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Quasi-particle dual mappings on $\{\widetilde{\mathbb{H}}_v\}$ carrier spaces for dynamical structures of $\mathcal{S}_{2n}$-invariant-based, integer-rank tensorial sets: A democratic-recoupling $\mathcal{S}_{2n}$-compatible overview of v-auxiliary labelling in superboson algebras of uniform multispin NMR ensembles

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The independent cardinalities of invariants (SIs) of the dual group and its $(2n)$-fold uniform spin ensembles are derived via $\mathcal{S}_{2n}$-decompositional approaches. The fundamental terms arise from character theory, whereas the $(2i < 2n)$ subsidary statistical subsets arise from arguments based on time-reversal symmetry (TRV) in the context of democratic recoupling – an approach consistent with a projective view and also with the nature of (Weyl) $(I \bullet I)_1 \cdots ()_i \cdots (I \bullet I)_n$ single pairwise exchange yielding TRV spin symmetry. In contrast to traditional $|D^0(\mathbf{U})|((\otimes SU(2))^{(2n)})$ formalisms, democratic sampling and recoupling now play important roles. As derived via superboson algebra, the dual tensorial properties of $[A\ldots]_{(2n)}$ uniform $2n$-fold NMR spin systems are seen also as fundamental in defining aspects of quantum computing via NMR analogues. Representational aspects of (quasiparticle) pattern algebras are given for superbosons over dual projective carrier subspaces of Liouville space. Hence an independent Lie-algebraic proof is derived of the fundamental "sign" structure of superbosons acting on $\{\sum_v \bigoplus_{\widetilde{\lambda}} \widetilde{\mathbb{H}}_v^{(\widetilde{\lambda})} \mid [\widetilde{\lambda}] \in \mathcal{S}_n;\ v \text{ aux.} \in SU(2) \times \mathcal{S}_n\}$ carrier subspaces. This constitutes a direct extension of earlier work [Physica A 198 (1993) 245]. The explicit SI-based tensorial v-auxiliary labels of the latter are defined via the dual action $\widetilde{\mathbf{U}} \times \mathcal{P}: \widetilde{\mathbb{H}} \to \widetilde{\mathbb{H}}\{\cdot \mid \widetilde{\mathbf{U}} \in SU(2), \mathcal{P}(\widetilde{\Gamma}) \in \mathcal{S}_n\}$ for the dual group and $[A\ldots]_n(\mathcal{S}_n)$ identical spin ensembles involving high degeneracies. Motivation for the work arose from certain fundamental quantum questions for dual group actions on *multiple invariant-based* systems, themselves subject to projective-compatible, $\mathcal{S}_n$ democratic recoupling. to graph-based results for such specialised uniform systems. Attention is drawn to various correspondences to geometric, quasiparticle (or superboson) and Lie-algebraic concepts for these systems, as being of topical interest both to quantum physics and to computing.

KEY WORDS: dual group $\mathcal{S}_{2n}$ invariants and analogous tensorial sets, $\mathcal{S}_n$-combinatorical decompositions, (super)boson mappings over (Liouvillian) carrier spaces of uniform NMR multi-spin ensembles, (Liouvillian) representational theory and Lie algebras of the dual group, $\mathcal{S}_{2n}$-invariants as auxiliary labels of $\widetilde{\mathbb{H}}_v$ carrier space, well-defined fundamental quantum entanglements

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1. Preamble

The value of transformational properties [1,2] as analytic relationships between distinct graphical recoupling schemes [3] is well established as an important part of both dual tensorial sets and quantum-Liouville tensorial NMR formalisms. On considering uniform n-fold NMR spin ensembles, one is concerned also with democratic recoupling [4], as a consequence of their adapted bases [5–20] being under (automorphic) $\mathcal{S}_n \downarrow \mathcal{G}$ spin symmetries – themselves based on specialised zeroth-order forms of Liouvillians (Hamiltonians). Within the latter, the $\{J_{AX}\}$ sets of couplings are weak compared to the various $J_{AA'}$, $J_{XX'}$ intracluster interactions. We shall restrict our discussion (without loss of generality) to the $[A]_{2n}$, $[AX]_{2n}$ NMR spin systems [6–11], for which a wider appreciation of (dual) tensors, and their dual group-based invariants (SIs) and projective techniques, all prove invaluable. In order to define the $\mathcal{S}_n$ auxiliary tensorial labels (or recoupled forms), a precise knowledge of the cardinality of these inherent SIs is necessary. Integer-rank tensorial formalisms themselves are prerequisites to, e.g., modern (operator-basis) studies of NMR evolution, of isotropic mixing-induced coherence transfer [14–20] or of intracluster-based spin relaxation processes. The automorphic spin symmetries defining spin subsystems represent extensions to known $\mathcal{GL}_n \supset \mathcal{S}_n \supset \cdots \supset \mathcal{G}$ chain properties [12,13], which are of wider conceptual significance to spectroscopy. These $\mathcal{S}_n$ chain properties utilised in the text are specific to *uniform multiple* spin systems, $[A]_n/[AX]_n$, whereas the optical spectroscopies are generally based on the othogonal groups and their distinct subduction scheme.

The purpose of this work is to address the nature of $\mathcal{S}_n$ projective models, and various related conceptual ideas, since dual group mapping has significantly contributed to the *foundations of quantum physics*, as well as yielding the prospect now of novel insights into topical *aspects of quantum computing*. Before proceding further, one should note the existence of strict group-theoretical limitations to simple analytic algebraic correlations between $\{3nj\}$-*graphical* formalisms [3] and the totally *democratic* $\mathcal{S}_n$ group-based forms [4]. Where such analytic forms exist, they are restricted to certain specific few-body systems whose recoupling may be characterised by (tridiagonal) Jacobian forms [4], for which eigenvalues are universally derivable. The *origins* of the (analytic) *disjuncture* between graphical and democratic recouplings (or chain sequences) in all other cases is simply due to the higher levels of degeneracy found in the generalised $[A\ldots]_{2n}(\mathcal{S}_{(2n)}) \mid 2n \geqslant 4$ type spin (sub)systems, all of which lie beyond the $\mathcal{S}_4 \downarrow \mathcal{D}_2$ automorphic group limit given originally by Galbraith [21] in his 1972 work. The origin of this limitation alternatively may be viewed as one arising from the overall system-dependence on *more than a single scalar invariant* for specific high n-fold spin symmetries of $[A\ldots]_{2n}/[A\ldots]_{(2n+1)}$: $(2n \geqslant 4)$ spin ensembles. This is an especially insightful view. One also notes that the admixture of graph theory for recoupling, or in defining SIs [22,23], to essentially projective (quasiparticle, or group subduction) methods for other quantum properties is neither tractable, or sufficiently general above $2n = 10$, to be useful in forming higher $\mathcal{S}_{2n}$ dual tensorial structures. This point also deserves wider recognition in the literature.

Despite the above limitations to democratic recoupling, $(SU(2)\times)\mathcal{S}_n$-based quasiparticle or analogous projective methods (over Liouvillian carrier space) offer novel physical insight into spin dynamics, once the impact of scalar invariant cardinalities (based on time-reversal invariance [22,23] and its numerical coefficients [24,25] of some specific model) is recognised. As the nature of *quantum entanglements* of quantum informatics and computing mirror certain fundamental aspects of n-fold NMR spin ensembles, the questions raised here are clearly of wider topical interest. The NMR systems of use in modelling quantum informatics (teleportation) typically include bases comparable to those under (dominant intracluster) (isotropic) coupling [22] or other (dipolar) isotropic interactions, $\widehat{\mathcal{L}} = [\widehat{H}_{\mathrm{sc}},\ ]_-$, discussed here.

An understanding of the specific role(s) of various projective methods in defining dual tensorial sets, their auxiliary labels and associated (independent) scalar invariant cardinalities, |SI|s, is of fundamental importance to quantum physics. No $\mathcal{S}_n$ projective formalism for the cardinality of the SIs has appeared previously in the literature. In addition, the fuller significance of augmented dual quasiparticle formal mapping [26–31] deserves to be more widely recognised as a powerful projective technique. It defines the Liouville space mappings as a closed superboson algebra [28] based on the dual mappings:

$$\widetilde{\mathbf{U}} \times \mathcal{P} : \widetilde{\mathbb{H}} \to \widetilde{\mathbb{H}}\big\{ D^k\big(\widetilde{\mathbf{U}}\big) \times \widetilde{\Gamma}^{[\tilde{\lambda}]}(v)(\mathcal{P}) \,\big|\, \widetilde{\mathbf{U}} \in SU(2), \mathcal{P} \in \mathcal{S}_n \big\}, \tag{1}$$

with the structured carrier subspaces here defined via the auxiliary democratic v-labels, as in section 6.2. Linkage of superboson algebra to Lie algebra is developed in the main text. Our earlier work stressed that superbosons are the equivalent of Wigner fundamental unit (super)operators; thus, they transform as irreps under the dual product group, $SU(2) \times \mathcal{S}_n$. Novel usage of additional $\mathcal{S}_n$ techniques [24,25,32–35] is stressed in deriving the independent SI cardinalities via certain explicit time-reversal coefficients with a democratic recoupling (sampling) context. This constitutes the specific purpose in reporting this work, in which we shall focus on various general aspects of the NMR of regular uniform (cage-like) spin ensembles, $[A\ldots]_{2n}(\mathcal{S}_{2n})$, for higher n-fold indices, in the range $2n \sim 12,\ 20$.

In addition to involvement in dual map actions, the role of $\mathcal{S}_n$-combinatorics in spin physics is examined, with the $\mathcal{S}_n$-group properties viewed as part of *algorithmic symbolic* computing [32–34]. In this context, the nature of general decompositional processes is important for its conceptual value for the invariants [24] and also in alternatively deriving the auxiliary label sets from subduction pathways of [25]. Here the specific role of the reduction coefficients generated from Yamanouchi stepwise $\mathcal{S}_n$-chain subduction processes [24,25,35] should be noted. Both of these mapping techniques are invaluable in defining the fundamental SI cardinality, e.g., as in the enumerations of section 4 below. Since the entanglements of quantum informatics and computing (teleportation) necessarily mirror certain fundamental (superpositional basis) aspects of n-fold NMR spin ensembles, the questions raised here are of wider topical interest. This point arises from the Liouvillian mappings involving explicit auxiliary labels, a point often overlooked in discussions of the foundations of quantum physics.

After a brief overview of additional context, including CNP weight properties isotopomers, section 3 gives a brief overview of some specialised forms of combinatorial functions for their pertinence to Weyl's TRV-based *pre-graph recoupling theory* view of scalar invariants. Subsequently, the fundamental components and the subsidary $(2i) < 2n$ statistical contributions to the number of independent scalar invariants for $2n$-fold identical spin ensembles under the dual group are considered in sections 4, 5, in terms of explicit mathematical decompositions; thereafter, section 5 focusses more especially on the role of certain bi-, quadra-partite $\mathcal{S}_n$ character sets of smaller related $\mathcal{S}_n$ groups (those associated with $\overline{((\ldots)(\ldots))}$ or $\overline{((\ldots)(\ldots)(\ldots)(\ldots))}$ block permutations which need be excluded from extended Weyl TRV models). The fundamental and corrective terms are discussed for a couple of specific $(2n)$ identical spin ensemble applications. Dual group representation theory is extended in sections 6.1, 6.2 and appendix A, particularly in relation to (super)bosons of pattern and Lie algebras. The final focus here is on the structure of the dual group carrier spaces, whether one is considering problems described in terms of Hilbert or Liouville space formulations. Section 7 summarises the correspondence between these algebras and certain standard NMR tensorial properties [1,2,14,15] as analytic transformational properties allied to graph recoupling schemes. Subsequently, section 7.2 focusses on the role of inner tensor products (ITPs) in the formation of integer-rank democratic dual tensorial sets. This serves to introduce section 8 which gives a brief overview of the inherent structure derived for these dual tensorial sets, with the discussion restricted to (integer) component k rank (alone) descriptions above $k = (n/2)$, essentially for reasons of generality. Our concluding remarks in section 9 focus on the generality of the techniques adopted here, on the role of geometric combinatorics in physics, as well as stressing the pertinence of (auxiliary) tensorial structure in discussing quantum computing and the foundations of quantum mechanics from a Liouvillian carrier space viewpoint.

The notation adopted throughout the text derives *directly from standard usage* of Sanctuary [1,3] and Biedenharn and Louck [2,26,27], all of whom have contributed to the foundations of quantum physics. Here quasiparticle formalisms (originally due to Biedenharn and Louck [26,27]) now in a recently extended Liouville space form, are of particular value to NMR spin dynamics [28]. Apart from the terms FG, and irreps/reps for finite groups and the now well-established Biedenharn shorthand for irreducible and generalised representations, the mnemonics used herein consists of SI (|SI|), TRV, YC and $\mathrm{Y}^m\mathrm{S}$, for scalar invariants and their cardinality, time-reversal invariance, Yamanouchi chains and permutational symbol, respectively. Certain additional mnemonics (of group theoretic or combinatorial origins), such as ITP, LR, SF, etc., are all carefully defined on first usage.[1] Finally for clarity, we stress that the $\tilde{\cdot}$ (tilded) quantities, labels kqv and projective action $\mathcal{P}$ all refer to Liouville space formalisms, whose democratic (as compared to graphical) recoupling (see section 7) is denoted by the alternative auxiliary set $\{\widetilde{\mathcal{V}}\}$ (compared to $\{\widetilde{\mathcal{K}}\}$) of integer rank tensor notation.

[1] With the exception of the mathematical terms $\lambda \vdash n$, $\doteqdot$ for respectively "number partition of n", and "defined as".

2. Initial specific contextual discussion

2.1. Dual group invariants and their tensorial sets

The scalar invariants defining uniform n-fold NMR spin ensembles under certain established types of (liquid, or mobile liquid-crystal mesophase, based) NMR Hamiltonians, may be interpreted in terms of either the implied $(\otimes SU(2))^{2n}$ decompositional formalism for the $|D^0(\mathbf{U})|$ frequency, or (equally and perhaps better) in terms of an appropriate $SU(2) \times \mathcal{S}_{2n}$ (or bipartite) dual group algebraic model. The essential role of time reversal symmetry factors [22,23] is retained in both approaches.[2] Clearly, the $SU(2) \times \mathcal{S}_{2n}$ restricted aspect of the dual group itself is fundamental to the study of (democratic-based) scalar invariants, since the $SU(2) \times \mathcal{S}_{2n}$ dependence holds *irrespective of* whether the $[A\ldots]^{(I_i)}_{(2n)}(SU(m) \times \mathcal{S}_{2n})$ spin system *actually pertains* to a uniform multiple spin-one-half ensemble, or to some *uniform higher* $SU(m \geqslant 2)$ unitary algebra. Hence, the actual number of independent scalar invariants (SIs) is a property of fundamental importance to (auxiliary) tensorial structure, with various interesting combinatorial properties.

For certain initial small $(2n\ (<\ 10))$ fold systems and within an "auf-bau" constructive process, Corio [22] utilised the early (i.e., pre-1950s graph theory) $(\otimes SU(2))^{2n}$ direct-product bracket (linear-recoupled) notation, adopted from Weyl [23], to estimate the number of independent scalar invariants. However, the invariants of uniform spin systems arise indirectly in dual-group quasiparticle mapping formalisms originally due to Biedenharn and Louck [26,27] in which mapping over a carrier space plays a fundamental role. In the context of stationary Liouvillians [3,14–20] of NMR spin dynamics (utilising integer-rank tensorial bases), a recent realisation of dual mapping over the Liouville-augmented carrier space-based superboson mappings of [28] explicitly involves the auxiliary SI-based labels. The main text sets out the necessary additional statistical (non-QP) mappings involved in deriving the cardinalities of uniform spin ensemble SIs at the kernel of this work. Generalised dual tensorial sets, as structures [29–31] with specific $\{\widehat{\lambda}\}$ Schur-function-based origins and specific finite group embedding properties are the subject of related work on the role of combinatorics in spin physics [22–38].

Dual group treatments of NMR are a logical conceptual consequence of Balasubramanian's discussion [6] of spin ensembles which exhibit permutational properties, in terms of group automorphisms. The latter arises directly from the nature of certain $\cdots \mathcal{S}_n \supset \cdots \supset \mathcal{G}$ chain properties. In contrast to conventional rovibrational spectral subduction chains (involving the orthogonal group) for uniform NMR ensembles, it is now the $\mathcal{S}_n$-based theoretical physics group-chain,[3] which is pertinent. Descriptions of spin ensemble properties and their democratic system invariants follow directly. The latter point stresses the fundamental difference in viewpoints between those of the present

[2] For technical reasons, the distinction between even and odd sets of spin operators is a cogent point in both types of modelling with the odd spin operator set derivable from the cardinality of the immediate preceding "even" indexed set.

[3] Rather than that containing the orthogonal group(s), as in other types of spectral problems.

author and earlier workers.[4] For an introduction to modelling via discrete mathematics and the $\mathcal{GL}_n \supset \mathcal{S}_n$ group properties, references [24,25,29–36] should be consulted. The conceptual linkages between $\mathcal{GL}_n$, $\mathcal{S}_n$ groups and the invaluable physics role of Schur functions, i.e., mapped on to restricted subgroup spaces, are now well-established ideas [12,13,29–34,36]. Subsequent interest [37,38] in the role of the $SO(5)$ group and its subgroups in quantum physics is of recent origin. Such developments are of specific pertinence to Liouville space descriptions of NMR spin dynamics, as the $SU(2) \times SU(2)$ group is a direct subgroup of $SO(5)$.

More general specific discussions of the value to physics of traditional combinatorial methods, and of the $\mathcal{S}_n$ group with its Young tableaux notation, may be found in the 1994 physics text due to Sternberg [39]. Full details of (Yamanouchi group-chain) subduction processes, in terms of Young tableaux, and comments on precisely how to implement the Littlewood–Richardson (LR) rule for outer product decompositions are given there. Examples of enumerative applications in wider chemical physics spin ensemble problems, or of various combinatorial ideas derived from [24,25,32–35], may be found in recent related works of ours [5,29–31,36], or else in the extensive body of CNP enumerative work, due to Balasubramanian [40].

2.2. Contrasts between NMR dynamical structure and CNP spectral weight aspects

The most fundamental question addressed in the present work concerns the consequences of the *multiple scalar invariant* nature of highly degenerate democatically recoupled quantum spin systems and the resultant *disjuncture* in graphical versus projective (or group-subduction-based) analytic models under these circumstances. This may help to explain the intractability of certain NMR ensemble systems, i.e., *beyond* those of the simplest $A[X]_3$, or $[A]_4$, $[AX]_4(\mathcal{S}_4 \downarrow \mathcal{D}_2)$ forms. This underlying difficulty in treating highly degenerate spin systems specifically beyond $\mathcal{S}_{n\geqslant 4} \downarrow \mathcal{G}$ has not been recognised adequately in, e.g., the general NMR literature. Its origin is due specifically to the presence of the *multiple invariants*, which are themselves essential to definitions of auxiliary aspects of tensorial sets associated with uniform n-fold spin ensemble systems.

Our concluding remarks focus on the practical effect of these multiple invariants within a spin ensemble, and on a recent (if limited) advance which may in part resolve such questions.[5] Rather, it presents aspects of theoretical physics which are effectively modelled by NMR, stressing the nature of dual group decomposition in finding the numbers of independent scalar invariants which define the auxiliary labels. The latter are associated with both dual tensors (bases) and with obtaining *simple-reducible* superboson carrier subspaces for quasiparticle formalisms. The conceptual material of the main text spans several distinct areas, and highlights specific contrasts to other (either graph-recoupled, or product basis) NMR work (i.e., involving commutation rules [42], or else,

[4] As compared to either Corio's 1962–1968 insights [7,8], or his later augmented views discussed in [22]. However, even Corio's earlier theoretical analysis [7] implies a role for combinatorics in spin algebras.

[5] For clarity, we stress that this paper is *not concerned* with Hilbert operator methods in spectral calculations, see [41].

the so-called isotropic mixing techniques [43,44], from the zero-order form of scalar interaction, in coherence transfer [14–20] or multiquantum properties of symmetry-adapted spin systems [45–49]).

An additional role for ITPs occurs in a range of examples [49] involving extended caged-type multispin ensemble CNP statistical spectral weighting. Here, the total spin symmetry versus orbital symmetry is governed by a product constraint in the form of

$$\Gamma^{\text{nucl. spin}}\begin{pmatrix}\text{fermion}\\ \text{boson}\end{pmatrix} \times \Gamma^{\text{ro-vib}}\big(SO(3) \downarrow \mathcal{G}\big) \to \begin{cases}\mathcal{A}_2\\ \mathcal{A}_1\end{cases}, \tag{2}$$

as noted in various (cycle-indexed based) works of Balasubramanian [40]. Except where indicated otherwise, only the nuclear spin symmetry properties, as derived from the analogous NMR Liouvillian view for dominant intracluster couplings set(s) as networks associated with an automorphic spin symmetry [6], are considered in the remainder of this paper. The interdisciplinary nature of NMR ensures that its models and applications draw extensively on concepts from theoretical physics with the latter including conceptual areas of both symbolic computing and discrete mathematics.

3. Beyond Weyl $(\widehat{\mathbf{I}} \bullet \widehat{\mathbf{I}})(\widehat{\mathbf{I}} \bullet \widehat{\mathbf{I}}) \cdots (\widehat{\mathbf{I}} \bullet \widehat{\mathbf{I}})$-bracket recoupling: SIs via $\mathcal{S}_{2n}$ combinatorics

Since Weyl's bracket dot-product notation [23] predates both graphical and democratic schemes for recoupling, it could hardly be expected to yield functional forms of a more general type. However, initially these bracket models corresponded directly to the $(2, \dots, 2)$ type of multinomial partition (not previously mentioned in the physical science or NMR literature, to our knowledge) where for integer values of $n/2$,

$$\begin{pmatrix} (n) \\ 2, 2, \dots, 2 \end{pmatrix} \Big/ (n/2)! \doteqdot \frac{n!}{2!\,2! \cdots 2!} \Big/ (n/2)!,$$

so that the evaluation of the $(2n) = 6$ specialised partition becomes

$$N_{\text{SI}}^{(6)} \equiv \begin{pmatrix} (6) \\ 2, 2, 2 \end{pmatrix} \Big/ 3! = 15,$$

a physical result, known from the earlier $(\otimes SU(2))^{(2n)}$ formalism [22] with its linear recoupling. Further cardinalities of independent scalar invariants for modest index arguments are in accord with a difference expression, *provided uniform spin time-reversal invariance* (TRV) symmetry involving democratic recoupling and sampling (extending Weyl pairwise views [21]) may be simply incorporated into the scheme. At or above $N_{\text{SI}}^{(12)}$, no overall scheme for the coefficients of the various structured multipartite components exists, to the best of our knowledge. As the Weyl scheme is neither a pure graphical (or a fully democratic [4,21]) form of recoupling, this is perhaps predictable.

As a simple example of the (extended Weyl) system, the $2n = 8$ case is interesting with its |SI| realised as

$$N_{\mathrm{SI}}^{(8)} \equiv \binom{(8)}{2,2,2,2}\Big/4! - \binom{(6)}{2,2,2}\Big/3! + 1 = 91. \tag{3}$$

In addition for the number of independent scalar invariants of the (highest acessible) $2n = 10$ case, the TRV-weighted form, e.g., becomes

$$N_{\mathrm{SI}}^{(10)} \equiv \binom{(10)}{2,2,2,2,2}\Big/5! - 3\binom{(8)}{2,2,2,2}\Big/4! - 2\binom{(6)}{2,2,2}\Big/3! + 3 = 603. \tag{4}$$

For these simple cases, the various weighting coefficients are simple integers, corresponding to the numbers of ways the (current) multinomial term can be inserted into the (left-hand) next higher $(2, 2, \ldots, 2)$ component with due allowance being made for time-reversal (i.e., single pairwise permutational effects). Such a stepwise progressive view is of much less assistance in the region $20 \leqslant (2n) \leqslant 60$, where new insight may be sought only from the projective properties of the dual group, rather than directly from the (possibly more restricted) traditional frequency of occurence of $\mathcal{D}^0(\mathbf{U})$ group representations. Clearly in discussing single pair-exchange processes, Weyl's bracket structure exhibits *linear* recoupling; thus it lacks the democracy associated with projective treatments of uniform spin systems. This point is important once one searches for |SI|s of $(2n) \geqslant 10$ and higher $2n$-fold ensemble systems. With its underlying geometric basis, polyhedral combinatorics is needed to visualise recoupling in a non-graphical democratic view for the uniform multiple spin ensembles discussed here.

4. $N_{\mathrm{total:SI}}^{(2n)}$ via $\mathcal{S}_{2n}$-projective map decompositions onto the $\mathbf{N}_f^{(2n)}$, $(\mathbf{N}'^{(2n)}_f)$ $\mathcal{S}_n$ fundamental(s) and a series of weighted $(2i) < (2n)$ $N_{\mathrm{SI}}^{(2i)}$ terms

Considering the number of scalar invariants (SIs) in terms of the dual group $SU(2) \times \mathcal{S}_{2n}$ leads one to the following mathematical decompositional view, where the Weyl time-reversal invariance (TRV) modifies the additional weighted $(2i)$-based (earlier total) components, derived from all $(i < n)$ total terms within the (two-part) statistical mapping expression:

$$\begin{aligned} N_{\mathrm{total:SI}}^{(2n)} \equiv \big(\mathbf{N}_f^{(2n)} - \mathbf{N}'^{(2n)}_f - \mathbf{N}''^{(2n)}_f\big) + \Big\{ & N_{\mathrm{total}}^{(2n-2)}\binom{n}{1}\Big(\overbrace{\big(\widehat{\mathbf{I}}\bullet\widehat{\mathbf{I}}\big)\cdots\big(\widehat{\mathbf{I}}\bullet\widehat{\mathbf{I}}\big)\big(\widehat{\mathbf{I}}\bullet\widehat{\mathbf{I}}\big)\,\mathbf{1}}\Big)^* \\ & + N_{\mathrm{total}}^{(2n-4)}\binom{n}{2}\Big(\overbrace{\big(\widehat{\mathbf{I}}\bullet\widehat{\mathbf{I}}\big)\cdots\big(\widehat{\mathbf{I}}\bullet\widehat{\mathbf{I}}\big)\,\mathbf{1}\,\mathbf{1}}\Big)^*/f_1(\mathrm{to})\cdots \\ & + N_{\mathrm{total}}^{(\ldots)}\binom{n}{n-2}\Big(\overbrace{\big(\widehat{\mathbf{I}}\bullet\widehat{\mathbf{I}}\big)\big(\widehat{\mathbf{I}}\bullet\widehat{\mathbf{I}}\big)\,\mathbf{1}\cdots\mathbf{1}}\Big)^* + 1\Big\}, \end{aligned} \tag{5}$$

where the * starred combinatorial arguments above are democratically sampled, while the f_i factors are the (now explicit) inverse (extended Weyl) TRV factors. Clearly, the

$(\widehat{\mathbf{I}} \bullet \widehat{\mathbf{I}})$ pairs are progressively replaced by **1**, unities in the $\{\cdot\}$ statistical weight portion of the above model. Comparison of the above dual group decompositions, initially for specific $n < 5$ SI values, yields a set of *identical* cardinalities for the independent SIs, which are totally consistent with the $(\otimes SU(2))^{(2n)}$ product approach via the $D^0(\mathbf{U})$ frequency product decomposition with its original linear recoupling and TRV forms:

$$\left|D^0(U)\right|\left(\left(\otimes SU(2)\right)^{2n}\right).$$

The specific form(s) used for the set of (initial) fundamental $\mathbf{N}_f$ terms, on considering the first few $N^{(2n)}_{\text{total:SI}}$ for $2, 4, 6, 8 \leqslant (2n)$ values, corresponds to another established theoretical physics mapping concept [50]. One notes also that $\mathbf{N}'^{(2n)}_f$, as corrective terms, arise from the need to exclude $(\overline{(\ldots)(\ldots)})$ or $(\overline{(\ldots)(\ldots)(\ldots)(\ldots)})$, etc., sector permutations, since only the lone bracket $(\widehat{\mathbf{I}} \bullet \widehat{\mathbf{I}})$ pairs are functional exchange arguments in the proper derivation, of time-reversal invariance defining the total number of independent SIs.

It will be seen that there is a subtle distinction between the $(\otimes SU(2))^{(2n)}$-based Corio–Weyl approaches and a truly democratic dual group viewpoint. This concerns the contrasts between the implied linear recoupling of Weyl brackets involving time-reversal invariance, as in Corio's essentially *unitary* presentation [22], and the dual *totally projective* views associated with $\mathcal{S}_n$ democratic recoupling. This novel view is shown in equation (5), where the bracket operator pairs in the Weyl–Corio view [22,23] imply a specific linear ordering in the recoupling of Weyl brackets, which is in direct contrast to the projective notation, above. In the latter, all $\widehat{\mathbf{I}} \bullet \widehat{\mathbf{I}}$ terms form part of a democratic (recoupled) model, reflecting the *uniform cage* view of these (identical) spin ensembles, e.g., as pertinent to ^{1}H dodecahedrane or $^{13}C_{60}$ fullerene and to polyhedral combinatorics. Further comments on the form of such overall models are deferred until the end of section 5.

5. Role of $\mathcal{S}_n,\ \mathcal{S}_{n/2}$ group characters in defining the $\mathbf{N}^{(2n)}_f,\ \mathbf{N}'^{(2n)}_f$ terms

By comparison of each new $(2n)$-based result in a series with the hierarchy of unweighted fundamental components (of left-hand $\{\cdot\}$ brackets of equation (5)) within the series of $(\otimes SU(2))^{(2n)}$ equivalent decompositions, it may be shown that the general-n sums of squares of $\mathcal{S}_n$ bipartite characters play a central role in defining the mathematical decomposition of the $2n$-fold product, via $N^{(2n)}_f$ as a sum over bipartite irreps (in the Butler 1971 irrep notation), as

$$\mathbf{N}^{(2n)}_f \equiv \sum_{\text{bipart }[\lambda]=[0]}^{[(n/2)]} \left(\chi^{[\lambda]}_{1^n}\right)^2(\mathcal{S}_n). \tag{6}$$

From this equation and analogous expressions for corrective terms on $\mathcal{S}_{n/2}$ (for non-TRV active $\overline{(\ldots)(\ldots)}$ block permutations of still higher $(2n)$ cases) particularly simple forms for all the fundamental terms of the hierarchy are obtained. The remainder of the problem (i.e., within the braced portion of equation (5)) is thus reduced to forms involving statistical weightings of preceding steps for the (overall) $N^{2(n-i)}_{\text{total:SI}}$ values. Hence, for the nearly maximal ($2n = 10$) spin ensemble, the full calculation now has the following combinatorial structure under the $SU(2) \times \mathcal{S}_{2n}$ dual group:

$$\left\{(42-0) + 91\binom{5}{1} + 15\binom{5}{2}\Big/2 + 3\binom{5}{3} + 1\right\} \equiv 603, \tag{7}$$

for $N^{(10)}_{\text{SI}}$, where the right-hand difference now refers to the earlier multinomial partitional view, a result derived in equation (4). The fundamental term and its correction for the $(2n) = 10$ case arise from the (bipartite irrep) expression

$$\mathbf{N}^{(10)}_f = \sum_{[\lambda]} \left(\chi^{[\lambda]}_{1^n}\right)^2 \equiv \left\{1^2 + 4^2 + 5^2\right\}(\mathcal{S}_5) \tag{8}$$

and the recognition that $N'^{(10)}_f$ vanishes identically here, as $(n/2)$ group index is not integer; hence, the respective terms become 42 and zero.

Further for the $((2n) = 12)$-fold spin ensemble, corresponding to simple icosahedral (natural group-embedded) spin symmetry, the fundamental component is now:

$$\begin{aligned} &\mathbf{N}^{(12)}_f \sim \left\{\left\{1^2 + 5^2 + 9^2 + 5^2\right\} \,\middle|\, \text{bipart char (set) } \in \mathcal{S}_6\right\} = 132, \quad \text{with} \\ &\mathbf{N}'^{(12)}_f \equiv |\mathcal{S}_3| \; (= 6), \end{aligned} \tag{9}$$

based respectively on the appropriate bipartite character (char) set and on the $N'^{(12)}_f$ corrective term of the corresponding $\mathcal{S}_{(n/2)=3}$ algebra – so as to evaluate (and thus exclude) $\overline{(\ldots)(\ldots)}$ versus $\overline{(\ldots)(\ldots)}'$ double-pair sector permutation. From these preliminaries, the number of independent SIs for this (even n value) $(2n) = 12$ (icosahedral-based cage) spin ensemble gives

$$\left\{(132-6) + 603\binom{6}{1} + 91\binom{6}{2}\Big/5 + 15\binom{6}{3}\Big/2 + 3\binom{6}{4} + 1\right\} = N^{(12)}_{\text{SI}}. \tag{10}$$

Hence, numerically one finds that the overall SI is given by $N^{(12)}_{\text{SI}} = 4213$, just as found on decomposing the $|D^0(U)|((\otimes SU(2))^{(2n)})$ expression for $(2n) = 12$. Thus, whether a purely linear or fully democratic explicit TRV model is adopted for the form of recoupling is not significant to the result of (low n) enumerations, i.e., this being so *provided* (*iff*) a corresponding series of *regular geometric solids* actually exists. $N^{(12)}_{\text{SI}}$ represents a limiting case to democratic recoupling and the dual group approach via uniform solid geometric (cage) models. Clearly, no intermediate component N_{SI} sets, or indeed suitable $\{f^{(2i)}_i\}$ Weyl TRV factors, are available in estimating the cardinality of $N^{(20)}_{\text{SI}}$ – only the $\mathcal{S}_{10}$-based fundamental term

$$N^{(20)}_f = \sum_{\text{bipart } \lambda}^{[10]} \left\{\chi^{[\lambda]}_{1^{10}}\right\}^2 = 16796, \tag{11}$$

Table 1

The fundamental $\mathbf{N}_f^{(2n)}$, $\mathbf{N}_f'^{(2n)}, \ldots, \sum^{(f)}$ terms and a set of statistical contributions over all $(2i) < (2n)$-based SIs to $N_{\text{total:SI}}^{(2n)}$, the total number of independent SIs. The $N_{\text{total:SI}}^{(2n)}$ values for the total numbers of independent scalar invariants obtained via a democratic, projective mapping approach over separate fundamental and TRV weighted components. Here, the fundamental components are over the complete $(2n)$ Weyl bracket range, whereas the statistically weighted contributions involve progressive bracket replacement by unities within the functional argument, together with the use of earlier $(2i)$-based |SI| values. The influence of Weyl TRV symmetry is evident in the factors (denominators) arising in this latter statistical portion of the calculation.

n	$\mathbf{N}_f^{(2n)}$	$-\mathbf{N}_f'^{(2n)}$	$-\mathbf{N}_f''^{(2n)}$	$\to \sum^{(f)}$	$N(.(.)(.)1)$;	$N((.).(.)11)$;	$N((..).111)$	$N((.)11)$;	$N(.11)$	$N_{\text{total:SI}}^{(2n)}$
2:	2			$= 2$:	1					3
3:	5			$= 5$:	$3\binom{3}{1}$	1				15
4:	14	2		$= 12$:	$15\binom{4}{1}$	$3\binom{4}{2}$	1			91
5:	42	0		$= 42$:	$91\binom{5}{1}$	$15\binom{5}{2}/2$	$3\binom{5}{3}$	1		603
6:	132	6		$= 126$:	$603\binom{6}{1}$	$91\binom{6}{2}/5$	$15\binom{6}{3}/2$	$3\binom{6}{4}$	1	4213[a]
7:	429	0		$= 429$:						(30,537)[b]
8:	1430	24	2	$= 1404$:						(227,475)[b]
10:	16796	119	0	$= 16,677$:						(6,192,443)[b]
12:	208012	714	6	$= 207,292$:						$(\ldots)$[b]

[a] The denominators 2 or 5 of the various combinatorial weighting terms here correspond to democratic TRV-based SI properties derived over regular geometric models.

[b] Not accessible under dual group projective mapping for lack of a $(2i) < (2n)$ progressive series of TRV factors and related solid-geometric models for $(2n) \geqslant 14$; this is essentially a mathematical limitation, comparable to Galbraith's earlier observation [21] concerning analytic constraints to multiple-scalar-invariant-based spin systems, with high degeneracies.

from the general $\mathcal{S}_{10}$ character algebra, and the initial correction

$$N_f'^{(20)}(\mathcal{S}_5) = \sum \left\{\chi_{1^5}^{[0]}\right\}^2 + \left\{\chi_{1^5}^{[1]}\right\}^2 + \left\{\chi_{1^5}^{[2]}\right\}^2$$

are accessible – as summarised in context in table 1.

In presenting specific views of time-reversal symmetry, under the dual group via expressions similar to equation (5) here, it will be observed that *beyond* the modest ensemble $(2n)$ values considered in [22] uniform model derivation of the (now explicit) TRV factors becomes non-trivial. Under democratic recoupling, the cause of this is clear. Some type of *regular solid-geometric model* is necessary in order to derive these f_i TRV-factors, but for $(2n) > 12$ uniform spin systems this is not mathematically attainable over the full progressive stepwise propagation, from the right-hand portion of equation (5). Indeed, whether Corio–Weyl type enumeration of the number of independent scalar invariants with its implicit TRV symmetry represents the full contraction for the actual specific numbers of independent scalar invariants – i.e., for uniform $(2n)$-fold ensembles, such as those corresponding to $[^1H^{12}C]_{20}$ dodecahedrane or higher regular cage isotopomers – still remains an open question. Since the $\mathcal{S}_{2n}$ group and unitary group approaches are necessarily interrelated views of the same physical phenomena, one may well question whether the *full purely unitary contraction* for SIs is reliable for highest $2n$ values, when derived via linear (or graphical) recoupling over these *uniform* spin ensembles representing polyhedral networks.

6. Quantum physics overview: Dual-group irreps and (super)bosons in a Lie-algebraic context

The properties described in equation (5) are those of the dual group inherent in spin and theoretical quantum physics, with its $(\mathbf{U} \times \mathbf{P})$ projective mappings acting over some $(SU(2) \times \mathcal{S}_n)$ carrier space. They are *not* simply a set of equivalence labels invoked for their *notational convenience*, as one frequently encounters, e.g., as in theories of electronic structure [51] and bonding. We shall discuss Hilbert, Liouville carrier spaces, their boson (superboson) mapping over these $\mathbb{H}$ (or $\widetilde{\mathbb{H}} \equiv \sum_v \widetilde{\mathbb{H}}_v$) carriers which via the SIs or v auxiliary labelling govern the actions of bosonic entities. The notation employed follows essentially from the standard forms adopted in [26–28]. The first subsection, on Hilbert space dual group representational aspects of boson pattern algebra, is given to set the material of the subsequent section in its proper conceptual context. In addition, an additional independent proof is given in appendix A for the representational structure of superbosons. This does *not invoke* now explicit calculations involving the Heisenberg super-generator(s) [28], or its right-derivation properties.

6.1. *Quantum physics via Hilbert space boson mappings*

In order to subsequently understand the representational aspects of Liouville space, it is first necessary to introduce some discussion of Hilbert space in terms of boson pattern algebras [26,27]. Since the scalar invariants whose independent cardinalities were derived in earlier sections apply directly to Hilbert formalisms, this subsection serves to link the two conceptual quasiparticle mappings of NMR interest. A totally general consequence of boson/superboson mapping is that it defines the completeness of irrep tensorial sets under the dual group [26,27], as in

$$\left\{ D^j(\mathbf{U}) \times \Gamma(\mathbf{P}) \,\middle|\, \mathbf{U} \in SU(2); \mathbf{P} \in \mathcal{S}_n \right\},$$

where the Gel'fand type pattern bases [26,27] arise from the (Hilbert) maps onto the conventional basis set, such as

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

The correspondence between the various Weyl, Gel'fand and boson-pattern algebraic notations is treated at length in [2,26,27]. Here, the Biedenharn and Louck defined $\{a_i\}$ bosons act as Wigner fundamental operators (WFO) [2], as in, e.g.,

$$\left\langle 1 \quad \begin{matrix} 1 \\ \binom{1}{0} \end{matrix} \quad 0 \right\rangle |jm\rangle \equiv \left[\frac{(j \pm m + 1)}{(2j+1)} \right]^{1/2} |j + 1/2, m \pm 1/2\rangle, \tag{12}$$

and a further expression obtained via the actions of the corresponding $(j + \Delta) = 0$ (zeroth shift term) boson:

$$\left\langle 1 \quad \begin{matrix} 0 \\ \binom{1}{0} \end{matrix} \quad 0 \right\rangle |jm\rangle \equiv (\mp)\left[\frac{(j \mp m)}{(2j+1)}\right]^{1/2} |j - 1/2, m \pm 1/2\rangle. \tag{13}$$

The unitary transformational properties arise from **U** rotational actions on members of the basis set:

$$\mathbf{U}|jm\rangle \sim \sum_{m'} \mathcal{D}^{j}_{m'm}|jm'\rangle; \tag{14}$$

similar transformations apply to **U** actions on the $\{\langle 2j\ [\cdot]\ 0\rangle\}$ Wigner fundamental (unit-tensor) operators (i.e., alias generalised bosons). All of these actions arise via the unitary rotations on an $\widetilde{\mathbf{n}}$ unit "celestial sphere":

$$\mathbf{U} \sim \exp\bigl\{-\mathrm{i}\phi\bigl(\widetilde{\mathbf{n}} \bullet (\sigma/2)\bigr)\bigr\}, \tag{15}$$

for ϕ some angle on $\widetilde{\mathbf{n}}$, and their Lie algebra, as realised via equations (6)–(12) of [27]. The full dual action, which now includes permutational forms (via Yamanouchi symbols), for the boson set on vacuum space (equations (32), (33) of [27]) arises from the fact that the **U** and **P** actually commute; the corresponding Liouvillian operators $\widetilde{\mathbf{U}}$ and $\mathcal{P}(\mathcal{S}_n)$ necessarily behave similarly. The scalar invariants associated with these bases (and WFOs) necessarily are of a form dictated by the dual group, where the latter includes both conventional eigenvalue sets via democratic recoupling and labelling associated with irreps (Young tables under $\cdots \supset \mathcal{S}_{n-i}$ chain), within the stepwise subduction [24,25,35] of the Yamanouchi chain $\mathcal{S}_n \supset \cdots \supset \mathcal{S}_2$.

For Hilbert space the role of a carrier space is especially straightforward [26,27], with permutational aspect of the basis described by a Yamanouchi symbol, so that in general one has

$$\bigl|(\bar{i}_1\bar{i}_2 \ldots \bar{i}_n)\colon jm\bigr\rangle \equiv \sum_{0:\widehat{k}_1 \ldots \widehat{k}_n}^{1} \left\langle \begin{pmatrix} 2j & 0 \\ j+m & \end{pmatrix} \right| \langle 1 \begin{bmatrix} \widehat{i}_1 \\ \widehat{k}_n \end{bmatrix} 0\rangle \cdots \langle 1 \begin{bmatrix} \widehat{i}_n \\ \widehat{k}_1 \end{bmatrix} 0\rangle \left| \begin{pmatrix} 0 & 0 \\ & 0 \end{pmatrix} \right\rangle \cdots$$

$$\cdots a^{(1)}_{2-\widehat{k}_1} \cdots a^{(n)}_{2-\widehat{k}_n}|0\rangle, \tag{16a}$$

or some equivalent form such as, from the standard properties,

$$\bigl|(\bar{i}_1 \ldots \bar{i}_n)\colon jm\bigr\rangle \equiv \sum_{0:\widehat{k}_1 \ldots \widehat{k}_n}^{1} \bigl\langle (2j\ 0)\bigr| \langle 1 \begin{bmatrix} \widehat{i}_1 \\ \widehat{k}_n \end{bmatrix} 0\rangle \cdots \langle 1 \begin{bmatrix} \widehat{i}_n \\ \widehat{k}_1 \end{bmatrix} 0\rangle \bigl|(0\ 0)\bigr\rangle \left| \begin{matrix} 1 & & 0 \\ & \widehat{k}_1 & \end{matrix} \right\rangle \otimes$$

$$\cdots \otimes \left| \begin{matrix} 1 & & 0 \\ & \widehat{k}_n & \end{matrix} \right\rangle, \tag{16b}$$

where the $(\bar{i}_1 \ldots \bar{i}_n)$ term, with $2 \equiv 0$ over $\{0, 1\}$, is the Yamanouchi symbol (Y^mS) [26, 27,39] corresponding to $[(n/2) + j,\ (n/2) - j]$, and $\langle 1\ [\cdot]\ 0\rangle$ are the standard bosons or WFOs, whose actions were described in equations (12), (13) above. The $\widehat{i}, \widehat{k}$ "hatted" quantities are ordered $(j+\Delta),\ (j+m)$ abbreviated indexed-terms – as defined in detail at the end of appendix A.1. Naturally, the orthonormal basis on left-hand (LH) side is within the usual constraints $(n/2 \geqslant j \geqslant 1/2, 0)$ and $-j \leqslant m \leqslant j$.

Hence, for $(\bar{i}_1 \dots \bar{i}_n)$ a Y^m symbol, the formal $\mathbf{P}(\mathcal{S}_n)$ projection, as the equivalent to the $\mathbf{U}$ action given above, then takes a form similar to that of equation (14), namely:

$$\mathbf{P}\big|(\bar{i}_1 \dots \bar{i}_n)\colon jm\big\rangle \equiv \sum_{(\bar{i}_1 \dots \bar{i}_n)'} \Gamma^{[(n/2)+j,(n/2)-j]}_{(\bar{i}_1 \dots \bar{i}_n)(\bar{i}_1 \dots \bar{i}_n)'}(\mathbf{P})\big|(\bar{i}_1 \dots \bar{i}_n)'\colon jm\big\rangle, \tag{17}$$

where the sum is taken over the primed Yamanouchi symbols and the Γs are irreps of the symmetric group (actions) associated with the dual group. This implies that the $\{|(\bar{i}_1 \dots \bar{i}_n)\colon jm\rangle\}$ set is a complete and irreducible set:

$$\big\{\mathcal{D}^j(\mathbf{U}) \otimes \Gamma^{[n/2+j,n/2-j]}(\mathbf{P})\big\},$$

within which $1/2$ (or 0) $\leqslant j \leqslant n/2$; this acts over some specific carrier space, such as

$$\mathbb{H} \equiv \bigoplus_{\lambda=(\cdot)} \mathbb{H}^{(n/2+j,n/2-j)}, \tag{18}$$

or more explicitly for the set components:

$$\begin{aligned}&\big\{\big|I(M=I)\big\rangle; \big|I(I-1)\big\rangle; \dots; \big|I(M=0)\big\rangle\big\}\\ &\quad\equiv \big\{[0]; \big\{[0]+[1]\big\}; \dots; \big\{[0]+[1]+\dots+[n/2-1]+[n/2]\big\}\big\},\end{aligned} \tag{19}$$

where we have utilised the Butler contracted (last digit of binary) permutational-irrep notation of [13], and where the inner ensemble $(i_1 \dots i_n)$ components of the basis have been suppressed for brevity. The individual component sets on the right-hand side here are simply Schur functions [29–31]. Thus, the left-hand basis of equation (16) may be represented as dual irreps in terms of certain specific Weyl and standard Young tableaux, with numerate forms set out in equation (56) of [26,27]. Furthermore, the absence here of any reference whatsoever to the auxiliary $v, \in SU(2) \times \mathcal{S}_n$ terms is in strong contrast to the following equivalent mapping over carrier space of the augmented spin spaces of section 6.2 below. Some consideration both, of how multispin bases are formed via recoupling, and of how such tensorial forms (rather than simple shift bases [52–54], or else generalised projective $\{|IM\rangle\langle IM|\}$ bases [55]) may be adapted to transform as irreps under the dual group is important, e.g., in proceeding from Hilbert space to subsequent Liouville space discussions of NMR spin dynamics.

We now turn to consider the equivalent actions of superbosons involving mappings over the augmented carrier space pertinent to NMR spin dynamics originally described [1,3,14,15] in terms of quantum-Liouville (QL) formalisms and simple tensorial basis sets established in the mid-1970s. The pertinance of superboson mappings to QL formalisms, with their correlation to the Biedenharn–Louck pattern algebras of Hilbert space, lies in its wider conceptual value for applications. In order to proceed further, the impact of the (Hilbert-space-defined) scalar invariants (SIs) on the augmented carrier space formalisms needs to be examined – essentially from the viewpoint of the retention of simple reducibility in established $SU(2) \times \mathcal{S}_n$ dual tensorial formalisms involving carrier subspaces.

6.2. Dual group superboson mappings pertinent to the QL tensorial formalisms

From the QL equation of [14,15], one may readily derive a dual group form as

$$-\mathrm{i}\hbar\dot{\phi}_q^k\big(v{:}\,[\widetilde{\lambda}]\big) \sim \sum_{k''q''v''} \langle\langle kqv[\widetilde{\lambda}]\big|\widehat{L}^{k'q'}(v')\big|k''q''v''[\widetilde{\lambda}]\rangle\rangle \phi_{q''}^{k''}\big(v''{:}\,[\widetilde{\lambda}]\big)(t=0), \tag{20}$$

for which the Liouvillian has the form (to zeroth order, i.e., as it occurs in systems with weak *intercluster* couplings compared to their dominant $\{J_{AA'}\}, \ldots$ intracluster interaction set(s)):

$$\widehat{L} \sim \big[\widehat{H}_{\mathrm{SC}}(\mathcal{A})^{(0)},\ \big]_-, \quad \text{or } \sim \big[\widehat{H}_{\mathrm{SC}}(\mathcal{A})^{(0)} + \widehat{H}_{\mathrm{DD}}^{\text{liq. cryst. media}}(\mathcal{A})^0,\ \big]_-,$$

as exemplified in [7–11,18–20] and [45–47], respectively. In the QL equation context, both the equivalent forms of bases,

$$\{|kqv\rangle\rangle\} \equiv \left\{\left|\begin{pmatrix}2k & 0\\ k+q & \end{pmatrix}\right\rangle\right\rangle\right\},$$

and the superboson or unit-tensor,

$$\big\{\langle\langle 2k\ [\cdot]\ 0\rangle\rangle\big\},$$

exhibit similar dual group transformational properties, beyond unitary aspects [1,3]. Further, these sets allow for the following Liouvillian form of mapping [28] over the now augmented carrier space, $\widetilde{\mathbb{H}} \equiv \sum_v\{\bigoplus_{(\cdot)} \widetilde{\mathbb{H}}_v^{(\cdot)}\}$, within the fundamental Liouvillian carrier-based mapping:

$$\widetilde{\mathbf{U}} \times \mathcal{P} : \widetilde{\mathbb{H}} \to \widetilde{\mathbb{H}}\big\{D^k\big(\widetilde{\mathbf{U}}\big) \times \widetilde{\Gamma}^{[\widetilde{\lambda}]}(v)(\mathcal{P})\,\big|\,\widetilde{\mathbf{U}} \in SU(2), \mathcal{P} \in \mathcal{S}_n\big\}. \tag{21}$$

Here the now explicit v labelling contains both the $\bar{v} = (k_1, \ldots, k_n)$ (field), as well as the recoupling labels or scalar invariant aspects. The new carrier space is clearly a direct sum of all suitable $\widetilde{\mathbb{H}}_v$ subcarrier spaces with $p \leqslant 2^2$ now describing the partite forms of $[\widetilde{\lambda}]$ irreps, and with

$$\widetilde{\mathbb{H}} \equiv \sum_v \bigoplus_{\widetilde{\lambda}} \widetilde{\mathbb{H}}_v^{(\widetilde{\lambda})}\big|[\widetilde{\lambda}] \equiv [\lambda] \otimes [\lambda']\big\},$$

and generating simply-reducible $\mathbb{H}_v$ subspaces, despite the non-SR properties of ITPs in general.

The equivalent inner tensor product as a function of k-rank (via the $\{j, j'\}$s of Hilbert space) is simply

$$\big\{[\widetilde{\lambda}]\big\} \equiv [n/2+j, n/2-j] \otimes \big[n/2+j', n/2-j'\big] \quad \forall\, \big(j \oplus j'\big) = k, \tag{22}$$

with j, j' as implied above. The specific forms of v-labelling are discussed in detail elsewhere [1,11]. Naturally, this expression is consistent with properties discussed previously [14–17], i.e., in terms of $\widetilde{X}_i$, X_i (Liouville/Hilbert space) class (cycle) operators over the $\mathcal{S}_n$ algebra for which one has

$$\widetilde{X}_i \mathcal{T}^{k,q}(v) \equiv X_i \mathcal{T}^{k,q}(v) X_i^{\dagger} \quad \forall \widetilde{X}_i, X_i \in \mathcal{S}_n, \tag{23}$$

where the equivalent (superoperator) $\mathcal{P}_\lambda$ projection action becomes

$$\mathcal{P}_{\widetilde{\lambda}} \mathcal{T}^{k,q}(v) \equiv \mathbf{P}_\lambda \mathcal{T}^{k,q}(v) \mathbf{P}_{\lambda'}^{\dagger} \quad \forall \left(\lambda \otimes \lambda'\right) = \widetilde{\lambda}. \tag{24}$$

This is in accord with the direct product nature of Liouville space, demonstrated in detail in [14–17] for the $\mathcal{D}^k(\widetilde{\mathbf{U}}) \times \widetilde{\Gamma}^{[\widetilde{\lambda}]}$ as irreducible representations (irreps) under the dual group. Naturally, there is a Liouvillian analogue to Yamanouchi-symbol-based transformations (i.e., matching equation (17) above).

For corresponding Liouvillian ladder operations as unitary group aspect of the dual group now in context of the superbosons (as defined in [24,25,28]) and with $\widehat{\mathcal{I}}_+ = [s_1\bar{s}_2,\ ]_-$; $\widehat{\mathcal{I}}_- = [s_2\bar{s}_1,\ ]_-$, one has the pair of expressions:

$$\widehat{\mathcal{I}}_\pm \overset{*}{y}\ (s_1 s_2) \longrightarrow \begin{matrix} (s_1^2) \\ (s_2^2) \end{matrix}, \tag{25}$$

and (retaining a consistent upper (lower) choice throughout) also that

$$\widehat{\mathcal{I}}_\pm \begin{matrix} (s_2^2) \\ (s_1^2) \end{matrix} \longrightarrow \begin{matrix} (s_1 s_2) \\ (s_2 s_1) \end{matrix}, \tag{26}$$

which serves to define a complete set underlying the ladder superoperators. Such actions necessarily derive from the Heisenberg super-generator formalism [28], i.e., as defined by the right-derivation-based [2,26,27] commutator properties:

$$\left[\left(\bar{s}_i^2\right), \left(s_j^2\right)\right]_- \equiv 2\delta_{ij} \quad \text{for } 0 < i, j \leqslant 2.$$

Equally, the direct product nature of Liouville space representations, in terms of Hilbert space irreps, allows for the alternative direct product decompositional definitions. These are comprised of direct sums, or direct differences, i.e., over the original boson structure to yield the superboson maps. This aspect of Lie-algebra-based representation theory was not explicitly mentioned in our 1993 paper [28]. Since this view yields a particularly direct confirmation of our earlier Heisenberg super-generator based maps, it deserves wider recognition. The appendix gives the specific details of these a forms of superboson mappings for the 8 non-trivial actions or representational correlations. For brevity, we shall largely omit further details of the adjoint bosons/superbosons and the structural sign question associated with equations (A1)–(A5), despite its importance in the context of Lie algebra [26–28]. More specific comments on the nature of superboson actions may be found from equations (50), (51) and [28, section 7]. Both [26,28] extensively discuss the fundamental orthogonalities (or invariant unit-operators) of bosons (superbosons) and their augmented Wigner/Racah algebras.

7. QL tensorial bases and graphical recoupling

7.1. Analytic transformations [3] for graph-based Liouville space formalisms

Naturally for $\mathcal{I}_\mu \equiv [I_\mu,\ ]_-$, the above superboson formulation is totally consistent with the various $\{\mathcal{I}_{\pm,0}\}$ actions on $\{|kqv\rangle\rangle\}$ bases given in [1–3,11,14–17], as expressed by

$$\mathcal{I}_\pm\ |kqv\rangle\rangle \equiv \left\{(k \mp q)(k \pm q + 1)\right\}^{1/2}\ |k, q \pm 1, v\rangle\rangle,\ \text{whereas}\ \overset{*}{y}\ \mathcal{I}_0|kqv\rangle\rangle \equiv q|kqv\rangle\rangle, \tag{27}$$

with the dot-product spin superoperator $\widehat{\mathcal{I}}^2 = [\widehat{I} \bullet \widehat{I},\ ]_-$ yielding

$$\widehat{\mathcal{I}}^2|kqv\rangle\rangle \equiv k(k+1)|kqv\rangle\rangle, \tag{28}$$

where the $\{|kqv\rangle\rangle\}$ bases here are explicit (outer) tensorial forms, rather than shift-bases [51].

The form of integer rank tensorial bases may be simply related to the frequently used $\{|IM\rangle\langle IM'|\}$ basis forms by standard transformations (here in the phase and the notation of [3,14,15]), such as

$$\mathcal{Y}^{k,q} \equiv |kq\rangle\rangle = i^k\big[(I)(k)\big]^{1/2}\sum_{MM'}(-1)^{I-M}\begin{pmatrix} I & k & I \\ -M & q & M' \end{pmatrix}|IM\rangle\langle IM'|, \tag{29}$$

(where for compactness the $(a)\doteq(2a+1)$ notation has been adopted), or its inverse:

$$|IM\rangle\langle IM'| = \big[(I)\big]^{-1/2}(-1)^{I-M}\sum_{k}^{2I}\sum_{q=-k}^{k}(-i)^k\big[(k)\big]^{1/2}\begin{pmatrix} I & k & I \\ -M & q & M' \end{pmatrix}\mathcal{Y}^{k,q}, \tag{29a}$$

while the tensorial form $T^{k,q}(1\ldots1)$ for the simplest spin ensemble may be cast into a recoupling expression, analogous to equation (29a), namely:

$$\begin{aligned}&\mathcal{T}^{k,q}\big(k'k''\big)\ \big(\equiv\big|kq(k_1k_2)\big\rangle\!\big\rangle\big)\\ &\quad\equiv \big[(k)(I_i)\big]^{1/2}\sum_{q'q''}(-1)^{k_1-k_2+k}(-1)^{k-q}\begin{pmatrix} k & k' & k'' \\ -q & q' & q'' \end{pmatrix}\mathcal{Y}^{k',q'}\mathcal{Y}^{k'',q''}.\end{aligned} \tag{30}$$

Further (unitary-based) graphical recoupling schemata involving, e.g., $\{T^k{}_{\{\widetilde{\mathcal{K}}\}}(111)\}$ etc., may be found in Sanctuary's early (1976) work [3] on the wider graphical schematic unitary group structures of Liouville space. Of special interest in the specific context of $\mathcal{S}_n$ auxiliary labelling of $|I^{\text{out}}M(\ldots)_\mathcal{V}\rangle\langle I^{\text{out}}M(\ldots)_\mathcal{V}|$, versus $T^{kq}_{\widetilde{\mathcal{V}}}(k_1\ldots k_n)$ bases for uniform ensembles in respectively Hilbert and Liouville spaces is the fact that there is no known analytic transformational relationship, in terms of either the democratic or Y^m-based projective *auxiliary labels* for higher indexed $SU(2) \times \mathcal{S}_{n\geqslant 4}$ -based systems. This observation is compatible with Galbraith's 1972 views on democratic recoupling [21] within multi-invariant-based systems.

Table 2
Some example representations for $\{T^{kq}(11\colon[\widetilde{\lambda}])\}$ dual tensors over the $(\alpha\alpha, (\alpha\beta + \beta\alpha)/2^{1/2}, \beta\beta;$ $(\alpha\beta - \beta\alpha)2^{1/2})$ adapted primary Hilbert set (after [16]). Note the coherence transfer implication to the representational structure of the $[\widehat{11}]$ symmetry breaking tensorial component. For the cardinalities of various adapted dual tensorial sets, see [11,17,36,57,58].

$$T^{11}(11\colon[\widetilde{11}]) \equiv \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \end{pmatrix} \Big/ 2^{1/2}$$

$$T^{22}(11\colon[\widetilde{2}]) \equiv \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \Big/ 2^{1/2}$$

$$T^{20}(11\colon[\widetilde{2}]) \equiv \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \Big/ 6^{1/2}$$

The value of purely unitary integer-rank tensorial bases and of $\sigma(t)$ density operator formalisms to NMR has been extensively studied in the 1980s and was reviewed in some detail, e.g., in Sanctuary and Halstead's works [3,14,15] and in other works [16,17] of that era. Here, we merely note that the entities of direct physical interest for NMR, and related techniques (e.g., nuclear acoustic resonance (NAR)) are the ϕ_q^k polarisations, or for NMR:

$$\phi_q^1(1\ldots1) \equiv \big\langle \mathcal{T}_q^{k=1}(1\ldots1)\big\rangle,$$

or, via suitable selective multiquantum COSY experiments [45], in which $q = 1$ processes are subjected to phase suppression, whereas their multiquantum analogues are now retained. In contrast, the solid state NAR is generally only concerned with $\phi_{\pm1}^2$ or $\phi_{\pm2}^2$ polarisations, as reviewed, e.g., by Fedders [56].

The form of dual symmetry bases in suitable adapted representations for a simple tractable NMR case, namely, the two $[A]_2$, is presented in table 2 to illustrate the above discussion, but such formal representations for more extended systems soon become somewhat intractable to display. Permutational actions applied to these representations are set out in [15, tables 8, 9], i.e., based on work first reported in [17]. An underlying fundamental theoretical reason for difficulty in handling dual group automorphic spin symmetry formalisms clearly derives from the lack of any direct general correspondence between graphical recoupling techniques [3] and projective formalisms [16,17], i.e., in all cases, *beyond* the $\mathcal{S}_2$ bases of equation (29) and the *few-body* system bases under $\mathcal{S}_3$ or $\mathcal{S}_4 \downarrow \mathcal{D}_2$, as originally discussed by Lévy-Leblond and Lévy-Nahas [4], and by Galbraith [21], respectively. It should be noted that the direct use, without tensorial recoupling over the full cluster, of multispin Lie algebras [20,42,44] totally ignores the existence of the essential underlying multiple scalar invariants. It is not to be recommended on the additional grounds of lack of generality – see Sanctuary's comments, in [1,14,15] and elsewhere, in the context of the analogous repetitive commutator evaluation question.

In addition to this fundamental theoretical question, Avent's (*mobile* liquid-crystal media) experimentally based work [45] highlights a further NMR problem. This is concerned with applying selective multiquantum techniques to spin systems of high automorphic spin symmetry under the $\widehat{L}_{\mathrm{SC}} + \widehat{L}_{\mathrm{DD}}^{\text{liq. cryst.}}$ Liouvillian. To date no way has been devised of differentiating between any pair of higher degenerate irreps (at or beyond $\mathcal{E},\ \mathcal{T},\ \mathcal{G},\ldots$, analogous $[n-m,m],\ m \leqslant n/2$) (multiquantal) spectral subspaces typical of $\mathcal{S}_6,\ \mathcal{S}_{12},\ \mathcal{S}_{20}$ or $\mathcal{S}_n \downarrow \mathcal{G}$ spin symmetries, *unless* they happen to have different maximal q projective bounds. Hence, it is questionable whether present NMR methods for generally identifying spectral features associated with specific spin symmetries and system invariants has proceeded much *beyond* the double resonance network tracing methods, as known in principle since the mid-1960s [59–61]. It is not enough just to supress all the non-$\mathcal{A}$ related lower-q multiquantal features, i.e., in more general problems than the liquid-crystal media simple $A[B]_3$ dipole–dipole-based one, considered in [45]. More progress has been made recently with the labelling aspects of the conceptual problem of describing democratic system invariants [24,25,30,35]. This development rests on an appreciation of the nature of group subduction in the Yamanouchi chain process. Recently, Chen et al. [62] considered various algebraic aspects of group subduction, but only for the rather small cubic groups and specifically based on the orthogonal, rather than the $\mathcal{GL}_n$ group chain.

7.2. *QL tensorial NMR as models of extended Biedenharn–Louck quantum physics under democratic recoupling and multiple invariants*

The initial discussion on auxiliary v's and scalar invariants under the dual group leads one to revise the earlier (graphical-based recoupling) $T^k_{\{\widetilde{\mathcal{K}}\}}(111\ldots)$ notation to now include the scalar invariants $\widetilde{\mathcal{V}}$, specifically in a democratic recoupling form [4,21] so on taking a further trace with the density operator:

$$\phi^k_{q\{\cdots\}}(v) \equiv \mathrm{Tr}\left\{\sigma \mathcal{T}^k_{q\ \{\widetilde{\mathcal{K}}\}}(v)\right\} \quad \text{or} \quad \phi^k_{q\{\widetilde{\mathcal{V}}\}}(v) \equiv \mathrm{Tr}\left\{\sigma \mathcal{T}^k_{q\ \{\widetilde{\mathcal{V}}\}}(v)\right\}, \tag{31}$$

where $\widetilde{\mathcal{V}} \in \mathrm{SI}(\mathcal{S}_n)$, or as $\in$ of a route: $\mathcal{S}_{n-1} \supset \cdots \supset \mathcal{S}_2$, as discussed respectively in sections 4, 6.2 and in [24,25,37,38]. Hence, the dual-group-based spin dynamics is governed by a more generalised form of von Neumann QL equation, which utilises basis sets of the form

$$\left\{\mathcal{T}^{k,q}{}_{\{\widetilde{\mathcal{V}}\}}(v)\right\} \equiv \left\{\left| W \times W_{\{\widetilde{\mathcal{V}}\}}\colon \begin{pmatrix} \square\square & & \square\square \\ \square\ldots & \otimes & \square\ldots \end{pmatrix} \right\rangle\!\!\right\rangle\Big\}, \tag{32}$$

in which the (LH) Weyl W table products are consistent with $SO(5) \supset SU(2) \times SU(2)$, and the right-hand product irreps (Young tableaux) are those of the inner tensor product

Table 3

The coefficients of some typical ITP ($\mathcal{S}_{12}$) decompositions over $\{[\lambda'']\}$ set (in dominance order [34]) within the $\lambda = n - i, i$ written $[i]$ in Butler's (1971) notation [12,13]. Only $\lambda \otimes \lambda'$ ITPs in (or close to) the *weak-branching* (WB) limit of $i \leqslant n/4$, which are general forms for high symmetric groups, are mentioned here; other specific ITP decompositions (of restrict $\mathcal{S}_n$ index form) are obtainable from symbolic algorithms, or from the package referred to in [32]. The initial $[n-1,1] \otimes [\lambda]$; ($[n-2,2] \otimes [n-2,2]$) ITPs are standard forms [49]. Note that for bipartite forms the nature of the ultimate decompositional components, as $[ii']$, totally reflects the form of $[i] \otimes [i']$ ITP under examination.

$[\lambda] \otimes [\lambda''](\mathcal{S}_{n\geqslant 12})$: reduction coefficients from decompositions over $\{[\lambda']\}$
0 1 2 11; 3 21 111; 4 31 22 211.; 5 41 32 311 221..; 6 51 42 411 33 321.222.;
7 61 52 511 43 421.331.; 8..
[2] [2] $\to$ 1121; 121; 1 1 1 0
[2] [3] $\to$ 0111; 220; 1 2 1 1 0; 1 1 1 0 .
[2] [4] $\to$ 0100; 110; 2 2 1 0 0; 1 2 1 1 0 .; 1 1 1 0 ..
[3] [3] $\to$ 1121; 221; 2 3 2 1 0; 1 2 2 1 1 0; 1 1 1 0 1 0
[3] [4] $\to$ 0111; 220; 2 3 1 1 0; 2 3 3 1 1 0; 1 2 2 1 1 10; 1 1 1 0 1 ..
Non/WB:
($[4] \otimes [4]$) $\to$ 1121; 221; 3 3 2 1 0; 1 4 3 2 1 0; 1 2 4 1 2 2 0 1.; . . 1 1 2 1. 1.; 1
$\mathcal{S}_{16}$: WB Lt:
$[4] \otimes [4]$ $\to$ 1121; 221; 3 3 2 1 0; 2 4 3 2 1 0; 2 3 4 1 2 2 0 1.; 1 2 2 1 2 1. 1.; 111010.1

(ITP) group,

$$[\lambda]\mathcal{S}_n \otimes [\lambda]\mathcal{S}_n \to \big(\{\ldots\}\mathcal{S}_{2n}\big) \downarrow \mathcal{S}_n \to \sum_{\widetilde{\lambda}'} c_{[\lambda],[\widetilde{\lambda}']}\big[\widetilde{\lambda}'\big](\mathcal{S}_n), \tag{33}$$

which generally span a non-simply reducible set. For clarity of notation in context of ITPs, the Liouville space irreps are denoted by $[\widetilde{\lambda}]$. Several examples of these $\mathcal{S}_{12\leqslant n\leqslant(20)}$-based ITPs [32–34,39], as components of equations (34) and (35) below, are given in table 3. For brevity therein, we have utilised the Butler $[\mu]$ ($\doteq [n-\mu,\mu]$) abbreviated irrep-notation [12,13]. The whole question of the general role of ITPs for high index, weak $\lambda \vdash n$ branched bipartite irreps in group structure has received algorithmic consideration recently [63].

The resultant tables from the bipart irrep ITP decomposition(s) necessarily span at most the sets of $p \leqslant 2^2$ part partitional forms. They are known to play an equally important role to Kostka coefficients in the structures (and inverse problem solutions [49]) associated with group embedding [5,36]. Various standard ITP decompositional maps were given elsewhere in the context of isotopomer statistical weight structures [5,40,49]. One way of representing more general $\{\widetilde{\mathcal{V}}\}$ system invariants beyond the few-body spin ensemble case has been suggested [24,25] recently, utilising the Yamanouchi group-chain subduction hierarchy [35]. To demonstrate these features, one first requires the $SU(2) \times \mathcal{S}_n$ dual irrep sets as functions of tensorial rank, as set out in a following section. Naturally, the reasons for our specific interest in both these mappings and their associated SIs for spin ensemble/systems arise from the ways in which they serve to define various distinct aspects of (dual group) tensorial sets. In turn, these bases allow one to define the properties of Liouville space, as utilised in multispin NMR evolution [10,11] and spin dynamics [1,2,14–20].

8. $\{T^k_{\{\widetilde{\mathcal{V}}\}}(111\ldots:[\widetilde{\lambda}])\}$ dual tensorial structure by rank alone

8.1. Outline derivation via Schur functions via Hilbert space properties

Dual tensorial sets are most conveniently derived [30] from Schur function (SF) descriptions of $SU(2)$ Hilbert space [7,8], i.e., based on simply-reducible Hilbert space 1 : 1 mappings over

$$\big\{\big|IM()\big\rangle\big\} \to a\big\{\{\widehat{\mu}\}a\big\}, \quad \text{for } \{\widehat{\mu}\} \equiv \{0\}, \ldots, \{n/2\}, \quad \text{as } M = I, I-1, \ldots, 0,$$

in order, for the bipartite Schur functions as a consequence of earlier relationship, equation (18), so that $|II(\ldots)\rangle, \ldots, |I0(\ldots)\rangle \equiv \widehat{\{0\}}, \ldots, \{\widehat{n}/2\}$, and more generally over the so-called reduced space – since the $\mathcal{S}_n$ group is a subgroup of the $\mathcal{GL}$ group. Hence, to obtain the tensorial space structure (here extending the ITP-based 1989 work [11] on $[AX]_4$, by both rank and q-projection) one evaluates successive minor skew-diagonal sums of products of SFs, i.e., starting the calculation from the maximal M forms, $M = I$, for the outermost integer k-rank. On restricting the presentation to the essential $\{T^k_{\{\widetilde{\mathcal{V}}\}}(v)\}$ component set(s) over *decreasing rank* with the help of the *strictly bipartite* Schur function products, from equations (12)–(15) [31] under (for its generality) a high n-index, weak $\lambda \vdash n$ (partitional) branching constraints, one obtains the following (outer) k-rank structure:

$$\Big\{\sum_{v,i} T^{k_{\max}-i}_{\{\cdot\}}(111\ldots)\Big\} \sim \Big\{\sum_i T^{k_{\max}-i}_{\{\cdot\}}(\ldots)\Big\}^v + \Big\{\sum_i T^{k_{\max}-i}_{\{\cdot\}}(\ldots)\Big\}^{v',v'',\ldots}. \qquad (34)$$

In terms of the final (reduction) coefficients of $\mathcal{S}_n$ reduced-space bipart Schur products (over dominanced-ordered irrep set $\mathcal{L}$ defined below), as detailed in [29], this becomes:

$$\big\{T^k_{\{\widetilde{\mathcal{V}}\}}(v)\big\}\big(SU(2)\times\mathcal{S}_n\big) \sim \begin{pmatrix} 1000; & & \\ 1100; & & \\ 1111; & & \\ 1111; & 110; & \\ 1111; & 111; & 11100; \\ \ldots; & & \end{pmatrix}^v \mathcal{L}(\mathcal{S}_n) + \begin{pmatrix} 0000; & & \\ 0100; & & \\ 1220; & & \\ 1442; & 310; & \\ 2483; & 650; & 24000; \\ \ldots; & & \end{pmatrix}^{\{\cdot\}} \mathcal{L}(\mathcal{S}_n), \qquad (35)$$

with the final $\{\cdot\}$ (superscript) labelling indicating that *all the remaining* $(v', v'', \ldots)$ auxiliary components are included (i.e., for *presentational* purposes) in this second factor (though belonging conceptually to a series of simply reducible subspaces), and where the irrep set

$$\mathcal{L}^{\dagger} \equiv \{[0], [1], [2], [11]; [3], [21], [111]; [4], [31], [22], [211], \ldots; \ldots\}\mathcal{S}_n \tag{36}$$

is given (after Sagan) in its full dominance order [34].

The products invoked here in deriving these $SU(2) \times \mathcal{S}_n$ tensorial set structures are those of strictly bipartite forms of Schur functions(SFs) for high indices – and consequently, in a weak $\lambda \vdash n$ branching limit – with the standard multiple usage of the Littlewood-Richardson rule replaced by a product decompositional mapping on subgroup restricted space [63] of some simply reducible(SR) SF set. These are subsequently decomposed onto irrep space by use of Young's rule [30,64] (and its non-simply reducible Kostka coefficients), with adequate sample total ITP decompositional processes being derived via independent symbolic group algebra to confirm the individual ITP results. It is important to stress the point about weak branching, as provides the generality in these and our earlier calculations [29,64]. Otherwise, the SF products would be tedious to evaluate. For higher branched (multipartite) forms, the SF mappings undoubtedly would be non-simply reducible and hence less accessible. The specific roles of the weakly-branched bipartite SF product maps onto SFs on restricted space and of the subsequent SF Young rule decompositions follow, e.g., directly from [29, equations (12)–(15)]. In addition for the auxiliary factors, an alternative way of representing the democratic invariant labels inherent in these dual tensorial sets exists via group subduction (chain) properties. These are outlined in table 4 for the specific case of $[A]_6$, of say $[A]_6X$, via the Yamanouchi chain properties of $\{[\lambda]\}(\mathcal{S}_6)$ irreps, and more generally via brief examples drawn from the $[A]_{12}(\mathcal{S}_{12})$ spin ensemble, as given in appendix A. A full description of the reduction coefficient sets derived from $\mathcal{S}_{12}$ irreps is available in related works of ours [24,25,30].

8.2. *An inherent limit to* $[A]_n(\mathcal{S}_n)$ *coherence transfer modelling*

It is long established [1] that the use of tensorial bases reduces the commutator problem of $|IM\rangle\langle IM|$ formalisms for weakly coupled systems [42–44] to well-established graph theory coefficients. For multiquantum processes of $[A\ldots]_n$ systems, a hierarchical approach to symmetry labelling has been suggested by Avent [45] and other workers [46], for examples based on either scalar coupling, or in the presence of both scalar and dipolar coupling in liquid crystal media [46,47]. Both here and in studies of isotopic mixing [44], or in other coherence transfer studies [16–20], the systems studied were under some modest order $\mathcal{S}_n \downarrow \mathcal{G}$ subgroup, e.g., $\mathcal{S}_4 \downarrow D_2$ as the highest order group to which the Galbraith's analytic restrictions concerning multi-invariant-based systems does not apply. In contrast to weakly coupled spin system of [14,15,19], the coherence transfer studies of Sanctuary [14], Temme [16], Listerud et al. [18] have all focussed on the role of $\phi_q^{k(=n-1)}(1\ldots1\colon [\widetilde{n-1}, 1])$ dominated (maximal multiquantum)

Table 4
The Yamanouchi chain (YC) derived democratic auxiliary labels, analogous to the known 15 independent scalar invariants of the $[A]_6(\mathcal{S}_6)$ system whose Liouvillian irreps are known, e.g., from the ITPs of [63]. The analogous YC reduction coefficient hierarchy for $\mathcal{S}_9$ irreps will be found in [24,25].

[6]	[5] ⊃ [4] ⊃ [3] ⊃ [2]
[51]	[5] ⊃ [4] ⊃ [3] ⊃ [2]
[51]	[41] ⊃ [4] ⊃ [3] ⊃ [2]
[51]	[41] ⊃ [31] ⊃ [3] ⊃ [2]
[42]	[32] ⊃ [31] ⊃ [3] ⊃ [2]
[42]	[41] ⊃ [31] ⊃ [3] ⊃ [2]
[42]	[41] ⊃ [4] ⊃ [3] ⊃ [2]
[411]	[41] ⊃ [4] ⊃ [3] ⊃ [2]
[411]	[41] ⊃ [31] ⊃ [3] ⊃ [2]
[33]	[32] ⊃ [31] ⊃ [3] ⊃ [2]
[33]	[32] ⊃ [31] ⊃ [21] ⊃ [2]
[33]	[32] ⊃ [22] ⊃ [21] ⊃ [2]
[321]	[32] ⊃ [31] ⊃ [3] ⊃ [2]
[321]	[32] ⊃ [31] ⊃ [21] ⊃ [2]
[321]	[32] ⊃ [22] ⊃ [21] ⊃ [2]

processes [48], which themselves draw on an initial subhierarchy immediately under that associated with the constants-of-motion. However, many NMR workers still utilise product bases even when their systems are actually strongly coupled, simply to avoid using fully recoupled tensorial bases. This is regreted, since there are inherent advantages to tensorial bases and represent an established theoretical technique for the calculation of most spectroscopic quantities. To appreciate the full dual group dynamical system structure of $[AX]_n$ or AX_n NMR spin systems, including their democratic recoupling which establishes their scalar invariant forms, use of dual tensorial bases is essential. The value of dual symmetry is highlighted in studies of the role of the auxiliary labels (defining the scalar invariants) in projective representational mapping, a property *only demonstrable* in the form of $\widetilde{\mathbf{U}} \times \mathcal{P}$ Liouville space (tensorial) actions [28], i.e., as indicated in equations (21)–(25). This physical observation constitutes a particularly insightful reason for the conceptual use of (democratically recoupled) tensorial bases, well beyond arguments, concerning their purely mathematical convenience, or the spectroscopic generality of such methods. Further in the context of phase-based selective multiquantum COSY techniques, the rank and quantal orders associated with specific irrep spin symmetry manifolds become significant selective physical labels as demonstrated in multiple quantum NMR, by Avent [45] in the 1980s.

This section has stressed the interdisciplinary nature of reduced space Schur function modelling as it applies to spin physics [29–31,36], or isotopomer statistical weightings (with latter equally derivable from ITP formation of biclusters comparable to the processes in equation (23)), and hence finally to NMR evolution [8–11,45–47], or coherence transfer processes [16–20,48] within $[A\ldots]_n(\mathcal{S}_n)$ ensemble systems. Only an absolute minimum of necessary theoretical background has been included here in order to outline the properties of uniform n-fold spin ensemble systems and their associated (democratic recoupled, invariant-based) auxiliary terms, which specify the form of $\widetilde{\mathbb{H}}_v$ carrier subspaces.

9. Concluding comments

In the main presention of these ideas, we have focussed on three aspects of the (independent) scalar invariants of uniform n-fold spin systems under the dual group and shown just how the interrelation between unitary and $\mathcal{S}_n$ component groups (of dual symmetry) yields valuable direct combinatorial insights into n-fold spin ensemble physics of NMR in mobile (or liquid crystaline) media, or likewise into the structures of dual tensors as NMR bases of some relevence to quantum informatics applications. The SIs associated with dual tensors necessarily incorporate the (non-explicit) time-reversal TRV-properties in Weyl's original approach [23] and the $|D^0(U)((\otimes SU(2))^{(2n)})|$ (linear-recoupling) enumerations [22]. TRV effects become explicit parts in projective dual group approach to SIs. A universal representational physics approach to auxiliary forms, via the Yamanouchi–Gel'fand chain (YC), was the subject of other recent work [24,25,35], as it represents a viable alternative auxiliary labelling to that derived from the standard Jucys graph theory as used by Sanctuary [3] in the mid-1970s. However, the numbers of distinct YC routes [24,25,35] possibly may be over-determined for higher index cases, i.e., compared to the numbers of independent SIs derived here. The specific purpose of our original enquiry into dual-group-based decompositional formalism for |SI|, and the related matters discussed in sections 2–5 above, was to confirm the actual values for $N_{\mathrm{SI}}^{(2n=12)}$, $N_{\mathrm{SI}}^{(2n=20)}$ pertinent to twelve-, twenty-fold dual group tensorial sets. Since other aspects of these tensorial structures have been derived in some detail elsewhere [29–31] (via $\{|IM()\rangle\}$ based *specialised bipartite* Schur function (product) decompositions over restricted $\mathcal{GL}_n$ subgroup spaces [63]), the present interest represented a final stage in understanding these foundations of physics. For individual ITPs one is necessarily considering SF products derived from (SF based) difference expressions [64] in the specific weak-branching (high index) limit indicated.

The form of table 1 and the nature of sections 4, 5 here both stress that at *least* the $\mathbf{N}_f^{(2n)}$, $\mathbf{N}_f'^{(2n)}$, ... fundamental components of SIs are accessible for *any* $(2n)$ index-value dual group. Modelling of TRV weightings over higher odd-valued (prime) n values (of $(2n)$) introduce certain difficulties from implicit underlying algebro-geometric considerations, i.e., concerning the *non-existence of progressive regular* geometric solids above $(2n) > 12$ apicial solids. The value of democratic recoupling for higher $(2n)$ fold (cage-like) spin ensembles has been stressed. The central portion of the paper and the proofs of the representational form of superbosons, as set out in appendix A, both highlight the existence of useful explicit correlations between NMR QL formalisms and combinatoricial aspects of theoretical physics, including aspects of $\mathcal{S}_n$-based decomposition. In the early sections of this work, it was shown how such concepts give an alternative projective route to the numbers of independent scalar invariants under impact of explicit TRV invariance (dual-group-based) factors. However, algebraic geometric considerations apply to higher index applications of the modified Weyl TRV theory for uniform spin ensembles, comparable to the Galbraith criteria [21] for the analytic use of democratic recoupling. The 1993 work on superboson mapping [28], which itself augments the original Hilbert space views of Biedenharn and Louck [2], should be consulted for fuller details, and additional discussion of orthonormality and other interesting properties of Wigner unit-tensors. Clearly, (dual group) carrier space maps [26,27] and unit-tensors [2] lie at the essential core of quantum physics related to *uniform* n-fold spin ensembles.

A remaining fundamental question concerns the realisation of $\{\widetilde{\mathcal{V}}\}$ democratic recoupling, either analytically or in terms analogous to graph-theoretical schemes, for $n \geqslant 4$ fold spin systems of high degeneracies as a result of their inherent multiple scalar invariant structure. This has remained a largely open question in the theoretical physics literature, to the best of our knowledge. However, perhaps some starting point from which to attack this long-standing high-degeneracy-induced problem associated with multiple scalar invariant systems may be seen in the recent work due to Chen et al. [62]. This actually treats a simpler $\mathcal{O}(3)$ based chain problem, involving cubic symmetries. Galbraith's contention [21] regarding these multiple invariant-based (Hilbert) spin systems clearly remains of primary theoretical importance, e.g., in helping to explain why perturbation theory in the alternative *strongly coupled limit* [65] has not developed further to include the $[A]_{n\geqslant 4}(\mathcal{S}_n)$ forms which underlie, e.g., the $[AB\ldots XY]$, $[ABCD\ldots]$ NMR spin systems. In addition, from other related work on uniform spin ensembles [57,58], it has been noted also that the number of possible spin-$1/2$ related mathematically determinable forms of $\mathcal{S}_n \downarrow \mathcal{G}$ Cayley-compatible (automorphic) group embeddings is strictly limited [66].

It is of some topical interest to view deceptive NMR spin systems [67] in a new role, as forms of *intercluster* $\{J\}$ interaction (graph-based) networks, which exhibit properties that approach those of certain analogous "small world" model networks [68]. Such general view is comparable to Balasubramanian's conceptual work [6] on NMR ensemble spin systems as (group-based) networks, i.e., as being analogues of automorphic (zeroth-order-based ensemble) spin symmetries. The inherent correspondence between super-positional (SP) bases and dual-group-adapted uniform spin ensemble bases implies that studies of tensorial structure and numbers of scalar invariants have specific pertinence to the foundations of quantum physics, and thus also to quantum informatics, as realised via recent experimental NMR physics and modelling [69–71]. On the basis of the role of auxiliary SI-based terms in dual tensorial bases for dynamical uniform spin systems (as the equivalent forms of (coherent) SP bases), the (unrestricted) dynamical process of teleportation in quantum computing is necessarily restricted to $n \leqslant 4$ equivalent nodes. This view is a consequence of theoretical physics arguments previously employed, i.e., in the context of democratic recoupling [21] and the natural of dual QP mapping presented above. Our penultimate point concerns the existence of relationships between geometric polyhedral combinatorics and democratic or projective-based recoupling, from the viewpoint of Landau-like $\mathcal{S}_n$ decompositional maps of the statistical portion of the calculations presented above. The statistical submodel is the origin of the constraint (previously noted in section 5) on defining the (dual) auxiliary tensorial labels for uniform ensembles of $\mathcal{S}_n$ indices of $2n \leqslant 12$. This is physically reasonable in ensemble NMR, since local spin symmetries will eventually dominate dual-group-based NMR Liouvillians derived from larger uniform polyhedral cage ensembles. No comparable constraint is explicitly associated with (simple Hilbert) CNP permutations as these are simply statistical weights.

Viewing QP mappings within a Liouvillian superboson perspective [28], and utilising the necessary decompositional statistical maps, has proved invaluable in presenting the above work. A final consequence is that the (dual group) $\mathcal{S}_{2n}$ invariants of democratically recoupled uniform multispin NMR spin ensembles are seen as essential forms of quantum entanglement (as being at the foundations of quantum theory) for the types of models discussed above. Indeed, the explicit carrier subspatial mappings and dynamical system structures as Liouvillian entities indicate that for these uniform spin ensemble and formalisms, there is now little real need to refer to any other forms of quantum entanglement.[6] In the Liouville structural view, the role of recoupling in furnishing system invariants as auxiliary labels (and disjunct subspaces in appropriate cases) is quite clear and precise, whereas in Hilbert space or product formalisms the possibility of presence of non-graphical recoupling and operator bases with (quasi-) $\mathcal{S}_{2n}$ invariants is often ignored. The latter is frequently the case in presentations discussing quantum computing which tend to restrict their views to Hilbert space AMX formalisms, despite Sanctuary [14] having shown the valve of superpositional operator bases in an analytic treatment of $\phi_1^1(11)$ coherence transfer.[7] By considerating uniform multispin models and focussing on (superboson) mapping, the work provides a rather precise view of quantum entanglements, even if their physical realisation under democratic recoupling may not be universally analytic, (or) global $(2n)$-ensemble properties of known cardinality, for reasons given above.

Strong additional support for our present *general-n limit* view concerning the nature of *uniform* $(j_1 \ldots j_{2n})$, or $(k_1 \ldots k_{2n})$, labelled (Hilbert or Liouvillian) tensorial sets of spin physics, i.e., as being subject to eventual indeterminacy in respect to their scalar invariant cardinalities is now available from a very recent mathematical physics study [72], due to Atiyah and Sutcliffe. They find in presenting the analogous simultaneous mappings associated with the formally-related $SO(3) \times \mathcal{S}_n$ double group, as compared to dual group of NMR spin physics of the main text here, that there is an inherent incompatibility between linear (graphical) recoupling of their extended unitary mapping in the presence of *uniform subset auxiliary labelling*, or other forms of degeneracy. The latter is shown to invalidate the simultaneous unitary and $\mathcal{S}_n$ mappings for some general-n limit, as predicted by Galbraith [21] in his group-theoretic discourse on *democratic recoupling* in the 1970s. The only valid conclusions which may be drawn in the NMR spin ensemble context is that the degeneracy associated with

[6] Or even to introduce EPR ideas [69–71].
[7] As compared to the ensemble dual group view of [16,17].

uniform auxiliary labelled dual tensors (under democratic recoupling) accordingly renders the $|D^0(\mathbf{U})((\otimes SU(2))^{2n})|$ simple unitary approach (and the four specific $2n \geqslant 14$, $(\ldots)^b|SI|_{\text{total}}$ values for uniform spin ensembles in the final column of table 1) physically invalid in the general n limit of these uniform auxiliary tensorial sets. This occurs because the full simultaneous mapping, either under the double group of [72], or under the dual group utilised in the main text, breaks down in the presence of such $(j_i, \ldots)$, *or* $(k_i, \ldots)$ degeneracy. This structural aspect of these (uniform) $SU(2) \times \mathcal{S}_n$ tensorial sets (for general n) has not been recognised in the quantum physics literature, apart from being implicit in Galbraith's views [21] of democratic recoupling. The presentation in section 5 above demonstrates how the linkage between algebraic geometry and combinatorics serves to confirm this group-theoretic result. The conceptual basis [72] for this important result was reported whilst this manuscript was already 'in press'.

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Appendix A. DP dual-group representations of superbosons

The direct product (DP) nature of the structure of Liouville space under the dual group allows one to realise the correlations between boson of the primary $\mathbb{H}$ carrier space and superboson over $\widetilde{\mathbb{H}}$ of the augmented spin space, as, e.g., in the following $SU(2)\times\mathcal{S}_n$ dual group mappings [64], for individual quasi-particle based on $k = 1$:

$$(a_1 \otimes a_1)_{(\oplus)} \longrightarrow \left(s_1^2\right) \longrightarrow \left\langle\!\!\left\langle 2 \quad \begin{matrix} 2 \\ \cdot \\ 2 \end{matrix} \quad 0 \right\rangle\!\!\right\rangle \tag{A.1}$$

for a (Liouvillian shift term) $\widetilde{\Delta} = 1$, $(k+q) = 2$ augmented shift and lower component, whereas

$$(a_1 \otimes a_2)_{(\oplus)} \longrightarrow (s_1 s_2) \longrightarrow \left\langle\!\!\left\langle 2 \quad \begin{matrix} 2 \\ \cdot \\ 1 \end{matrix} \quad 0 \right\rangle\!\!\right\rangle \tag{A.2}$$

for corresponding $q = 0$ superboson, and finally

$$(a_2 \otimes a_2)_{(\oplus)} \longrightarrow \left(s_2^2\right) \longrightarrow \left\langle\!\!\left\langle 2 \quad \begin{matrix} 2 \\ \cdot \\ 0 \end{matrix} \quad 0 \right\rangle\!\!\right\rangle \tag{A.3}$$

for $q = -1$ or $(k+q) = 0$ superboson with the same shift term as in equations (A1) and (A2) and where these outer left-/right-hand forms are generic described as being of

$$\left\{\langle 2j \begin{bmatrix} \cdot \\ \cdot\cdot \end{bmatrix} 0\rangle\right\} : \left\{\langle\langle 2k \begin{bmatrix} \cdot \\ \cdot\cdot \end{bmatrix} 0\rangle\rangle\right\}$$

Hilbert, or Liouville space, forms, respectively. Here the upper (lower) segment components of the double Gel'fand shape are respectively:

$$(j+\Delta), \left\{\left(k+\widetilde{\Delta}\right)\right\} \text{ or } \widehat{i}_{(\cdot)}, \qquad \left\{\widetilde{\widetilde{\widehat{i}}}_{(\cdot)}\right\} : \left((j+m), \left\{(k+q)\right\} \text{ or } \widehat{k}_{(\cdot)}, \left\{\widetilde{\widetilde{\widehat{k}}}_{(.)}\right\}\right).$$

The form of ordering (over a boson, superboson field) for the subscript indices are those pertinent to equations (16a) and (16b) of the main text.

Likewise, the adjoint bosons (superbosons) (of zero upper segment representational form) exhibit similar form with variation in the upper portion of the inner-$[\cdot]$ portions, as in the generalised set of adjoint boson mappings:

$$\left\{ (\bar{a}_i \otimes \bar{a}_{i'}.)_{(\oplus/\ominus)} \longrightarrow \left(\bar{s}_i^2\right) \longrightarrow (\text{sign})\langle\langle 2 \begin{bmatrix} 0 \\ \cdot \\ \cdot\cdot \end{bmatrix} 0\rangle\rangle \right\},$$

for suitable i, i' labels and sign; here decomposition of $\otimes$ (left-hand side) may involve *either* $\oplus$ or $\ominus$ non-trivial evaluations of resultant superboson representation(s). This approach provides more direct insight into the sign aspects of adjoint superbosons than was possible in the earlier work [28].

Hence, one finds the following pair of superboson, derived as indicated, map onto the related pattern bases:

$$\begin{matrix} (\bar{a}_1 \otimes \bar{a}_1)_\oplus \\ (\bar{a}_2 \otimes \bar{a}_2)_\oplus \end{matrix} \longrightarrow \begin{matrix} (\bar{s}_1^2) \\ (\bar{s}_2^2) \end{matrix} \longrightarrow (\pm)\left\langle\!\!\left\langle 2 \begin{matrix} 0 \\ \binom{0}{2} \end{matrix} 0 \right\rangle\!\!\right\rangle \tag{A.4}$$

and

$$(\bar{a}_1 \otimes \bar{a}_2)_\ominus \longrightarrow (\bar{s}_1\bar{s}_2) \longrightarrow (+)\left\langle\!\!\left\langle 2 \begin{matrix} 0 \\ 1 \end{matrix} 0 \right\rangle\!\!\right\rangle, \tag{A.5}$$

for the increasing ordering of adjoint forms shown. Hence overall, there are eight non-trivial superbosons within the set, with the negative external sign in the mapping applying only to the subset: $\{(\bar{s}_2^2), (\bar{s}_2\bar{s}_1)\}$. On this premise, it follows that the actions of the following superboson subsets:

$$\begin{matrix} (s_1^2) & (\bar{s}_1^2) \\ (s_2^2) & (\bar{s}_2^2) \end{matrix}, \quad \text{and} \quad \begin{matrix} (s_1 s_2) \\ (\bar{s}_1\bar{s}_2) \end{matrix}$$

(consistently using *all* upper (lower) options throughout left-/right-hand sets) are respectively:

$$\begin{matrix}(s_1^2)\\(s_2^2)\end{matrix}\left|\begin{pmatrix}2k & & 0\\ & (k+q) & \end{pmatrix}\right\rangle\!\!\right\rangle \longrightarrow \left[\frac{(k\pm q+1)}{(2k+1)}\right]^{1/2}\left|\begin{pmatrix}(2k+2) & & 0\\ & (k+q+{}^{2}_{0}) & \end{pmatrix}\right\rangle\!\!\right\rangle, \quad (A.6)$$

while,

$$\begin{matrix}(\bar{s}_1^2)\\(\bar{s}_2^2)\end{matrix}\left|\begin{pmatrix}2k & & 0\\ & (k+q) & \end{pmatrix}\right\rangle\!\!\right\rangle \longrightarrow (\pm)\left[\frac{(k\mp q)}{(2k+1)}\right]^{1/2}\left|\begin{pmatrix}(2k-2) & & 0\\ & (k+q-{}^{2}_{0}) & \end{pmatrix}\right\rangle\!\!\right\rangle, \quad (A.7)$$

whereas one finds (respectively) that:

$$\begin{matrix}(s_1 s_2)\\(\bar{s}_1\bar{s}_2)\end{matrix}\left|\begin{pmatrix}2k & & 0\\ & (k+q) & \end{pmatrix}\right\rangle\!\!\right\rangle \longrightarrow (+)\left[\begin{pmatrix}k-q+1\\ k-q\end{pmatrix}\Big/(2k+1)\right]^{1/2}\left|\begin{pmatrix}(2k\pm 2) & & 0\\ & (k+q\pm 1) & \end{pmatrix}\right\rangle\!\!\right\rangle. \quad (A.8)$$

On considering $[A\ldots]_n$ n-fold spin ensembles, the action of bosons/superboson on members of the basis sets of dual group irreps are naturally restricted to the bounds associated with the scalar invariant (auxiliary) labelling of the specific $\{\widetilde{\mathbb{H}}_v\}$ carrier subspaces. Additional comment on the more technical theoretical physics properties, such as various forms orthonormality and descriptions of the nature of the Wigner fundemental (super)operators (alias, the unit tensor operators based on Racah step-functions) will be found in [28], while details of the nature of the $\{\widetilde{\mathcal{V}}\}$ set(s) may be found in [24,25,30]. The correspondence between Gel'fand patterns and Weyl tables takes an especially simple form – see, e.g., equation (18) in Biedenharn's 1979 discussions [26].

Appendix B. $SU(2)\times\mathcal{S}_{12}$ $(\ldots\mathcal{S}_{20})$ YC reduction and FG embeddings

B.1. The twelve-fold YC-based invariants via a reduction hierarchy

The stepwise Yamanouchi-based subduction (YC) hierarchy introduces the $(n-2)$ correct number of labels. It also acts to retain the impact of the characters of the original irreps subsequently as constraints at each step, i.e., on the sum of the products of derived reduction coefficients and associated subduced characters. The following examples, over the coefficient sets of (for brevity) limited portions of the irrep hierarchy, should suffice to demonstrate these YC constraints, for (generally non-simply reducible) reduction coefficient sets within

$$\mathcal{S}_{12}\supset\cdots\supset\left\{c_{[\lambda']}\left[\lambda'\right]\right\}\mathcal{L}'(\mathcal{S}_{10})\supset\cdots\supset\left\{c_{[\lambda'']}\left[\lambda''\right]\right\}\mathcal{L}''(\mathcal{S}_6)\supset\cdots\supset\{c_{[2]},c_{[11]}\}(\mathcal{S}_2),$$

which from specific initial irreps gives rise to following reduction coefficients under the YC process:

$$[11,1]\to\{2,1,0,0;\ldots\}\mathcal{L}'(\mathcal{S}_{10})\to\{6,1,0,0;\ldots\}\mathcal{L}''(\mathcal{S}_6)\to\{10,1\}\mathcal{L}(\mathcal{S}_2)\quad (B.1)$$

$$[8,4] \to \{0,0,1,0;2,0,0;1,\ldots\}\mathcal{L}' \to \{15,20,1,0;5\}\mathcal{L}'' \to \{200,75\}(\mathcal{S}_2)$$
$$\text{for } \chi^{[8,4]} = 275, \tag{B.2}$$
$$[8,22] \to \{0,0,1,1;0,1,0;0,0,1\}\mathcal{L}' \to \{30,40,15,15;0,1\}\mathcal{L}'' \to \{420,196\}$$
$$\text{for } \chi^{[822]} = 616, \tag{B.3}$$

and, as a final example,

$$[444] \to \{\ldots\}\mathcal{L}' \to \{0,0,9,5;10,16,0;5\}\mathcal{L}'' \to \{252,210\}(\mathcal{S}_2) \quad \text{for } \chi^{[444]} = 462. \tag{B.4}$$

As labels for the scalar invariants, only the number of distinct routes contributing to the labelling over this hierarchy which terminate on the $[2](\mathcal{S}_2)$ irrep need be considered. In view of overdeterminacy, the intermediate self-associate irreps are largely excluded from the initial portions of these route maps, also. Fuller details of the complete set of YC maps under the $\mathcal{S}_{12}$ group are the subject of related work [30]. Table 4 of the main text exemplifies the independent SI labelling via Yamanouchi-chain-derived route maps originating from various $\mathcal{S}_6$ group irreps.

B.2. $\mathcal{S}_{20} \downarrow \mathcal{I}$ natural finite group embeddings

In certain contexts, such as for the liquid-crystal media, dipole–dipole NMR spectra of dodecahedrane, additional group embedding mappings are needed. Such properties may be derived from comparisons of invariance-derived models with either ITP forms, or (Kostka coefficient generating) SF decompositional maps [29–33,36,49,64]. The propagation of these enumerative mappings is based on recursive hierarchical forms [5] from the weakly branched $\lambda \vdash$ forms of irreps in dominance order; for $\mathcal{S}_{20} \downarrow \mathcal{I}$ examples of group embedding, we consider the following:

$$[19,1] \to \{0,2,1,1,1\}\Gamma(\mathcal{S}_{20} \downarrow \mathcal{I}),$$
$$[18,2] \to \{5,11,17,6,6\}\Gamma \quad \text{for } \chi^{[18,2]} = 170, \tag{B.5}$$
$$[18,11] \to \{1,11,12,11,11\}\Gamma \quad \text{for } \chi^{[18,11]} = 171, \tag{B.6}$$
$$[17,3] \to \{15,65,75,50,50\}\Gamma \quad \text{for } \chi^{[17,3]} = 950, \tag{B.7}$$
$$[17,21] \to \{30,126,162,96,96\}\Gamma \quad \text{for } \chi^{[17,21]} = 1920, \tag{B.8}$$
$$[17,111] \to \{20,67,81,46,46\}\Gamma \quad \text{for } \chi^{[17,111]} = 969, \tag{B.9}$$
$$[16,4] \to \{75,249,318,174,174\}\Gamma \quad \text{for } \chi^{[16,4]} = 3705, \tag{B.10}$$
$$[16,31] \to \{180,754,933,574,574\}\Gamma \quad \text{for } \chi^{[16,31]} = 11305, \tag{B.11}$$
$$[16,22] \to \{145,505,655,360,360\}\Gamma \quad \text{for } \chi^{[16,22]} = 7600. \tag{B.12}$$

These bi- (or multi-) partite mappings (extending those of [49]) define components of the structure of simple Hilbert (or Liouville) carrier spaces of $[^{12}CH]_{20}$ dodecahedrane. The bipartite-based mapping may also be of value in describing endohedral $[A]_{20}X$ spin systems. The spin statistical weight problem for the uniform $[^{13}CH]_{20}$ dodecahedrane molecule is clearly one derived via fermionic nuclear spin subproblems, for its further representational (Hilbert space) form, concerned with isotopomer statistics. NMR biclusters needs to be considered in some detail for each specific bicluster ensemble system in regard to the relative magnitudes of the intra/inter couplings, since use of inner tensor products (here of the bipartite irreps) implies that the inter-cluster $\{J_{\mathrm{H}^{13}\mathrm{C}}\}$s, of dodecahedrane example above, are much less significant in magnitude than those of the $\{J_{\mathrm{HH}}\}$ set. This is often not the case for ring (and hence, cage) molecules. Hence, the use of the specific $\mathcal{S}_{20} \downarrow \mathcal{I}$ automorphic NMR spin symmetry in terms of product constructs for the highest $2n$ valued uniform bicluster needs to be approached with due caution [67].

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