ensemble weightings of clusters, or cage-molecules. The mathematical determinacies of these, obtained here for higher m-valued SU(m) × $S_{12} \downarrow \mathcal{I}$ group embeddings, are compared with that of an established group embedding, in order to collate the spin physics of $[^{11}\text{BH}]_{12}^{2-}(\text{SU}(2(m \leq 4)) \times S_{12} \downarrow \mathcal{I})$ with that for $[^{10}\text{BH}]_{12}^{2-}(\text{SU}(m \leq 7) \times ..)$ -analogue. The most symmetrical form of $[(^{10}\text{BH}) (^{11}\text{BH})]_6^{2-}((\mathcal{S}_6 \otimes \mathcal{S}_6) \downarrow (\mathcal{S}_3 \otimes \mathcal{S}_3))$ anion provides a pertinent example of the SU(m > n) × $S_n \downarrow \mathcal{G}$ physics discussed in [10]. Retention of determinacy in the two $S_{12} \downarrow \mathcal{I}$ cases is correlated to the completeness of the 1:1 bijective maps for natural embeddings of automorphic dual group NMR spin symmetries. The Kostka transformational coefficients of a suitable model (S_n module, Schur fn.) play a important role. Our findings demonstrate that determinacy persists (to SU(m ~ n/2) × S_n branching levels) more readily for embeddings derived from (automorphic) finite groups dominated by odd-permutational class algebras, such as the above $S_{12} \downarrow \mathcal{I}$, or the SU(m ≤ 3) × $S_6 \downarrow \mathcal{D}_3$ case discussed in [16a,15,3d], compared to other examples – (e.g. as respectively, in press, and in [17b]): SU(m) × $S_8 \downarrow \mathcal{D}_4$, SU(m) × $S_{10} \downarrow \mathcal{D}_5$. Generality of the symbolic algorithmic difference approach is stressed throughout and the corresponding dodecahedral SU(m) × $S_{20} \downarrow \mathcal{I}$ maps are outlined briefly – for the wider applicability of SF-difference mappings, or of comparable S_n -symbolic methods, (e.g.) via [7].

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1 Introduction

The search for physical insight into nuclear identicalspin ensemble properties of automorphic dual group spin symmetries, such as the ro-vibrational (R-V) weighting inherent in (exclusive) isotopomeric clusters, begins by considering the role of Cayley's theorem [1] for (automorphic) finite-group natural embeddings in specific symmetric groups. This has a strong inherent theoretical association with the regular-polyhedral lattice-point structure [2,3]which governs nuclear permutation. Physical insight into the latter is governed by the contention (due to Balasubramanian [4] in the early 1980s) that nuclear spin symmetry constitutes an automorphic (dual group) symmetry. On the basis of appropriate (rotational/permutational) finite group algebras, the spin symmetry is related to the specific hierarchical $\{J_{ij}\}$ subset structure of the spin-spin interactions in NMR.

In the present work, spin symmetry is applied to higherspin isotopomers in order to understand spin-ensemble weighting (via the complete nuclear permutations(CNP)) of R-V spectra, and also the determinacy question for natural group-embeddings involving the icosahedral group [3,5]. The latter $S_n \downarrow \mathcal{I}$ natural subduction has been examined via certain established S_n algorithms of symbolic computing [6,7], in the context of S_n -group representational theory [8,9].

From Casimir-invariant studies [10] on $S_6 \downarrow S_3$ related NMR spin systems, Sullivan and Siddall-III deduce – irrespective of both the Cayleyan criterion [1,3] and the intermediate $SU(m \leq n) \times S_n \downarrow \mathcal{G}$ embedding determinacy – that at the highest branching levels, represented by $SU(m > n) \times S_n \downarrow \mathcal{G}$, retention of determinacy is no longer possible. This result is clearly consistent with a symbolic mathematical ($\lambda \vdash n$ partitional) viewpoint [11], where the use of m-branching levels greater than 1^n , for permutational index-n, implies the introduction of degeneracy. Physical insight into

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the intermediate $3 \leq m \leq n$ SU branching aspects of natural embeddings [5] have attracted recent attention for their importance in nuclear spin weighting constraints, *i.e.*, *via* spin algebras, imparted to R-V spectroscopic investigations of cage-molecules [12–14] and symmetrical clusters. The importance of natural finite group-embedding in molecular spectroscopy was first recognised in the work of Galbraith and Cantrell [12]. As a property of nuclear spin ensembles, the topic subsequently has become of wider spectroscopic significance [13–19]. Recent interest in an everincreasing range of clusters, each with a potential wealth of (exclusive single-isotope based) isotopomers [14,18], has given a greater cogency to the topic.

Here, we shall focus on the automorphic nuclear spin symmetries of exclusive single-isotope $[A]_n$.. systems which govern the weight-constraints imparted to R-V spectra. Thus for all such fermion (boson) isotopomeric $[A]_n(\mathcal{S}_n \downarrow \mathcal{G})$ systems, the constraint that:

$$\Gamma(\mathrm{SU}(m) \times \mathcal{S}_n \downarrow \mathcal{G} : \text{nucl. spin}) \times \Gamma^{\mathrm{3space; R-V}} \equiv \mathcal{A}_{2 \ (1)}$$
$$|\text{as } [A]_n \text{ a fermion (boson) system}\},$$

determines the spin-ensemble weighting. Since the icosahedral group embedded into $SU(m) \times S_{12}(_{20,60})$ may well exhibit contrasting mathematical determinacies according to both their (permutational) type, or to the $(\lambda \vdash n)$ SU(m) -branching level associated with its embedding, the CNP properties, and (equally) the NMR automorphic spin symmetries [10], are of definite physical and mathematical interest.

A number of theoretical considerations related to polyhedral lattice vertex-point modelling of nuclear spin symmetries [15–18] are invaluable for the physical and conceptual insight they provide -i.e., irrespective of whether one is considering Cayleyan type embeddings [15], or highly $\lambda \vdash n$ -branched non-Cayleyan forms. For further details of the nature of S_n symbolic computational algorithmic (SCA) modelling applied to the original (but much more limited) $SU(2 \le m < 5) \times S_n \downarrow \mathcal{I}$ processes (of Eqs. (24-32) below) which define the spin-3/2 containing $[^{11}BH]^{2-}_{12}$ anion, the reader is referred to various fuller discussions and tabulations, given in earlier works [3,5] of ours. The corresponding $[^{10}B]^{2-}_{12}$ anion is of interest from the extended level of partitional branching it imparts to the dual automorphic group. The present work sets out the most general branched $SU(m) \times S_{12} \downarrow \mathcal{I}$ forms and their weights, in the context of the earlier $SU(m \leq 3) \times S_6 \downarrow D_3$ (Cayleyan) case and in contrast to the dominant even permutational-cycle embedded groups, such as $\mathcal{S}_8 \downarrow \mathcal{D}_4$.

2 Discussion: Group-based relationships via combinatorics: A general role for $\{ \triangle \Lambda_{.,\lambda'} \}$ Kostka-based difference maps: hierarchical (maximal) set properties under $S_n \downarrow G$

Prior to discussing more explicit aspects of group embedding, it is necessary first to make some general remarks and give a summary of certain "algorithmic-generators" properties of symbolic \mathcal{S}_n encoding. For reasons associated with the convergence of the (decompositional) coefficients to their standard maximal weak-branching values in the systemic forms of such sets, and in particular for the convenient difference mapping relationships over a minimal number of non-vanishing terms, it is advantageous to proceed via a Young's third-rule approach [5,6]. This is one choice, rather than (e.g.), utilising inner tensors to recursively generate the comparative algebras on the \mathcal{S}_n and the subduced group spaces. The less regular, highly non-simple-reducible nature of reduction coefficient decompositional sets of the inner tensors (ITPs) [6,9], as obtained (e.g.) via multiple Littlewood-Richardson (L-R) rule applications for $12 \le n \le 18$ cases, mitigates against their use here as generators in the general higher-branched $(\lambda \vdash n)$ cases. The fact of their slower convergence to a *maximal* reduction coefficient set, even for modestly branched bipartite forms, somewhat impedes their use as "combinatorial-generators" of parallel full and subduced symmetry relationships in the more general case. In other (subsequently derived) work, we discussed the origins and occurrence of *maximal sets* for ITPs associated with higher index- $n \sim 20$ fold symmetric groups as compared to the level of *bipartite* irrep $\lambda \vdash n$ branching. Here, the value of the SYMMETRICA symbolic computing package [7] in studies involving generators (*i.e.*, beyond known general $\otimes [n-1,1]$ forms) will be noted.

In the earlier work [5] on the SU $(m \leq 4) \times S_{12} \downarrow \mathcal{I}$ forms of embedding arising from [19, 20] $[A]_{12}(S_{12} \downarrow \mathcal{I})$ identical spin ensembles of proton, deuteron, or ¹¹B, as $(I_i \leq 3/2)$ -NMR nuclei of 12-fold cage clusters, we utilised equivalent procedures (*i.e.* as formulated by Sagan [6]) to those of symbolic algorithmic (SC) computing of Kohnert et al. [7]. These are concerned with simple group modules, or their analogous Schur functions (fns.) (SFs) of an appropriate multipartite form characterised by their corresponding monomial cardinality. These entities owe much of their subduced/restricted space properties to such spin ensembles being viewed as vertex lattice-point networks, after the Erdös *et al.* [2]. Such a viewpoint of S_n encoding properties is especially helpful for the Cayleyan (or closely-related) forms based on $\mathcal{D}_{3(5)}, \mathcal{O}, \mathcal{I}$ (automorphic) groups. Only for the $SU2 \times S_n$ cases are the encodings directly physical correlations, rather than mathematical quantities (i.e., SFs) into which the latter are subsumed. In such structures, it follows that the module- or Schur fn. models themselves provide physical insight via their decomposition properties over $\mathcal{L}^{\dagger} \equiv \{ [\lambda] \}$ set – from initial component irrep [n] down towards λ_{SA} in dominance order. Such properties of modules (SFs) are implicit in the third variant of Young's rule [6,7] (YR-III). Hence via well-established enumeration techniques, one obtains:

$$\lambda \to \bigoplus_{\lambda'}^{\text{(enm.)}} \Lambda_{\lambda,\lambda'}[\lambda'], \qquad (1)$$

on the basis of semi-normal standard tableaux (sst), where the unprimed and primed λ s refer respectively to the contents and the shape tableaux properties. The Kostka coefficients $\Lambda_{\lambda,\lambda'}$, or $K_{\lambda,\lambda'}$ (both the latter, and the forms on the right of following equation, are given in Sagan's notation [6]) are clearly:

$$\Lambda_{\lambda,\lambda'} \equiv (\mathrm{sst})^{\lambda'}(\lambda). \tag{2}$$

Beyond the tabulated relationships given in the earlier $(i.e. SU(m \leq 4) \times$ -based) work, it is physically insightful to invoke hierarchical difference "combinatorial generators" based on the YR-III rule For the symmetric group from n = 10 to n = 20 (and upwards) the full power of these relationships is seen on recognising the occurrence of maximal subsets of Kostka coefficients associated specifically with lower (weak) $\lambda \vdash n$ branching, which for higher indiced S_n groups are *independent* of n. Other reduction coefficient sets for sufficiently high-indexed symmetric groups have been shown to exhibit similar maximal subsets, provided one is concerned specifically with weak $\lambda \vdash n$ branching:

$$\Lambda_{\lambda,\lambda'}^{(\max'l)} \equiv \{(sst)^{\lambda'}(\lambda)\}_{(weak \ \lambda \vdash n)}.$$
 (3)

Specific indexed S_n group-module decompositions in themselves are still valuable, but the maximal subsets for high n and weak $\lambda \vdash n$ branchings (WBs) are particularly convenient aspect of YR-III decompositions to utilise in applications. To summarise the (WB) methods (based on both decompositional forms) used here on the basis of the earlier work [3–5], we give the following totally general "combinatorial generators" for symmetric group/subgroup properties in general, namely $\forall n \geq 2(\mu + \mu')$ – here with μ' being the other integer (sum of such integers) of the lefthand " parts-of-n", or first of the righthand SFs (or modules), below:

$$[n - (\mu + 1), \mu 1] \Leftrightarrow \{n - (\mu + 1), \mu 1\} - \{n - \overline{\mu, \mu} - 1, 1\} - [n - (\mu + 1), \mu + 1] - [n - \mu, \mu], for \ \mu \ge 2, \quad (4)$$

$$[n - (\mu + 2), \mu 2] \Leftrightarrow \{n - (\mu + 2), \mu 2\} - \{n - (\mu + 2), \mu + 1, 1\} - [n - \mu - 1, \mu, 1] - [n - \mu, \mu],$$
for $2 \le \mu$, (5)

$$[n - (\mu + 3), \mu 3] \Leftrightarrow \{n - (\mu + 3), \mu 3\}$$

$$- \{n - (\mu + 3), \mu + 1, 2\} - [n - (\mu + 2), \mu 2)]$$

$$- [., (\mu - 1)3] - [n - \mu - 1, \mu 1] - [., (\mu - 1)2]$$

$$- ([., (\mu - 2)3]) - [n - \mu, \mu] - [., (\mu - 1)1]$$

$$- ([., (\mu - 2)2]) - [n - \mu + 1, (\mu - 1)]$$

$$- ([., (\mu - 2)1]) - ([., \mu - 2]),$$
for $\mu \sim 4$, or with extra terms (5), (6)

$$[n - (\mu + 2), \mu 11] \Leftrightarrow \{n - \mu - 2, \mu 11\} - \{n - (\mu + 1), \mu - 1, 11\} - 1[n - (\mu + 2), \mu + 2] - 2[., (\mu + 1), 1] - [., \mu 2] - 2[n - (\mu + 1), (\mu + 1)] - 2[., \mu 1] - [n - \mu, \mu],$$
for $\mu \ge 2$, (7)

within their respective decompositional coefficients under Young's rule, as in the *specific maximal* Kostka set of weakly-branched $\{\Lambda_{i,i'}\}^{\text{maxl.s}}$ (as *e.g.*, under $S_{12\leq n(\sim 20)}$). Hence, $2\Sigma_{\mu,\mu'} \leq n$ of $\lambda \sim n - \Sigma_{\mu\mu'}$ (partition) over an implied dimensionality balance yields:

$$[n-3,21] \equiv \{\widehat{n-3,21}\} - \{\widehat{n-2,11}\} - [n-3,3] - [n-2,2], \tag{8}$$

$$[n-4,31] \equiv \{n-4,31\} - \{n-3,21\} - [n-4,4] - [n-3,3],$$
(9)

$$[n-5,41] \equiv \{\widehat{n-5,41}\} - \{\widehat{n-4,31}\} - [n-5,5] - [n-4,4].$$
(10)

$$[n-4,22] \equiv \{\widehat{n-4,22}\} - \{\widehat{n-4,31}\} - [n-3,21] - [n-2,2],$$
(11)

$$[n-5,32] \equiv \{\widehat{n-5,32}\} - \{\widehat{n-5,41}\} - [n-4,31] - [.,22] - [n-3,3] - [n-3,21] - [n-2,2],$$
(12)

$$[n-6,33] \equiv \{n-6,33\} - \{n-6,42\} - [n-5,5] - [.,41] - [n-4,31] - [n-3,21] - [n-2,2], where /[\lambda]_{left}/, \triangle SFs, \Sigma_{[\lambda]_{right}}:$$
(13)

$$/[\lambda]_{\text{left}}/(S_{12}) \rightarrow \{320; 891; 1408; 616; 1925; 1650\},\$$

as sets over equations (8-13) above,

$$\label{eq:second} \begin{split} / \triangle (SF) s / \to \{ 528; 1320; 1980; 990; 3960; 4620 \}, \\ \text{so necessarily,} \end{split}$$

$$\Sigma_{[\lambda]_{\text{right}}} \to \{208; 429; 572; 374; 2035; 2970\};$$
(14)

$$\begin{split} [n-4,211] &\equiv \{n-4,211\} - \{n-3,111\} \\ &- [n-4,4] - 2[.,31] - [.,22] \\ &- 2[n-3,3] - 2[.,21] - [n-2,2], \quad (15) \\ [n-5,311] &\equiv \{n-5,311\} - \{n-4,211\} \\ &- [n-5,5] - 2[.,41] - [.,32] \\ &- 2[n-4,4] - 2[.,31] - [n-3,3], \quad (16) \\ [n-5,221] &\equiv \{n-5,221\} - \{n-5,311\} \\ &- [n-5,32] - [n-4,31] - 2[.,22] \\ &- [.,211] - [n-3,3] \\ &- 2[.,21] - [n-2,2], \quad (17) \end{split}$$

where now the cardinalities of these final three *dif-ferences* SFs, $\triangle(SF)$ span: {4620, 9900, 7920}(\mathcal{S}_{12}); ({51300, 251940, 155040}(\mathcal{S}_{20})). These accord with the detailed balance of the known cardinalities of the $\chi^{[\lambda]}_{1n}$ characters (and monomials), given in references [5,9b].

Naturally, these and further specific forms for both low and general partitional branching are open to confirmation from matching of decompositional processes available in the SYMMETRICA symbol computing package [7]. Further details for n = 12, n = 20 specific symmetric groups (beyond Refs. [5,11]) in intermediate- and high $(\lambda \vdash n)$ branching regimes will be found in Appendices A1, A2. As a contrasting alternative view (for completeness), we give some of the simpler decompositional mappings based on (bipart) inner tensorial product *maximal reduction coefficient* sets, which naturally have more component coefficients and converge more slowly to to the maximal sets of n-independent YR-III forms. Thus one finds that:

$$\begin{split} & [n-\mu-1,\mu 1] \longrightarrow ([n-1,1] \otimes [n-\mu,\mu]) \\ & - [n-\mu+1,\mu-1] - [n-\mu,\mu] \\ & - [n-\mu,\mu-1,1] - [n-\mu-1,\mu+1], \\ & \text{for } \mu \leq (n/2-1), \end{split} \tag{18} \\ & [n-4,22] \longrightarrow ([n-2,2] \otimes [n-2,2]) \\ & - [n-4,4] - [.,31] \\ & - [n-3,3] - 2[.,21] - [.,111] \\ & - 2[n-2,2] - [.,11] - [n-1,1] - [n], \\ & \text{for } 2 \leq ((n/2)-2), \end{aligned} \tag{19} \\ & [n-3,111] \longrightarrow ([n-2,11] \otimes [n-1,1]) \\ & - [n-3,21] - [n-2,2] - [.,11] \\ & - [n-1,1], \text{ for } 3 \leq ((n/2)-3), \\ & \text{else generally}, \end{aligned} \tag{20} \\ & [n-\mu-2,\mu 11] \longrightarrow ([n-2,11] \otimes [n-\mu,\mu]) \\ & - [n-\mu-2,(\mu+1),1] - [n-\mu-1,(\mu+1)] \end{split}$$

$$-2[., \mu 1] - [., (\mu - 1)2] - [n - \mu - 1, (\mu - 1)11] - [n - \mu, \mu] - 2[., (\mu - 1)1] - [., (\mu - 2)11] - [n - \mu + 1, \mu - 1] - [., (\mu - 2)1], for 2 < \mu < ((n/2) - 2).$$
(21)

Simple tractable ITP decompositional difference relationships (*i.e.* over a conveniently restricted number of terms, *i.e.*, close to simple-reducibility (SR)) are more limited however under (multiple) L-R processes, as simple wellordered development over a set of *minimal*-valued reduction coefficients is not a general characteristic of even bipartite ITP decompositions, though at high-enough *n*index values a *maximal (vs. n) set* of reduction coefficients will exist. This arises from the comparability of the Young and L-R rules, highlighted by Sagan [6]. In order to stress the *generality* of the "combinatorial-generator" approach (especially in respect of these higher index-*n* and standard maximal coefficient subsets), the appendix material sets out some analogous initial $S_{20} \downarrow \mathcal{I}$ subductions, based on generator equations (4-16; 18-20).

Finally in this section, we stress the bi-directionality of mappings under $SU(m) \times S_n$ or $\ldots \times S_n \downarrow \mathcal{G}$ (dual groups) associated with $\lambda \vdash n$ modelling and algebraic combinatorics. Aside from specific properties arising from higher spin or $SU(m \geq 3) \times \ldots$ aspects of these algebras, in general the automorphisms between point groups and spin symmetries with the involvement of some intermediate combinatorial-based mappings constitutes a closed cyclic form, in principle; thus, it may utilised to establish a purely group theoretical relationship. That this is so is a consequence of the general bi-directionality of automorphisms. It establishes and justifies the role of "group theory via algorithmic algebraic combinatorics" as an equal counterpart to Kerber's (1991) overview [8] of "algebraic combinatorics *via* finite group actions".

2.1 Overview of additional $SU(m \geq 3) \times \mathcal{S}_n \downarrow \mathcal{G}$ embedding criteria

On comparing the determinacy question for the $\mathrm{SU}(m \leq 6) \times S_6 \downarrow \mathcal{D}_3$ embedding system with that for the icosahedral mappings in the context of $[^{11}\mathrm{B}]_{12}$ or $[^{10}\mathrm{B}]_{12}$ ensembles, such as those inherent in the $\mathrm{SU}(4) \times$ and $\mathrm{SU}(7) \times S_{12} \downarrow \mathcal{I}$ permutational problems, it has been suggested [15] that even where Cayley's theorem applies, once $\mathrm{SU}(m \geq 3) \times$ branchings are considered [16], it is only a *necessary condition*. Hence, in mathematical physics terms, it is no longer a *sufficient* general-criterion on its own to apply *beyond* the $\mathrm{SU}(2) \times S_n \downarrow \mathcal{G}$ level.

The completeness of strictly (1:1) bijective mapping for natural subduction is an important indication of retained determinacy, as it implies the existence of the requisite number of independent relationships. For group structures of the \mathcal{G} non-icosahedral groups, such determinacy is inherently correlated to "self-associacy (SA) retention under subduction", a property typical of Yamanouchi chain of \mathcal{S}_n embedded groups. The latter are known for their universal determinacy, irrespective of the SU($m \leq n$) branching level [15,16] associated with the \mathcal{S}_n -irrep. As an example of such (non- $\mathcal{I} \sim \mathcal{A}_5$) chain subduction properties with SA retention, the following chain forms will suffice:

$$[321]_{SA}(\mathcal{S}_6) \to \{[32] + [311] + [221]\}_{SA} \\ \to 2\{[31] + [22] + [211]\}_{SA} \\ \to 2\{[3] + 3[21] + [1^3]\}_{SA} \text{ over}, \qquad (22)$$

$$\mathcal{S}_6 \supset \mathcal{S}_5 \supset \ldots \supset \mathcal{S}_3 \ldots$$

We have suggested now that such a property applies to non- \mathcal{I} natural embeddings also, and that its occurence is one sufficient criterion to guarantee determinacy for such highly branched $\mathrm{SU}(m) \times S_n \downarrow (\mathcal{G}(\not\equiv \mathcal{I}))$ (subduced) algebras- corresponding to specific isotopomeric clusters [16]. As a example one notes how the group chain properties for the $S_6 \downarrow \mathcal{D}_3$ case develop over:

$$\begin{pmatrix} [51]\\ [42]\\ [411]\\ [33]\\ [321] \end{pmatrix} \rightarrow \begin{pmatrix} 0 \ 0 \ 1 \ 0 \ 0 \\ 1 \ 0 \ 1 \ 0 \ 2 \\ 0 \ 1 \ 0 \ 2 \ 1 \\ 0 \ 2 \ 0 \ 1 \ 0 \\ 0 \ 0 \ 2 \ 2 \ 2 \end{pmatrix} (\mathcal{S}_6 \downarrow \mathcal{O}) \rightarrow \begin{pmatrix} 0 \ 1 \ 2 \\ 3 \ 0 \ 3 \\ 1 \ 3 \ 3 \\ 0 \ 3 \ 1 \\ 2 \ 6 \end{pmatrix} (\mathcal{S}_6 \downarrow \mathcal{D}_3),$$

$$(23)$$

as a natural subduction process, where the last rows correspond to SA forms *throughout* the group embedding process. Further the intermediate group \mathcal{O} here is related directly to the final Cayleyan-embedded form *via* an *induced symmetry* group relationship, a question discussed in Section 5 (below). On questions arising from the algebras of group em- rebedding, we would just stress that:

i) mathematical determinacy simply implies a freedom from degeneracies, or alternatively simple multiples, in the mappings arising from natural subduction processes, whereas,

ii) retention of determinacy to $SU(m \leq n)$ branching level (or self-associacy (retention) for non- \mathcal{I} groups) implies that a process involves a complete set of independent relationships up o SU(n/2) level, and thereafter is governed simply by properties derived from $\otimes 1^n$ irrep (inner product) multiplication. Naturally, the latter is an inherent part of \mathcal{S}_n group structure. As a sequal to the above, there is one further underlying question of interest to those readers with specific group theoretical interests. Namely, "is it only odd-permutational cycle/class-structured finite groups which allow for determinate embedding right upto the m = n limit, as identified in reference [15] with the $\mathcal{S}_6 \downarrow (\mathcal{D}_3 \equiv \mathcal{S}_3)$ case?" A further point we shall return to in a later section. Finally, we stress the notation adopted here in all the natural subductions and mappings: *i.e.*, $\dot{\Gamma}$ (as a final right-hand term) is a (unit) column-vector, as in references [3,5] with the standard form [20] for the icosahedral group being: $\hat{\Gamma}(\mathcal{I})^{\dagger} \equiv \{\mathcal{A}, \mathcal{G}, \mathcal{H}, \mathcal{T}_1, \mathcal{T}_3\}.$

2.2 Symbolic S_n -encodings for $S_n \downarrow \mathcal{I}$ maps via "combinatorial generators"

The study of various appropriate (multicoloured) regularpolyhedral lattices provide the basis for the following incremental-m SU(m) sets of bijective mappings – from reference [5] (omitting much of the detail), within the notation given therein:

$$[11,1] \Longleftrightarrow \{-,-,1,1,1\} \mathring{\Gamma}(SU(2) \times \mathcal{S}_{12} \downarrow \mathcal{I}), ..$$

$$[6,6] \Longleftrightarrow \{10,10,14,2,2\} \mathring{\Gamma},$$
(24)

where clearly this is not a Cayley-embedded form, such as described elsewhere [3] for $SU(2) \times S_{60} \downarrow \mathcal{I}$. Additional features for the twelve-fold deuteron spin-one cluster arise from mapping such as:

$$[10, 11] \iff \{0, 4, 3, 4, 4\} \hat{\Gamma}(SU(3) \times \mathcal{S}_{12} \downarrow \mathcal{I}), ..$$

$$[5, 43] \iff \{35, 136, 183, 103, 103\} \hat{\Gamma}.$$
(25)

$$[4, 44] \iff \{17, 34, 39, 19, 19\}\check{\Gamma},$$
 (26)

where the $\chi^{[\lambda]}_{1^n}$ principal characters respectively span, {11, {..}, 132}; {55, {..}, 2112, 462}. For the SU(4) × $S_{12} \downarrow \mathcal{I}$ embeddings arising from the $[^{11}B]_{12}$ cluster, the mappings take on the following forms, which includes a typographic correction to $[5,...] \iff {..}\hat{\Gamma}$ subset of reference [5]:

$$[9,1^{3}] \iff \{5,12,14,7,7\}\hat{\Gamma}(SU(4) \times S_{12} \downarrow \mathcal{I}), ...$$
$$[6,2^{3}] \iff \{43,131,166,88,88\}\hat{\Gamma}; \text{ and}$$
(27)
$$[5,511] \iff \{36,99,135,63,63\}\hat{\Gamma}.$$
(28)

$$[5, 421] \iff \{94, 387, 475, 293, 293\}\check{\Gamma},$$
 (29)

$$[5, 331] \iff \{76, 278, 354, 200, 200\} \dot{\Gamma},$$
 (30)

$$[5, 322] \iff \{63, 297, 360, 234, 234\}\check{\Gamma},$$
 (31)

$$[4, 431] \iff \{42, 198, 240, 156, 156\}\hat{\Gamma},$$
 (32)

where now,

$$\{\chi^{[\lambda]}{}_{1^n}\} \equiv \{165, \{..\}; 1925, 1485, 5775, 4158, 4455, 2970\},$$
(33)

with the (SU(4) × ..) final self-associate (SA) (dual-group) irrep-mapping given as equation (43) below. After these necessary preliminaries, we now turn to dual group higher branchings and embeddings specifically associated with the $I_i = 3$ boron-10 component spin-ensemble of the borohydride anion.

3 Completeness of $(SU(m \le (n/2)) \times S_{n=12} \downarrow I)$ -dual-group bijective maps

Both the above and the higher $SU(m) \times ...$ mappings were obtained using (recursive) hierarchical encoding techniques of references [5, 6, 11].These are simply based on projective decompositions and use of the standard Young's rule [6,7] to give the Kostka, or reduction, coefficients [6,8,9,11] for the non- $SU(2) \times S_{12}$ -modules (SFs), which yield models for the higher-spin isotopomers. Beyond the SU(4) $\times S_{12} \downarrow \mathcal{I}$ subset of mappings, with their pertinence to the $[^{11}B]_{12}$ isotopomeric cluster given earlier [5], one needs to arrive at all the strictly bijective mappings in dominance order (from n (= 12)) prior to (and including), (or, $\succeq [\lambda_{SA}]s$ in mathematical terms) the further self-associate S_n irreps [621⁴] and [53211] to give a complete-enough picture to understand the $SU(7) \times S_{12} \downarrow \mathcal{I}$ determinacy question for the regular $[^{10}B]_{12}$ cluster, as a polyhedral point-lattice network [2]. It is this aspect of the ¹⁰B-borohydride (anionic) ensemble, and its associated SU(5 $\leq m \leq 7$) $\times S_{12} \downarrow \mathcal{I}$ algebras, which is the principal focus of this work. No other comparable highly branched determinate dualgroup subduction algebras have been reported to date for specific SU(3 $\ll m \leq (n/2)$) $\times S_{n \gg 6} \downarrow G$ natural embeddings, despite some earlier investigations [17] of $\ldots \times S_n \downarrow \mathcal{D}_{(n/2)}$ systems.

From the $\{\Lambda_{\lambda,\lambda'}\}$ Kostka coefficient sets of further higher-branched simple S_n -modules as lattice encodings [2] over a sequence of SCA-difference enumerations (see Appendix), it follows that the SU(5).. subset spans: above):

$$[81^4] \Longleftrightarrow \{7, 21, 31, 14, 14\} \dot{\Gamma}(\mathrm{SU}(5) \times \mathcal{S}_{12} \downarrow \mathcal{I}), \quad (34)$$

$$[721^3] \iff \{28, 116, 144, 86, 86\}\hat{\varGamma},\tag{35}$$

$$[631^3] \iff \{65, 248, 307, 184, 184\}\hat{\Gamma},$$
 (36)

$$[62211] \iff \{50, 238, 288, 187, 187\}\hat{\Gamma},$$
 (37)

$$[541^3] \iff \{59, 232, 299, 173, 173\}\dot{\Gamma},$$
 (38)

and the one remaining SA-irrep mappings accords with equation (42) below. In these newly-reported SU(5)-branched mappings, the principal characters now span the following (5-fold) subset:

$$\chi_{1^{12}}^{[\lambda]} \to \{330, 1728, 3696, 3564, 3520\}.$$
(39)

For the SU(6) branchings, the only two dual-group irrep mappings possible are:

$$[71^5] \iff \{7, 31, 35, 26, 26\}\dot{\Gamma},$$
 (40)

of cardinality 462, and the first of the SA-irrep mapping, equation (41) below.

What is striking about the complete sets of mappings is their strictly 1:1 bijective quality down to $\lambda_{\text{SA}} \vdash n$. This property of the mappings is retained in this specific $S_{12} \downarrow \mathcal{I}$ case *irrespective* of the branching depth. This is a new and strongly physics-related property. Its importance arises from the fact that it implies a strict independence of the complete set of relationships contained over all the above SU(2)-SU(6) subset mappings, and thus of the complete algebra. The occurence here of a series of (new) prime numbers as coefficients for the resultant icosahedral irreducible representations (irreps) serves to stress the strong virtues of odd-permutational class-operator algebras, in the context of 1:1 bijective mapping. Hence finally, the extended hierarchical calculations via $\Delta \Lambda_{.,\lambda'}$ relationships (*i.e.*, beyond those of Ref. [5]) yield:

$$[6, 21^4]_{SA} \iff \{41, 138, 185, 97, 97\}\dot{\Gamma},$$
 (41)

$$[5, 3211]_{SA} \iff \{129, 508, 653, 379, 379\}\Gamma$$
, and (42)

$$[4, 422]_{SA} \iff \{65, 174, 245, 109, 109\}\hat{\Gamma},$$
 (43)

whose respective S_{12} group characters are simply:

$$\{\chi_{1^{12}}^{[\lambda]}\} = \{3564, 7700, 2640\}.$$
(44)

These final additions to the 1:1 mappings yield the *complete* subduced algebras to $SU(m = n/2) \times ...$ forms, and thus implicitly up to the Sullivan and Siddall(-III) limit [10] form, $SU(m = n) \times S_n \downarrow \mathcal{I}$.

All the SU $(n/2 \le m < n)$ branchings beyond [4422]_{SA} are defined inherently now via the structure of the S_n group itself predictably as "involutions about" its self-associate irrep subset. Hence the specific SU $(7) \times S_{12} \downarrow \mathcal{I}$ results naturally span the following subset (*i.e.*, starting from forms based on the results given in Eqs. (40, 35)

$$[61^6] \longleftrightarrow [1^{12}] \otimes [71^5],$$

$$[521^5] \longleftrightarrow [1^{12}] \otimes [721^3], \tag{45}$$

 $[431^5] \iff \{32, 139, 171, 106, 106\}\hat{\Gamma},$ (46)

$$[4221^4] \iff \{46, 158, 204, 113, 113\}\hat{\Gamma},$$
 (47)

$$[3321^4] \iff \{27, 127, 158, 100, 100\}\hat{\Gamma},$$
 (48)

where the last three cases come from $1^{12} \otimes [\lambda]$, for $[\lambda] = \{[7221], [7311], [732]\}$, respectively).

Even for a twelve-fold identical $I_i = 9/2$ spin cluster as a model over a point-lattice polyhedral network [2,3], such ensembles still correspond to SU(m)-branching levels below the maximally-determinate $SU(m = 12) \times S_{12} \downarrow \mathcal{I}$ form. Thus they necessarily must be determinate, on the basis of the number of independent relationships implicit in the above 1:1 bijectivity already exhibited by the mapping. This itself is a consequence of the total lack of degenerate, or simple multiple entries (of earlier components), over the full $SU(m \leq 6 \ (= n/2)) \times S_{12} \downarrow \mathcal{I}$ sets of observed mappings, as derived via (suitably-ordered) direct, or symbolic SCA-, techniques. A further explicit weighting, now involving modules (SFs) distributed on $\{|IM\rangle\}$ space, as in Tables 1, 2 of reference [5a] (for 12fold clusters of deuterons or ¹¹B) (or as in an earlier specific discussion of these aspects [21]), is too lengthy to setout here. For the full $[{}^{\mu}BH]_{12}{}^{2-}$ anions the full total (product) weights follows directly, on forming all possible inner products between the $\Gamma(\mathrm{SU}(2) \times \mathcal{S}_{12} \downarrow \mathcal{I})$ and appropriate $\Gamma(\mathrm{SU}(m) \times \mathcal{S}_{12} \downarrow \mathcal{I})$ results, discussed above. A distribution of the SU(m)-partitional model forms as monomial SFs (or S_n -modules) over $\{|IM\rangle\}$ -space should be included in the final weightings assigned to isotopomeric clusters. However, since the distribution of monomial SF models on M(SO(2)) (of $\{|IM\rangle\}$) projective aspects are not strictly involved in the determinacy question, they are not given explicitly here for brevity.

4 Some contrasts within $[\mu^{=10}B]_{12}$ -related spin ensembles

In addition to stressing the importance of strict bijective nature of the mapping, we now note that both the $[^{\mu}B]_{12}$, ($\mu = 10$, or $\mu = 11$) (all identical nuclei) isotopomeric clusters yield totally determinate natural embeddings. In addition, it is of some spectroscopic interest to point out on the specific basis of Sullivan and Siddall-III earlier Casimir invariant study [10], that the (equimix) isotopomer $[(^{10}BH)(^{11}BH)]_6(\otimes \mathcal{S}_6 \downarrow (\mathcal{S}_3 \otimes \mathcal{S}_3))$ -derived in one sense from icosahedral symmetry as an enveloping group for the 12-identical spin clusters-includes an indeterminate embedding. This arises from the latter's $[^{10}B]_6$ isotopomeric (partial) cluster. It is a direct consequence of its SU(7)-branching now having m-values of SU(m) $\times S_6 \downarrow S_3$ *greater than* that of its symmetric group index, n. This occurs despite the full range of all $m \leq n$ embeddings being determinate forms of spectroscopic interest, *i.e.* associated with the $S_6 \downarrow S_3$ mappings, as given in references [15,16]. The latter is of some interest, both in the context of the classic work by Galbraith *et al.* [12,13] and of more recent work on icosahedral cage forms [18–20,22–24].

Naturally, much of the recent interest in $S_n \downarrow \mathcal{I}$ natural embedding has been driven by work on C_n fullerenes, and (in particular) on their spectral and their structural (cage) properties. Interest in the ¹³C_n cage-clusters and their RV weight properties dates from the work of Balasubramanian [19,22] and from similar work [18] on (alternative) [H(²H)¹²C]₂₀ dodecahedranes – at present restricted to the $SU2(3) \times S_n$ algebras. For an overview of the correlation between the \mathcal{O}_n orthogonal and S_n permutational symmetries, the 3-space work of Butler and King [25] and Wybourne's use [26] of restricted space SFs should be consulted. Similar concepts govern (*e.g.*) a more recent work [27] of ours.

5 A role for induced symmetry in determinacy problems

From the structure deduced here for the $S_n \downarrow \mathcal{I}$ naturally embedded algebras, it would appear that the icosahedral group may be S_n -embedded in a determinate fashion right up to the highest branching levels of physical interest, $SU(10) \times S_{12}$, and that this may not be limited only to the $S_{12} \downarrow \mathcal{I}$, since $S_{60} \downarrow \mathcal{I}$ is a known Cayleyan determinate embedding [3a, c, e, 22]. This is seen as a consequence of both the structure of the lower group's class algebra, in generating prime-number subduction coefficients in such processes, and the example corresponding to the $m \ll n$ Sullivan and Siddall criterion [10]. Both effects work in favour of $S_n \downarrow \mathcal{I}$ determinacy.

In the context of induced symmetry, the question arises of whether a direct intermediate group to a Cayleyan embedded subgroup plays a role in determinacy as in the finite group chain:

$$\mathcal{S}_6 \supset \mathcal{O} \supset \mathcal{D}_3, \text{ for } /\mathcal{D}_3 / = 6,$$
 (49)

of equation (23) – as discussed in a wider context elsewhere [28]. Whilst its ability to retain determinacy as a guaranteed property is not proven in an analytic sense, as a corollory to the chain properties the logic for its viability appears irrefutable.

6 Concluding remarks

All of the above reinforces the view that the study of nuclear spin effects on spectral properties via the dual group and its multicolour $(\lambda \vdash n)$ SF-like models yield valuable physical insight into cage-cluster RV statistical weighting problems, not otherwise accessible. Historical parallels may be drawn with the role of recouplings including spin momenta (and associated specific particle-type statistics) in the early shell models of quantum physics in several distinct fields from 1930s. Indeed, the use of SFs in the former contexts for mapping onto restricted group spaces is seen as part of a long (atomic) physics tradition [25–27], now with applications in molecular physics, e.g. in defining the structure of $SU(2) \times S_n$ tensorial sets, which encompass S_n invariants [29,30] and insightful inter-group co-operativity [31]. These aspects are adjuncts to the form of carrier spaces for Liouville space (super)boson mappings [32]. The presentation of this work has stressed the value, both of Kostka decompositional reduction coefficient sets and of the hierarchical difference properties of SF models, as generators in the physics of higher dual groups which are related to certain sets of identical spins of cage-isotopomers. One notes that this example of $m \sim n$ SU(m) branching with higher indices for $S_n \downarrow \mathcal{I}$ is of strong phys-ical interest, comparable to the earlier $S_6 \downarrow \mathcal{D}_3$ case set out in reference [10]. Certain wider generalities are stressed. These include the need for additional criteria for the determinacy of natural embeddings into specific (higher unitary/ \mathcal{S}_n) dual groups, for which parallels with the universal determinacy of Yamanouchi groupchains provide insight. Essentially, such guides would resolve this conceptual question for all non-icosahedral embeddings.

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Appendix A: Generalised weak-branching (high-index $S_{n\sim 20} \downarrow G$) cases: role of $\{ \triangle \Lambda_{.,\lambda'} \}$ Kostka sets in recursive process

Earlier work (e.g. Tab. 1 of Ref. [5b], in contrast to specific S_{12} mappings of Tab. 2 therein) has established the $\lambda \vdash n$ weak-branching limit for YR decompositions of SFs (or, simple modules). It is this limit which enhances the generality of the application of recursive hierarchy-based generators from YR (or selective ITPs), such as those given as equations (4-17; 18-20) in the text. Since an extended set of such generalised YR decompositional mappings based on $20 \sim n \leq 24$ is incorporated into recent subsequent work [27], it is not given explicitly here. Certain additional group-embedding maps involving the \mathcal{I} group are available – on the basis these exhanced weaking-branching subsets

of Kostka coefficients occurring at $n \sim \geq 20^{-1}$, namely:

$$[16, 211] \implies \{180, 765, 945, 585\}\hat{\Gamma},$$

over $\{1145, -45, 0, 0, 0\}\check{C},$ (50)
 $[15, 32] \implies \{915, 3705, 4620, 2790\}\hat{\Gamma},$

$$\{55575, -45, 0, 0, 0\}\breve{\mathcal{C}},\tag{51}$$

$$[14, 42] \Longrightarrow \{3811, 14921, 18732, 11114\}\dot{\Gamma}, \{223839, 315, 0, 4, 4\}\check{C},$$
 (52)

$$\begin{array}{l} [14,33] \Longrightarrow \{2041,8412,10411,6371\}\dot{\varGamma}, \\ \{125970,-290,42,0,0\}\breve{\mathcal{C}}, \mbox{ via } \otimes [n-1,1] \\ (53) \end{array}$$

$$[12,71] \Longrightarrow \{6276, 25194, 31470, 18918\}\check{\Gamma},$$

over $\{377910, -90, 0, 0, 0\}\check{C},$ (54)

$$[11, 81] \Longrightarrow \{6884, 27556, 34460, 20672\} \check{\Gamma},$$

$$\{413440, 0, -20, 0, 0\}\breve{\mathcal{C}},\tag{55}$$

$$[10,91] \Longrightarrow \{4611, 18483, 23079, 13866\}\check{\Gamma}, \{277134, -42, 15, -6, -6\}\check{\mathcal{C}},$$
(56)

where $\check{C}^{\dagger} \sim \{C_2, C_3, C_5, C_{5'}\}$ is the class vector and $\check{\Gamma}(\mathcal{I})$ retains its earlier definition as a vector. These seven forms extend the $S_{20} \downarrow \mathcal{I}$ correlative mappings for this non-Cayley group embedding beyond those to be found in reference [18].

Appendix B: Specific model decompositionson S_{12} -irreps at intermediate branching

Here, we restrict the simple $S_{n=12}$ module (or SF) examples to those additional to the SU($m \leq 4$)-branched sets of reduction coefficients given in Table 2 of reference [5], so that the higher branched forms yield:

$$: 6222 : \longrightarrow \{1363; 7, 8, 1; 6, 9, 6, 3, 0; \\3, 6, 6, 3, 3, 0; 1, 2, 3, 1, 1, 2, 0, 1, 0\}\mathcal{L}$$
(58)

$$: 541^{3} : \longrightarrow \{1476; 8, 11, 4; 8, 12, 5, 6, 1; 7, 12, 6, 6, 2, 1; \\3, 9, 6, 6, 1, 2, 1, 00; 3, 3, 1, 2, 1\}\mathcal{L}$$
(59)

$$: 5322 : \longrightarrow \{1363; 8, 8, 1; 8, 11, 6, 3, 0; 6, 10, 9, 4, 3; \\2, 6, 7, 3, 3, 4, 0, 1, 0; \\3, 1, 2, 2, 0, 1, 1\}\mathcal{L}$$

$$(60)$$

$$53211 : \longrightarrow \{1486; 11, 14, 4; 11, 17, 9, 9, 1; \\ 8, 17, 14, 11, 6, 2; 4, 10, 11, 8, 6, 8, 2, 1, 1; \\ 4, 3, 3, 4, 1, 2, 1, 1\} \mathcal{L}$$

$$(61)$$

with the difference maps (of specific $|\Delta^{:\lambda:}|$ cardinalities) as single-digit Kostka reduction coefficient sets (omitting

comma separators), given by:

$$: 541^{3} :- : 631^{3} :, |\Delta| = 55, 440 \longrightarrow \{0000; 000; 10000; 330000; 26330000; 33121\}\mathcal{L}$$
(62)

$$: 5322 :- : 6222 :, |\Delta'| = 83, 160 \longrightarrow \{0000; 100; 22000; 343100; 14422200; 3122011\}\mathcal{L}$$
(63)

$$: 53211 :- : 541^{3} :, |\Delta"| = 166, 320 \longrightarrow$$

$$\{0010; 330; 35430; 158541; 11525611; 10220211\}\mathcal{L}.$$

$$(64)$$

The specific symbolic algorithm for the third form of Young's rule has been setout in the text by Sagan [6], or may be found as equation (5) of reference [3d]. The need to proceed sequentially from the least $\lambda \vdash n$ -branched models in such difference decompositional mapping will be clear from the above. The \mathcal{L}^{\dagger} vectorial space of the \mathcal{S}_{12} group may be shown to span the ordered set of $\{[\lambda']\}$ irreps (omitting leading elements of the (regular) subsequences):

$$\begin{split} \mathcal{L}^{\dagger}(\mathcal{S}_{12}) &= \{ [12], [, 1], [, 2], [, 11]; [9, 3], [, 21], \\ &[, 1^3]; [8, 4], [, 31], [, 22], [, 211], [, 1^4]; \\ &[7, 5], [, 41], [, 32], [, 311], [, 221], [, 21^3], \\ &[1^5]; [6, 6], [51], [, 42], [, 411], [, 33], [, 321], \\ &[, 31^3], [, 222], [, 2211], [, 21^4]_{\text{SA}}, [, 1^6]; \\ &[5, 52], [5, 511], [5, 43], [5, 421], \\ &[5, 331], [5, 322], [5, 3211]_{\text{SA}}, [5, 31^4], [5, 2221], .; \\ &[4, 44], [4, 431], [4, 422]_{SA} \}. \end{split}$$

Much of the work reported here (with the exception of Eqs. (6, 7, 21)) essentially *pre-dates* the author's explicit use of the Bayreuth Math. Inst.'s general S_n -symbolic package, Symmetrica [7].

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