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On $SU(2) \times \mathcal{S}_{n\geqslant 12}$ dual-group tensorial sets and carrier spaces in the multiple invariant physics of multiquantum NMR. II. $\{\mathcal{S}_{12} \supset \cdots \supset [2]\mathcal{S}_2\}$ pathways from Yamanouchi monomial reductions as $[A]_{12}$ democratic $\mathcal{S}_n$-invariant labels

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The transformational and Liouville carrier space (LCS) properties of dual tensorial bases for $[A\ldots]_n$ NMR spin systems are considered within the quantum physics of (super)boson quasiparticles, where the (contracted) auxiliary labels of $SU(2) \times \mathcal{S}_n$ tensors are derived from the $\mathcal{S}_n$-based scalar invariants (SIs). Beyond both the $\{s_i^2\}$ (super)bosons mappings of pattern-algebra [F.P. Temme, Physica A 198 (1993) 245] and the (outer) k-rank based sub-structure of LCS (e.g., in terms of $\mathcal{S}_{12}$ irreps [F.P. Temme, J. Math. Chem. 27 (2000) 111 (this issue)]), now (cf. Jucys recoupling) we consider the dual group physics role of the $\{\widetilde{\mathcal{V}}\}$ auxiliary terms of the (SI-related) democratic sets for all the $\geqslant$ 4-fold multispin systems, as obtained via the $\mathcal{S}_{n-1} \supset \cdots \supset ([2])\mathcal{S}_2$ Yamanouchi–Gel'fand chains (YGCs). The simple reducibility of LCS derives from the explicit role of such auxiliary labels in dual mapping. The full monomial YGC reduction coefficient sets, and their related sum rule, are given here for $SU(2) \times \mathcal{S}_{12}$ tensorial sets and the distinctness of individual reduction pathways is demonstrated. Recent enumerative work on SIs [F.P. Temme, J. Magn. Reson. (2000) (to appear)] (extending [P.L. Corio, J. Magn. Reson. 134 (1998) 131]) gives expressions for the numbers of independent $\mathcal{S}_{12}$ ($\mathcal{S}_{20}$) SIs for icosa-(dodeca)hedral spin ensembles. The search for additional insight into multiquantum evolution (or coherence transfer) from the use of $\{\mathcal{T}^{kg}_{\widetilde{\{\mathcal{V}\}}}(1_1, \ldots, 1_n; [\widetilde{\lambda}])\}$ dual bases motivates this work – cf. that of [M.C. Carravetta et al., J. Magn. Reson. 134 (1998) 131; B.C. Sanctuary, Molecular Phys. 55 (1985) 1017]. Studies of SIs, and of the origins of Cayley's group embedding theorem, highlight the need to retain the $\mathcal{S}_n$ group in quantum physics involving spin ensembles, cf. Corio's $\mathcal{O}(3)$ viewpoint. A recent lattice-point model of 12-fold cage isotopomers, now for general multipartite forms, has demonstrated that *universal mathematical determinacy* (a property for which YGCs are especially noted) also prevails in $SU(m) \times \mathcal{S}_{12} \downarrow \mathcal{I}$ natural group embedding [F.P. Temme, Eur. Phys. J. 11 (1999) 177].

1. Introduction

In the study of multispin ($[A]_n$), $[A]_nX$, or $[AX]_n$ type NMR systems [12,16, 23,24,40,44,63] in liquid (or mobile liquid crystal) media, it is valuable to focus on certain essential symmetry-related questions. These are important because they serve to define the nature of the model spin system, and yield some fuller physical insight into their spin dynamics. Prominent amongst these are the number of scalar invariants (SIs) [14] which underlie the auxiliary label set in dual-group-based formalisms. Some knowledge of the form of these SIs is necessary, in order to define suitable multispin tensorial bases and understand various aspects of their transformational properties. Indeed, the specific properties of dual tensorial bases impart some additional meaning to NMR studies of spin dynamical processes [39], such as multiquantum evolution, or coherence transfer, even when there exist earlier spin dynamical treatments in the framework of simple (inner) *SU*(2)-related formalisms. Experimentally, it is well known that COSY-based multiquantum filtering phased-pulse techniques [2,18] (MQF) are of considerable value in understanding the multiquantum evolution, or coherence transfer processes of multispin ensemble systems, including those exhibiting some form of spin symmetry. From the theoretical perspective of contractive recoupling, naturally the requisite $n-2$ auxiliary labels of $v = (1_1, \ldots, 1_n)\{\ldots\}$ n-fold systems, derived from the SIs (under the dual group), play a central role in the use of tensorial formalisms, since they reflect the inherent structure of Liouville space as known from superboson mapping techniques. The conceptual reason for treating NMR spin dynamics via such formalisms (rather than by other methods) is that these are general spectroscopic or theoretical techniques [36] with well-known properties. Under dual group symmetry [1,5–7,34,41,42,49,50,52,54,58], the inner *SU*(2)-based $\{k_i\}$ set of v (or corresponding $(i_1, \ldots, i_n)$ of Hilbert space) retain their status as *good quantum numbers*, under the action of complete nuclear spin permutation for the type of NMR spin ensemble system discussed here.

In earlier work [50,52,54], we have examined the structure of Liouville space under various *SU*(2) $\times$ $\mathcal{S}_n$ dual algebras, because of the physical insight such applications impart to specific non-symmetry-breaking forms (in an $\mathcal{S}_n$ permutational sense) of quantum Liouville equations (QLEs). Here we utilise the automorphic (finite subgroup) symmetries arising from a complete set of nuclear spin permutational (CNP) operations [12,16,23,24,50,52,54], applied to a spin cluster. The resultant irreps under the dual group are of value, both in discussing nuclear spin spectral statistical weightings of cage isotopomeric clusters (as mentioned in [58]) and in understanding the various ($[A]_n$), $[A]_nX$, or $[AX]_n$ types of NMR spin systems [2,12,14,16,18,23,24,36,39,50,52,54,58]. The immediately preceding article [58] has set out some of the initial dual tensorial basis aspects, namely those which specifically pertain to 12-fold (Liouvillian) symmetry under the *SU*(2) $\times$ $\mathcal{S}_{12}$ dual group. In this paper [58], a symbolic algorithmic derivation (based on Schur functions) was utilised to obtain the $\{p \leqslant 4\}$ partitioned (tensorial) irrep subsets, as functions of the outer k rank (alone). The value of such an approach is that it allows one to under-

stand *the role of carrier spaces* in quantum physics, a viewpoint not generally adopted in discussing NMR problems. The use of dual tensorial bases in NMR applications naturally implies that the specific form of Liouvillian is dominated by its intracluster interactions [2,12,14,16,18,23,24,50,52,54] (as in the above case of $SU(2) \times \mathcal{S}_{12}$ spin symmetry discussed in [58]), whereas all the component intercluster terms of the $\{J_{AX}\}$ set are small, by comparison.

For $[A\ldots]_n$-derived spin systems evolving under either purely scalar or both scalar and isotropic dipolar interactions, the dynamical properties may be studied most conveniently in terms of the dual group bases and in the QL formalism. However, such Liouvillian bases have some inherent essential operator (and carrier space) physics of their own. Within spin ensemble dynamics, the former arise via the (outer) spin-operator-based $\{kqv\}$ labelled angular momentum properties [1,5–7,34,36,39,41,42,49] associated with Liouville space, as in

$$\begin{aligned} &\widehat{\mathcal{I}} \bullet \widehat{\mathcal{I}}|kqv\rangle\rangle \equiv k(k+1)|kqv\rangle\rangle, \quad \text{for } \widehat{\mathcal{I}} \equiv \big[\widehat{\mathbf{I}},\big]_-, \\ &\widehat{\mathcal{I}}_0|kqv\rangle\rangle \equiv q|kqv\rangle\rangle, \end{aligned} \tag{1}$$

where k is the outer tensorial rank and q its conventional z-projection. An underlying, equally general transformational property [5,34,39,41,42,49] applies to Liouville space as a product-space, namely that

$$\mathcal{X}(\Gamma)|kqv\rangle\rangle\mathcal{X}(\Gamma)^\dagger \equiv \sum_{\mu'} \widetilde{\mathcal{X}}_{\mu'}(\Gamma)\big|kqv(\mu')\big\rangle\big\rangle, \tag{2}$$

for $\mathcal{X}_\mu, \widetilde{\mathcal{X}}_{\mu'}$ projective (class/cycle) operators (or their characters) of some (dual) group action, in respectively Hilbert and Liouville space. This property significantly enhances the utility of dual group algebras and projective methods. One of these, the physics of (super)boson pattern-algebra [6,7], plays an especially important role in defining the structure of Liouville space. Both (super)boson algebras and the nature of Wigner unit-operators (as applied to Liouville space) deserve to be better known, in the context of quantum-physics-based ideas discussed, e.g., by Biedenharn and Louck [6,7].

Since some of these wider physics topics have been surveyed in detail elsewhere, see, e.g., [54,58], we give only brief commentaries here. The purpose of several gedanke-experiments (discussed in [50–52,54,58]) was to define $[A]_n(X)$, $[AX]_n$ spin clusters as NMR systems [5,12,16,23,24,34,41,42,49] in a way which allows precise answers to the following insightful questions:

(a) What is the nature of the mechanism which allows for the retention of simple reducibility (SR) of $SU(2)$ symmetry for NMR over dual group-formulated Liouville space?

(b) How can one understand the correlation of similar properties, in a general sense, between the two common quantum mechanical spaces?

(c) And also, just *how* do the two distinct groups of the dual group established an interactive mode of communication?

In this context, we stressed in [58] that the auxiliary labels (defining the scalar invariants) for Liouvillian carrier space of boson mapping are now explicit parameters of the (projective) mapping, in contrast to their merely implicit role over the simple carrier space of $\{|I\overline{M}(i_1,\ldots,i_n)\rangle\}$ Hilbert space [1,6,7]. The answers to the questions that were posed above appear in discourses given in papers [50,52,54] for (a), or else from equation (2) for (b), and finally in respect of (c), in our 1992/1993 work [51].

The nature of the above comments stress the well-known inseparability of quantum physics modelling, or their applications, from the fundamental symmetry principles inherent in descriptions of the actual phenomena. Spectroscopies at their most fundamental level exhibit certain similarities or correlations, but the question of *what* does, or does not, constitute an *observable* is only rarely of significance to the actual quantum physics. Recent developments (set out in [58]) have been focused on the role of the *highest n-indexed $\mathcal{S}_n$* CNP-based systems from the viewpoint [35] of group structure, as part of algorithmic combinatorial physics via group actions [26,27]. In such research areas, a number of well-established discrete mathematics techniques have proved to be invaluable. Progress via some suitable symbolic computational method [26,27] is then possible. Of the various libraries available for such purposes, the SYMMETRICA package [27] is quite general and only requires a modest level of C-language skill to allow for its direct application to problems of scientific interest. In practice, much of the detailed work reported in [58] only required the use of symbolic computation, as an additional check on various component decompositions as combinatorial enumerations. The use of sum-rules and direct (hand) enumeration was adequate in analysing YGC reduction processes reported herein.

The present work extends our view of the $\{[\widetilde{\lambda}](\mathcal{S}_{n(=12)})\}$ set of irreps (given in [58]) by considering the forms of $\mathcal{S}_n$ encoding and certain symmetry reduction coefficients of pertinence to the definition of democratic $\mathcal{S}_n$-invariants. This necessitates considering all the ($p \leqslant 4$) branched forms of the irreps generated in [58]. Such views of what underlies the SR property of the dual group over Liouville spin space (to be found in [50,52]) lifts the idea of recoupling, from being one governed by constrained formalisms of $\{\widetilde{\mathcal{K}},\ldots\}$ recoupling based on $(1_1,\ldots,1_n)$ and somewhat arbitrary choices implicit in diagrammatic techniques of graph theory [25,36], into new realms. There it provides a proper $\mathcal{S}_n$-democratic-based formalism which is comparable to (super)boson mapping techniques. Such mapping properties are clearly beyond the $(\otimes SU(2))^n$-based views adopted by Corio [14]. In consequence, they constitute one important focus of the present work, in which the specific use of the $\mathcal{S}_n$ group, its irreps, and its democracy are established at the outset. This framework leads to the following equivalence relationship between graphical and dual-group-based tensorial sets:

$$\left\{T^{kq}_{\{\widetilde{\mathcal{K}},\ldots\}}(v)\right\} \equiv \left\{T^{kq}_{\{\widetilde{\mathcal{V}},\ldots\}}\left(1_1,\ldots,1_n : \left[\widetilde{\lambda}\right]\right)(\mathcal{S}_n)\right\} \tag{3}$$

(as indicated in [58]), where $\{\widetilde{\mathcal{V}}\}$ is a set of labels derived from the democratically defined scalar invariants, discussed in sections 2–4. In contrast to the usage adopted here

and in [58], previous $\mathcal{S}_n$ symmetry chain reduction schemes have been *restricted* to resolving more general particle-physics labelling problems, i.e. those involving reduction coefficients (RCs). These topics are extensively covered in the theoretical works of Sullivan [46] and Chen [10]. In addition, a concise mathematical summary of the nature of YGC chains and their associated properties may be found in Sternberg's (1994) monograph [45].

The focus in the present work is on generalised $\mathcal{S}_n$-democratic properties of dual-group-based spin systems and their underlying $\mathcal{S}_n$-invariants (i.e. beyond the few-body analogues of explicit quantum physics systems derived by Lévy-Leblond and Lévy-Nahas [30] in the mid-1960s). It was shown via the explicit quantum algebra of [30] that the democratic and graph theoretic results for the three-body case differ only by a $6j$-coefficient. Further direct analytic algebraic treatment over generalised $n \geqslant 4$-fold spin (many-body) interactions (unless they happen to correspond to the $\mathcal{S}_4 \supset \mathcal{D}_2$ ($\supset \mathcal{C}_2$) subgroups [20]) are not feasible for a rather specific mathematical reason associated with higher degeneracies. The basis for this *fundamental insight* lies in a group theoretical argument, originally due to Galbraith [20]. He pointed out that the *degeneracy of higher permutational* symmetries implies that such systems were governed by *more than a single* system invariant. Hence, the number of (independent) invariants (SIs) in NMR systems is of greater physical significance than the discussion in the previous $O(3) \downarrow \mathcal{G}$-based Hilbert space work [11,13,14] would suggest (see also works of H. Weyl, E.P. Wigner cited in [14]).

Naturally, the retention of Balasubramanian's ideas concerning the role of automorphic spin symmetry in NMR [3] (and hence, the role of the $\mathcal{S}_n$ group in spin physics, as a subgroup of $(\mathcal{G})\mathcal{L}_n$), is central to our physical understanding of the nature of carrier spaces, and thus, of dual projective mapping in *either* Hilbert, or Liouville, space. As a consequence of Cayley's theorem [10], all the conventional finite symmetry groups are clearly subgroups of the $\mathcal{S}_n$ group, *rather than being directly derived* from the $(S)\mathcal{O}(3)$ group. Hence it is noted that $[AX]_n$ NMR cluster problems with their automorphic $\mathcal{S}_n \downarrow \mathcal{G}$ symmetries necessitate the retention of the $\mathcal{S}_n$ group on two quite *independent* grounds. The first is as a result of the necessity to retain simple reducibility properties under dual group actions for mappings over Liouville space, as discussed in an earlier discourse [52]. An additional reason is discernable on considering the $\mathcal{S}_n$ index-based form of Cayleyan theorem for mathematically determinable finite group embeddings into particular $\mathcal{S}_n$ groups, as it here applies to spin symmetries based on *SU*(2) bipartite algebras. For group embeddings involving other types of irreps under the *wider SU*$(m) \times \mathcal{S}_n$ dual symmetry, which approach the *maximal multipartite branching* levels of [47], the criterion given from this theorem is *necessary*, but in itself *not sufficient to ensure* mathematical determinacy.

After an overview of Yamanouchi–Gel'fand chain (YGC) properties and a brief comment in section 2 on the nature of the auxiliary labels in the context of dual group projective actions, section 3 of the paper turns to the central focus of work, the tabulation of the monomial reduction coefficients over the YGC-hierarchy. Here we consider specifically the $\{\mathcal{S}_{11} \supset \cdots$ (stepwise down to) $\cdots \supset \mathcal{S}_2\}$ YG process,

within a sum-rule, and note that only the [2]($\mathcal{S}_2$) terminating routes are pertinent to the SI auxiliary labelling, discussed here. Section 4 sets out specific illustrations of chain labelling for scalar invariants, in the context of actual enumerations of their gradually extending cardinality for modest symmetric groups with indices $n \leqslant 6$, i.e. in accord with other work in the area of the number of possible independent forms for $[A]_n$, for $n = 12,\ 20$ (see [54]). A brief overview on the consequences of the two distinct types of Liouvillian transformation, and of their impact on the nature of Wigner unit-(super)operators in such spaces, follows in section 5. In a penultimate section 6, we consider a couple of NMR applications [9,17,31–33,38,48] which serve to highlight the pertinence of $\mathcal{S}_n$ democratic recoupling formalisms; for a contrasting overview of state space nuclear spin statistical weightings, in the CNP spin aspects of isotopomers [4,21,53,55,59,62], the reader is referred to our remarks in [58].

In order to relate different approaches to the study of SIs of spin ensembles, we stress here that group-theoretical correlations [8] are known between the group chain embeddings involving the $\mathcal{O}(n)$ and those for $\mathcal{S}_n$ groups (see equation (6) of [58]). Rather surprisingly, the nature of the linkage between these separate chains is not as well known as the importance of the topic to molecular physics might suggest. In addition to incorporating more recent work on SIs [56,60], brief mentions are accorded the topics of group structure, as observed by symbolic computing via high-index decompositions [61] of inner products, and the potentially technologically significant question of the role of projective *decompositions*, as applied to the NMR density matrices [37] in the context of potential processes for NMR modelling [15,19,22,28,29,43] of *quantum computing*.

2. Quantum physics of NMR on tensorial operator bases: Dual projective maps having explicit auxiliary labels

In order to correlate this work with discussions of related areas, we set out some of the background (i.e. of [50,54] which should be read in the context and the *existing notation* of [1,5–7,34,39,41,42,49]) briefly here, in order to make the cogency of the use of YGC pathways as system invariants clear to the reader. Naturally, the presentation for Liouville space is based on the ($p \leqslant 4$)-partite irrep set of the preceding paper [58]. For the space of dynamical quantum processes, one needs to introduce first the (NMR) density matrix, from which the quantum Liouville equation (QLE) (equation (5) below) follows directly [5,34,39,41,42,49]:

$$\sigma(t) = \sum_{k=0}^{k_{\max}} \sum_{q=-k}^{k} \phi_q^k(v:t) \mathcal{T}^{kq}_{\{\widetilde{\mathcal{V}}\}}(1_1, \ldots, 1_n), \tag{4}$$

$$(-\mathrm{i}) d_{(t)} \phi_q^k(v) = \sum_{k'q'v'} \big\langle\big\langle kqv \big| \widehat{\mathcal{L}} \big| k'q'v' \big\rangle\big\rangle \phi_{q'}^{k'}\big(v'^{t=0}\big); \tag{5}$$

the form of the auxiliary terms includes the dual group partitional irreps once automorphic spin symmetry is adopted. For a typical $\widehat{\mathcal{L}}$ Liouville operator (or superoperator) acting on a spin ensemble system whose evolution is dominated by the zeroth order intracluster interaction terms (as presented in [58]), with $\widehat{\mathcal{L}} \equiv [\widehat{H}^{(0)} + \widehat{H}_1, \cdot]_-$, analogous $\mathcal{S}_n$-partitioned forms exist to those given above in equations (4), (5). One notes here, in the context of $\{\mathcal{T}^{kq}(v)\} \equiv \{|kqv\rangle\rangle\}$ being a (dual) tensorial basis set, within which the ks now are of integer rank defining the range of the $-k \leqslant q \leqslant k$ projections, that the v terms of the density matrix include all the remaining $(1_1, \ldots, 1_n)\{\widetilde{\cdot}\}$ auxiliary terms, under either a conventional graphical, or democratic, recoupling criteria. The $\phi_q^k(v)$ terms of the QLE above are NMR coherences (or polarisations for $q = 0$) and represent a set of time-dependent coefficients which correspond to the *physical observables* of spin dynamics. In NMR applications, these dynamical techniques naturally require the use of some initial $t = 0$ condition.

For NMR evolution and a number of similar processes, a further symmetry arises from the additional permutational properties of $[A \ldots]_n$ type systems. This allows the use of dual group projective mapping over the v-designated subspaces of the full Liouvillian carrier space $\widetilde{\mathbb{H}}$, as an augmented form compared to the original simple Hilbert space boson algebraic mappings of Biedenharn and Louck [1,6,7]. Over the full $\{\widetilde{\mathbb{H}} \equiv \bigoplus \widetilde{\mathbb{H}}_v\}$ carrier space, dual group projective actions may be represented by the following mapping:

$$\widetilde{\mathbf{U}} \times \mathcal{P} : \widetilde{\mathbb{H}} \to \widetilde{\mathbb{H}}\big\{\mathcal{D}^k\big(\widetilde{\mathbf{U}}\big) \times \widetilde{\Gamma}^{[\lambda]}(v)(\mathcal{P}) \,\big|\, \widetilde{\mathbf{U}} \in SU(2); \widetilde{\Gamma}^{[\lambda]}(v), \mathcal{P} \in \mathcal{S}_n\big\}, \tag{6}$$

based on superboson algebra, with the $D^k(\widetilde{\mathbf{U}})$ (Liouvillian) transformations as defined in equation (17) of section 5. One notes that there is a direct correspondence here to the graphical recoupling properties (hereafter referred to as SJG properties), discussed in Sanctuary's 1976 paper [41] on Jucys-like generalised spherical tensors under $SO(3) \equiv SU(2)$ (alone) for NMR spin dynamics; the treatment of $\widetilde{\mathbf{U}}$ rotational ($SU(2)$ group) actions given in [39,41] is necessarily identical to that implied herein. It is the permutational projective mapping aspects which distinguish the two presentations. Papers [54,58] discussed the contrasting case of group actions inherent in the use of dual tensors and gave the *dimensionalities* associated with the full and subspatial forms of (rank-alone) dual group carrier spaces. In terms of Schur functions, a more general *square construction* based on certain *skew-diagonal* summations was presented in our *immediate preceding* paper [58]. This approach gives the $k = k_{\max} - i$ sub-spatial dimensionalities in terms of a set of $\chi_{1^{2n}}^{[2n-i]}\mathcal{S}_{2n}$ (bipartite) characters, via equation (21) of [58]. A further important point to note here is that the subspatial auxiliary $(k_1, \ldots, k_n)\{\widetilde{\mathcal{V}}\}$ forms in Liouville space mappings are now explicit parameters of the mapping; this contrasts strongly with the original mappings over simple Hilbert carrier space. Naturally, these $\bar{v} = (1_1, \ldots, 1_n) : \widetilde{\mathcal{V}}$ auxiliary labels are closely related to the system scalar invariants (SIs) and are necessary features of the augmented dual mapping which ensure the retention of simple reducibility over the dual carrier space. This point was stressed first in our papers [50,52] of a decade ago.

From SJG theory applied to Liouville space recoupling [36], the number of auxiliary labels is two less than the number of inner ($k_i \leqslant 1$) ($k_1, \ldots, k_n$) $SU(2)$ spin labels. Indeed, the completeness of both the dual group irrep set and of the $\{\widetilde{\mathbb{H}}_{(1_1,\ldots,1_n)\{\widetilde{\mathcal{V}}\}}\}$ carrier subspaces arise from the fuller description of the democratic $\mathcal{S}_n$ SIs. The quantum physics imparted by these SI labels is an *essential* focus of the present work. One notes that the derivation of SI labels utilises an additional type of symbolic encoding, i.e. *distinct* from the earlier algorithmic combinatorical encodings based on Schur functions and their decompositions invoked in [58]. In the specific case discussed here, the algorithm is taken over the full $\mathcal{S}_{11} \supset \cdots \supset \mathcal{S}_2$ Yamanouchi–Gel'fand chain (YGC) utilising the complete set of $\mathcal{S}_{12}$-based, $p \leqslant 2^2$ (quadra-partite) irreps, derived in [58]. Before moving on to discuss the specific details of the full $\mathcal{S}_{12}$ YGC process, we would stress that the above mappings essentially come from the study of certain *quasiparticles* (called superbosons to underline their relationship to the Hilbert space mapping formalism of [1,6,7]), themselves defined by an augmented form of Heisenberg generator (see [52]), namely, $[\bar{s}_i^2, s_j^2]_- = 2\delta_{ij}$. In this context, retention of the *right-derivation* properties [1,52] is essential to this fundamental generator description of $\{s_i^2\}$-bosons as superoperators. In addition to the simpler aspects [60] of Lie algebras, some understanding of the nature of double Gel'fand patterns and of the general role of ladder operators in quantum mechanics is central to the material given in this section. Such concepts are central to the study of $\{s_1^2, (s_1 s_2), s_2^2\}$ s-bosons, and their corresponding adjoint $\bar{s}$-bosons, $(\{\bar{s}_1^2, (\bar{s}_1 \bar{s}_2), \bar{s}_2^2\})$, sets.

3. An overview of generalised YGC properties

Whilst the general outline of the Yamanouchi–Gel'fand chain process for small n-indexed symmetric groups consists of surveying all possible node-removal processes [10,46] (as in the introductory overviews given, e.g., in Sternberg's text [45]) from the irrep(s) of the preceding indexed group, use of the process to yield the distinct v labels for the system invariants focuses on the descending *routes* (pathways/flightpaths) for chain subduction. Each of these may be shown to be *distinct*. One notes in this context the nature of the following illustrative stepwise subduction process:

$$\begin{aligned}[10,2] \to \big\{[10,1] + [9,2]\big\} \to \big\{[10] + 2[9,1] + [8,2]\big\}(\mathcal{S}_{10}) \\ \to \cdots \to \big\{3[9] + 3[8,1] + [7,2]\big\} \to \big\{6[8] + 4[7,1] + [6,2]\big\}(\mathcal{S}_8), \end{aligned} \quad (7)$$

and that of the similar processes derived from treating the [444]($\mathcal{S}_{12}$) irrep of figure 1. All such YGC processes are subject to a condition of *detailed balance* at *each stage* of the subduction process, so that the general criterion

$$\chi_{1^n}^{[\lambda]} \equiv \sum_{[\lambda']} \Lambda_{[\lambda']}^{(n-i)} \chi^{[\lambda']}(\mathcal{S}_{n-i}) \quad (8)$$

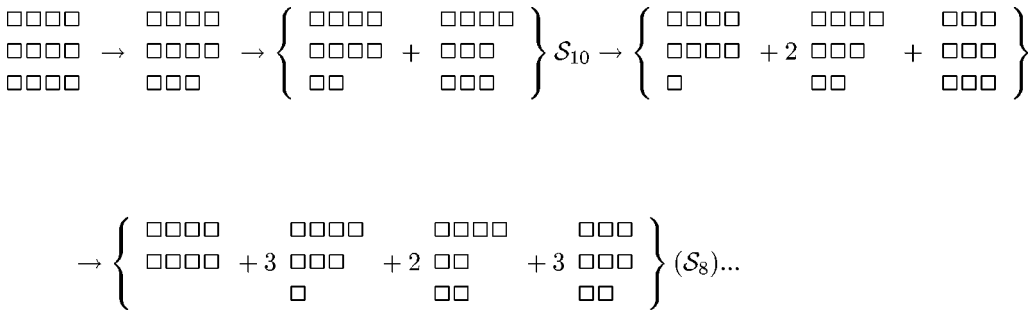

Figure 1. Schematic view of the initial stepwise Yamanouchi–Gel'fand chain subduction process for [444]($\mathcal{S}_{12}$), down to the $\mathcal{S}_8$ subset. Full details of the remaining chain subduction steps are given in table 2.

holds $\forall(n-i) \geqslant 2$, where the $\Lambda^{(n-i)}_{[\lambda']}$ are the reduction coefficients at the $(n-i)$th stage. On limiting discussion for illustrative purposes to the interim $\mathcal{S}_8$ and final stages, both of equation (7) and for figure 1 (as box forms of a graphical representation), the (outer-most) detailed balances are given by respectively

$$\begin{aligned} &\text{for } \chi^{[10,2]}_{1^{12}}: \quad 54 = (6+28+20)(\mathcal{S}_8) \supset \cdots \supset (45+9)(\mathcal{S}_2), \\ &\text{for } \chi^{[444]}_{1^{12}}: \quad 462 = (14+210+126+112)(\mathcal{S}_8) \supset \cdots \supset (252+210)(\mathcal{S}_2), \end{aligned} \tag{9}$$

where the latter numbers are the final monomial reduction coefficients for the full YGC subduction onto the [2], [1^2] set of $\mathcal{S}_2$ irreps.

A complete demonstration of the distinctness of each route, down to these terminal YGC chain $\{[\lambda]\}\mathcal{S}_2$ set, would require a more detailed listing than is possible here. Suffice it to note that their *total* number of *routes, or pathways*, from any specific *initial irrep* of character $\chi^{[\lambda]}_{1^n}$ (here of the $\mathcal{S}_{12}$ group) must equal (from equation (8)) the sum of the [2], [1^2] terminal monomial reduction coefficients. These are set out in some detail over the full $\{\lambda \vdash (12) \mid \forall p \leqslant 4\}$ in tables 1 and 2 (with the retention for illustrative purposes of the intermediate symmetric groups $\mathcal{S}_{10}$, $\mathcal{S}_6$, etc.). Naturally the sumcheck, as a detailed-balance criterion, has been applied to all of these reduction coefficient subduction results. A full description of *each invariant* requires the listing of the full intermediate irrep routes inherent in the subduction process, which finally leads to [2]($\mathcal{S}_2$). For convenience of presentation and brevity in handling $\mathcal{S}_{12}$ group properties in the text, we essentially give only the monomial reduction coefficients (RCs) here, and not the detailed sets of route maps derived from them. However, the RC sets demonstrate the nature of the decompositional map, with the $\{[\widetilde{\lambda}]$, for $\lambda \vdash n \mid p \leqslant 4\}$-partite forms of the initial irrep, completely defining the process tabulated here. The route maps terminating in [2] are those specific to the *explicit* mapping labels, as derived from the $\mathcal{S}_n$-invariants (SIs); they are *only* found in Liouville space descriptions of dual group projective actions, as a consequence of the mappings associated with equation (6).

Table 1

The Yamanouchi $\mathcal{S}_{12} \supset \cdots \supset \mathcal{S}_2$ stepwise subduction process for ($p \leqslant 4$)-part irrep set $\{[11,1],\ldots,[7,1^5]\}$.

	$\mathcal{S}_{11} \supset$																		
	[11] . . .				83 . . .			74 . . .					65 . . .						
[12]	1	0																	
[11, 1]	1	1	0																
[10, 2]	0	1	1	0															
[10, 11]		1	0	1															
[9, 3]			1	0	1														
[921]			1	1	0	1													
[9111]				1	0	0	1												
[8, 4]					1	0	0	1											
[831]					1	1	0	0	1										
[822]						1	0	0	0	1									
[8211]						1	1	0	0	0	1	0							
[81^3]							1	0	0	0	0	1							
[75]								1	0	0	0	0	1						
[741]								1	1				0	1					
[732]								0	1	1			0	0	1				
[7311]								0	1	1			0	0	0	1			
[7221]								0	0	1	1		0	0	0	0	1		
[721^3]								0	0	0	1	1	0	0	0	0	0	1	
[71^5]								0	0	0	0	1	0	0	0	0	0	0	1

	$\mathcal{S}_{10} \supset \cdots \supset$																		
	10 . . .				73 . . .			64 . . .					55 . . .						
[12]	1																		
[11, 1]	2	1																	
[10, 2]	1	2	1																
[10, 11]	1	2	0	1															
[9, 3]	0	1	2	0	1	0													
[921]	0	2	2	2	0	1	0												
[9111]	0	1	0	2	0	0	1												
[8, 4]	0	0	1	0	2	0	0	1											
[831]	0	0	2	1	2	2	0	0	1										
[822]	0	0	1	1	0	1	0	0	0	1									
[8211]	0	0	1	2	0	2	2	0	0	0	1								
[81^3]				1	0	0	2	0	0	0	0	1							
[75]					1	0	0	2					1						
[741]					2	1	0	2	2				0	1					
[732]					1	2	0	0	2	2			0	0	1				
[7311]					1	2	1	0	2	0	2		0	0	0	1			
[7221]					0	2	1	0	0	2	2		0	0	0	0	1		
[721^3]					0	1	2	0	0	0	2	2	0	0	0	0	0	1	
[71^5]					0	0	1	0	0	0	0	2	0	0	0	0	0	0	1

	$\mathcal{S}_6$										
	6 . . .				33 . . .			222 . . .[1^6]			
[12]	1										
[11, 1]	6	1									
[10, 2]	15	6	1	0							
[10, 11]	15	6	0	1							
[9, 3]	20	15	6	0	1						
[921]	40	30	6	6	0	1					
[9111]	20	15	0	6	0	0	1				
[8, 4]	15	20	15	0	5						
[831]	45	60	30	15	6	6					
[822]	30	40	15	15	0	6		1			
[8211]	45	60	15	30	0	6	6	0	1		
[81^3]	15	20	0	15	0	0	6	0	0	1	
[75]	6	15	19	0	9	0					
[741]	24	60	60	20	24	14	0	0			
[732]	30	75	60	40	15	30	0	5	0		
[7311]	36	90	60	60	15	30	15	0	5	0	
[7221]	30	75	40	60	0	30	15	6	6	0	
[721^3]	24	60	20	60	0	15	30	0	6	6	
[71^5]	6	15	0	20	0	0	15	0	0	6	1

Table 1
(Continued.)

$\mathcal{S}_5$						$\mathcal{S}_4$					$\mathcal{S}_3$			$\mathcal{S}_2$			
5...			311...			4	31	2^2	211	1	3	21	1^3	2	11	$\sum = \chi^{[\lambda]}$	$[\lambda]$
1						1					1			1		1	[12]
7	1	0				8	1				9	1		10	1	11	[11, 1]
21	7	1	0			28	8	1			36	9		45	9	54	[10, 2]
21	7	0	1			28	8	0	1		36	9	1	45	10	55	[10, 11]
35	21	7	0	0		56	28	7	–		84	35	–	119	35	154	[9, 3]
70	42	7	7	1		112	56	8	8		168	72	8	250	80	320	[9, 21]
35	21	0	7	0	1	56	28	0	8	1	84	36	9	120	45	165	[9, 111]
35	35	20	0	0	0	70	55	20	0	0	125	75	0	200	75	275	[8, 4]
105	105	42	21	6	0	210	168	48	27	0	378	233	27	611	260	891	[8, 31]
70	70	21	21	7	0	140	112	28	28	0	252	168	28	420	196	616	[8, 22]
105	105	21	42	7	7	210	168	28	56	7	378	252	63	630	315	945	[8, 211]
35	35	0	21	0	7	70	56	0	28	8	126	84	36	210	120	330	[8, 1111]
21	34	28	0	–	–	55	62	28	0	0	117	90	0	207	90	297	[7, 5]
84	140	98	34	14	0	224	272	112	48	–	496	432	48	928	480	1408	[7, 41]
105	175	105	70	35	0	280	350	140	105	–	630	595	105	1225	700	1925	[7, 32]
126	210	105	105	35	20	336	420	140	160	20	756	720	180	1476	900	2376	[7, 311]
105	175	70	105	42	21	280	350	112	168	21	630	630	189	1260	819	2079	[7, 221]
84	140	35	105	21	42	224	280	56	168	48	504	504	216	1008	720	1728	[7, 2111]
21	35	0	35	0	21	56	70	0	0	–	126	126	84	252	210	462	$[7, 1^5]$

Table 2
The Yamanouchi process applied to remaining $\lambda \vdash (n = 12)$ irreps, i.e. of four-part (or less).

	$\mathcal{S}_{11} \supset$			$\mathcal{S}_{10} \supset \cdots \supset$			$\mathcal{S}_6 \supset$
	[65] . . .	551 . . .	443	64 . . .	55 . . .	442 . . . 443 . . . 42^3	6 . . . 33 . . . 222 . . .
[6,6]	1	0		1 0	1		1 5 9 0 5 0
[651]	1 1	0 1		2 1 0	2 2 0		5 30 54 14 30 14 0
[642]	0 1 1	0 1 0		1 2 1 0	0 2 2 0		9 54 90 45 45 54 0 9 0
[6411]	0 1 0 1 0	0 0 1 0		1 2 0 1 0	0 2 0 2 0		10 60 90 60 45 54 19 0 9
[633]	0 0 1 0 0	0 0 0 1 0		0 1 1	0 0 2 0 0	0 0 1 0	5 30 45 30 20 40 0 10 0
* *							
[6222]	0 1	0 0 0 0 0 0 1		0 0 1 1 0	0 0 0 0 2 0	0 0 0 0 0 1 0	5 30 30 45 0 40 20 15 15
[62211]	0 0 0 0 1 1		0 1 0	0 0 1 2 1	0 0 0 0 2 2	0 0 0 1	9 54 45 90 0 60 60 15 30 15 0
$[621^4]$	0 1 1		0 1	0 0 0 1 2	0 2 2	0 0 0 0 1	5 30 15 60 0 20 60 0 15 30 5
$[61^6] \equiv [71^5] \otimes [1^{12}]$							
[552]		1 1 0			1 2 1 0	1	0 14 45 19 30 30 0 5 0
[5511]		1 0 1 0			1 2 0 1 0	0 1	0 15 45 24 30 30 9 0 5
[543]		0 1 0 1	1 0		0 1 2 0	2 0 2 0 0	0 14 54 30 40 61 0 16 0
*							
[444]			1 0			1 0 1 0	0 0 9 5 10 16 0 5 0

Table 2
(Continued.)

$\mathcal{S}_5 \supset$							$\mathcal{S}_4$					$\mathcal{S}_3$			$\mathcal{S}_2$			
5	41	32	311	221	21^3	1^5	4	31	22	21^2	1^4	3	21	1^3	[2]	[11]	$\sum = \chi_1^{[\lambda]_{12}}$	$[\lambda]$
6	14	14	0	0	0	0	20	28	14	–	–	48	42	–	90	42	132	[66]
35	98	98	28	14	0	0	133	224	112	42	–	357	378	42	735	420	1155	[651]
63	189	189	99	63	0	0	252	477	252	162	–	729	891	162	1620	1053	2673	[642]
70	210	189	133	63	28	0	280	532	252	224	28	812	1008	252	1820	1260	3080	[6411]
35	105	105	70	50	0	0	140	280	155	120	–	420	555	120	975	675	1650	[633]
35	105	70	105	70	35	0	140	280	140	210	35	420	630	245	1050	875	1925	[6222]
63	189	105	210	105	105	15	252	504	210	420	120	756	1134	540	1890	1674	3564	[62211]
35	105	35	140	35	105	35	140	280	70	280	140	420	630	420	1050	1050	2100	$[621^4]$
																		$[61^6] \equiv [71^5] \otimes [1^{12}]$
14	78	105	49	35	0	0	92	232	140	84	–	324	456	84	780	540	1320	[552]
15	84	105	63	35	14	0	99	252	140	112	14	351	504	126	855	630	1485	[5511]
14	98	155	91	77	0	0	112	344	232	168	–	456	744	168	1200	912	2112	[543]
0	14	35	21	21	0	0	14	70	56	42	–	84	168	42	252	210	462	[444]

4. $\{\widetilde{\mathcal{V}}\}(\mathcal{S}_n)$ democratic label sets for the scalar invariants

4.1. Numbers of independent SIs for $2n \leqslant 6, \ldots, 12, 20$ via Weyl bracket formalism

For even number of spins in (say) an $[A]_{2n}$-based ensemble system, the cardinality of independent SIs, discussed elsewhere [14,60], reduces to establishing the fundamental $N^{(2n)}_{f:\,\mathrm{SI}}$ component and then including suitable combinatorially weighted forms for all the lower (previously established) $N^{(2n')}$ terms. As pointed out by Corio [14] in his unitary-group-based $|SU(1)|((\otimes SU(2))^{2n})$ notation, a small modification has to be included to allow for Weyl time-reversal symmetry (TRS). For the $N^{(10)}_{(\mathrm{SI})}$ case [56], this only applies to the $\binom{(i)}{2}$ weighted (lower) components where (i) $(<n)$, the number of actual Weyl brackets (each containing a pair of spin operators), is odd; this property is a consequence of noting that, e.g.,

$$\big(\widehat{I}_A \bullet \widehat{I}_B\big)\big(\widehat{I}_C \bullet \widehat{I}_D\big) \equiv \big(\widehat{I}_C \bullet \widehat{I}_D\big)\big(\widehat{I}_A \bullet \widehat{I}_B\big),$$

or other single interchanges of Weyl bracket components, are equivalent.

More recently [56,60] in a dual group context, the underlying fundamental component $N^{(2n)}_{f:\,\mathrm{SI}}$ terms themselves have been given as a more convenient form being defined (here for $2n$ spin operators) as a sum over all the bipartite characters for the half-index specific $\mathcal{S}_n$ group. On noting that the bipartite characters are simply difference between combinatorials, the underlying fundamental terms of the series for $2n = 6, 8, 10, 12, \ldots$ and $2n = 20$ are open then to enumeration, the results being that

$$N^{(2n)}_{f:\,\mathrm{SI}} \equiv \big\{\{5, 14, 42, 132\};\ 16796\big\},$$

respectively, for the set of $2n$ values indicated above. From these $N^{(2n)}_{f:\,\mathrm{SI}}$ terms and the Weyl TRS-modified [14] weighting process [56,60], or otherwise, it is straightforward to show that in consequence there must be

$$\big\{N^{(2n)}_{(\mathrm{SI})}\big\} \equiv \{15,\ 4213,\ \text{and } \leqslant 13{,}327{,}978\}$$

independent scalar invariants for the $2n = 6,\ 12,\ 20$-fold spin ensembles, respectively. Further specific details may be found in table 1 of [56]. Finally, we would stress that these are "independent" SIs, whereas it is possible that the YGC process discussed below could furnish *over*-determined sets of SI labels for $2n \gg 8$-fold $[A]_{2n}$ spin ensembles.

4.2. SI labels via YGC route-maps $\mathcal{S}_{n-1} \supset \cdots \supset [2]\mathcal{S}_2$: Illustrative $\mathcal{S}_{\leqslant 6}$ examples

On considering encoding of SIs from $\mathcal{S}_{n-1} \supset \cdots \supset \mathcal{S}_2$, one finds for irreps of $n = 4, 5$ indexed democratic systems down as far as the initial self-associate form(s) under $\mathcal{S}_n$:

$$\begin{aligned} \big([4]\big) &\to \big\{[3];[2]\big\}, \\ \big([31]\big) &\to \big\{[3];[2]\big\}, \\ \big([31]\big) &\to \big\{[21];[2]\big\}; \end{aligned} \tag{10}$$

whereas the five-fold case yields

$$\begin{aligned}
\big([5]\big) &\to \big\{[4];[3];[2]\big\},\\
\big([41]\big) &\to \big\{[4];[3];[2]\big\}\\
&\to \big\{[31];[3];[2]\big\}\\
&\to \big\{[31];[21];[2]\big\},\\
\big([32]\big) &\to \big\{[31];[3];[2]\big\},\\
\big([32]\big) &\to \big\{[31];[21];[2]\big\}.
\end{aligned} \tag{11}$$

Within a criterion that *no* SA irrep, or $\lambda \vdash n : p \geqslant 3$ partitioned form, may include a subsequent lower-indexed SA irrep in its pathway to [2], there are 3 and 6 *independent scalar invariants*, respectively, for these systems, in accord with established operator-product-based results [14].

Similarly, for the $[A]_6\mathcal{S}_6$ spin cluster within the above criteria, one finds that there are now 15 *independent* SIs or allowed pathways to [2], over the following compacted set, or hierarchies:

$$\big([6] \text{ or } [51]\big) \to \big\{[5];[4];[3];[2]\big\}, \tag{12}$$

$$\begin{aligned}
\big([51] \text{ or } [42]\big) &\to \big\{[41];[4];[3];[2]\big\}\\
&\to \big\{[41];[31];[3];[2]\big\}\\
&\to \big\{[41];[31];[21];[2]\big\},
\end{aligned} \tag{13}$$

$$\begin{aligned}
\big([42] \text{ or } [33]\big) &\to \big\{[32];[31];[3];[2]\big\}\\
&\to \big\{[32],[31];[21];[2]\big\},
\end{aligned} \tag{14}$$

$$\begin{aligned}
\big([411]\big) &\to \big\{[41];[4];[3];[2]\big\}\\
&\to \big\{[41];[31];[3];[2]\big\},
\end{aligned} \tag{15}$$

$$\big([321]\big) \to \big\{[32];[31];[3];[2]\big\}. \tag{16}$$

Corio [14] has set out the precise equivalently labelled operator forms (as in Sanctuary–Jucys graph (SJG) theory [25,36]) for the three cases (of equations (10), (11) and (12)–(16)) discussed above.

The number of forms for the independent SIs grows rather rapidly beyond six-fold spin stage for $[A\ldots]_n$ clusters. However, from the earlier discussions of the role of auxiliary labelling of carrier subspaces in [52] and Corio's work [14], it follows that $p \geqslant 5$ branched partite initial irreps, in general, are excluded from the SI labelling sets.

5. Intensive structure of Liouville space, an introduction

As a consequence of the recognition in [52] of the precise form of $\widetilde{\mathbf{U}}$-transformations – discussed originally in the graphical context of SJG recoupling theory [25,36]

– of Liouvillian tensorial (integer k rank) bases, via

$$\mathcal{D}^{j}(\mathbf{U})|kqv\rangle\rangle\mathcal{D}^{j'\dagger}(\mathbf{U}) = \sum_{q'} \mathcal{D}^{k}_{qq'}\big(\widetilde{\mathbf{U}}\big)\big|kq'v\big\rangle\big\rangle, \tag{17}$$

it follows that individual quasiparticles of Liouville space, superbosons, are associated with certain generalised double Gel'fand pattern structures, cf. Hilbert space views [1, 6,7], with $\widetilde{\Delta}$ being a (pattern) shift operator in the Liouvillian form of Wigner–Eckart theorem (see [52]), now within (with minor adjust of k, q notation here to K, Q in superboson maps, for clarity in a further relationship below) K integer, $-K \leqslant Q \leqslant K$, frequently with $K = 1$, so that both K, Q of Liouville space are integer. In the following mapping relationships, the (Liouvillian) pattern structures are shown enclosed in double brackets:

$$s_1^2 \to \left\langle\left\langle\left(\begin{pmatrix} 2K & K+\widetilde{\Delta} \\ & K+|Q| \end{pmatrix} 0\right)\right\rangle\right\rangle, \tag{18}$$

$$s_2^2 \to \left\langle\left\langle\left(\begin{pmatrix} 2K & K+\widetilde{\Delta} \\ & K-|Q| \end{pmatrix} 0\right)\right\rangle\right\rangle, \quad \text{or} \tag{19}$$

$$s_1^2 \to \left\langle\left\langle\left(\begin{pmatrix} 2 & 2 \\ & 2 \end{pmatrix} 0\right)\right\rangle\right\rangle, \tag{20}$$

$$s_2^2 \to \left\langle\left\langle\left(\begin{pmatrix} 2 & 2 \\ & 0 \end{pmatrix} 0\right)\right\rangle\right\rangle, \tag{21}$$

$$(s_1 s_2) \to \left\langle\left\langle\left(\begin{pmatrix} 2K & K+\widetilde{\Delta} \\ & K+0 \end{pmatrix} 0\right)\right\rangle\right\rangle, \quad \text{or} \tag{22}$$

$$s_1 s_2 \to \left\langle\left\langle\left(\begin{pmatrix} 2 & 2 \\ & 1 \end{pmatrix} 0\right)\right\rangle\right\rangle. \tag{23}$$

Based on the standard operator-to-boson mapping realisations

$$\big\{\widehat{\mathcal{I}}_+, \widehat{\mathcal{I}}_0, \widehat{\mathcal{I}}_-\big\} \equiv \big\{s_1\bar{s}_2, \big(\bar{s}_1 s_1 - \bar{s}_2 s_2\big), s_2\bar{s}_1\big\}, \tag{24}$$

one has (for $\widehat{\mathcal{I}}_\mu \equiv [\widehat{\mathbf{I}}_\mu, \cdot]_-$) the following ladder-operator properties (whose initial commutator vanishes *unless* the index $i = 1, 2$ is correlated respectively with signs $\mp$):

$$\big[\widehat{\mathcal{I}}_\mp, s_i^2\big]_- \equiv s_1 s_2,$$

or conversely for specific order noted,

$$\big[\widehat{\mathcal{I}}_\pm, s_1 s_2\big]_- \equiv \begin{cases} s_1^2, \\ s_2^2. \end{cases} \tag{25}$$

Naturally, the $\widehat{\mathcal{I}}_{+,0,-}$ (super)operators act on the Liouvillian $\{|kqv\rangle\rangle\}$ bases in a manner consistent with the well-known standard $\{kq\}$ ladder operations set out in equations (6)

and (17)–(19) of [52]. For the equivalent non-pattern algebraic formulation the reader is referred to [39,41,42,49].

The purpose of stressing the above is to introduce the *intensive* properties of Liouville space [52], its Clebsch–Gordan (CG) coefficients and various ideas connected with Wigner–Eckart (WE) theorem applied to tensorial forms [36,39] of this space. Most notable of these are:

(a) that the Wigner fundamental (super)operators are simply the CG coefficients (of Liouville space), which as in [1,6,7,36] may themselves be recoupled;

(b) that a specialised form of WE theorem exists, within which

$$T^{KQ}(v)|kq\rangle\rangle \equiv \sum_{\widetilde{\Delta}} \big\langle\big\langle K+\widetilde{\Delta}\big\|T^{K}\big\|K\big\rangle\big\rangle \times \left\langle\left\langle\left(\begin{pmatrix} 2K & K+\widetilde{\Delta} \\ K+Q & 0 \end{pmatrix}\right)\right\rangle\right\rangle |kq\rangle\rangle, \tag{26}$$

where the $\langle\langle \ldots ||T^{K}|| \ldots\rangle\rangle$ is a reduced matrix element of the Liouville space formalism;

(c) that the concept of an invariant unit ($\underset{\sim}{\widetilde{\mathbb{I}}}^{k}_{\widetilde{\Delta}}$) operator(s) is associated with a characteristic step function, which plays an important role in the algebra;

(d) hence, the idea of the so-called *intensive structure* is inherent in a wide range of properties. It has its greatest impact on the nature of orthogonality and in the analogous *invariant unit operator* properties, with some of these being applied over the individual $\widetilde{\mathbb{H}}_{(1_1 \ldots 1_n)\{\widetilde{\mathcal{V}}\}}$ subspaces.

On account of the discourse given in [54], we shall restrict explicit discussion to brief illuminations of the more accessible concepts. In particular, we omit almost all reference to the *adjunct quasiparticle* properties altogether, since they are set out at length elsewhere [52] and only add one further conceptual point to the underlying theory, namely in relation to the question of signs which arise from the structure of semi-simple Lie algebras [1,6,7].

In order to stress the dual projective aspects of boson-pattern algebras applied to Liouville space, one notes the equivalent form for permutational projections (based on $\widetilde{\mathcal{Y}}, \widetilde{\mathcal{Y}}'$ being Yamanouchi symbols) to equation (2); this is then clearly

$$P|kqv\rangle\rangle P^{\dagger} = \sum_{\widetilde{\mathcal{Y}}' \equiv \widetilde{(i_1,\ldots,i_n)}'} \mathcal{P}\big(\widetilde{\Gamma}\big)_{\widetilde{\mathcal{Y}}'\widetilde{\mathcal{Y}}} \big|kq\big(\widetilde{\mathcal{Y}}' \equiv \widetilde{(i_1,\ldots,i_n)}'\big)\big\rangle\big\rangle. \tag{27}$$

In the context of *class projective* formulations, explicit examples of the above permutation operation applied to $\{|kqv\rangle\rangle\}$ bases were given in [41,42,49]. Finally in this

section, we give a couple of explicit illustrative examples (from $SU(2) \times \mathcal{S}_4$) of double Gel'fand pattern-algebra shape sets, namely that for the initial triply degenerate form,

$$\left[\widetilde{31}\right] \equiv \left\{ \left(\begin{array}{ccccccc} & & & 2 & & & \\ & & 4 & & 0 & & \\ & 4 & & 4 & & 0 & \\ 4 & & 4 & & 4 & & 0 \\ & 4 & & 4 & & 0 & \\ & & 4 & & 0 & & \\ & & & k+q & & & \end{array} \right) : \left(\begin{array}{ccccccc} & & & 2 & & & \\ & & 4 & & 0 & & \\ & 4 & & 4 & & 0 & \\ 4 & & 4 & & 2 & & 0 \\ & 4 & & 4 & & 0 & \\ & & 4 & & 0 & & \\ & & & k+q & & & \end{array} \right) \right.$$
$$\left. : \left(\begin{array}{ccccccc} & & & 2 & & & \\ & & 4 & & 0 & & \\ & 4 & & 4 & & 0 & \\ 4 & & 4 & & 0 & & 0 \\ & 4 & & 4 & & 0 & \\ & & 4 & & 0 & & \\ & & & k+q & & & \end{array} \right) \right\}, \tag{28}$$

and now, in contrast, the doubly degenerate irrep double Gel'fand forms become

$$\left[\widetilde{2^2}\right] \equiv \left\{ \left(\begin{array}{ccccccc} & & & 2 & & & \\ & & 4 & & 0 & & \\ & 4 & & 2 & & 0 & \\ 4 & & 4 & & 2 & & 0 \\ & 4 & & 2 & & 0 & \\ & & 4 & & 0 & & \\ & & & k+q & & & \end{array} \right) : \left(\begin{array}{ccccccc} & & & 2 & & & \\ & & 4 & & 0 & & \\ & 4 & & 2 & & 0 & \\ 4 & & 2 & & 0 & & 0 \\ & 4 & & 2 & & 0 & \\ & & 4 & & 0 & & \\ & & & k+q & & & \end{array} \right) \right\}; \tag{29}$$

finally, the $[\widetilde{211}]$ irreps clearly correspond to

$$\left[\widetilde{211}\right] \equiv \left\{ \left(\begin{array}{ccccccc} & & & 2 & & & \\ & & 2 & & 0 & & \\ & 4 & & 2 & & 0 & \\ 4 & & 4 & & 2 & & 0 \\ & 4 & & 2 & & 0 & \\ & & 2 & & 0 & & \\ & & & k+q & & & \end{array} \right) : \left(\begin{array}{ccccccc} & & & 2 & & & \\ & & 2 & & 0 & & \\ & 4 & & 2 & & 0 & \\ 4 & & 2 & & 2 & & 0 \\ & 4 & & 2 & & 0 & \\ & & 2 & & 0 & & \\ & & & k+q & & & \end{array} \right) \right\}$$

$$: \left\{ \left(\left(\begin{array}{ccccc} & & 2 & & \\ & 2 & & 0 & \\ 4 & & 2 & & 0 \\ 4 & 2 & & 0 & 0 \\ 4 & & 2 & & 0 \\ & 2 & & 0 & \\ & & k+q & & \end{array} \right) \right) \right\} . \tag{30}$$

6. Applications of dual tensors and their projective decompositions

The type of NMR applications to which this work applies are those which are concerned with multiquantum evolution (or coherence transfer). The recent work of Carravetta et al. [9] on $[AX]_n[AB]_n$, $2 \leqslant n \leqslant 4$ on the octo- (or certain tetra-) fluoronaphthenes, where spin cluster is subject to tumbling within a liquid-crystal medium (as reviewed, e.g., in [17,32]), is typical. In the actual examples given in [9,16,17,32], the interactions include *both* intramolecular (isotropic) dipolar $\overline{D}_{ij}$ coupling components and J_{ij}^{iso} indirect interactions. In addition here, the $\mathcal{S}_4 \downarrow D_2$ subduction from the structure of the zeroth-order (cluster) Hamiltonian implies that the SI-based recoupling aspects are wholly tractable [20] in these circumstances. The $[AX]_4(\mathcal{S}_4)$ or $[A]_4[X]_2(\mathcal{S}_4 \downarrow \mathcal{D}_2)$ systems with large magnitude intracluster interactions could offer a greater chance of meaningfully exploring Corio's (1999) suggestion [14] that small *quartic* spin–spin interactions (mentioned in his study of SIs) *may possibly exist*. By contrast to Corio's remarks [14], it is suggested that other, e.g., $(AA'A''A''')$, NMR cluster-based systems would be more suitable than the well-known symmetrised $AA'XX'$ system cited by him, since the four-fold quantum processes of this latter case would correspond to the constants-of-motion, and therefore, in general, would not contain any detailed information. (To study possible quartic interactions, larger isochronous spin systems should be investigated, where the interaction does not correspond to the constants-of-motion of the system. The complexity of four-fold $AA'A''A'''$ symmetrised cluster system NMR spectra, especially for isotropic dipolar Liouvillians, could help to explain why such interaction has not been detected previously.)

For systems involving simple scalar interaction systems, the question of the nature of coherence transfer under J_{ij} interactions of the Liouvillian within (mono)cluster systems [48] follows on conceptually directly from the (1985) Laplace-transform formulation of AB or AX spin systems by Sanctuary [39,38] and a later specialisation of the AB formulation to $[A]_2$ (or else to a coherent superpositional (CSP) basis) problems [48]. Whilst Listerud et al. [31,33] utilise a number-type notation, which is analogous to the $\mathcal{S}_3$-box notation, their work *does not* actually consider *either* the nature of democratic recoupling (as in the few-body Hilbert quantum physics formalism of [30]), or the SJG-based invariant structure of their strongly-coupled total $[A]_3$ system, despite the authors' formal Liouvillian viewpoint in the work. A recent dis-

cussion [54] of various NMR applications in similar contexts should be consulted for its overview of experimentally focused work. Further material on the mathematical chemistry of dual group nuclear spin problems may be found in [41,42,49], or else in works which discuss the mathematical determinacy of natural group embeddings [4,21,53,55,59,62].

As a final ancillary brief comment to the discussions of this section, it is of topical interest to note that certain *decompositional* aspects of NMR density matrix descriptions are similar to both to that invoked in the multiplet projection treatments of $\sigma(t)$ in the 1983 Sanctuary work [37] and to ideas concerned with the comtempory role of the density matrix in recent NMR modelling of *idealised quantum computing*. This topic is both extensive [15,19,22,29,43] and developing at a fast pace. Although the quantum computing gate processes are concerned directly with $\mathcal{D}^k(\widetilde{\mathbf{U}})$ rotations, to date the systems used to model the phenomena have been restricted to AX, AMX, or $AMPX$ weakly coupled systems involving quasi-pure states and an action described in the inner *SU*(2) product basis literature as an entanglement [15,19,22,29,43]. Whilst it would seem that NMR model systems (within known theoretical group properties) may have yet wider technological significance in the future, it is not clear to date whether $[A]_n(X)$, or $[AX]_n$ NMR cluster systems with their natural dependence scalar invariants (alias, entanglements), or indeed their overall (dual) tensorial formalisms, have a role to play in conceptually modelling quantum computing processes.

7. Concluding remarks on $SU(2) \times \mathcal{S}_n$ based spin systems

The work has stressed how the proper democratic invariants, based on $p \leqslant 4$ part $\lambda \vdash n$ irreps, are derived using YGC subduction route maps, starting from the dual projective properties given in the rank-alone formalism of our related paper [58]. To place the sets of independent scalar invariants in a wider physics context, we have emphasised the role of transformational properties and the pertinence of (Liouvillian subspatial) boson (double) pattern algebras.

Our conceptual encoding approach, based on Schur functions and YGC subduction, has yielded a model pertinent to certain recent experimental-focused NMR work, such as that of Corio [14], or the work of Avent [2] and Carravetta et al. [9] based on COSY NMR techniques utilising modern ideas on multiquantum detection [2,18]. The ideas presented here also correlate well with various underlying aspects of the theoretical physics of many-body problems, besides stressing for transformational properties the disjunction between graphical and projective techniques which occurs once a spin system is determined more than a single invariant, and thus subject to high degeneracy.

The fuller value of Yamanouchi–Gel'fand chains (based on pre-self-associate initial $\mathcal{S}_n$ irreps), and their associated reduction coefficients, in describing the scalar invariants has been recognised, as offering some new physical insight into a long-standing problem in dynamics. The ($\mathcal{S}_{n-1} \supset \cdots \supset \mathcal{S}_2$) labellings given here avoid the inherent ambiguities (even for 3, 4 spin clusters) of Jucys graph theoretical systems, concerning the auxiliary labels of quantum physics. Illustrations of several complete

independent SI sets, to respect of their YGC-based labelling and the cardinality of their independent forms, have been given in the earlier discussion. In addition, our treatment of YGC labelling for system invariants has focussed on the $[A\ldots]_{12}(\mathcal{S}_{12})$ spin system(s) and their extensive set of SIs. In our approach, we have utilised many of the fundamental tensorial properties, referred to in [58], as well as Weyl time-reversal symmetry, other aspects of pre-1972 physics, and several of NMR-based ideas, e.g., those cited by Corio [14].

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Appendix A. Outline of YGC-based subduction route maps, derived from $[11,1]$, $[10,2]$ irreps

The hierarchical route-map structure, showing the distinctness of each route, which use in invariant labelling necessarily ends on [2], is set out in the two examples; these are the 10 and 45 distinct route maps derived from $[11,1]$, $[10,2]$, respectively, with the former spanning:

$$\left\{\begin{array}{cccccc} 11 & 10 & 9 & 8 & \ldots & 2 \\ 10,1 & 10 & 9 & 8 & \ldots & 2 \\ 10,1 & 9,1 & 8 & 7 & \ldots & 2 \\ & & & & & \\ 10,1 & 9,1 & 8,1 & \ldots & 2,1 & 2 \end{array}\right\},$$

totalling 10 routes in all to [2].

In contrast, for $[10,2]$, one finds

$$\left\{\begin{array}{llllllll}
10,1 & 10 & & & & & 2 & \\
10,1 & 9,1 & 9 & & & & 2 & \\
 & & & & & 2,1 & 2: & \text{sum } 9 \\
9,2 & 9,1 & 9 & & & & 2 & \\
 & 8,2 & 8,1 & 8 & & & 2 & \\
 & 8,2 & 7,1 & 6,1 & 6 & & 2 & \\
 & & & & 3,1 & 2,1 & 2: & \text{sum } 8 \\
\text{etc.} & & & & & & \multicolumn{2}{l}{\text{subseq. seqs. summing to } 7,6,5,4,3} \\
9,2 & 8,2 & 7,2 & \ldots & 3,1 & 3 & 2 & \\
9,2 & 8,2 & 7,2 & \ldots & 2,2 & 2,1 & 2: & \text{sum } 2
\end{array}\right\},$$

or, $2{+}3{+}\cdots{+}9$: totals to 45 routes in all. Clearly even attempting to record the simpler cases in hierarchical route forms is rather tedious and impractical. Once the significance of the reduction coefficients is accepted, as being in $1:1$ correspondence to the distinct hierarchical component routes, the direct presentation is no longer necessary.

Appendix B. Illustrative additional mappings: $\mathcal{S}_{12} \supset \cdots \supset \mathcal{S}_5 \supset \underline{\mathcal{A}}_5$

As a corollary to the mappings of tables 1, 2, we note the following mapping over $\Gamma'(\supset \cdots \supset \mathcal{S}_5 \supset \mathcal{A}_5) = \{\mathcal{A}, \mathcal{G}, \mathcal{H}, (\mathcal{T}_1 + \mathcal{T}_3)\}$, as being distinct both from the full YGC and natural embedding [57] processes:

$$\begin{aligned}
[11,1] &\to \{7,7,0,0\}\Gamma', \\
[10,2] &\to \{21,7,1,0\}\Gamma', \\
[10,11] &\to \{21,7,0,1\}\Gamma', && \text{(B.1)} \\
[93] &\to \{35,21,7,0\}\Gamma', \\
[921] &\to \{70,42,8,7\}\Gamma', && \text{(B.2)} \\
\left[91^3\right] &\to \{35,22,0,7\}\Gamma', && \text{(B.3)} \\
[84] &\to \{35,35,20,0\}\Gamma', \\
[831] &\to \{105,105,48,21\}\Gamma', \\
[822] &\to \{70,70,28,21\}\Gamma', && \text{(B.4)} \\
[8211] &\to \{105,112,28,42\}\Gamma', \quad \text{down to} && \text{(B.5)} \\
[75] &\to \{21,34,28,0\}\Gamma', \\
[741] &\to \{84,140,112,34\}\Gamma', \\
[732] &\to \{105,175,140,70\}\Gamma', && \text{(B.6)} \\
[7311] &\to \{126,230,140,105\}\Gamma', \\
[7221] &\to \{100,196,112,105\}\Gamma', \quad \text{finally to} && \text{(B.7)} \\
[552] &\to \{14,78,140,49\}\Gamma', && \text{(B.8)}
\end{aligned}$$

$$[5511] \to \{15, 98, 140, 63\}\Gamma', \tag{B.9}$$

$$[543] \to \{14, 98, 232, 91\}\Gamma',$$

$$[444] \to \{0, 14, 56, 21\}\Gamma'. \tag{B.10}$$

At the time of writing, there is no known molecular physics role for these extended chain mappings.

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