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Indistinguishability in DR n-fold point-sets & their $\mathcal{S}_n$-invariant dual projective mappings: limitations imposed on Racah–Wigner algebras for Liouville spin dynamics of $[A]_n X$ multi-invariant NMR systems**

B. C. Sanctuary

Department of Chemistry, McGill University, 801, Sherbrooke West, Montreal, P. Que., Canada H3A 2K6
E-mail: Bryan.Sanctuary@McGill.ca

F. P. Temme*

Department of Chemistry, Queen's University, Kingston, ON, Canada K7L 3N6
E-mail: temmef@tantalus.chem.queensu.ca

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The theoretic implications of democratic recoupling (DR) over identical point sets with their related $\tilde{\mathbf{U}} \times \mathcal{P}(\mathcal{S}_n)$ group actions defining Liouvillian (super)boson projective mapping on carrier space(s) is re-examined in the context of $[A]_n X$, $[AX]_n(SU(2) \times \mathcal{S}_n)$ (model) spin systems. In such identical point set (DR) scenerio, graph theoretic recoupling with its **direct** Racah–Wigner algebra (RWA) for $n \geq 3$ is disallowed [Atiyah, Sutcliffe, 2002,Proc. R. Soc., Lond., **A458**, 1089], in favour of dual group actions (over a carrier space) and DR which yields a set of $\tilde{v}\mathcal{S}_n$ invariant-labelled disjoint carrier subspaces [Temme, 2005, Proc. R. Soc., Lond. **A461**, 341] in formalisms that define the $\{T^k_{\{\tilde{v}\}}(11..1)\}$ 'set completeness', based on group invariants and their cardinality, $|SI|^{(n)}$ as [2006, Mol. Phys., submitted MS]. Even for tensorial properties of three-fold mono-invariant spin/isospin systems, many particle indistinguishability (identicality) poses various problems for subsequent direct use of RWA. The value of Lévi-Civitá democratic (super) operator approach is that it generates auxilary cyclic commutation properties permitting realistic extended form of RWA usage. This Lévi-Civitá -based method is restricted however to three-fold identical spin problems, similar to that of Lévy-Leblond and Lévy-Nahas [1965, J. Math. Phys., **6**, 1372]; higher index $SU(2) \times \mathcal{S}_{n\geq 4}$ based problems require novel $\mathcal{S}_n$ quantum physics solutions. The purpose of this communication is to stress the need for (group) compatibility between

* Corresponding author.
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spin symmetry of the specific problem and the algebra adopted to solve it–i.e. prior to regarding any particular (group) problem as being physically non-analytic.

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1. Introduction

In addition to standard Racah–Wigner algebraic (RWA) graph-theoretic approaches to recoupled tensorial sets of spin physics [1] and Liouvillian NMR [2], which largely excludes automorphic $\mathcal{S}_n$ (FG) spin symmetries [3, 4], it is important to recognise the $\mathcal{GL}_n \supset \cdots \supset (\mathbf{U}_n) \supset \cdots \supset \mathcal{S}_n$ subductional subgroup chains and Schur duality [5] underlying tensorial set properties, as well as the extensive range of symbolic $\mathcal{S}_n$-algorithmic combinatorial techniques [6–9] that apply to dual group tensorial sets. Naturally, the full treatment of $[A]_n X$, $[AX]_n$ Liouvillian spin system as problems involvingmultiple spin identicality and its DR-related point sets draws in Weyl ideas on time-reversal invariance (TRI) in spin physics [10, 11], as well as on $D^1(\mathbf{U}) \otimes D^1(\mathbf{U}) \otimes \cdots \otimes D^1(\mathbf{U})$ -based bijection [12] for the rank multiplicities, alias the coefficients of fractional parentage (CFP) forms of graph schemata [13], to define the group invariants [scalar invariant (SI)] implicit in $\tilde{\mathbf{U}} \times \mathcal{P}(\mathcal{S}_n)$ group actions. These are important in describing $\{T^k_{\{\tilde{v}\}}(11..1)\}$ *tensorial set completeness* as part of (super)boson mapping over the invariant-labelled carrier subspaces [9] associated with Liouville spin dynamics.

In order to extend the general analytic approaches of multiple spin NMR, beyond the transformational aspects touched on in Listerud et al. [14] and the single invariant three-fold solutions given by Lévy-Leblond and Lévy-Nahas [15]–who utilised the Lévi-Civitá-defined cyclic commutator properties in their mid 1960s seminal analytic theoretical physics work-, to the general case with the implications of matching the actual solution techniques employed in obtainin solutionsneeds to nature of the (indistinguishability)problem. An appropriate approach is one that involves $\mathcal{S}_n$ techniques to accord with identical multipoint set structure, which Atiyah and Sutcliffe [16] refer to in discussing both the applicability and the specific limitations (i.e. under *particle indistinguishability*) of graph theoretic techniques. One of the alternative approaches is called for in treating multispin ensemble NMR [11–17] which draws on role of TRI in many-particle spin physics, in the context of (super) boson pattern algebra and its quasiparticle mapping formalisms [8, 9, 18]. Naturally, such (dual) group theoretic projective views stem from earlier Hilbert space presentations due to Louck and Biedenharn [8]. The purpose of this short communication is to stress the power and value of these mapping techniques as Liouvillian formalisms and their value in handling NMR related inner DR- tensorial set problems involving indistinguishability over point-sets.by invoking Various examples of physical interest are given here (drawing ondiscussions in refs. [12, 16–20] to avoid an overly abstract presentation.

2. Context: group invariants for use in subsequent mapping techiniques

Various examples of the difficulty of handling the indistinguishability aspects of many-body problems are known, including those within the orthogonal and/or graph theoretic scenerios of the early Galbraith 1971 paper [19] concerning a group-theoretic proof of *non-analytic* forms arising in the treatment of the four-body vibrational spectroscopic problem; more recently a certain inappropriateness to the use of quasi-geometric modelling for TRI-based invariant cardinalities or $|SI|^{(2n)}$ has been noted here [9, 17]. Direct use of Weyl's original specific TRI-criteria [10] yields an elegant solution to this problem [20] in terms of specific sum of particular *even* $\chi_{1^n}^{<\lambda>}$ (reduced) characters. Such direct forms as this $\mathcal{S}_n$ character analysis informs our views and served to initiate these remarks on the role of combinatorics [21–23] and TRI [24] in NMR and related forms of spin physics.

Clearly, the technique used to analyse $SU(2) \times \mathcal{S}_n(SU(m) \times \mathcal{S}_n)$ spin physics needs to reflect the permutational (phenomological) nature of such problems. For example the $|SI|^{(2n)}$ invariant cardinality here is treated as a group invariant property so that (e.g.) for ensemble NMR of $[^{19}F]_{36}[C]_{60}$ polyfluoro-fullerene [22], with its $|SI|^{(36)}$ seen as derivable [20] via TRI and (sub) group characters (chars) [5], it follows (e.g.) that for n *even* indices:

$$|SI|^{(36)} = M^{(0)}(SU(2) \times \mathcal{S}_{36}) \text{ for } M^{(0)} \text{ initial portion of multiplicity set}$$
$$.. = \chi_{1^{36}}^{<0>} + \chi_{1^{36}}^{<2>} + \chi_{1^{36}}^{<22>} + \chi_{1^{36}}^{<2^3>} + \cdots + \chi_{1^{36}}^{<2^{15}>} + \chi_{1^{36}}^{<2^{16}>} + \chi_{1^{36}}^{<2^{17}>}. \quad (1)$$

Hence on utilising the standard hooklength numerical processes of ref. [7], this expression reduces to following numerical form:

$$\begin{aligned}
&1 + 594 + 104160 + 8023575 + 322,858305 + 7,461,614160 + 104,830,165440 \\
&+926,623,783799 + 5,252,774,741490 + 19,233236,745700 + 45,320,499, \\
&677300 + 67,694,635,250400 + 62,260,952,153600 + 33,587,326,836000 \\
&+9,809,631,964800 + 1,348,824,395160 + 65,770,848990 \\
&+477,638700 = 245,613376,802185, \qquad (1b)
\end{aligned}$$

a result obtainable with equal validity from a sum over $(M^{(i)})^2(SU(2) \times \mathcal{S}_{18})$ (a Z_{22} -like) relationship; this itself is derived by bijective mapping [12] over a hierarchy of lower indexed $\{M^{(ii)}\}$ set of values. Hence it follows that:

$$|SI|^{(36)} = \sum_{i=0}^{18} (M^{(i)})^2 (SU(2) \times \mathcal{S}_{18})$$
$$.. = (1,730787)^2 + (4,805595)^2 + (6,857307)^2 + (7,596144)^2 + (5,860206)^2$$
$$+(4,276350)^2 + (2,787966)^2 + (1,626322)^2 + (847382)^2 + (392598)^2$$
$$+(160548)^2 + 57324^2 + 17595^2 + 4539^2 + 951^2 + 153^2 + 17^2 + 1, \quad (2b)$$

i.e. with an identical numerical value for full sum of squares. It is noted that the inter-related nature of $\otimes SU(2)$ schemes and $\mathcal{S}_n$ combinatorics are an important aspect of (automorphic) NMR spin symmetries. Likewise, these specific techniques [12] yield the most direct access to the $\mathcal{S}_{60}$ group invariant cardinality for ${}^{13}C_{60}$ fullerene of cageo-fullerene NMR spin systems.

Explicit representative forms of the various individual invariants $\tilde{v}$ (for modest indices) are available via the following (subgroup) subductional irrep chain hierarchies, which all terminate with the simplest invariant irrep [2]($\mathcal{S}_2$), with from particle physics symmetry:

$$\tilde{v} \equiv \left\{ [\lambda](\mathcal{S}_n) \supset [\lambda'](\mathcal{S}_{n-1}) \supset .. \supset [2](\mathcal{S}_2) \right\}, \quad (3)$$

for all group (subgroup) respectively $\lambda, \lambda', \dots \geq \lambda_{SA}, \geq \lambda'_{SA}..$ over the complete hierarchy, where the λ_{SA} (etc.) irreps are the (tableau-based) self-associate irrep(s) for a specific symmetric (sub)group. From these considerations, the invariant cardinality and the forms of these specific component subduction-chain-realised invariants [18] are now recognised as fully defined dual group properties. In passing, one notes that the multiple higher magnitude spin problems retain the $SU(2) \times \mathcal{S}_n$ over group symmetry for its invariants, whilst drawing on the various (λ) Schur function decompositional combinatorial map properties-involving Kostka coefficient set (derived from the symmetric group being a subgroup of the general linear group). The underlying tensorial structures [21] draw on the various branching rules under specific automorphic spin symmetries.

3. Liouvillian dual mapping techniques and tensorial set completeness

Many of the details of standard $\tilde{\mathbf{U}} \times \mathcal{P}(\mathcal{S}_n)$ dual group actions over $\tilde{\mathbb{H}}$ Liouvillian carrier space have been discussed in earlier work [9,20] which defined these actions as:

$$\tilde{\mathbf{U}} \times \mathcal{P}: \tilde{\mathbb{H}} \longrightarrow \tilde{\mathbb{H}} \left\{ D^k(\tilde{\mathbf{U}}) \times \tilde{\Gamma}^{[\tilde{\lambda}]}(\tilde{v})(\mathcal{P}) | \tilde{\mathbf{U}} \in SU(2); \mathcal{P} \in \mathcal{S}_n; \tilde{v}, \mathcal{S}_n \text{invariant} \right\}, \quad (4)$$

within which:

$$\tilde{\mathbb{H}} \equiv \oplus \, \tilde{\mathbb{H}}_{\tilde{v}} \quad (5)$$

defines via the specific invariants the full carrier space, as a set of *disjoint carrier subspaces* yielding the form:

$$\left\{D^k(\tilde{\mathbf{U}}) \times \tilde{\Gamma}^{[\lambda]}(\tilde{v})(\mathcal{P})\right\}, \text{ over specific labelled components of } \{\tilde{\mathbb{H}}_{\tilde{v}}\} \quad (6)$$

that in term provides an elegant criteria for dual inner DR tensorial set *completeness*. Clearly, this is comparable to basis completenessgiven in combinatorial terms, by the 1979 Biedenharn and Louck Hilbert space formalism [8]:

$$\sum_{j}^{\mathrm{Max}/j=n/2} D^j(\mathbf{U}) \times \Gamma^{[(n/2)+j,(n/2)-j]}, \quad \text{for } j \geq (1/2), 0, \quad (7)$$

but with the difference that for Hilbert formalism this does not contain any explicit invariant dependence. As explicit examples of the subductional chains representing the group invariants for $\mathcal{S}_3$ and $\mathcal{S}_4$ are:

$$[21] \supset [2]; \quad (8)$$

$$\{[31] \supset [3] \supset [2]; [31] \supset [21] \supset [2]; [2^2] \supset [21] \supset [2]\}, \quad (9)$$

whereas the sixfold elements of the $\mathcal{S}_5$ hierarchy are given by:

$$[41] \supset [4] \supset [3] \supset [2]; [41] \supset [31] \supset [3] \supset [2]; [41] \supset [31] \supset [21] \supset [2];$$
$$[32] \supset [31] \supset [3] \supset [2]; [32] \supset [31] \supset [21] \supset [2]; [32] \supset [2^2] \supset [21] \supset [2], \quad (10)$$

noting both the restriction to $\lambda \geq \lambda_{SA}$ condition mentioned above, and that the chain based on the outermost constant-of-motion clearly is omitted here. For $(2n+1)$ odd -indicies, the invariant cardinality is only obtained via bijection techniques with (e.g.) $|SI|^{(2n+1)}$ for 5 and 7 being of value 6 and 36, respectively.

One further important point in the mapping [8] and comparability of $SU(2)$versus $\mathcal{S}_n$ distinct properties deserve to be mentioned here. This concerns the Hilbert and Liouville space $(y = (i_1..i_n);\ (or\, \tilde{y} = \widetilde{(i_1..i_n)})$ Yamanouchi-labelled purely $\mathcal{S}_n$ transformations of (inner) DR tensorial sets, with:

$$P\colon |y : jm> \longrightarrow \sum_{y'} \Gamma^{[n/2+j,n/2-j]}_{y',y}(P)\ |y'\colon jm>, \quad (11)$$

from the (Hilbert) exposition in ref. [8] the contrasting Liouvillian transformational processes: and

$$\mathcal{P}\colon |\tilde{y} : (\tilde{v})kq >> \longrightarrow \sum_{\tilde{y}'} \tilde{\Gamma}^{[\tilde{\lambda}]}_{\tilde{y}'\tilde{y}}(\tilde{v})(\mathcal{P})|\tilde{y}' : (\tilde{v})kq >>, \quad (12)$$

for all $[\tilde{\lambda}] = [\lambda] \otimes [\lambda']$, which is now explicitly labelled by a specific group invariant of the full $\{\tilde{v}\}(\mathcal{S}_n)$ set.

4. Concluding comments on the spin indistinguishability RWA problem

From the discussion above, it will be clear that there is a need for the symmetry group compatibility between the inherent spin symmetry and that implicit in the methods utilised to analyse the problem. Likewise, prior to making any designation of non-analytic form to a problem involving many spin indistinguishability, it is essential to seek an approach based on symmetry compatibility. The Lévy-Leblond and Lévy-Nahas studies [15] highlight this point, since here while the direct initial simple RWA approach fails due to presence of democratic recoupling of the three-fold spin/isospin problem, a full analytic (Hilbert space) solution is possible,once the *democratic Lévi-Civitá operator* under $\mathcal{S}_3$ (with its additional cyclic commutators), is incorporated into the analysis. The corresponding four-fold spin problem remains to date an unresolved open question, noting that the corresponding orthogonal versus $\mathcal{S}_4$ symmetries has been shown by Galbraith's 1971 group theoretic proof to be non-analytic [19]. However, this is a quite separate question from unitary vs (automorphic) symmetric group compatibility underlying the corresponding four (or greater) -fold identical spin problems. It is clear however that Atiyah and Sutcliffe views [16] distinguishing simple point, from identical point-, sets–(e.g.) in inner tensorial set formation- implies that graph theoretic techniques and their associated RWA have distinct limitations for systems essentially involving democratic recoupling as a property associated with spin indistinguishability.

In earlier discussions, the problematic nature of utilising Liouville-based RWA in the presence of invariant-labelled disjoint carrier subspaces (associated with multi-invariant-based problems) has been stressed. However, it is the absence of any suitable generalised democratic operators beyond the Lévi-Civitá tri-indexed form which is just as important an inhibition to developing any further full dual symetry-adapted type of RWA, or forms of analysis based on the symmetric group to accord with the $\mathcal{S}_n$-dominant structure of dual tensorial sets,beyond the simplest $[A]_2(\mathcal{S}_2)$ case [23],with its inaccessible anti-symmetric coherence domain associated with J interaction. The general $SU(m) \times \mathcal{S}_n$ tensorial sets and their subduction to some automorphic FG draw on general properties of (λ) Schur functions [5b,6,7,21], as structure that may be decomposed onto Kostka coefficient-weighted ordered {[λ]} irrep sets.

The direct conclusions for the spin emsemble studied in Para II is that, while TRI (or T invariance as a part of wider particle symmetry studies [24, 25]) and $SU(2) \times \mathcal{S}_n$ (super) boson projective methods are invaluable in demonstrating the completeness of inner recoupled dual tensorial sets, the full formulation of spin dynamical analysis of such ensemble NMR problems is constrained by difficulties of treating democratic recoupling beyond the three-fold spin problem. Whether the incompatibility of RWA to DR multi-invariant-defined dual tensorial sets is simply an 'open question' or implies that such DR problems are inherently non-analytic–i.e., beyond ascertaining the invariant cardinality and dual tensorial basis completeness–remains until a further proof is forthcoming, equivalent to that given in ref.[19] for the orthogonal case. From the above discussion, it should be clear that graphic recoupling, or conventional RWA quantal methods based on such explicit forms of recoupling, may not be directly utilised in the presence of multispin indistinguishability point sets and DR. Hence other ($\mathcal{S}_n$ group-based) algebraic methods [20] must be sought. Unfortunately the NMR community frequently overlook [26] both the graph recoupling and the spin indistinguishability under DR. Details of earlier specific unitary group-labelled Hilbert methods for general magnitude nuclear spins may be found in the work of Siddall-III [27, 28].

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