n-Body democratic recoupling and role of Schur Fn. products on S_n , a NMR dual-group view pertinent to coherence-transfer

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For automorphic spin symmetries over isotopomer networks defining both NMR coherence transfer and cage-cluster ro-vibrational (RV) weighting phenomena, the role of Schur functions (SF) and their SF products (SFP) (restricted to S_n) is re-evaluated, beyond that typical of atomic physics. It is seen now as being equally applicable to molecular physics. Our special focus here is on the SU2 × S_n dual group for its importance in replacing (Jucys) recoupling schemata by generalised S_n democracy invariants, which ensure the retention of simple reducibility (SR) of carrier spaces for superboson mappings, under $\widetilde{U} \times \widetilde{P}(\Gamma)$ actions over Liouville space, i.e., as in Physica A 198 (1993) 245. SFP mapping onto S_n and simple Young rule SF mappings onto $\{[\lambda]\}(S_n)$ sets are developed in the high *n*-index, weak-branching limit and utilise known similarities in the algorithms for the Young and Littlewood–Richardson rules. Over discrete k rank, from k = n (down), the $\sum_v \{/T^k(v)/\}k$ -set orders are related to the \supseteq ordered bipartite $\chi_{12n}^{[\lambda]}(S_{2n})$ characters.

1. Introduction

The central role of Schur functions (SFs) in subduction chains in the group theory of atomic physics has been established, for example, by Wybourne [36] in 1970s and subsequently extended [6,18]. However, the use of SFs in the context of molecular physics of clusters or isotopomers has been largely neglected. For dual group SU2 × S_n implicit in NMR coherence transfer or evolution, whose automorphic structures have been discussed by Corio [11] and Balasubramanian [1], SFs and their SF product decompositions on S_n provide a systematic way of deriving dual group tensorial sets. Here we are concerned with automorphic polyhedral modelling over spin networks inherent in non-magnetically equivalent $[AX]_n[AB]_n$ systems whose intra-cluster $\{J_{ij}\}$ zeroth order interactions give rise to their spin symmetry [1,11] and to S_n -networks. Similar considerations govern descriptions of the complete nuclear permutation (CNP) aspects of nuclear spin weighting for rovibrational spectroscopy of cage-isotopomers [2,3]. The recoupling schemata underlying such *n*-body problems with their high multiplicities may be treated de-

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mocratically at the outset, by taking a permutation-over-a-field viewpoint [29] and establishing the latter's system-invariants from combinatorial considerations. These are seen as analogous to the known hierarchies of distinct pathways over $(S_i \supset \cdots \supset S_2)$ Yamanouchi chains, as discussed, e.g., by Chen [7] in his particle-physics text.

Additional motivation for this work will be found in the structure of projective carrier spaces of Liouville space, in which the generic v label becomes an explicit aspect of (superboson) mappings under $U \times P(\Gamma)$ actions [29]. From this, the form of tensorial sets is derivable in principle from SFP decompositions onto the restricted space $SF(S_n)$ [34] set. Of necessity, these constitute [36] a subset of the mappings onto the $GL(n, \mathbb{C})$ group. The early Hilbert space formalisms of Levy-Leblond [16] and others [13] introducing a (limited few-body) democratic recoupling formalism to replace the unitary projective schemata, such as that given, e.g., in work of Sanctuary [20,21], has influenced us to seek the now general S_n -invariants of the dual group algebra. These invariants strongly augment a recent projective view of the carrier space structure of Liouville space in terms of superboson pattern algebras [29], for reasons mentioned later. Many of the purely combinatorial aspects are considered in a general high *n*-index, weak-branching (WB) limit of SFP mappings, this being seen as a consequence of the algorithmic similarity noted by Sagan [19] between the Young and Littlewood–Richardson (L-R) rules. The differences in the *n*-index values of the S_n -weak-branching limits under these two classic enumerative rules is the subject of other work [28,30,31].

The physical motivation for discussions of the n-2 set of labels governing S_n -invariants is that they define the carrier subspaces over which $\widetilde{U} \times \widetilde{P}(\Gamma^{[\widetilde{\lambda}]})$ act; they are essential for any systematic treatment of general dual group tensorial sets, beyond either the (Cartesian) tensor views of Coope et al. [10], or the SU2 × S_3 -based NMR coherence studies of Listerud et al. [17] and others [21,25]. Naturally, the use of dual-group space for spin-dynamic processes is not limited to NMR evolution; it is also pertinent to wider discussions, e.g., of rotational tunnelling. However, in true dynamic processes the standard ansatz of quantum mechanics applies and the coherent superpositional bases, carrying a pseudo-partitional label [17], are distinct from the stationary spin symmetry inherent in cluster systems [8].

After a survey of $U \times P(\Gamma)$ actions over the \mathbb{H} carrier space of Liouville space in section 2, we discuss the role of SF, SFP decompositions, section 3. Techniques involved in forming tensorial sets and their k-dependant dimensional properties are considered in section 4. Subsequently, the S_n -invariants of dual group recoupling schemata are reviewed in section 5, in the context of Yamanouchi S_n -chains. Various applications of these concepts to NMR and to ro-vibrational (RV) isotopomer weightings are discussed in the concluding section 6. For completeness, some outline of ladder operators on Liouville space (also referred to as shift operators in the mathematics lit.) and of $\{\mathbf{s}_i^2\}$ superbosons related to certain fundamental Wigner operators (alias 3*j*-coefficients) are given in an appendix.

2. Projective mappings within superboson algebra

On extending the Biedenharn and Louck Hilbert space formalisms [4,5] into augmented spin space for dynamical processes under \widetilde{U} rotational action

$$D^{j}(U)|kqv\rangle\rangle D^{j}(U)^{\dagger} = \sum_{q'} D^{k}_{qq'}(\widetilde{U})|kq'v\rangle\rangle,$$
(1)

(from equation (17) of Sanctuary's 1985 work [22] and from the $\widetilde{U} \times \widetilde{P}(\widetilde{\Gamma}^{[\lambda]})$ rotational/permutational analogous action, within the fundamental superboson mapping [29] defined on the Liouvillian carrier space ($\widetilde{\mathbb{H}}$) by

$$\widetilde{U} \times \widetilde{P} : \widetilde{\mathbb{H}} \to \widetilde{\mathbb{H}} \{ D^k(\widetilde{U}) \times \Gamma^{[\lambda]}(v) \, \big| \, \widetilde{U} \in \mathrm{SU2}, \, \widetilde{P}(\Gamma) \in S_n \},$$
(2)

one finds that under the dual group $SU2 \times S_n$ the invariant aspects of the generic v terms over n-2 terms are explicit aspects of the mapping, which gives raise to a hierarchy (direct sum) of labelled carrier (sub)spaces

$$\widetilde{\mathbb{H}} \equiv \bigoplus_{v} \widetilde{\mathbb{H}}_{v}.$$
(3)

As in the analogous Hilbert space formalism [4,5], the pattern algebra serves to define the analogous (3j)-coefficients, which are none-other than the fundamental Wigner operators of Liouville space [29], or (respectively)

$$\mathbf{s}_{\binom{1}{2}}^{2} \equiv \left\langle \left\langle \left(\begin{array}{cc} 2 & 0 \\ 0 & 0 \end{array} \right) \right\rangle \right\rangle; \quad \mathbf{s}_{1}\mathbf{s}_{2} \equiv \left\langle \left\langle \left(\begin{array}{cc} 2 & 0 \\ 1 & 0 \end{array} \right) \right\rangle \right\rangle. \quad (4)$$

Identifying the superbosons with a sequence of Q values allows a more general formalism to be invoked

$$\left\{ \mathbf{s}_{1}^{2}, \mathbf{s}_{1}\mathbf{s}_{2}, \mathbf{s}_{2}^{2} \right\} \Leftrightarrow \left\langle \left\langle \left(\begin{array}{cc} 2 & 0 \\ 2 & 0 \\ 1 + Q \end{array} \right) \right\rangle \right\rangle;$$

$$\left\{ \overline{\mathbf{s}}_{1}^{2}, (-)\overline{\mathbf{s}}_{1}\overline{\mathbf{s}}_{2}, (-)\overline{\mathbf{s}}_{2}^{2} \right\} \Leftrightarrow \left\langle \left\langle \left(\begin{array}{cc} 0 & 0 \\ 2 & 0 \\ 1 - Q \end{array} \right) \right\rangle \right\rangle,$$

$$(5)$$

respectively, as $\{Q = 1, 0, -1\}$. The associated signs here are a structural part of the corresponding Lie algebra of SU2 × SU2 group, as discussed by Hughes [14] in terms of the corresponding Casimir invariants (and in its role as a subgroup of the SO(5) group).

Further, the structure of nuclear spin permutational fields under $SU2 \times S_n$, from simple bipartite SF differences in the context of equations (1) and (2) naturally leads to a consideration of tensorial sets under dual group in terms of SF products and

their decompositional properties on the restricted space of S_n group. Wybourne in the 1970s [36] has stressed the existence of isometries between (outer (or inner)) SF products on $GL(n, \mathbb{C})$ space and the analogous (outer (inner)) [λ] tensor products on S_n space. Our present concern is with the restriction of SF, SFP from $GL(n, \mathbb{C})$ to some subset on space of the S_n symmetric group – this being a direct conceptual extension of the group subduction properties of SFs referred to in [36]. These properties have wide implications both for RV isotopomer weightings and for all problems involving S_n networks in chemical physics. The value of these ideas in understanding physical applications is a prime motivation for this work.

3. Schur Fn. Product mappings onto SF (on S_n) subsets

For SFs written as $\{\widehat{n-\mu}, \mu\}$ bipartite products on a restricted $\mathcal{GL}_n \supset S_n$ space

$$\{\widehat{\lambda}\} \otimes \{\widehat{\lambda}''\} \to \sum_{\lambda'} (\mathbf{\Lambda}_{\otimes, \{\lambda'\}}) \{\widehat{\lambda}'\} (S_n), \tag{6}$$

where the subscripted (Λ_{-}) s are the reduction coefficients, and where now the *p*partite resultant SF subset clearly will not be constrainted to simply bipartite forms. It is convenient in the interests of discussing generalised mapping relationships to introduce a high-*n* index limiting behaviour corresponding to weak-branching (WB) in the initial bipartite SFs. The origin of such properties may be traced to algorithmic similarities [19] between Young's rule (in its third form) and the Littlewood–Richardson rule, as used in duple applications for the establishment of inner tensor products (ITPs), particularly for lower *n* general-partitioned forms of SFs or irreps. There is no difficulty in recognising that (over a product space) the SF-subset (being mapped onto) will span $p \leq 2^2$ -(maximal) partite forms for products of initial bipartite WB forms. Further, since one is considering only SU2 × S_n SF mappings, it is taken that (at least for weak-branchings) the SF S_n -space mapped onto is *simply-reducible*, as well as being a *subset* of a GL(n, \mathbb{C}) group set. In addition, departures from the SF product WB limit lead to sub-subsets of the latter.

Utilising various general forms in [36] and invoking dimensional considerations for strictly bipartite initial SFs, one finds that for a high enough *n*-index to give the WB limit, referred to above (and dropping hat symbols specifically in the numerate SFs of equations (7)–(16) below), the mappings onto the *restricted* S_n space become

$$\{n-2,2\} \otimes \{n-2,2\} \to \{\{n-4,22\} + \{n-3,111\} + \{n-2,2\}\},$$
(7)

whereas the subsequent product maps onto subset

$$\{n-3,3\} \otimes \{n-3,3\} \rightarrow \{\{n-6,33\} + \{n-5,221\} + \{n-4,211\} + \{n-3,3\}\}.$$
 (8)

Similarly, the WB dissimilar SF products yield restricted space mappings of the form

$$\{n-2,2\} \otimes \{n-3,3\} \to \{n-5,32\} + \{n-4,211\} + \{n-3,21\},$$
(9)

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$$\{n-2,2\} \otimes \{n-4,4\} \to \{n-6,42\} + \{n-5,311\} + \{n-4,22\},$$
(10)

$$\{n-3,3\} \otimes \{n-4,4\} \to \{n-7,43\} + \{n-6,321\} + \{n-5,221\} + \{n-4,31\}, (11)$$

noting that in the WB limit and for bipartite products, these are simply-reducible (SR) mappings. Proofs of these relationships are possible from equations (7) and (8) via either high-indexed S_2 -plethysms given by Esper [12], or else via either reverse-ITP hierarchical calculations, or the use of symbolic computing algorithmic approach, as developed by Kohnert et al. [15].

Clearly the SF products in the WB limit surveyed here (or in $[\lambda] \otimes \cdots$ ITP formation where the SR property is not retained) are associated with the implied subduction chain

$$S_n \times S_n \supset S_{2n} \supset S_n, \tag{12}$$

and necessarily will be for a distinctly higher *n*-index than that associated with the simple SF (or simple S_n -module) decompositional mappings for ($p \leq 4$)-partite forms, discussed in earlier work [28,31], e.g.:

$$\{n - 4, 31\} \quad (1221; 21 -; 11) \rightarrow ()\mathcal{L},$$
 (13)
$$\{n - 4, 22\} \quad (1231; 22 -; 111)$$

$$\{n-4, 211\} \to (1343; 341; 1211)\mathcal{L},$$
 (14)

where \mathcal{L} spans the $\{[\lambda]\}\$ set in standard dominance order, from [n]. Also one finds that the $\{n-5,\ldots\}$ SF mappings are of the form

$$\{n-5, 32\} \to (1231; 32-; 221-; 111)\mathcal{L},$$
 (15)

$$\{n - 5, 311\} \quad (1343; 441; 3411 -; 1211) \rightarrow () \mathcal{L}, \qquad (16) \{n - 5, 221\} \quad (1353; 561; 3532 -; 12211)$$

within the Sagan generalisation [19] of Young's rule (in its third form), or as an explicit symbolic algorithm:

$$\left\{\widehat{\lambda}\right\} \to \bigoplus_{\lambda'} (\mathbf{\Lambda}_{\lambda,\lambda'})[\lambda'](\mathbf{S_n}),\tag{17}$$

where the unprimed λ s refer to the "contents" (sets of ones, twos, etc.) and the running primed subscript refers to the "shape" of boxes into which the "contents" are fitted in the enumerative process. Naturally, the subscripted ($\Lambda_{-,\lambda'}$)s of both equations (6) and (17) are the reduction coefficients, which occur in various physics applications [7].

4. Applications of SF, SFPs on S_n : dual tensorial sets via combinatorics

4.1. Illustrative generalised bipartite $ITPs(S_n)$

On writing the ITP components, of the Latin square underlying dual tensorial structure, for the complete $SU2 \times S_n$ tensorial set, as

$$[n-\mu,\mu] \otimes [n-\mu',\mu'] = (\{n-\mu,\mu\} - \{n-\mu+1,\mu-1\}) \times (\{n-\mu',\mu'\} - \{n-\mu'+1,\mu'-1\}), \quad (18)$$

one finds that $[n-2,2] \otimes [n-4,4]$ in the WB limit becomes

$$[n-2,2] \otimes [n-4,4] = \{n-2,2\} (\{n-4,4\} - \{n-3,3\}) - \{n-1,1\} (\{n-4,4\} - \{n-3,3\}).$$
(19)

By utilising the above properties and writing the result in terms of their appropriate (Λ_{-}) reduction coefficient matrices, one has mappings onto the \succeq dominance-ordered [19] (branched) restricted SF-sets:

$$[n-2,2] \otimes [n-4,4] \to (0000;000;001(-1)0;0(-1)(-1)1000;00100000) \left\{ \left\{ \hat{\lambda} \right\} \right\}, (20)$$

$$[n-2,2] \otimes [n-4,4] \to (0010;110;22100;1211000;1110000) \{ [\lambda] \},$$
(21)

both under S_n , as the final group of the implied chain subduction of equation (11). These ITPs are the building blocks from which Liouville space structure as one aspect of dual tensorial sets are derived. More formal theoretical views of $SU2 \times S_n$ tensorial structure are be found in, e.g., the double coset formalisms of Sullivan [23].

4.2. Dimensionality of $\{T^k(v)\}$ tensorial sets

Simple combinatorial consideration of the permutational field as

$$v = (k_1, k_2, k_3, \dots, k_i, \dots, k_n), \quad \forall k_i \leq 1, \text{ positive},$$
(22)

serves to define the order of the total $0 \leq k \leq n$ rank-based tensorial space of the $\{T^k\}(SU2 \times S_n)$ set as

$$\sum_{kv} / \left\{ T^k(v) \right\} / = \binom{2n}{n}.$$
(23)

By contrast, the subspaces for the full range of vs and a specific rank k (alone) simply take the form of the principal character of an appropriate bipartite irrep of the corresponding S_{2n} group, as set out in [34]. This is in keeping with the SF properties discussed by Wybourne [36], although *no actual* application to molecular physics, or restriction of the $GL(n, \mathbb{C})$ group to S_n , SFP-subset, is given in this classic physics text.

5. S_n invariants of $(p \leq 2^2)$ -part tensorial sets: democratic recoupling

We restrict discussion here to two simple examples of Yamanouchi chain subduction process in generating totally distinct, reduction pathways [7] under SU2 × S_n and NMR evolution [21,25] or coherence transfer processes [17]. The distinctness which leads to these S_n invariants is a consequence of standard commutator $[\mathcal{I}^2, \mathcal{I}_0]_-$, which applies to NMR evolution and to spin coherence transfer. The examples considered here are limited to the inner symmetry chain subduction derived from [n - 1, 1] and [n - 6, 33] irreps, where we shall take $S_n = S_9$, for brevity:

$$[8,1] \to \{[8] + [7,1]\} \to \{2[7] + [6,1]\} \to \dots \to \{5[4] + [31]\} \\ \to \{6[3] + [21]\} \to \{7[2] + [11]\},$$
(24)

with reduction coefficients 7:1, whereas the self-associate irrep $[333]_{SA}$ yields

$$[333] \rightarrow [332]_{SA} \rightarrow \{ [322] + [331] \}_{SA} \rightarrow \{ 2[321] + [222] + [33] \}_{SA}$$

$$\rightarrow \{ 5[31] + 6[22] + 5[211] \} \rightarrow \{ 5[3] + 16[21] + 5[111] \}$$

$$\rightarrow \{ 21[2] + 21[11] \}_{SA}$$
 (25)

and an equal pair of reduction coefficients of 21, whose sum is simply $\chi_{19}^{[333]}(S_9)$.

Hence over the n-2 labelled hierarchy in the two examples above, there are, respectively, 8 and 42 distinct pathways. For reason discussed elsewhere [7,35], the number of distinct invariant label sets are likewise 8 and 42 for the irreps [8,1] and [333], respectively, in agreement with the known $\chi_{19}^{[\lambda]}$ principal characters. The retention of SA property over full chain of S_n groups is proof of the retention of mathematical determinacy for S_n embedding in the internal spin symmetry, as discussed by Sullivan [24] in the mid-1980s. More recently, it has been utilised as a guide to the properties of specific natural group-embeddings and their mathematical determinacy [9,32,33].

6. Concluding comments

We have sketched some significant roles for SFs and combinatorics in generating tensorial sets under the dual group $SU2 \times S_n$ and in context of the existence of generalised democratic recoupling schemes under the internal Yamanouchi symmetry chain, rather than some Jucys-type diagrammatic recoupling scheme, as presented, e.g., in [20]. The methods used here are based on the tractable properties of (SU2) bipartite SFs on S_n space for a subset of (SU(m)) dual group tensorial sets, classically treated under the wider aspects of Schur–Weyl duality [23] and general ITP formation.

The earlier limitation of S_n -democracy to single invariant few-body problems [13, 16] has been lifted by recognising the significance of Yamanouchi chain subduction in the context of system invariants. The latter realisation is totally consistent with

arguments presented by Chen in his 1987 particle-physics group theory text [7]. These concepts are valuable keys to the wider understanding of the dual group, its utility and the value of permutations-over-a-field in molecular physics network (or isotopomer) problems. In addition to providing the structure of tensorial sets and thence the nature of weighting of RV spectra of cluster-like molecules, the foregoing is closely associated with ideas on the double Gel'fand pattern basis of Liouville space [26,28,29], on extending the Hilbert space ideas of Biedenharn and Louck [4,5]. Some outline of the former is given in appendix A2 below.

From arguments presented in a discourse on NMR coherence transfer over S_n networks [21] there is a clear role for the now explicit v terms (alias invariants or
recoupling terms) of the projective dual actions [26–29]; the factorisation of coherence
transfer matrix in the strongly coupling (or cluster) limit which mixes $\phi^0(11)$ and $\phi_0^1(11)$ in the two-spin case [21,25] is no longer so physically transparent in other
NMR presentations treating these problems [17,37], i.e., in ways that tend to exclude
the full cluster of NMR automorphism, or the strong-*J*-limit, in coherence transfer
phenomena.

Appendix A1. (Super)bosons: ladder operations on Liouville space

These are governed by commutators of the appropriate (shift) superoperators with the members of (super)boson set [29], as in

$$\left[\mathcal{I}_0, \mathbf{s}_i^2\right]_- \Leftrightarrow (\pm) \mathbf{s}_i^2 \quad \text{(for } i = 1, 2: \text{ in order}), \tag{26}$$

$$\left[\mathcal{I}_{+}, \mathbf{s}_{2}^{2}\right]_{-} \Leftrightarrow (\mathbf{s}_{1}\mathbf{s}_{2}) \Leftrightarrow \left[\mathcal{I}_{-}, \mathbf{s}_{1}^{2}\right]_{-}, \tag{27}$$

whereas, in contrast for consistent upper (lower) choices,

$$\begin{bmatrix} \mathcal{I}_{\pm}, \mathbf{s}_1 \mathbf{s}_2 \end{bmatrix}_{-} \Leftrightarrow \begin{pmatrix} \mathbf{s}_1^2 \\ \mathbf{s}_2^2 \end{pmatrix}, \qquad \begin{bmatrix} \mathcal{I}_0, \mathbf{s}_1 \mathbf{s}_2 \end{bmatrix}_{-} = \emptyset \quad (\text{a null space}). \tag{28}$$

The equivalent forms for the $\{\overline{s}_1^2, \overline{s}_1 \overline{s}_2, \overline{s}_2^2\}$ set with the appropriate sign changes are simply

$$\left[\mathcal{I}_{0}, \overline{\mathbf{s}}_{\binom{1}{2}}^{2}\right]_{-} \Leftrightarrow (\mp) \overline{\mathbf{s}}_{\binom{1}{2}}^{2}, \tag{29}$$

$$\left[\mathcal{I}_{+},\overline{\mathbf{s}}_{1}^{2}\right]_{-} \Leftrightarrow (-)\overline{\mathbf{s}}_{1}\overline{\mathbf{s}}_{2} \Leftrightarrow \left[\mathcal{I}_{-},\overline{\mathbf{s}}_{2}^{2}\right]_{-},\tag{30}$$

$$\left[\mathcal{I}_{\mp}, \overline{\mathbf{s}}_1 \overline{\mathbf{s}}_2\right]_{-} \Leftrightarrow (-) \left(\frac{\overline{\mathbf{s}}_1^2}{\overline{\mathbf{s}}_2^2}\right). \tag{31}$$

The zeroth \mathcal{I}_0 commutator with $\overline{\mathbf{s}}_1 \overline{\mathbf{s}}_2$ also maps onto a null space; in all these properties, the standard relationships for \mathcal{I}_{μ} : { $\mu = +, 0, -$ } are implied:

$$\{\mathcal{I}_+, \mathcal{I}_0, \mathcal{I}_-\} \equiv \left\{ (\mathbf{s}_1 \overline{\mathbf{s}}_2), (\overline{\mathbf{s}}_1 \mathbf{s}_1 - \overline{\mathbf{s}}_2 \mathbf{s}_2), (\mathbf{s}_2 \overline{\mathbf{s}}_1) \right\}.$$
(32)

Further, we note that concept of *right-derivation* property [4,5,29] is central obtaining a self-consistent set of ladder-operations. Thus [29] replaces sections 5 and 6 of an initial report [26]. The (–) negative signs in the sets of \bar{s}_i^2 of equation (5) are part of the structure of the underlying Lie algebra for the SU2 × SU2 group (of Liouville space), as defined by its Casimir invariants [14] and discussed in the main text.

Appendix A2. Double Gel'fand patterns for bases and fundemental Wigner operators

A number of ideas concerned with Δ and Q changes for the (superboson) pattern algebras were the subject of earlier investigations, e.g., in sections 5–7 of [28] and sections 7,8 of [26] (where the unbracketted $\mathbf{s}_i^{\rm ii}$) terms on the right of equations (7.9), (7.11), (7.13)–(7.16) should read $\mathbf{s}_i^{2(ii)}$. Here we restrict presentation to a minimal outline to clarify matters and give general view of a couple of aspects of k = 4 rank dual tensors, including

$$T^{k=n,q}((11\dots 1_n): [\lambda] = n), \qquad \{T^{k=n-1,q}((11\dots l_n): [\lambda] = 31)\},\$$

$$\{T^{k=n-2,q}((11\dots 1): [\lambda] = 22)\},\$$

which the two latter 3(2)-fold degenerate dual irreps, respectively, span the following (even) pattern algebras:

$$\left\{ \begin{pmatrix} 2 & 2 & 0 \\ 4 & 2 & 0 \\ 6 & 4 & 2 & 0 \\ 4 & 2 & 0 \\ 4 & 2 & 0 \\ 4 & 0 & 0 \\ k+q \end{pmatrix} : \begin{pmatrix} 2 & 0 & 0 \\ 4 & 2 & 0 \\ 2 & 0 & 0 \\ k+q \end{pmatrix} : \begin{pmatrix} 2 & 0 & 0 \\ 2 & 0 & 0 \\ 2 & 0 & 0 \\ 2 & 0 & 0 \\ 2 & 0 & 0 \\ k+q \end{pmatrix} \right\},$$
(33)

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$$\left\{ \begin{pmatrix} & & 2 & & & \\ & 4 & & 0 & & \\ & 4 & 2 & & 0 & \\ & 4 & 2 & & 0 & \\ & 4 & 2 & & 0 & \\ & 4 & 2 & & 0 & \\ & 4 & 2 & & 0 & \\ & 4 & 2 & & 0 & \\ & 4 & 2 & & 0 & \\ & 4 & 2 & & 0 & \\ & 2 & & 0 & & \\ & & k+q & & \end{pmatrix} \right\}.$$
 (34)

Finally, from expression (51) of [29] for Yamanouchi permutational-indexed Liouvillian bases, $|(i_1i_2...i_n): kqv\rangle\rangle$, one notes that the equivalent equation for \mathcal{P} transformational properties is simply

$$P|(i_1\dots i_n)kqv\rangle\rangle P^{\dagger} \equiv \sum_{y'\equiv (i_1\dots i_n)'} \widetilde{\Gamma}_{y'y}^{[\lambda]}(\mathcal{P})|(i_1\dots i_n)'kvq\rangle\rangle,$$
(35)

within constraints implied by equation (2) and the detailed forms from equation (21) of [28].

Note added in proof

Further discussion of sections 3 and 4.1 material is given in subsequent work, which used the SYMMETRICA symbolic computing package of ref. [15].

References

- [1] K. Balasubramanian, J. Chem. Phys. 78 (1983) 6358.
- [2] K. Balasubramanian, Chem. Phys. Lett. 182 (1991) 257.
- [3] K. Balasubramanian, J. Phys. Chem. 97 (1995) 4647.
- [4] L.C. Biedenharn and J.D. Louck, in: *The Permutation Group in Physics and Chemistry*, Springer Tracts in Chemistry (1979).
- [5] L.C. Biedenharn and J.D. Louck, *Angular Momentum in Physics*, Math. Encyclopaedia Series, Vols. 8,9 (Cambridge University Press, Cambridge, 1985).
- [6] P.H. Butler, *Point Group Symmetry Applications: Methods and Tables* (Plenum Press, New York, 1981).
- [7] J.Q. Chen, Group Representation Theory for Physicists (World Sci., Singapore, 1988).
- [8] C. Cohen-Tannoudji, B. Dui and F. Lalöe, *Quantum Mechanics* (Hermann–Wiley, Paris, 1977) p. 252.
- [9] J.P. Colpa and F.P. Temme, Canad. J. Phys. (1998), to be published.
- [10] J.A.R. Coope, J. Math. Phys. 11 (1970) 1591 and references therein.
- [11] P.L. Corio, The Structure of High-Resolution NMR (Academic Press, New York, 1966).
- [12] N. Esper, J. Math. Comput. 29 (1976) 1150.
- [13] H.W. Galbraith, J. Math. Phys. 12 (1972) 782.
- [14] J.B.L. Hughes, J. Math. Phys. 24 (1983) 1015.
- [15] A. Kohnert, A. Lascoux and A. Kerber, J. Symbolic Comput. 14 (1993) 195.
- [16] J.M. Levy-Leblond and M. Levy-Nahas, J. Math. Phys. 6 (1965) 1372.
- [17] J. Listerud, S.J. Glaser and G.P. Drobny, Molec. Phys. 78 (1993) 629.

- [18] J. Paterna, R.T. Sharp and P. Winternitz, J. Math. Phys. 19 (1978) 2362.
- [19] B.E. Sagan, *The Symmetric Group: Its Representations, Combinatorial Algorithms and Symmetric Functions* (Wadsworth Math., Pacific Grove, CA, 1991).
- [20] B.C. Sanctuary, J. Chem. Phys. 64 (1976) 4352.
- [21] B.C. Sanctuary, Molec. Phys. 55 (1985) 1017.
- [22] B.C. Sanctuary, J. Magn. Reson. 61 (1986) 116.
- [23] J.J. Sullivan, J. Math. Phys. 19 (1978) 1674, 1683; 24 (1983) 424.
- [24] J.J. Sullivan, J. Math. Phys. 24 (1983) 2542.
- [25] F.P. Temme, J. Magn. Reson. 83 (1989) 383.
- [26] F.P. Temme, J. Math. Phys. 32 (1990) 1964.
- [27] F.P. Temme and J.P. Colpa, Molec. Phys. 73 (1991) 953.
- [28] F.P. Temme, Z. Phys. B 88 (1992) 83; 89 (1992) 335.
- [29] F.P. Temme, Physica A 198 (1993) 245.
- [30] F.P. Temme, Coord. Chem. Rev. 143 (1995) 161.
- [31] F.P. Temme, Molec. Phys. 85 (1995) 883; 86 (1995) 981.
- [32] F.P. Temme, J. Math. Chem. 20 (1996/1997) 311; 21 (1997) 373.
- [33] F.P. Temme, J. Math. Chem. 24 (1998) 133.
- [34] F.P. Temme, Chem. Phys. (1998), submitted.
- [35] F.P. Temme, Physica A (1997/1998, to be published).
- [36] B.G. Wybourne, Symmetry Principles and Atomic Spectroscopy (Wiley, New York, 1970).
- [37] J. Zhou, L. Li and C. Ye, Molec. Phys. 86 (1995) 1173.