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Beyond simple point sets to the indistinguishable point-set tensorial limits of R–W algebras: multiple G-invariants and the carrier-map-based quantal-basis completeness of uniform NMR spin systems

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Abstract

Augmented quasiparticle (QP) mappings, as applied to indistinguishable point sets of (Liouvillian) democratic-recoupled (DR) tensors, provide for a 1:1 invariant labelling of the underlying (disjoint) dual projective map carrier subspaces, where the Liouville pattern basis set is defined via superboson unit-tensor actions on a null space, $|\emptyset\rangle\rangle$. The co-operative-action Liouville algebras described here imply parallel limitations to Jucys graph recoupling and its related Racah–Wigner (R–W) algebras once DR indistinguishable point tensorial sets are involved, as in non-SR $\mathcal{S}_n, n \geqslant 4$ dominant (NMR) spin symmetry. The importance of $\mathcal{S}_n$ G-invariants, as labels for disjoint carrier subspaces in such automorphic spin symmetries, arises from their essential role in defining the quantal-completeness of indistinguishable point sets. From the established properties of augmented-QPs as super-bosons (Temme 2002 *Int. J. Quantum Chem.* **89** 429) (i.e., beyond the earlier Hilbert-space-based Louck and Biedenharn boson pattern views), insight into Atiyah and Sutcliffe's (A–S) assertions (Atiyah and Sutcliffe 2002 *Proc. R. Soc.* A **458** 1089) on the limitations of graph recoupling theory to distinct point sets is obtained. This clarifies the wider *analytic intractible* of automorphic DR spin systems—beyond the Lévi–Civitá cyclic-commutation (R–W) approach (Lévy-Leblond and Lévy-Nahas 1965 *J. Math. Phys.* **6** 1372) which holds for a mono-invariant problem. For (rotating-frame) density matrix approaches to $[A]_n, [A]_n(X)$ and $[AX]_n(SU(2) \times \mathcal{S}_n)$ (dual) NMR systems, the focus is necessarily on the specialized nature of *indistinguishable point sets* within multiple invariant-theoretic-based, dynamical spin physics. Here, the GI(s) (GI-cardinality) constitute an important part of the dual irrep set, $\{D^k(\tilde{\mathbf{U}}) \times \tilde{\Gamma}^{[\lambda]}(\tilde{v})(\mathcal{P})\}$, with combinatorics, as a central facet of invariant theory, playing a crucial role in the concept of 'quantal completeness' and the impact of A–S's assertion on the existing NMR tensorial physics. Clearly, the role of Liouvillian Yamanouchi projection, now as disjoint subspatial-based transformational properties, defines such DR bases and their unit tensors. A brief outline is given of the structure of augmented general-indexed Lévi–Civitá superoperators with their multiple GI-labelled carrier subspaces.

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List of Abbreviations Employed

CFP	(SU(2))-based coefficient of fractional parentage
DR	democratic recoupling
G-, GI	group/group invariant
$\mathbb{H}$	a superboson carrier space
L–C	Lévi–Civitá form
$\hat{\mathbf{L}}$	a Liouvillian
QP	Quasiparticle
R–W	Racah–Wigner (algebra)
SR	(in mathematics context) simply-reducible
TRI	time-reversal invariance
YM	Yamanouchi terms (as $\mathcal{S}_n$ labellings)

$(\lambda \vdash n)$, is a number partition; $|\tilde{\emptyset}\rangle\rangle$ and $|kqv\rangle\rangle$ represent, respectively, a null and its corresponding Liouville space basis. Wybourne suppressed leading-part notation employed in $\langle r_2 r_3\rangle S_n$ irrep and $\chi^{\langle\cdot\rangle}$ character notation.

$\mathbf{Z}(\mathbb{C})$ and $\mathbf{Z}(\mathbb{R})$ represent complex and real algebras, whereas $\mathbf{Z}_{n0}$, etc notations refer to graph schemata; $\tilde{\Delta}$ is a (Gel'fand) (L) shift.

1. Preamble

The theories associated with geometry-phase, quantum-rotational tunnelling or nutational spectral (and similar) aspects of NMR spin dynamics [1–3] are notable for the depth and range of the theoretical formalisms on which they draw. These include Jucy–Vanagas sanctuary and related recoupling theories [3, 4], TCP/TP (or time-reversal) invariance [4, 6, 7], and not infrequently also gauge-invariance [1] well established in quantum-rotational tunnelling. Because the nature of the quantum description changes in NMR, i.e., from one pertinent to open driven system(s), in the pulsed cycle, to one involving classic closed conserved system(s) in the evolution or relaxational period(s), spin dynamics and its formalisms [7–12] remain of considerable interest. In strong contrast to other spectroscopic techniques [13], NMR spin dynamics explicitly draws on the unitary group defined $\mathbf{Z}(\mathbb{C})$ algebras [10] pertinent to Magnus expansions. In addition, for analytic progress in handling many NMR problems and their associated model spin dynamics [3], some appreciation of applicable mathematics [14–18] pertinent to (inner recoupled) (abstract $\hat{\mathbf{L}}$-induced automorphic [8]) tensorial (point) sets is required. Naturally, the feasibility (wreath-product) group [9], typical of early rotomer NMR studies, provides models for much of reaction dynamics. However, the model spin symmetries considered here are those of direct Liouvillian-structure-based automorphic NMR spin symmetries. They are of specific interest on account of being derived from uniform spin-based *indistinguishable point sets and because they draw on invariant-labelled disjoint carrier subspaces* in their treatment of superboson set projective mappings [11]. Because R–W algebras are based on $\mathbf{Z}_{n0}$-linked chains of graph-based 3j/6j coefficients [10], $SU(2) \times \mathcal{S}_n$ automorphic spin symmetries by their inherent nature question the limits of R–W algebras and its general applicability to (rotating-frame) dual group NMR problems [19–22].

Whilst the nature of tensorial formalisms for *distinguishable point sets* (spins) and their unitary graph-recoupled tensors are well established [3, 10], the contrasting forms for dual group-based generalized uniform point tensors [11], whether derived via democratic recoupling (DR) [12, 13] or via dual unit tensors (Hilbert boson pattern algebras of [11]) are less well defined. A recent assertion given by Atiyah and Sutcliffe [14] (A–S) stresses that explicit recoupling procedures (and in consequence the established Racah–Wigner (R–W) treatment of the matrix formalisms in NMR spin dynamics [3, 4]) are strictly limited to *distinguishable point* sets. This raises two further interesting general questions: namely 'what form of applicable mathematics is proper and pertinent cf to *indistinguishable dual group*-based identical point sets' and/or their related generalized $\mathcal{S}_n$ DR-based pure spin tensorial sets, and the related question for Liouvillian higher n-fold abstract spin spaces of the nature of generalized forms of Lévi–Civitá operators? To the best of our knowledge, no $n \geqslant 4$ indexed permutational-group analogue (for identical point sets) to R–W algebra of [10] is known, which retains generally applicable to matrix descriptions of abstract automorphic space spin physics once *multi-invariant DR point sets* become a dominant feature. One suspects that the standard Lévi–Civitá form with its first intimations of DR non-graphical recoupling is a specific form restricted to 3-fold point highest mono-invariant forms of problem [12]. The need for the explicit treatment of auxiliary labels in Liouville space formalisms assists one here, by making one ask further precise fundamental questions that concern the nature of the underlying indistinguishable point-set-induced limitations to R–W algebra, once both DR and multi-fold invariant structures are involved. It is these questions essentially in a superboson pattern mapping-on-Liouvillian-carrier-space scenario [11–16] which provides the essential motivation for this paper with its combinatorial, discrete mathematics and density-matrix formalism bias.

In considering such indistinguishable point sets, our approach necessarily focuses on the physics of (Liouville) projective carrier (sub)spaces derived from (automorphic) dual group actions as projective mappings, where these constitute a superboson pattern (as unit-tensors) algebras [15]. Clearly, this viewpoint represents an augmented view of the classic Hilbert boson mapping formalism given by Louck and Biedenharn [11]. It is the need for these carrier subspaces to be defined by invariant designations [19–22], as well as dual group actions that gives a cogent insight into the persistence of an 'open problem' in automorphic-structured (NMR) spin physics. Knowledge of the underlying $\mathcal{S}_n$ combinatorics [16–19], of generalized $(\otimes D^{k=1}(\mathbf{U}))^n$ (Liouvillian $SU(2)$) CFP-schemata [3] and their cardinalities, i.e., based on [5, 6]) of multiple invariant $\mathcal{S}_n$ group action-defined NMR systems [11, 15], are all necessary precursors to any real understanding of indistinguishable point-set-based limitations inherent in applicable R–W algebras, once the basis is restricted to an automorphic abstract pure spin form.

2. Contrasting Hilbert and Liouville views of non-SR co-operative $SU(2) \times \mathcal{S}_n$ algebras

The utility of the graphical propagative Jucys–Vanagas diagrammatic recoupling theory to DR multiple spin NMR systems (in contrast to earlier form [3, 4]) is essentially limited to a single example. In this case, the *mono-invariant* Lévi–Civitá (L–C) operator as a DR interaction acts on a (general uniform I_i) 3-spin ensemble. This then generates additional cyclic commutation relationships which elegantly resolves [12] the specialized matrix structure derived under R–W analysis to yield a Jacobean tri-diagonal form[1]. Beyond this single established example, specific (combinatorial) features of Liouvillian NMR tensorial formalisms (cf Hilbert-space views) arising in DR (*integer* $\{k_i\}$) point sets necessarily must draw on the physics of $SU(2) \times \mathcal{S}_n$-based indistinguishable (inner recoupled) tensorial sets, now with the inclusion of their explicit auxiliary labelling. The latter clearly spans the various multiple component $\mathcal{S}_n$ group invariants. It is these additional explicit labels which are fundamental to treating the (Liouvillian) 'quantal-basis set-completeness' condition, because the (dual) permutation group (in contrast to that of the simple $SU(2)$ case) is intrinsically a non-simply-reducible (SR) group [15–20]. Hereafter, the role of group invariants and their inherent cardinalities, *beyond both the restricted mono-invariant 3-spin system* [12] *above and earlier Hilbert-space conditions*, equation (5) is central to extending quantum-Liouville formalisms to non-trivial automorphic $[A]_n(X)$, $[AX]_n$ NMR spin systems.

One should first stress that the superboson formalism (as a pattern algebra over augmented quasi-particles cf earlier pattern algebra [11]) is closely correlated with the corresponding *inner recoupled unit tensors*, here denoted by $\langle\langle(2k\,{}_{k\pm q}^{\cdot}\,0)\rangle\rangle$, in sense that, e.g.,

$$\left(s_1^2\right) \equiv \left\langle\left\langle\begin{pmatrix} 2k & 2 & 0 \\ & k+q & \end{pmatrix}\right\rangle\right\rangle \tag{1}$$

with

$$\left(s_1^2\right) \mid \tilde{\emptyset}\rangle\rangle \to \left| \begin{pmatrix} 2k & 2 & 0 \\ & k+q & \end{pmatrix}\right\rangle\right\rangle \tag{2}$$

as a component of basis set, ($\equiv |kqv\gg$), with the link between Liouville space and the earlier simple Hilbert-space formalism in terms of group action provided by the group actions,

$$\tilde{\mathbf{U}}\left\langle\left\langle\begin{pmatrix} 2k & 2 & 0 \\ & k\pm q & \end{pmatrix}\right\rangle\right\rangle \equiv \mathbf{U}\left\langle\left\langle\begin{pmatrix} 2k & 2 & 0 \\ & k\pm q & \end{pmatrix}\right\rangle\right\rangle\mathbf{U}^{\dagger}. \tag{3}$$

In consequence, the equivalent Liouvillian between-ness representations, based on 2k, are, e.g., at most 2-unit multiples of the simple Hilbert-space forms, as indicated in [15].

In this context, it the structure of dual projections over carrier space(s) (inherent in augmented or Liouvillian quasi-particle mappings) that play a special role in the (Liouville space) logic, one which is quite distinct from that in the Louck–Biedenharn 1979 Hilbert-space formalism [11]. Now, it is the dual projective carrier space that yields a necessary condition for the *completeness of DR Liouvillian tensorial sets*. This arises because the dual group formal mapping is now over a set of *disjoint carrier subspaces* [15]. Hence, the simple combinatorial equation for (dual) Hilbert spin space completeness is replaced by a formal carrier space mapping specific to invariant-based indistinguishable multi-point sets, below, with the role of invariant labels as important as that of the group irreducible representations (irreps) themselves. Hence, invariant theory is seen as an essential part of group theory once automorphic Liouvillian NMR spin systems considered.

One further key issue arises here, namely the substantive cardinality associated $\mathcal{S}_n$ group invariants [5–7, 19, 20]—a facet of invariant theory and the class structure of group theory

[1] As indicated above the limitation of L–C operators within some mono-invariant scenario to at-most $\mathcal{S}_3$-fold permutational DR problems represents an equivalent origin to many of the questions posed here concerning DR identical integer-rank unit tensorial sets.

itself. It also explains in part why the Liouvillian spin dynamics of *extended identical multi-spin* NMR systems has not been adequately understood to date, despite an earlier recognition [15] of salient features of carrier space for (augmented) QP Liouvillian projective mappings. Naturally, the (dual group) set logic here arises in the context of both classic groups and permutation groups being explicit subgroups of the $\mathcal{GL}_n$ group [13]. Recent progress in the development of $\mathcal{S}_n$ theory, its algorithmic combinatorics as part of symbolic computing [16–18] has had significant impact on physics applications based on combinatorics, including those of [19–22] of more recent times. The fuller role of disjoint subspaces in the dual algebras of the $[A]_n(X)$, $[AX]_n$ DR NMR systems (cf earlier (or related) work [18–22]) and their purely abstract spin space NMR dynamics application has not been explicitly addressed earlier, despite these formal mappings derived from group actions being set out in earlier discussions of superbosons as augmented quasiparticles [15].

3. Role of dual projective mappings over carrier (sub)spaces

3.1. Context: quasi-particle Hilbert projections

Prior to discussing Liouvillian projective mappings, one needs to establish the (cf) notation(s) involved and to highlight the contrasting properties under group actions first in the simple Hilbert spin space case and subsequently for spin dynamics formalisms. Hence, the original Louck, Biedenharn work on primary Hilbert-space QP projection over a carrier space [8] and their pertinence to Gelf'and (shape) algebras are referred to, before introducing (augmented) quasiparticles ('QP bosons') and their analogous (integer rank) unit tensors [10]. In particular, the SR simple unitary and dual projective mappings derive from the **U** (simple) and $\mathbf{U} \times P$ (dual) group actions that yield the distinct projective mappings:

$$\mathbf{U} : \mathbb{H} \longrightarrow \mathbb{H}\{D^j(\mathbf{U})|\mathbf{U} \in SU(2)\} \tag{4}$$

for j half-integer rank, and (below) over indistinguishable point sets (alias Hilbert DR tensorial sets) represented by

$$\mathbf{U} \times P : \mathbb{H} \longrightarrow \mathbb{H}\{D^j(\mathbf{U}) \times \Gamma^{[\lambda]}(P)|\mathbf{U} \in SU(2);\ P \in \mathcal{S}_n\} \tag{5}$$

in which λ is a typical (two-part) permutational group irrep. One notes here that the completeness of the Hilbert dual group irreps was defined by the simple combinatorial expression,

$$\sum_{j}^{\max j=n/2} D^j(\mathbf{U}) \times \Gamma^{[(n/2)+j,(n/2)-j]}, \qquad \text{for} \quad j \geqslant (0)(1/2). \tag{6}$$

In these Hilbert-space sets of mappings, there is clearly *no explicit reference to the group invariants or their cardinality*, simply because the orthogonality of R–W algebra is already defined by standard conditions [8].

3.2. Contrasting (L) projective maps over invariant-labelled carrier subspaces

For the comparable augmented QP (Liouville-space superboson) (pattern algebra) spans the following further sets:

$$\left\{s_1^2, s_1s_2, \ldots, s_2^2\right\}; \qquad \left\{\bar{s}_1^2, \bar{s}_1\bar{s}_2, \ldots, (-)\bar{s}_2^2, \text{(its adjoint subset)}\right\} \tag{7}$$

based on (cf to simple Hilbert QPs) integer rank k unit-tensor intensive augmented-QP forms, and, e.g., (Liouvillian) SU(2) ($k = 1; k \geqslant q \geqslant -k$) (ordered) structures:

$$\left\{\left\langle\left\langle 2 \overset{2}{\underset{k+q=2}{\cdot}} 0 \right\rangle\right\rangle : \left\langle\left\langle 2 \overset{k+\tilde{\Delta}=2}{\underset{k+q=1}{\cdot}} 0 \right\rangle\right\rangle : \left\langle\left\langle 2 \overset{2}{\underset{0}{\cdot}} 0 \right\rangle\right\rangle\right\} ; \left\{ .. ; \left\langle\left\langle 2 \overset{k-\tilde{\Delta}=0}{\underset{k-q=1}{\cdot}} 0 \right\rangle\right\rangle ; .. \right\},$$
$$\textit{for } \tilde{\Delta}, \textit{ integer} \leqslant k, \qquad (8)$$

or similarly for generalized multispin integer rank Gelf'and forms and their associated tensorial set bases. Clearly, these derive from augmented QPs, as unit tensor(s) acting on **null** (L) bases and yield similar transformational properties for both unit operators and related (Liouville) pattern bases. Strong distinctions exist between the simple/distinct point set unitary and dual group actions (on indistinguishable point sets) as projective mappings, with the form

$$\tilde{\mathbf{U}} : \tilde{\mathbb{H}} \longrightarrow \tilde{\mathbb{H}}\{D^k(\tilde{\mathbf{U}}) | \tilde{\mathbf{U}} \in SU(2)\} \qquad (9)$$

retained for distinguishable (non-identical) spin or point sets, or the single $SU(2)$ spin case, whereas the indistinguishable point set case is defined by explicit invariant-labelled (augmented) dual mappings:

$$\tilde{\mathbf{U}} \times \mathcal{P} : \tilde{\mathbb{H}} \longrightarrow \tilde{\mathbb{H}}\{D^k(\tilde{\mathbf{U}}) \times \tilde{\Gamma}^{[\lambda]}(\tilde{v})(\mathcal{P}) | \tilde{\mathbf{U}} \in SU(2); \mathcal{P} \in \mathcal{S}_n, \tilde{v}\, \mathcal{S}_n \text{ group invariant}\}; \qquad (10)$$

not only the dual group irreducible representations (irreps) given here but also $\tilde{v}$ is now a specific retained label (rather than just an auxiliary label, as in distinct point set graph-recoupling theories). Further, because the $\tilde{v}$ *invariants underlying the indistinguishable (Liouvillian) point sets* induce a set of disjoint carrier subspaces over which the augmented QPs now act, the augmented carrier space is defined by its invariant-labelled subspaces:

$$\tilde{\mathbb{H}} \equiv \oplus_{\tilde{v}} \tilde{\mathbb{H}}_{\tilde{v}}, \qquad (11)$$

in contrast to the Hilbert-space form. Naturally, the full extent of these disjoint subspaces (subsets) is itself defined by the cardinality of the $\mathcal{S}_n$ group invariants, with the (Liouville) set 'quantal-completeness' governed by the dual representations:

$$\sum_{\tilde{v}} D^k(\tilde{\mathbf{U}}) \times \tilde{\Gamma}^{[\lambda]}(\tilde{v})(\mathcal{P}) \equiv \oplus_{(\tilde{v})} T^k_{\{\tilde{v}\}}(1..11), \qquad \text{for} \quad \tilde{v} \in \mathcal{S}_n \text{ invariant set}, \qquad (12)$$

where the RH form over integer rank k stresses that the 'like' inner-tensorial properties from density matrix formalisms with each specific invariants contributing a $\delta_{\tilde{v}\tilde{v}'}$ further orthogonality condition, which applies over all the specific disjoint carrier subspaces. Analogous subspatial $\tilde{v}$-augmented-Yamanouchi $\mathcal{S}_n$ group projective actions defined via

$$\mathcal{P} : |\tilde{y} : (\tilde{v})kq\rangle\rangle \equiv \sum_{\tilde{y}'} \tilde{\Gamma}^{[\lambda]}_{\tilde{y}'\tilde{y}}(\tilde{v})(\mathcal{P}) |\tilde{y}' : (\tilde{v})kq\rangle\rangle, \qquad \text{for} \quad \tilde{y} = (\tilde{i}_1 \ldots \tilde{i}_n) \qquad (13)$$

provide the Liouvillian $\mathcal{S}_n$ group formal transformational properties. These now derive from ($m \leqslant 4$)-(word)partite $[\tilde{\lambda}]$ Liouvillian irreps implicit in $[\tilde{\lambda}] = [\lambda'] \otimes [\lambda'']$—where the (tilded) $\tilde{y}$'s are derived (Liouvillian) (augmented) Yamanouchi formal symbols, noting that the decreasing leading component lexical order $\mathcal{S}_6$ irrep set, e.g., corresponds (see, e.g., [23]) to Yamanouchi (YM) series:

111111; 111112; 111122; 111123; 111222;
<u>111223</u>; 111234; 112233; 112234,

where the underlined YM label corresponds to the self-associate (self-conjugate) [321] irrep. Naturally, the range of Yamanouchi symbols and their transformational results applicable in Liouville space derive from non-SR $\otimes[\lambda]$ product forms (as cf to SR $D^k(\tilde{\mathbf{U}})$ (Edmonds) rotations) which characterize the distinctions observed between *indistinguishable* (dual) spin point sets, i.e. from the contrasting simple distinct unitary point sets, in which graph recoupling and R–W algebra suffice to define the (distinct $\{k_i\}$)-based inner tensorial sets.

3.3. Invariant labelling of carrier subspaces for $[AX]_n$ bis-augmented systems

Since the above paragraph does not encompass all possible types of NMR spin systems, additional specific labelling arises in handling the group invariants of $[AX]_n$ spin systems. Naturally, the resultant invariant cardinalities are evaluated as products of the $\tilde{v}, |GI|^{(n)}$ original terms of the separate spin clusters, which extends the impact of the original non-SR considerations. Hence, for the above bis-model system with $n = 4$ identical spins associated with each cluster, each contributes its own three monocluster invariant label subset, which in the spirit of J–Q Chen's earlier work [23] becomes

$$\{[31] \supset [3] \supset [2]; [31] \supset [21] \supset [2]; [2^2] \supset [21] \supset [2]\}, \tag{14}$$

but one requires nine resultant product-type invariants to fully define the range of bis-cluster-based disjoint carrier subspaces, $\tilde{\mathbb{H}}(\otimes)$.

4. $\mathcal{S}_n$ invariants and their cardinality as TR-based Weyl properties

A direct statement of the cardinalities of $\mathcal{S}_{2n}$ invariants is available (without the need of quasi lattice points used previously [16] from a careful reading of Corio's 1998 work [6], augmenting Weyl classic discussion [5] of the role of time-reversal invariance (TRI) in theoretical physics [7] and the latter's views of the interrelationship between TRI and permutations, specifically over $(\hat{\mathbf{I}} \bullet \hat{\mathbf{I}})$, $(\hat{\mathbf{I}} \bullet \hat{\mathbf{I}})$ pairs of enbracketted scalar products. This then gives (as shown using direct hooklength character enumeration in [19] in some detail) the group invariant cardinality in terms of a specialized sum of (even) group characters [19] (in the $\mathcal{S}_n$ group form of reduced-Wybourne notation of [16]) as

$$|GI|^{2n} \equiv \chi^{\langle 0\rangle}_{1^{2n}} + \chi^{\langle 2\rangle}_{1^{2n}} + \cdots + \chi^{\langle 2(n-1)\rangle}_{1^{2n}}, \tag{15}$$

a closed analytic result[2], consistent with numerical results derived from a corresponding SU(2) unitary group $(\otimes D^{k=1}(\tilde{\mathbf{U}}))^n$ recursive bijection scheme for the *coefficients of fractional parentage CFP*(i) coefficients; clearly the zeroth component here is simply the scalar (or group) invariant cardinality discussed elsewhere—e.g., as equation (4) of [20]. This procedure itself is simply an augmented more direct discrete mathematics view of the earlier Chen–Moraal–Snider formalism [3]. The cardinalities derived by this stepwise recursive bijection are naturally a result of an end-of-chain addition (or $\mathbf{Z}_{n0}$) process, whereas taking the sum of squares of *CFP*(i) over the nth full set is similar to a $\mathbf{Z}_{22}$-based process. In contrast to the original bijective mapping, one should stress that the sum of CFPs on 'n' only yields the single '$2n$'th-based *CFP*(0) value shown underlined in equation (16).

To exemplify these processes, the $n = 5, 6, 10, (11), 12, 20$ (etc) sequence are of interest in respect of the bijection and sum-of-squares unitary processes, with second column

[2] The number of invariant tensors arising under polynomial tensor-contraction is a different $\mathcal{GL}$ group-based (even) char-sum result.

containing the $|GI|^{(n)}$ cardinalities indicated by n-fold bold-face indices:

n:	$C(0)$								$C(i)$				
5:	6	15	15	10	4	1							
6:	15	36	40	29	15	5	1						
$\cdots$:													
10:	<u>603</u>	1585	2025	1890	1398	837	405	155	45	9	1		
11:	1585	4213	5500	5313	4125	2640	1397	605	209	55	10	1	
12:	<u>4213</u>	11298	15026	14938	12078	8162	4642	2211	869	274	66	11	1
..:													
20:	<u>13, 393, 689</u>	37, 458330	54, 237210	61, 430895	59439429	50, 779476	38, 882740						
		26, 876830	16, 818610	9, 528500	4, 877300	4, 877300	2, 246465						
				925395	338010	108186	29849	6935	1310	190	19	1	

(16)

to yield (from the full CFP set of [20]) the $n = 40$-based <u>17, 047, 255, 430, 494497</u> primary GI cardinality result for component Liouvillian of the heterfullerene $[A]_{20}[X]_{40}$ exocluster Liouvillian (of ${}^{11}B_{20}{}^{13}C_{40}$)—here for typographic reasons we have staggered the rows of terms given for highest index value—whereas the $|GI|^{(60)}$ for group invariant of spin exocage ${}^{13}C_{60}$ fullerene if required may be derived, e.g., via $n = 15, 30, 60$ CFP sequence, with the character-sum expression equation (15) providing useful check on the bijection-derived intermediate results. For modest values of $2n \leqslant 30$ indices, the hooklength enumerative calculation of group characters is particularly convenient. It has been traditional to depict actual symmetric group invariants in terms of Chen *et al* [23] stepwise subgroup route-map hierarchies, as in equation (14). Fuller discussion of these techniques and examples of their resultant cardinalities may be found in the earlier cited works. Usage of Chen-type subgroup hierarchies as evaluative tool soon becomes rather tedious; likewise use of full $\mathcal{S}_n$ character tables above order 14,16 is not practical and rapid 'n' expansion of $\lambda \vdash n$ soon slows symbolic computing evaluations [18], whereas hooklength $\chi^{\langle,\rangle}_{1^n}$ s of equation (15) are simple to obtain.

5. Discussion in the Liouville NMR system context

Consideration of $3n$-j or $3n$-k recoupling techniques up to 6, 12, 18-j (k) concatenated symbols only confirms that such methods and matrix representational evaluations based on them are essentially graph diagrammatic forms that do not properly allow for DR and $\mathcal{S}_n$ induced *indistinguishable point sets*. The problem of Liouvillian basis sets themselves being multi-invariant labelled, implied in the above GI-cardinality analysis, further complicates the problem. Even for the early mono-invariant Hilbert-space *indistinguishable three spin* problem[3], discussed in [12, 19, 20], Lévy-Leblond and Lévy-Nahas's elegant Lévi–Civitá's operator method [12] was only able to find a tractable general solution for the three identical general spin problems $[A]_3^{(I_i)}$ basically on account of the existence of a Jacobean tridiagonal form. The latter arose from a set of cyclic commutator conditions imposed by the (mono-invariant space-based) Lévi–Civitá operator, typical of another 1960s work [3]. The use of more generalized permutational DR recoupling operators, structured over multi-invariant subspaces as implied above, to extend the restricted solution obtained from the conventional Lévi–Civitá operators remains to date an unproven approach, since it requires one to obtain simultaneous eigensolutions over the full set of invariant-labelled subspaces. Even the inner-product structure inherent in the full $[AX]_3$ bicluster NMR problem is likely just enough to destroy the analytic tridiagonal eigensolutions found for the simple $[A]_3$ case [12]. Whilst

[3] Largely overlooked in recent NMR work [22] unfortunately, together with the fact of the $[A]_3$ case being a specialized maximal mono-invariant form.

further more general insight into applicable mathematical reformulation of various $[A]_n$, $[AX]_n$ spin dynamical problem is required here, from a strictly NMR perspective, there are technical reasons why former mono-cluster automorphic spin symmetry systems are of little pertinence or interest. This arises because (from simple $[A]_2$ system [24]) the $[\tilde{n}]$ symmetric subspace has been long recognized as a *null space*, whilst examinations of any other subspace of such NMR dynamical problems are beyond the bounds of the technique, since no initial $\phi_q^k([\lambda \neq n])(t = 0)$ non-symmetric coherences can be generated by NMR pulse methods. The role of the $\mathcal{S}_n$ group in NMR spin problems was set out originally by Balasubramanian [8] back in 1983. The use of apparatus of group chain-irreps and their subduction reduction coefficients, including their $\mathcal{S}_n \supset \mathcal{S}_{n-1} \supset \cdots \supset \mathcal{S}_2$ stepwise subgroup chain properties as convenient ways of presenting specific component group invariants, may be traced to the extended particle physics writings of Chen *et al* [23]. However, the nature particle physics also shows a similar general avoidance of indistinguishable particle point set-based problems to that found in electronic structure areas. Hence, despite the wealth of new $\mathcal{S}_n$ algorithmic methods of symbolic and discrete mathematics [16–20], as yet they have not been assimilated into applicable mathematics for use in treating *indistinguishable point set* problems, beyond the simple Lévi–Civitá methods invoked in the earlier-cited work [12]. Because electronic structure problems retain their real spatial coordinates, and particle physics its distinct particle labelling, indistinguishable point-set problems are rare outside NMR. However one such case is known, namely that of an analogous automorphic four-body conventional spectroscopy problem; on symmetry grounds, this was held by Galbraith [13] in the 1970s to be non-analytic but no mention was made of the constraints inherent in applying graphical R–W algebras to implicit $\mathcal{S}_n$ algebras.

One further notable spin property of interest arises in (single J_{AX}-based) monocluster $[A]_n, [A]_n(X)(SU(2) \times \mathcal{S}_n)$ systems; it have been established that SU(2) NMR clusters have an innate ability to undergo *renormalization* to a subset of SU($m > 2$) problems, in accordance with the effective commutator-based intra-cluster interaction non-observability rule, known from the existing spin physics literature [25].

6. Concluding remarks

A recent assertion given by Atiyah and Sutcliffe [14] has provided impetus to the re-assessment of earlier density-matrix tensorial set formalisms [3] in the context of *indistinguishable point sets*. By pointing out that generalized-indexed forms of Lévi–Civitá (super)operator(s) (over $\mathcal{S}_n$ dual tensorial sets) are based on similar $\tilde{\mathbb{H}}_{\tilde{v}}$ invariant-labelled disjoint subspace constraints, the physics of indistinguishable point sets has been extended into the realm of $\mathcal{S}_n$-invariant theory and $\mathcal{S}_n$-combinatorics. The projective carrier space mapping methods utilized here provide an in-principle overview of the intrinsic structure of these more generalized Lévi–Civitá Liouville-operators applicable to wider indistinguishable point tensorial set problems, noting here that the presence of multi-invariant-labelled disjoint subspaces of itself may simply require one to seek simultaneous eigensolutions over all such subspaces. Much conventional physics has yet to use even the advanced intrinsic structures of Liouvillian (spin) dynamics, e.g., involving direct eigenfrequency solutions. This fact alone provides one with a further definitive reason for stressing the value of such Liouvillian algebras and mappings, as areas within which invariant (-subspace) labelling are totally explicit. The utility of carrier space mapping techniques employed here is particularly evident, e.g., in the ease with which they link Liouvillian spin-alone-spatial properties to their Hilbert analogues.

An explicit role for combinatorics, employing the elegance of (Rota) *invariant theory*, has been obtained in discussing the physics of dual tensorial sets and describing its 'quantal-basis set completeness' condition, for indistinguishable point sets characteristic of $\mathcal{S}_n$ automorphic NMR spin symmetries. Various pointers to the nature of further applicable algebras has been given, which allow for the replacement of graph-based R–W hierarchies on treating the remaining 'open problem', that of matrix representations based on *indistinguishable point sets*-defined abstract spin-alone space dual tensors. As presently constituted, the algebra of induction/subduction reduction-coefficients under $\mathcal{S}_n$ group chains of [23] does not appear directly suitable for a generalized reformulation of the outstanding open problem, which is viewed here as a form of applicable mathematics. However, DR-recoupled indistinguishable point sets clearly deserved their own form of appropriate algebra—comparable to our earlier Liouville-space study [15] of non-SR group co-operability in terms of carrier space mapping. Beyond any invariant theoretic view of quantal basis completeness, the above discourse represents some conceptual overview on how to replace R–W theory if one should wish to treat DR dual tensor problems that involve indistinguishable point sets.

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