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Communication

Time-reversal-based $SU(2) \times \mathscr{S}_n$ scalar invariants as (Lie Algebraic) group measures: a structured overview of generalised democratic-recoupled, uniform non-Abelian $[AX]_n$ NMR spin systems, as abstract $\mathscr{S}_n \supset \mathscr{S}_{n-1}../U_n \supset U_{n-1}..$ chain networks

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Abstract

The physics of dual group scalar invariants (SIs) as (Lie algebraic) group measures (L-GMs) and its significance to *non-Abelian* NMR spin systems motivates this overview of uniform general-2n $[AX]_{2n}$ spin evolution, which represents an *extensive addendum* to Corio's earlier (essentially restricted) view of Abelian spin system SU(2)-based SI-cardinalities. The $|D^0(\mathbf{U})|((\otimes SU(2))^{(2n)})|SI|$ values in [J. Magn. Reson., 134 (1998) 131] arise from strictly linear recoupled time-reversal invariance (TRI) models. In contrast, here we discuss the physical significance of an *alternative polyhedral combinatorics approach* to democratic recoupling (DR), a property inherent in both the TRI and statistical sampling. Recognition of spin ensemble SIs as being L-GMs over *isomorphic algebras* is invaluable in many DR-based NMR problems. Various $[AX]_n$ model spin systems, including the $[AX]_3$ *bis odd-odd parity* spin system, are examined as direct applications of these L-GM- and combinatorial-based SI ideas. Hence in place of $|SI| = 15$ (implied by Corio's $|D^0|((\otimes SU(2))^{2n})$ approach), the *bis* 3-fold spin system cardinality is seen now as constrained to a *single invariant on an isomorphic product* algebra under L-GMs, in accord with the subspectral analysis of Jones et al. [Canad. J. Chem., 43 (1965) 683]. The group projective ideas cited here for DR (as cf. to graph theoretic views) apply to *highly degenerate non-Abelian* problems. Over dual tensorial bases, they define models of spin dynamical evolution whose (SR) quasiparticle superboson carrier (sub)spaces are characterised by SIs acting as explicit auxiliary labels [Physica, A198 (1993) 245; J. Math. Chem., 31 (2002) 281]. A deeper $\mathscr{S}_{2n}$ network-based view of spin-alone space developed in Balasubramanian's work [J. Chem. Phys., 78 (1983) 6358] is especially important, (e.g.) in the study of spin waves [J. Math. Chem., 31 (2002) 363]. Beyond the specific NMR SIs derived here, there are DR applications where a sporadic, still higher, 2n-fold regular uniform spin ensemble exhibits a topological FG duality to some known modest $|SI|^{(2i<2n)}$ cardinality—in principle providing for the (sparce) existence of other $|SI|^{(2n)}$ DR-based values.

Keywords: Dual group non-Abelian NMR invariants; Democratic recoupling; Post-Weyl time-reversal invariance; S_n chains as invariants; Lattice point/polyhedral combinatorics in NMR invariant cardinality

1. Introduction

The subspectral analytic properties of isochronous multiple spin systems, AA′XX′, (AA′A″), AA′A″XX′X″, (e.g.), represents a longstanding classic area of NMR endeavour [1–3]. Certain theoretical physics concepts, including (e.g.) democratic recoupling [3] and aspects of group invariants [4] exert a significant impact on our recent understanding of the corresponding intra cluster-J dominated $[A]_n, [AX]_n$ spin systems, though to date the dependance of *uniform* multispin system NMR properties on such considerations has not been as widely recognised by the NMR community as it deserves. With the extensive recent development of cluster-based nanoscience, it is timely to re-examine the impact of theoretical physics concepts on a range of $[AX]_n$ type (automorphic) NMR spin systems [5–7], whether under

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even ($2n$), or odd ($2n+1$) indices. Naturally such studies are equally important in the realm of uniform sub-rank (dual) tensorial sets, and their completeness [8,9] as (e.g.) operatorbases of the Liouville equation. To appreciate in a systematic way the origin of the properties exhibited by these uniform sub-rank spin systems, one needs to consider their scalar invariants [1,4], parity [2], dual projective [5–11] and/or recoupling [10,12] properties. The nature of many-body interactions [3,8,13] implicit in democratic recoupling makes a significant impact on our specific understanding of both NMR evolution and relaxation processes [12,14,15] once *uniform* sub-rank multispin cluster systems are considered. For reasons based on their specific inherent quantum physics interest (and their previous neglect by the NMR community), we focus on *uniform multispin systems* described in terms of (multipole) tensorial formalisms [12]. The latter involve the use of (operator)bases involving uniform subrank-based auxiliary labels [9,12,14]. To illustrate the general NMR significance of the work reported here and to describe the various formalisms involved, brief informative overviews of various pertinent NMR subtopics are given in the initial paragraphs. Naturally these include the following topics: the role of time-reversal invariance in group invariants [4], the nature of both democratic recoupling and tensorial properties in NMR, and (as a comment in Section 2) several ideas associated with quasiparticle carrier space [9] properties of Liouville space; essentially in the context of democratic recoupling [3]. A brief introduction to multipole density-operator methods [10–12] in various post-1976 formalisms pertinent to NMR spin dynamics is included in Section 3 for completeness. Compared to shiftbase or product base approaches, formalisms utilising tensorial basis sets [10–12,15] allow strong physical interpretations to be associated with both (dual) mapping actions. They allow important roles for tensorial rank/auxiliary labelling involving invariants. These are all too frequently absent from discussions which draw on other NMR formalisms.

The primary motivation for the present study is to gain insight into the structure of *uniform non-Abelian* NMR multispin systems and their augmented $[AX]_{2n}$ bicluster forms. For reasons of tensorial completeness, this is considered in terms of their group invariants and $|SI|^{(2n)}$ cardinalities (or else via their external augmented $|SI|^{(2n:\otimes)}$ values), where the former are typical group measures of Lie algebra. These invariants, as analogues of graph-invariants [10c] of Abelian symmetries, form an important part of the structure of dual tensors and their completeness, a topic touched on given in Sections 2 and 3. Subsequently, Sections 4 and 5 introduce several distinct aspects of post-Weyl TRI-based $|SI|^{(2n)}$ modelling. Subsequently, Section 6 focuses on the dual projective properties. After initially considering the nature of invariance sets in state and Liouville spaces, the SIs as group measures are discussed in the context of dual quasiparticle mapping. To retain some brevity in the subsequent Secs., we set out here the full range of nmemonics utilised in the text, namely: DR, TRI, and SIs are utilised, respectively, for *democratic recoupling*, *time-reversal invariance*, and *scalar invariants*; likewise, the mnemonics FG, SR, and SA are used to denote *finite groups*, and the algebraic properties, *simply-reducibility and self-associacy*—in a tableaux sense. For *dual tensorial sets and Lie algebraic group measures*, we introduce the terms DTS and L-GM. In addition, we utilise tilded symbols for Liouvillian analogues of Hilbert space properties. Finally, the $\tilde{\chi}_{1^n}^{[\lambda]}\mathscr{S}_n$ characters (or 'chars' in mathematics texts) in Eqs. (10)–(14) will be slightly abbreviated for typographic convenience. This is possible here without introducing any ambiguity in the notation for the Eqs., since we merely omit the 1^n subscript labels from expressions involving $\chi_{1^n}^{[\lambda]}$ characters, or 'char' symbols.

2. Initial context

In an otherwise informative discourse [1] on the properties of various multiple spin systems, Corio appears to overlook the existence of more general *uniform* spin systems, as well as the *inherent limitations* present in $2n \geqslant 8$-fold *purely linear-recoupling* aspects of Weyl's original treatment [4] of time-reversal invariance (TRI) present in certain Abelian spin systems. The use of projective dual group properties (cf. [1]) has the advantage of being equally pertinent to Abelian spin problems and to non-Abelian $[A]_{2n}$ *uniform* multiple spin systems, i.e., for $2n \geqslant 8, 10$. It also avoids the restrictive recoupling conditions inherent in [1]. Accordingly, this allows for the use of more general treatments of uniform $[AX]_{2n}$ systems, such as those examined in this report. Whilst considering the structure imparted to the $\underline{\underline{\mathscr{H}}}$ Hamiltonian representation by zeroth-order scalar coupling, the 1998 work of Corio [1] gives no recognition to the theoretical significance [5] of extended $(\mathbf{I}\cdot\mathbf{I})$ scalar spin interactions as analogues of S_n-defined group actions over permutational networks [6]. The earlier Corio orthogonal group approach to the structure [7] of $\underline{\underline{\mathscr{H}}}$, is presented in analytic *spectral invariants* (1960s) terms. However, the idea of group actions and $\mathscr{S}_n$ networks allows one a deeper insight into the special (abstract) nature of automorphic NMR spin symmetry [5–7] arising from *dominant intra*-cluster couplings—cf. to that of analogous isochronous multispin system. The quantal physics of the former also necessitate some discussion of their relationship to boson (superboson) quasiparticle dual group mapping [8,9]. On utilising the Liouville operator $\hat{\hat{\mathscr{L}}} \equiv [\hat{\mathbf{H}},]_-$ (specifically over $\{|kqv\rangle\rangle\} \equiv \{T^{kq}(v)\}$ integer rank tensorial operator bases [10–12]) to describe evolution processes, certain important quantum physics questions arise. These are a specific consequence of the central role played by system scalar invariants (SIs) in dual projective mapping. An earlier (1993) work of ours [9] shows precisely how such dual projective mappings over a carrier space arise in the general context of superboson quasiparticle (QP) algebra. This more recent formalism (see Eq. (2) below) derives naturally from *simple reducibility* (SR) considerations, and is itself a (Liouvillian dual group) augmentation [9] of earlier Hilbert space ideas, originally due to Biedenharn and Louck [8].

For general, higher-indexed *uniform* NMR systems, the role of these group invariants is clearly defined by various $SU(2) \times \mathscr{S}_n$ dual group actions over an abstract spin space, with $[A]_n$ ensemble dual projections being discussed conveniently in the terms of *quasiparticle superbosons* acting over (quantal) carrier spaces [8,9], or alternatively in conventional terms, either as of $D^k(\tilde{\mathbf{U}})$ $SO(3)$ representations, or else via dual group as $\tilde{X}_{c:i}$ class (finite group (FG)) actions pertinent to invariance over Liouville space. In terms of (simple) SO(3) representations, these Liouvillian properties are defined by:

$$D^k(\tilde{\mathbf{U}}) \equiv D^j(\mathbf{U})|kqv\rangle\rangle D^{j\,\dagger}(\mathbf{U}), \tag{1a}$$

where the k label here defines the integer rank(s) of Liouville space $T^{kq}(v)$ tensors—in contrast to the half-integer increment-based js of Hilbert space. The auxiliary label(s) here, $v = (k_1..k_n)\{..\}$, span a full set of uniform sub-rank k_is and other related (recoupling) labels. Naturally under the $SU(2) \times \mathscr{S}_n \downarrow \mathscr{G}$ dual group(s), the FG projection properties of Liouville space involve the class (augmented) invariance properties $\tilde{\chi}_{c:i}(= tr\tilde{X}_{c:i})$ realised over $\{i = E, ., ., (C_2)\}(\mathscr{S}_n \downarrow \mathscr{G})$, set of an earlier joint work [11] via the analogous FG expression:

$$\tilde{X}_{c:i} \equiv X_{c:i}|kqv\rangle\rangle X^{\dagger}_{c:i}, \tag{1b}$$

for (respectively) $\tilde{X}_{c:i}, X_{c:i}$ as ith FG class operators of Liouville (or state) space algebras, on the basis of inherent (dual group) tensorial properties. Naturally over the augmented space, the corresponding $\tilde{\mathscr{P}}_{\tilde{\mu}}$ projections [11,12] draw on standard methods of traditional finite group theory, so that the Liouvillian representation(s) (irrep(s)) simply become: $\tilde{\Gamma}(\mathscr{S}_n \downarrow \mathscr{G}) = \sum_{\tilde{\mu}} \tilde{\mathscr{P}}_{\tilde{\mu}}(\mathscr{S}_n \downarrow \mathscr{G})$. The use of density operator methods in NMR, NQR, and related techniques has had a long history, dating from the 1950s. In the form of Liouville (super)operators acting over an appropriate $\{.\}$-defined $\{|kqv\rangle\rangle\} = \{T^{kq}_{\{.\}}(v = (k_1..k_n))\}$ tensorial sets of NMR operator bases, these methods has been known since the mid 1970s. Detailed overviews of these NMR (NQR) multipole formalisms and their applications may be found in [10–12]. Specific details of the formalism and its phase properties vary somewhat according to one's choice of tensorial bases for the density operator [10,12], as well as on the possible inclusion, as here, of dual (automorphic) spin symmetry [5,6,9–11]. The *uniform* sub-rank bases of more general $[A]_{2n>4}$ uniform spin ensembles require one to draw on some additional (including democratic recoupling) concepts in order to treat such systems in terms of suitable density operator formalisms. Central to any discussion of democratic recoupled (DR), uniform sub-rank multispin systems is the specialised nature of group invariants, and their use in place of either the existing graph invariants [10c] or $\{\tilde{K}_{ij}, ..\}$ (Jucys) labels within v. Applications in NMR of earlier aspects of recoupling have been extensively treated in (e.g.) the Sanctuary and Halstead review [12]. Irrespective of whether one is considering uniform $\{T^{jm}(j_1..j_n)\}$ state space, or (as here) $\{T^{kq}(k_1..k_n)\}$ Liouvillian bases, the group invariants constitute essential properties of these non-Abelian spin systems. They clearly complement the role of contrasting graph schematics in analytic spin dynamics involving Abelian systems.

It is important to note here that neither graph schematics or group invariants (alias SI-cardinalities) of the contrasting recoupling schemes are subject to any sort of augmentation on simply mapping analogous systems from Hilbert space onto Liouville space. In this respect recoupling and DR-based properties are distinct from the invariance properties discussed in Section 6.1 below. This much is clear from earlier work [12], in which only the $j_1, .., \{K_{ij}\}; k_1, .., \{\tilde{K}_{ij}\}$ formal labels change on mapping from state to Liouville space. Indeed, this lack of (internal) spin-spatial-based augmentation contrasts strongly with the changes to the basis dimensionality and to the various $\{\chi_{c:i}(\mathscr{S}_n \downarrow \mathscr{G})\}, (\{\tilde{\chi}\})$ invariance properties over automorphic group algebras implicit in Eq. (1b). Amongst the most important properties attributed to uniform k_i Liouville spaces, which is central to any discussion of DR, is that of mathematical *simple reducibility* (SR) over a superboson carrier space. It is essential to the *completeness* of all dual algebras. Realising this SR property in any specific case naturally requires some detailed knowledge of the dual group invariants, which define the underlying DR-based uniform multispin system. The dual group-based SI-cardinality contributes to a precise definition of the corresponding dual tensorial sets (DTS) and their completeness, as defined below in terms of group actions. The SIs as v auxiliaries demonstrate this requisite property via:

$$\{D^k(\tilde{\mathbf{U}}) \times \tilde{\Gamma}^{[\tilde{\lambda}]}(\mathscr{P})(v)|\tilde{\mathbf{U}} \in SU(2); v, \mathscr{P} \in \mathscr{S}_n\}, \tag{2a}$$

both of which derive from quasiparticle superboson mapping [9] over distinct $\tilde{\mathbb{H}}_v$ carrier subspaces. This view of the SR structure of DTS is based on acknowledging the explicit role of the group invariant auxiliary label v, as a part of $\tilde{\mathbf{U}} \times \mathscr{P}$ dual actions over a carrier space. These group actions are expressed by the formal mapping:

$$\tilde{\mathbf{U}} \times \mathscr{P} : \tilde{\mathbb{H}} \to \tilde{\mathbb{H}}, \quad \text{for } \tilde{\mathbb{H}} \equiv \sum_v \tilde{\mathbb{H}}_v, \tag{2b}$$

which, as part of a mathematical formalism [9], usually precedes the $\{..|..\}$ set expression of Eq. (2a). Clearly, the difference between Liouville and state space dual mapping actions arises from v invariant being an *explicit* map parameter only in the former case, as set out in Eq. (2a). In a distinct contrast to simple $|jm\alpha> \rightarrow |kqv\rangle\rangle$ interspatial mappings, any consideration of uniform multispin $[A]_n$, mono- to bipartite $[AX]_n$ system maps draws on the Lie algebraic aspects of group invariants over isomorphic product algebras. Since the form of these maps define the properties of bipartite clusters representing the $[AX]_n$ enhanced uniform NMR spin ensembles, they constitute a strong motivation for this analytic work on SIs. Hence, it is important to recognise now that these SIs or group invariants are actually group measures in a Lie-algebraic sense.

The central defining role played by forms of DR recoupling in many-body theory of mathematical physics [3,13] underlies much of the $\mathscr{S}_n$ (topological-based) modelling employed in this work. From the above comments, the reader will appreciate that some understanding of quasiparticle quantum formalisms (treated within the physics of many-body problems [3,13]) is central to any cogent study of DR within *uniform* multiple spin systems. An excellent recent overview (with wide literature citation) of many-body interactions by Atiyah & Sutcliffe [13] is especially helpful in placing the topic in a wider context. In addition to its survey of the field, it points out the specific algebraic contrasts between Abelian and non-Abelian systems, distinctions which also apply to the analogous automorphic NMR spin symmetries [5] discussed here. Clearly, the structure of $\underline{\underline{\mathscr{H}}}$ for uniform multiple spin NMR (and hence its related $\langle\langle kqv|\hat{\mathscr{L}}|k'q'v'\rangle\rangle \equiv \langle\langle..|[\hat{\mathbf{H}},|..\rangle\rangle]_-$ (evolutionary) matrix representation) is characterised generally by high levels of degeneracy. For higher uniform higher $(2n)$ systems, the use of either linear recoupling-based $\otimes SU(2)$-based Weyl–Corio techniques [1,4], or alternative forms of graphical recoupling or graph invariants, are seen as *totally inappropriate*. In principle, all graphical, $\otimes SU(2)$-based approaches are strictly limited to Abelian non-degenerate spin systems—a point all too frequently overlooked in the literature [1,14]. Hence the pertinence of our use of the full dual projective group-theoretic approach here in treating DR-based automorphic non-Abelian (*uniform* subrank k_i) multispin ensemble NMR problems and their associated properties.

In our subsequent discussion of recoupling applied to time-reversal phenomena, we also note the existence of distinct limitations to the use of Weyl's linear-chain recoupling view of TRI invariance (e.g.) over $(\mathbf{I}\cdot\mathbf{I})_{i'}(\mathbf{I}\cdot\mathbf{I})_{j'}(\mathbf{I}\cdot\mathbf{I})_{k'}..$ bracket structure, when they are applied for example to (uniform) higher $(2n)$-indexed ensemble problems. In Weyl's original TRI concept [4], only the *single* $(\mathbf{I}\cdot\mathbf{I})_{i'}(\mathbf{I}\cdot\mathbf{I})_{j'}$, or similar $i'k'$, $j'k'$, -pairwise operator-bracket permutations contribute to the time-reversal properties. In contrast, *none* of the various possible higher $((..)(..))_{i'}$ vs $((..)(..))_{j'}$ *block* permutations formally contribute to Weyl's formulation of TRI. In the present DR treatment, this Weyl criterion is explicitly retained, so as to exclude higher bracketted exchange terms. In the detailed presentation (Section 3. below), this leads to the inclusion of certain sub-algebraic-based (quadra (or higher)partite-based) terms, whose essential purpose is to ensure the *exclusion of all such higher-block* permutational contributions.

There is also an urgent need to recognise the value of various general $\mathscr{S}_n$ approaches to the role of DR in spin physics. In subsequent Secs. various algorithmic and symbolic computational views are applied to the treatment of *uniform* multiple spins (sub)sets of non-Abelian $[A]_n$, or $[AX]_n$ NMR systems. Prior to examining the specific focus of the work, a novel (Laudau-like) approach to the SI cardinality of rather general *uniform sub-rank* NMR spin systems, it is first necessary to outline a few aspects of NMR formalisms, in order to stress the practical motivation for the study. The central conceptual idea, the inclusion of DR into theory of group invariants, necessarily draws on the roles of dual group mapping and of polyhedral combinatorics (as a lattice point set-based technique) in defining the sets of SIs. The latter are simply one further aspect of dual projective formalisms. Prior to examining these questions, a clear understanding of the general nature of DR-based TRI contributions arising from the various indexed $(\mathbf{I}\cdot\mathbf{I})$ operator pairs [4] is needed.

3. Multipole density operator Liouville formalisms

The use of a normalised density-operator (NMR) technique over tensorial operatorbasis sets, with its retention of the property of rotational invariance, is a well-established approach to NMR [8,10–12]. Here the $\rho(t)$ is expanded via (in general) $\sum_i \phi_i(t)T^{(i)}$, or else in terms of $\sum_{kqv}\phi_q^k(v)(t)T^{kq}(v)$ multipole sum with ϕ_q^k as coefficients. Subsequently, this formalism is applied to spin evolution (development) under various specific conditions, or to relaxation via the Liouville (differential) Eq., with:

$$i\hbar\dot{\rho}(t) \equiv \hat{\hat{\mathscr{L}}}\rho - i\hat{\hat{\mathscr{R}}}\rho, \tag{3}$$

where the v, α labels associated with Liouville and Hilbert space bases (referred to above) are analogous auxiliary forms spanning the remaining labels and invariants. Thus, the uniform three spin ensemble bases (e.g.) are, respectively:

$$T^{jm}(\alpha) \equiv |jm\alpha\rangle \equiv |jm\overbrace{\{\mathbf{K}_{ij}\},\overline{v}=(j_1j_2j_3)}\rangle, \tag{4a}$$

for a state space tensor, and

$$T^{kq}(v) \equiv |kqv\rangle\rangle \equiv |kq\overbrace{\{\tilde{\mathbf{K}}_{ij}\}, \tilde{\tilde{v}} = (k_1k_2k_3)}\rangle\rangle, \tag{4b}$$

for the Liouville space analogue, as described below. Here the $\hat{\hat{\mathscr{L}}}, \hat{\hat{\mathscr{R}}}$ terms in Eq. (3) are, respectively, the Liouville and relaxation superoperators [12]. The auxiliary braced segments (commonly labelled α, v) of Eq. (4) contain (respectively) the recoupling and system scalar invariant terms appropriate to each type of basis and the $\overline{v}, \tilde{\overline{v}}$ specific invariants—only for this single specific case are the actual embracketted j_i, k_i sets (used elsewhere for the field of sub-ranks) notationally identical to the actual invariants. The nature of the recoupling schemes, as graph or system invariants, are common (except for the specific rank notation) to both state and Liouville spaces and *are not themselves subject to* ($\otimes$ *product*) *augmentation*, on introducing mappings from state space to the related $\{|kqv\rangle\rangle\}$ space. In addition, a close correspondence exists between established quantum mechanics and the more recent differential Eq. approach of Eqs. (3–7) to NMR, NQR (or NAR) spin problems. A number of aspects of spin dynamics in terms of differential eqs. (in a rotating frame) have been discussed elsewhere [10–12]. A more restricted Liouvillian in which relaxation processes are ignored is frequently adopted, so that the Schrodinger viewpoint then yields:

$$i\hbar\underline{\dot{\hat{\phi}}}(t) = \underline{\underline{\hat{\hat{\mathscr{L}}}}}\ \underline{\phi}(0), \tag{5}$$

with $\hat{\hat{\mathscr{L}}}$ being either time-dependent or, as in certain evolution processes, time-independent. In either case, $\hat{\hat{\mathscr{L}}} = [\hat{\mathbf{H}},]_-$ acts over the full $\{|kqv\rangle\rangle\}$ basis set. The corresponding $\phi^k_q(v)(t)$ polarisations are simply the (Liouvillian) *expectation values* of analogous tensorial components of the operator basis:

$$\langle\langle T^{kq\dagger}(v)\rangle\rangle \equiv tr\{\rho(t)T^k_q(v)\} \equiv tr\{T^{kq}(v)^\dagger\rho(t)\}, \tag{6}$$

where for example the $\phi^0(11), \phi^1_1(11)$ polarisations of the tractable AX, and $[A]_2$ problems correspond respectively to the dot and cross-product terms. Explicit Hilbert space matrix representations of the (simpler) $T^{kq}(v)$s themselves may be readily evaluated, as in Eqs. (32)–(34) of [11a]. The latter gives a detailed discussion of evolution for the various polarisations inherent in the $[A]_2$ spin system. For such time-independent $\hat{\hat{\mathscr{L}}}$ problems, formal linear algebraic solutions exist such as the alternative general form:

$$\underline{\hat{\phi}}(t) = \exp(-\mathrm{i}\hat{\hat{\mathscr{L}}}/\hbar)\underline{\phi}(0), \tag{7a}$$

where the vector of polarisations are taken over rank k, component q and suitable auxiliary v labellings. For $\hat{\hat{\mathscr{L}}}$ time-independent case, diagonalisation over the associated augmented spin space operatorbasis set yields interesting quantal physics. This may be seen most generally in terms of the λ_k eigenvalues and $\mathscr{T}_{\{..\}}$ row (column) transformational eigenvectors, which are generated in the course of numerical diagonalisation. It follows that a physical formal solution [12] exists in terms of $\hat{\phi}_l(v)(t), \phi_k(v)(0)$ (part of LH/RH $\underline{\phi}$ pair of vectors) within the linear algebraic expression:

$$\phi_l(t) \equiv \sum_{jk} \mathscr{T}_{lk} \exp(\mathrm{i}\lambda_k t/\hbar)\mathscr{T}^{-1}_{kj}\phi_j(0). \tag{7b}$$

One further theoretic comment on the wider structure of Eq. (3) is called for here, as it highlights the general importance of the role played by SIs, group invariants and auxiliary terms within Liouville density operator formalism. On adopting various reasonable assumptions made in the work of Happer [14] or others [15], cited by Sanctuary and Halstead [12], it follows then that relaxation in these formalisms are governed by various distinct $\overline{T}_{\{k..\}}$ relaxation times, which themselves arise from a block-diagonal structural form, e.g. as in:

$$(1/\overline{T}_{\{..\}})(vv')\ \delta_{kk'}\delta_{qq'}, \text{ with argument } \{..\} = kq, \text{ or } k. \tag{8}$$

In addition under the extreme narrowing condition, the $\mathscr{R}$ matrix reduces to a scalar quantity. From the discussions in [12,14], it is noted especially that *each rank and auxiliary-labelled* $(1/\overline{T}_{\{k.\}})(vv')$ process is completely distinct from any other rank/invariant-based generalised relaxation time. Similar $\{vv'\}$ auxiliary based block-diagonal structures exist in a number of other NMR, NQR contexts. Some further mention is given in the appendix of precisely how the $\{\hat{\phi}^k_q(v)\}$s behave, so as to furnish a tractable analytic view of NMR cluster spin dynamics.

4. Post-Weyl DR views of uniform spin ensemble TRI and SIs of non-Abelian spin symmetries

The overall structure of DR uniform non-Abelian multispin evolution (as a Liouville space spin dynamical process), and its associated dual projective features, lie well beyond those discussed (e.g.) in [10–12]. Apart from their convenience in analytic work, tensorial Liouville (rather than Hilbert, or non-tensorial product) space is retained here for another reason. System invariants and their properties derived via $\{|kqv\rangle\rangle\}$ formalisms also serve to *define the precise nature* of the dual carrier (sub)spaces [9] implicit in quasiparticle mapping over tensorial bases. Thus some of our initial concern will be with the quantum physics of superbosons with its explicit invariant-labelled carrier space—cf. to that of Hilbert quasiparticle dual maps over their simple $\mathbb{H}$ boson carrier space. With their explicit use of (dual) group invariants in retaining the simple reducibility (SR) [9] of (Liouvillian) $SU(2) \times \mathscr{S}_n$ dual carrier spaces ($\tilde{\mathbb{H}}$) for uniform $[A]_n$ spin systems, these mappings plays a vital role in Liouville descriptions, cf. [12–15], which is quite specific to scalar evolution and certain simple relaxation processes. Clearly the dual tensorial, invariant-related $\overline{v}$ auxiliary labels of $\tilde{\mathbb{H}} \equiv \sum_{\overline{v}} \tilde{\mathbb{H}}_{\overline{v}}$ Liouvillian carrier subspaces arise from a set of specific dual group invariants and their (independent) $|SI|^{(..)}$ cardinalities. In contrast to various typical EPR (paradox), or other ambiguities associated with simple Hilbert space (e.g., with respect to distinctions between their local vs global properties) which arise as a result of neglect in its quantal structures of the role of system invariants (and frequently even the presence of recoupling within $\{|jm..\rangle\langle jm..|\}$ (product) basis sets), we stress here in passing that the corresponding label-rich, dual group-based, Liouvillian augmented abstract spin space is essentially free from the majority of these difficulties. This is a direct consequence of the v-defined SR approach that we advocated a decade ago now [9]. From the outset, the dual group superboson mapping considerations (and its associated labels for the system invariants) are incorporated into the spin-alone quantal physics. Naturally, consideration of the role of SIs follows immediately, as being central (i.e., in the sense of being *both necessary and sufficient*) so as to define the structure of the *carrier space* and also the *completeness of its associated algebra*. Various novel concepts arise from detailed examinations of the nature of DR recoupling in quantum physics. Of these, the use of topological modelling over lattice point sets is especially helpful in describing non-Abelian automorphic NMR spin symmetries. Indeed, the techniques adopted will be seen here (i.e., in Section 5) as a rather convenient approach to the inclusion of lattice point sets and other elements of (polyhedral) topology into $\mathscr{S}_n$ combinatorics applied to NMR. Our main focus in this research is on applying the dual group-based concepts, inherent in DR, to general ($2n$)-indexed uniform spin systems and their NMR spin dynamics. In this regard, the ideas presented here augment Corio's strictly Abelian $\otimes SU(2)$ (1998) approach [1]. The latter restricted SU(2) view (cf. DR views) allows realisation of the SI cardinality of $(2n+1)$, odd spin systems directly from the $|SI|^{2n}$ of the preceding ($2n$)-indexed (linear recoupled) case. However, the more generalised ($(2n+1) > 7$), non-Abelian *uniform* $[A]_{2n+1}$, $[AX]_{2n+1}$ DR-modelled systems differ strongly in this regard. Accordingly, these more general SI models may not be used to characterise the subsequent $|SI|^{(2n+1)}$s for odd DR uniform spin systems. Indeed on account of certain topological geometric constraints and the lack of any sequence of regular odd-indexed lattice point sets in topology, how to treat $(2n+1) \geqslant 11$-fold uniform spin ensembles under DR remains essentially an open question.

Before considering the general-($2n$) physics of $[AX]_{2n}$ spin systems and their (dual group) scalar invariant cardinality, $|SI|^{(2n)}$, we first draw attention to the existence of a contrasting, limited-analytic approach, which exists quite aside from the initial $\otimes SU(2)$ linear recoupling-based views, due to Corio [1]. It focuses on the linear recoupled $(\mathbf{I}\cdot\mathbf{I})$ operator pairs of Weyl TRI formalisms [1,4] to yield a rth-fold bipartitite combinatorical (functional) view [16] in the form:

$$|SI|^{(2n)} = \{((2r)!)/(2!..2!2!)\}/r!, \text{with the inclusion of r-fold 2! entries.} \tag{9}$$

In physics applications, one clearly sets $n = r$ and observes that the highest possible (linear recoupled) analytic example is then $(2n) = 6$, with the $|SI|$s restricted to the following two cases: $|SI|^{(4)} = (4!/2!2!)/2!$ and $|SI|^{(6)} = (6!/(2!2!2!))/3!$, or 15. Thereafter, the inherent linearity-over-pairs condition implicit in Eq. (9) inhibits further application of this formalism to *uniform* multispin NMR systems, or analogous dual tensorial sets. This occurs because, once there are more than 3 Weyl bracket pairs [1,4], the various (internally permuting) (spin operator)-pairs of the TRI model can no longer exhibit pair indistinguishability, except for single pair exchange.

In the context of $\mathscr{S}_n$ representations [17] and group chain determinacy, two further points arise which are of particular note. These naturally concern the distinction, between the $(\otimes SU(2))^{2n}$ approach to SIs under TRIs for spin systems under a single (Abelian) group, and the wider uniform sub-rank dual group views. The insightful reader will notice that the main specific consequence of replacing Weyl linear recoupling (or sampling) by DR modelling is that the latter then allows for the use of quite general polyhedral combinatorial techniques. These clearly include the concept of FG projective actions over lattice point sets. In the context of regular solid geometries, this powerful idea accords well with both DR and the *uniform* nature of non-Abelian spin ensembles in terms of their k_i sub-ranks. The specific nature of such mapping onto lattice point sets of regular topological polyhedra is treated in Section 5 below. Whilst the methods of *induced symmetry* (as they apply to group representations) are well established [17–20], the recent work of Bowden [19] is interesting for its use of further induced symmetry techniques to demonstrate the nature of certain simple unitary transformations. Although restricted to date to (at most) the *Abelian* C_6 *cyclic* group, this work certainly deserves wider recognition. It represents a useful contribution towards resolving a fundamental question in applying group theory to physics, namely how best to derive various group-based analytic transformations. As yet, the methods reported in [19] may *not be applied* to transformations involving non-Abelian (automorphic spin) symmetries, or to spin systems governed by *multiple invariants*. From the established mathematical physics literature [3], the derivation of analytic transformational forms for these cases will recognised as largely an *open* *question*, a condition essentially caused by the presence of multiple invariants. Indeed, the progress reported to date in the treatment of multiple invariant-based systems and their $|SI|^{(2n)}$ descriptions, is possible only because a range of combinatorial, projective mapping and group measure-based techniques have been utilised—as indicated (e.g.) in Section 5. To fully appreciate the specific nature of SI concepts—i.e., initially as applied to the NMR spin physics of $AA'XX' \equiv [AX]_2$, $AA'MM'XX' \equiv [AMX]_2$ and then, beyond Corio's work [1], $AA'A''XX'X'' \equiv [AX]_3$—one needs to demonstrate first that one further significant group concept applies to DR-based SIs, namely that they constitute valid *group measures*. It is this Lie algebraic property which allows the interrelated SIs (of Section 6.1) to have an equal validity over isomorphic algebras [20], or direct product algebras. The ability to extend mono-cluster SIs into the realms of $|SI|^{(2n)}(\otimes)$ augmented SI calculations, which involve practical non-Abelian NMR bicluster problems is an important conceptual result. It arises exclusively from the concept of SIs (or group invariants) being (Lie) group measures. The importance of this group property is demonstated by its further direct application to (e.g.) the six spin $[AX]_3$ system, where the concept is essential for the retention of analytic forms. These define the subsystem's state-space spectral invariants of this *odd-odd parity* system, in accord with the work of Jones et al. [2]. Despite the importance of Lie group measures, one finds no mention of them either in [1], or in earlier NMR reviews [5–7,12].

For completeness in regard to the DR aspects of this work, the reader's attention is drawn to the value of other methods based on lattice point sets [21] (e.g.) from our earlier discussion of the *mathematical determinacy of* $\mathscr{S}_n \downarrow \mathscr{G}$ *group embeddings* in NMR spin symmetry. Interest in these properties arose initially from our concern with Cayley's theorem and the latter's relationship to Voronoi duals [22]. Full mathematical determinacy clearly implies that the *complete set of all possible* $\mathscr{S}_n \downarrow \mathscr{G}$ group embeddings [23] correspond to unique 1:1 correlations, i.e. bijective mappings. Hence, the mathematical determinacy of FG (multipartite) embeddings involving the $SU(m) \times \mathscr{S}_n$ group irreps lies well beyond the remit of standard $SU(2) \times \mathscr{S}_n \downarrow \mathscr{G}$ Cayley group-embedding criteria. To date, the nature of these additional multipartite-based embeddings may be approached only by demonstating that the individual correlative maps, within the full set of pre-self associate (SA) bijective mappings, are distinct [24] and encompass all levels of multipartite subduction processes allowed by the specific $SU(2I+1) \times \mathscr{S}_n(\downarrow \mathscr{G})$ group. Some further appreciation of the nature of $\mathscr{S}_n$ combinatorial algorithms [25] and their decompositional processes is invaluable, in order to understand both induced symmetry [17–20] and certain concepts associated with automorphic groups of NMR.

5. Group theoretic views of DR-based TRI in terms of Lattice point sets and $\mathscr{S}_n$ polyhedral combinatorics

For the present topological-based purposes (referred to herein as polyhedral combinatorics [26]), it suffices to draw on standard $\mathscr{S}_n$ theoretic views [27] of the independence of variables within polynomial expressions. As an approach to physical modelling of uniform spin problems, it naturally incorporates both democratic sampling and DR recoupling into the structure of the augmented TRI viewpoint. This is studied here purely for its contribution to $|SI|^{(2n)}$ cardinality. For initial convenience, we follow Weyl [4] in restricting consideration (at least initially) to even-indexed ensemble problems. Any polyhedral combinatorial approach is necessarily quite specific to *uniform* spin ensembles and their analogous uniform DTS. The cardinalities obtained arise within the framework of a pair of separate submodels. Of these, the first of these submodels give rise to the fundamental portion $\mathbf{N}_f^{(2n)}$ (shown under an over-brace), whereas the other type of contribution has a statistical origin. This part incorporates the previously obtained $2i < 2n$ total $|SI|^{2i}$s, now as a sequence of *total* cardinalities which are referred to here as $\mathbf{N}_{\text{total}}^{(2i)}$s. The development of the overall model is realised in a specific general context of uniform k_i tensorial spin physics treated under DR. The viewpoint adopted is based on *regular* topological lattice point sets. In addition, as the magnitude of $(2n)$ in this sequential treatment becomes large, it is essential to restrict TRI component SI-enumeration to $(\mathbf{I}\cdot\mathbf{I})_{i'}(\mathbf{I}\cdot\mathbf{I})_{j'}$ "pair" exchanges with the exclusion of all quadra-partite (or higher multiple embracketted) exchange processes. This is accomplished by subtracting certain lower $\mathscr{S}_{n'}$ model sum terms involving progressively higher partite forms. As discussed elsewhere [28], the requisite correction terms involve sums over various $\mathscr{S}_{n'}$ algebras with (integer) $n' = n/2, n/4, ..$ indices, now taken over all suitable (equal/less than) specific multipartite $(\chi^{[\lambda]})^2$s.

We now give a few examples, Eqs. (10)–(14), over the sequential set of SI-enumerations for the $[A]_{2n}$ uniform DR spin ensembles—noting the abbreviated $\chi^{[\lambda]}$ forms used here for brevity in discussing the 1^n based characters. In terms of these submodels, these polyhedral democratic sampling/recoupling-based $|SI|$ calculations take the following forms for specific cases:

$$|SI|^{(4)} = \overbrace{(\chi^{[2]})^2 + (\chi^{[11]})^2}(\mathscr{S}_2) + \{1\} = 3, \tag{10}$$

$$|SI|^{(6)} = \overbrace{(\chi^{[3]})^2 + (\chi^{[21]})^2}(\mathscr{S}_3) + \left\{3\binom{3}{1} + 1\right\}_{stat.w} = 15, \tag{11}$$

$$|SI|^{(8)} = \overbrace{((\chi^{[4]})^2 + (\chi^{[31]})^2 + (\chi^{[22]})^2)(\mathscr{S}_4) - ((\chi^{[2]})^2 + (\chi^{[11]})^2)(\mathscr{S}_2)} + \left\{15\binom{4}{1} + 3\binom{4}{2} + 1\right\}_{stat.w} = 91; \quad (12)$$

eventually one obtains the final 12-fold $|SI|$:

$$|SI|^{(12)} = N_f^{(12)}(\text{via } \mathscr{S}_6 : \mathscr{S}_3) + \left\{603\binom{6}{1} + 91\binom{6}{2}/5 + 15\binom{6}{3}/2 + 3\binom{6}{4} + 1\right\}_{stat.w}, \quad (13)$$

in which the various pre-combinatorial coefficient terms of the statistical portion arise as self-consistant integer terms. These integers are associated with the series of $\mathbf{N}_{\text{total}}^{(2i)} \equiv |SI|^{(2i)}$ terms for all $2i < 2n$. Naturally, the latter incorporates the prior fundamental terms, where each of these is a sum of squares of bipartite characters on $\mathscr{S}_n$ together with a subtractive term representing a sum of squares of quadra- (or higher) partite characters on some smaller group algebra(s), e.g., over all equal, or less than (notionally) 4-partite $(\chi^{[\lambda]})^2$s of $\mathscr{S}_3$ in the present example. The purpose of this last subsum(s) acts to exclude the Weyl non-allowed terms from contributing to the augmented TRI model. Hence for $|SI|^{(2n=12)}$, the fundamental model contributes:

$$\mathbf{N}_f^{(12)} = \overbrace{\{(\chi^{[6]})^2 + (\chi^{[51]})^2 + (\chi^{[42]})^2 + (\chi^{[33]})^2\}(\mathscr{S}_6) - \{(\chi^{[3]})^2 + (\chi^{[21]})^2 + (\chi^{[111]})^2\}(\mathscr{S}_3)} = 132 - 6, \quad (14)$$

with the first subset of group characters is clearly limited to bipartite forms. Hence the overall $|SI|^{(12)} = \mathbf{N}_{\text{total}}^{(12)} (= \mathbf{N}_f + \{..\}_{statw})$ cardinality becomes:

$$|SI|^{(12)} = 126 + 4087 = 4213. \quad (15)$$

Certain additional technical details concerning these various $(\chi_{1^n}^{[\lambda]})^2$ sums for generally accessible $\mathbf{N}_f^{(2n)}$ are given elsewhere [28]. In addition, we note for clarity that the Eq. immediately below Table 1 of [28a] should have included all the higher (quadra-) partite forms, except for the single 5-part $[1^5]$ irrep—one line of this Eq. in the earlier publication was omitted in error. The reader's attention is drawn to a further aspect of the denominators in the statistical submodel, Eq. (13) above. These constitute self-consistent primes within specific polyhedral topologies. They occur in these combinatorical models of TRI essentially on account of the intimate linkage between algebra and (topological) geometry.

The regular topological geometries [29,30] and their lattice point sets also highlight a further consequence of the *sequential* enumeration process, as now viewed in terms of the statistical submodel. Clearly by its nature, this type of modelling, as it applies to higher general (2n)- indexed uniform spin ensembles or analogous dual tensorial sets, is constrained by its underlying *regular* solid geometry. Thus, $|SI|_{\text{total}}^{(2n>12)}$ higher SI cardinalities become (for the most part) inacessible, or indeterminate. This occurs for a simple reason, namely the lack of further components to the sequence of *regular* topologies used to model $\mathscr{S}_{2n}$ group properties. One notes from Eq. (13) that all of the preceeding $\mathbf{N}_{\text{total}}^{(2i<2n)}$ terms make a contribution to the statistical submodel. It is only possible to circumvent this topological constraint in a few instances, where (e.g.) it may be shown that the specific highly degenerate $\mathscr{S}_{2n}$ case corresponds to one of the rare sporadic higher regular groups which are interrelated by means of FG dual topology and isomorphic algebras. Providing the lower indexed isomorphic-related SI-cardinality is known, the higher $2n$ based $|SI|^{(2n)}$ value may be obtained then simply by using the $\otimes$ product group measure property. Otherwise, all further $|SI|^{(2n>12)}$ values would be non-analytic, and thus indeterminate. Despite this last constraint implicit in 3-space, the conceptual value of FG topological duality is invaluable in much of the subsequent discussion. This occurs because FG duality provides the precise basis for the central assertion of this work, that SIs as *group invariants are group measures* in a Lie algebraic sense and provide the SI cardinalities of the bipartite NMR clusters.

6. Liouvillian FG-projections: specific applications of L-GM measures to DR uniform multipole NMR

6.1. Applications based on explicit invariance algebras

Prior to considering L-GMs and their direct product (bicluster) augmentation, a brief reference is made to other related projective techniques pertinent to Liouvillian applications. As an illustration, the $\mathscr{S}_3$ uniform spin-(1/2) is discussed, together a mention of uniform spin-1 $SU(3) \times \mathscr{S}_3$ NMR problems. In accordance the earlier discussion, the initial focus here is on the contrasting dual projective view of non-Abelian (invariance) algebras. By analogy with state space, the Liouvillian irreps of the $[A]_3(\mathscr{S}_3)$ spin-(1/2) monocluster ensemble arise directly from $tr\tilde{X}_{c:i}$s ($\tilde{\chi}_{c:i}$, here for $i = E, C_2, C_3$) invariance terms, i.e., over the char set $\{64, 4, 16\}$. From

Table 1
Uniform $SU(2) \times \mathscr{S}_3$ adapted NMR operator bases in a compact form, with the $\overline{(..)}$ notation denoting that the irreps shown are derived via signed sums over some particular dissimilar sub-rank auxiliary labels of the same type- i.e. 100, or 110

Multiplicity:	$\{T^k(k_1k_2k_3 : [\tilde{3}])\}$	:	Multiplicity:	$\{T^k(k_1k_2k_3 : \widetilde{[21]})\}$	:	Multiplicity:	$\{T^k(k_1k_2k_3; \widetilde{[\overline{111}]})\}$
7	$T^{3q}(111 : [3])$						
5	$T^{2q}(\overline{110} : [3])$	:	5	$T^{2q}(\overline{110} : [21])$			
		:	5	$T^{2q}(111 : [21])$			
3	$T^{1q}(\overline{110} : [3])$	:	3	$T^{1q}(\overline{110} : [21])$			
3	$T^{1q}(\overline{100} : [3])$	:	3	$T^{1q}(\overline{100} : [21])$			
		:	3	$T^{1q}(111 : [21])$	:	3	$T^{1q}(111 : [111])$
1	$T^{0}(\overline{110} : [3])$	:	1	$T^{0}(\overline{110} : [21])$			
1	$T^{0}(000 : [3])$	:			:	1	$T^{0}(111 : [111])$
20		:	20		:	4	

Overall dimensionality: 64

(cf. to analogous Liouville space work, reported in [10,31,32], especially (e.g.) Table 1 of [31].) The corresponding state space tables and problem sets given in [33] are also of specific interest in the present context.

use of the group algebra, one obtains (by analogy with the $SU(2) \times \mathscr{S}_2$ based Eqs. of Sanctuary and Temme [11c]) the total system irreps as:

$$\tilde{\Gamma}_{[3]} = \{\tilde{\chi}_E + 2\tilde{\chi}_{C_3} + 3\tilde{\chi}_{C_2}\}/6, \tag{16a}$$

$$\tilde{\Gamma}_{[21]} = \{2\tilde{\chi}_E - 2\tilde{\chi}_{C_3}\}/6, \tag{16b}$$

$$\tilde{\Gamma}_{[111]} = \{\tilde{\chi}_E + 2\tilde{\chi}_{C_3} - 3\tilde{\chi}_{C_2}\}/6. \tag{16c}$$

From these Eqs., it is clear that total irrep spans $\sum \tilde{\Gamma} = \{20, 20, 4\}\Gamma_0$, where Γ_0 refers to the {[3],[21],[111]} *unit column* irrep set. The main conceptual value of the latter is that it allows one to realise the 3-fold spin-1/2 $\mathscr{S}_3$ adapted Liouvillian tensorial bases under $SU(2) \times \mathscr{S}_3$ dual automorphic NMR spin symmetry simply by inspection. Thus, the set of dual tensorial forms over various $\{k_1k_2k_3\}$ sets is as given (in context of [31–33]) in Table 1. The value of this view of uniform spins is that it clearly retains the DR aspects inherent in the dual group; in addition, it represents a view analogous to an earlier classic scalar invariant study, that due to Lévy–Leblond and Lévy–Nahas [3a] based on uniform subranks over state space. The Liouvillian DTS given in Table 1 extend the earlier analogous $\mathscr{S}_2$ Liouville space tables [11a,11c,12a]. Ref. [11a] also gave the state space matrix representations of the earlier (Liouvillian) dual tensors. Unfortunately, because of its focus on certain technical unitary transform properties—including the use of CFP techniques under a single SI-, the 1994 Liouville space work of Listerud et al. [32] (in which the $\mathscr{S}_3$ structures play the role of effective unitary labels) does not mention the underlying theoretical physics associated with DR [3], involving *uniform* k_i tensorial subrank labelled system under the dual group. The work reported in [32] is only possible, because it is based on a single SI. On setting aside the constants of motion, this $\mathscr{S}_3$ group invariant clearly corresponds to the single induced symmetry chain $[21] \supset [2]$, a fact omitted from the original paper. The present use of projective techniques and quasiparticle mapping under the full dual group and its DR should yield a more physically insightful approach, precisely because some effort has been made here to put the problem into its wider proper theoretical context [3,8,9].

The corresponding $[AX]_3$ bicluster problem is one of some immediate NMR interest, because it is open to further investigations on the basis of the bicluster (isomorphic) augmentation processes given in Eqs. (17–21) below. In terms of projection over the invariance algebra, it exhibits the Liouvillian irreps shown in Eq. (17b) simply on the basis of the $(\tilde{\chi}_i)^2$ numerical factors of the direct product invariance set:

$$\{\tilde{\chi}_i(\otimes)\}\text{over } \{i = E, C_3, C_2\}$$
$$\equiv \{4096, 16, 256\}, \text{ over the } \tilde{\chi}(\otimes) \text{ algebra.} \tag{17a}$$

Naturally the corresponding irrep set follows directly as:

$$\tilde{\Gamma}(\otimes) = \{864, 1360, 561\}\Gamma_0, \quad (17b)$$

with the completeness of these inter-related spaces being based on the respective $\tilde{\chi}_E : (\tilde{\chi}_E)^2$ values.

The equivalent uniform spin-one $[A]_3^{(I_i=1)}$ ensemble, whose state space irrep spans $\Gamma = \{10, 8, 1\}$, follows directly from the additional Liouvillian invariance algebra. This spans:

$$\{tr\tilde{X}_i : \text{over} i = E, C_3, C_2\}^{(I_i=1)} \equiv \{729, 9, 81\}. \quad (18a)$$

With $\Gamma_0 \equiv \mathscr{A}_1, \mathscr{A}_2, \mathscr{E}$, the total irrep for the 3-fold uniform spin-one system then becomes:

$$\tilde{\Gamma}^{(I_i=1)} = \{165, 240, 84\}\Gamma_0. \quad (18b)$$

In contrast to Table 1, the $SU(3) \times \mathscr{S}_3$ dual tensorial sets $\{T^{6q}(v), \ldots, T^0(v')\}$, encompass the following set of auxiliary labels:

$$v, v', \ldots = \{222; 221; 220; 211; 210; 200; 111; 110; 100; 000\}. \quad (19)$$

These uniform threefold $I_i = 1$ operator bases are still of fairly modest dimensionality, 729. From their correspondence to the classic 1965 work on three-spin symmetry of Jones et al. [2], one concludes that two further distinct basis sets could well be of particular interest to the NMR community, namely those for trideuto- 1,3,5-trifluorobenzene, and its 2,4,6-trideutero-1,3,5-triazine analogue. The former is clearly a $\Gamma^{(I_i=1)}(\mathscr{S}_3) \otimes \Gamma^{(I'_i=(1/2))}(\mathscr{S}_3)$ spin problem. The pure bis 3-fold spin-one spin system exhibits an interesting distinct feature in being of even-even parity, in contrast to the odd-odd parities of the original pure bis 3-fold spin-1/2 system of [2]. On utilising the respective $tr\{\tilde{X}_i : E, C_3, C_2\}$ invariance subsets for these further bipartite cluster spin systems, one obtains the following respective invariance sets: $tr\{\tilde{X}_i(\otimes)\} \equiv \{46656, 36, 1296\}$, *else* $tr\{\tilde{X}_i(\otimes)^{I_i, I'_i=1}\} \equiv \{531441, 81, 6561\}$. These in turn defines the corresponding overall irreps. Hence,

$$\tilde{\Gamma}(\otimes)^{(I_i=1:I'_i=(1/2))} \equiv \{8436, 15540, 7305\}\Gamma_0, \quad (20)$$

defines the overall irrep over Liouville space of the mixed bipartite system, in contrast to the $\chi_E(\otimes) =$ 531241-dimensioned, bis pure spin-one (bi)cluster system. The irreps of the latter span:

$$\tilde{\Gamma}(\otimes)^{(I_i,I'_i=1)} \equiv \{91881, 177120, 85320\}\Gamma_0, \quad (21)$$

in agreement with the stated dimensionality.

6.2. DR and LGM-defined SIs for bicluster NMR systems

On invoking the Lie algebra concept that SI invariants constitute actual group measures, further induced symmetry or projective techniques become available for use in auxiliary label (or recoupling) aspects of NMR spin physics. In a sense, these techniques complement those based on either invariance algebra or dual quasiparticle mapping. However, there are certain important differences from the latter, since the $|SI|$s represent recoupling-based (not invariance-based) properties. As noted in the context of graph invariant schemes [12] and elsewhere, recoupling over $\{k_i\}$s (whether for linear or DR forms) simply mirrors the analogous forms over state space $\{j_i\}$s, *without* there being any (internal) map-based augmentation implied between the corresponding state and Liouville space recouplings. Induced symmetry arguments are invaluable in the context of invariants and their cardinality. Hence it follows that the four and fivefold spin invariants in either space are governed by their inherent subduced symmetry chain sets. To implement this observation it is first necessary to omit the chain derived from the constant(s)-of-motion from consideration. For the above monocluster spin systems, the group invariants are represented by (otherwise $v, v'v''$ labelled) subsets of irrep chains which span:

$$\{SI; SI'; SI''\}(\mathscr{S}_4) \equiv \{[31] \supset [3] \supset [2]\}; \{[31] \supset [21] \supset [2]\}; \{[22] \supset [21] \supset [2]\}, \quad (22)$$

and the six pre-SA/SA $\mathscr{S}_5$ component subsets:

$$\{[41] \supset [31] \supset [21] \supset [2]\}; \{[41] \supset [31] \supset [3] \supset [2]\}; \{41 \supset [4] \supset [3] \supset [2]\}, \quad (23)$$

$$\{[32] \supset [31] \supset [3] \supset [2]\}; \{[32] \supset [31] \supset [21] \supset [2]\}; \{[32] \supset [22] \supset [21] \supset [2]\}, \quad (24)$$

respectively. One has necessarily excluded the initial tripartite SA-irrep based chain-sequence here; clearly, this is justified on account of the SIs or group invariants being exclusively $SU(2) \times \mathscr{S}_n$ properties.

Further discussion of enhanced cardinality here refers specifically to the external type inner product process implicit in L-GM properties. Practical NMR applications of the latter are as part of bicluster formation—rather than to any internal mapping property of more theoretical interest. On utilising the known SI-cardinalities for any of the simple spin ensembles, the responding overall bis system $|SI|^{(n':\otimes)}$ cardinality follows directly, with the actual invariants being represented (as below) as suitable products of chain sequences. Hence for the n'-indexed systems $[AX]_2, [AX]_3$, and for the specific $[AX]_4(\mathscr{S}_4 \downarrow D_2)$ case, (as one subset of a more general $[AX]_4(\mathscr{S}_4)$ NMR system [11b]), one finds that the SI-cardinalities over the isomorphic direct product algebras (themselves based on unit (component) $|SI|^{(n')}$) all correspond to the L-GM algebra:

$$\{|SI|^{(n')} \otimes |SI|^{(n')}\}(\mathscr{G} \otimes \mathscr{G}) = |SI|^{(n':\otimes)} = 1. \quad (25)$$

Indeed, the central logic of this relationship taken in the context of earlier theoretical work [3b] clearly defines the full extent of monoinvariant-derived augmented bis cluster spin systems in NMR. It is interesting to note that this includes the *bis* 3-fold spin system, discussed by Jones et al. [2] in the mid-1960s and, in a Liouville space context, by Listerud et al. [32] more recently. In contrast to the three examples above, the *bis* 4-, 6- and 10-fold $[AX]_{2n}$ spin systems (e.g.) differ, since each represents distinct monocluster cardinalities for NMR spin problems which are defined by *multiple invariants*. On the basis of Galbraith's mathematical physics conclusions [3b] concerned with the group theoretic nature of DR, all these higher-indexed monocluster NMR systems all lack conventional *closed analytic descriptions*, comparable to [11a,32]. Since such multiple invariant constraints to non-Abelian systems have been well established [3] from research of the period 1965–1972, in the following paragraph we shall confine ourselves to a brief review of applications of the LGM concepts in obtaining augmented $|SI|^{(n':\otimes)}$s for bipartite $[AX]_n$ spin systems.

For each of the three specific monoclusters mentioned above, augmentation to practical bicluster systems involves analogous logic in deriving the explicit $|SI|^{(n':\otimes)}$ cardinalities over isomorphic direct product algebras, based on this L-GM concept. As an example of L-GM based mapping for a system defined by multiple group invariants, we consider the formation of the higher spin symmetry $[AX]_4$ system. The resulting bipartite spin cluster system is defined by the invariant cardinality:

$$|SI|^{(4)} \otimes |SI|^{(4)} = |SI|^{(4:\otimes)} = 9. \quad (26)$$

This is seen to arise from the 3-fold initial monocluster cardinality. Using all possible v, v', v'' chain sequences from Eq. (22) (*et seq.*) above, generates specific pairings (with ordering retained), which now represent the new set of invariants for the augmented spin system. Thus, the invariants of $[AX]_4$ are represented by:

$$\{vv, vv', vv''; v'v, v'v', v'v''; v''v, v''v', v''v''\}. \quad (27)$$

Similarly, the SI-cardinality associated with $[AX]_6$ is defined by:

$$|SI|^{(6)} \otimes |SI|^{(6)} = |SI|^{(6:\otimes)} = 15 \times 15 = 225, \quad (28)$$

Clearly both cases represent direct products over suitable isomorphic algebras being used to define the cardinality associated with mono → bi-partite cluster mapping. Analogous detailed consideration of the (ordered) induced chain sequence products as useful representations of the bicluster invariants is not given here for brevity. Finally, the corresponding overall *bis* tenfold spin system cardinality, as $|SI|^{(n'=10:\otimes)}$, exhibits a resultant magnitude for the number of these independent SIs of 363,609. This arises directly from $|SI|^{(10)} = 603$ being the number of invariants defining the monocluster. Because of the mathematical physics property of analytic indeterminacy inherent in all these multiple SI-based spin systems, little if any further progress would seem possible in describing the spin dynamics of these bipartite system, *unless of course* the analysis incorporated the invariants in such a way that distinct subsectors could be associated with each invariant. Whilst this insight is novel in the present context, it is somewhat analogous to the multi-structured physics of relaxation, as obtained from auxiliary labelled *intensive tensorial* theories of multi-mode relaxation, e.g., in work due to Happer [14] dating from the 1970s. Since the use of $|SI|^{(n':\otimes)}$ terms (and induced symmetry sequence products) arises from L-GM defined DR recoupling-based properties, specific to (dominant intra $J_{AA'}, J_{XX'}, ..$-based) uniform spin systems, any analogue to multi-mode type analysis is not a *direct group theoretic* simplification, i.e., in the sense intended by Galbraith [3b]. As far as the present author is aware, no actual multimode (non-relaxation) analytic spin dynamics calculation, or analogous transformation, have appeared to date. The form of such analyses for some suitable ($\geqslant 4, 5$) spin systems (i.e., *beyond* the conventional mono-SI work given in [32]) in principle represents an interesting non-trivial open question.

7. Discussion and general conclusions

Experimental multiquantum studies for irrep-selective NMR evolution were reported by Avent [34] in the mid-1980s. However, they were restricted to discrimination between the possible distinct irreps of the single invariant based $A[B]_3$ spin system which did not involve (multiple) irreps of high degeneracy, such as those discussed in the Sec. above. For conceptual completeness here, as well as for its clarity in the context of Corio's recent discussion [1] in terms of orthogonal symmetries, it is important to stress that any method of obtaining SIs, which are ultimately based on SO(3) homomorphic mapping onto SU(2), is constrained. In principle, it is simply not applicable to NMR spin systems involving high degeneracy, such as those exhibited by uniform ($2n$)-fold $[A]_{2n}, [AX]_{2n} \forall 2n \geqslant (4)5, 6$ uniform spin systems. For these specialised uniform j_i/k_i sub-rank set systems, only DR dual group models using topological-based combinatorial methods are viable. As shown in Section 5, such models arise via the (recursive) Landau-Lifschitz [27] generalised approach to the (properly independent) variables of polynomials and so provide a basis for determining the fundamental components, $\mathbf{N}_f^{(2n)}$ under DR. The $\mathbf{N}_{\text{total}}^{(2i<2n)} = |SI|^{(2i)}$ series of components (the right-hand numerical terms contributing to the statistical submodels in Eqs. (11)–(13)), plays an important role in modelling, because they limit the extent of the DR sequential statistical submodel. This effect occurs for geometric reasons arising from the known limits to regular topological polyhedra. Indeed despite the known existence of *higher stellate* (non-convex) I_h 3-space forms, the maximal *regular convex hulls* (solids) known are the icosahedron and its FG dual; for this reason alone, the extant of the sequential even series mentioned above is limited. Since further statistical submodels, beyond those given in Eqs. (10)–(13), are undefined, equally the polyhedral combinatorial modelling over lattice point sets is interrupted also at the point, $2n \geqslant 14$, for lack of any viable sequential statistical contribution. Little further progress is possible in defining either further monocluster SIs, or the $|SI|^{(2n)}(\otimes)$ invariants for higher $[AX]_{2n}$ (uniform) NMR systems, or their associated dual tensorial sets. One uniform multispin monocluster exception is predicted on the strength of recognising the central role played by FG duality in the context of group measures over isomorphic algebras, a concept reported in Section 6.2 above. On topological grounds, it is clear that even where further possibly quasiregular polyhedra actually occur beyond the $(2n) = 12$-indexed SI example treated here, they are of rather sporadic occurrence. In addition their treatment would require the presence of a definite FG-topological duality linkage to furnish any further $|SI|^{(2n)}$ value for a still higher uniform spin ensembles. Hence, treatment of a new monocluster ensemble system in terms of its independent $|SI|^{(2n)}$ cardinality, as obtained via a *higher sporadic regular* topology and isomorphic algebra, is the subject of separate applied mathematical focussed work [35]. Conceptually it is of interest to note here exactly how originally one recognised that SIs (group invariants) are indeed Lie algebraic group measures [20].

For historical context, we stress that no mention of the concept of group measures, or of the need *to distinguish between multiplicity-free and non-Abelian* spin systems, was made in Corio's original discussion [1] of $(\otimes SU(2))^{2n}$ based SI cardinality for Abelian spin symmetries. Corio also leaves a further essential question unresolved. This concerns the nature of more general $(2n)$-bis system SI cardinalities. Because these properties generally define tensorial completeness, they play a specific essential role within the quantal physics of spin dynamics of uniform non-Abelian bipartite spin ensembles. Hence the lack in [1] of any statement on the specific role of SIs as group measures (acting over isomorphic direct product algebras) is a serious omission. This additional Lie-algebraic concept had to await recognition of a more explicit formalism in the Russian theoretical physics literature [20], before it could be introduced into descriptions [28] of NMR spin symmetry [11,31], as a proof that SIs are group measures. This viewpoint essentially rests on the role of topological FG duals as seen in a specific comparison of the $(2n) = 6, 8$-based $[A]_{2n}$ system $|SI|^{(2n)}$ values. The central role here in NMR of SIs as group measures (as well as important distinctions between the Abelian, or non-uniform, $(\otimes SU(2))^{(2n)}$ based (degeneracy-free) examples [1] and the higher $(2n)$-based *uniform* $\{j_i, k_i\}$ DR recoupled spin systems) is quite fundamental to the modelling reported in this work. Indeed, the DR-derived $|SI|^{(..)}$ cardinalities determine the structure and completeness of uniform, higher $(2n)$ based dual tensorial sets, also. No description of them could be complete without a precise knowledge of the independent SI cardinalities and bipartite mapping. Even discussions of the nature of non-multiplicity-free NMR spin systems, derived from simpler uniform spin ensembles, benefit from the use of a tensorial operator-basis approach. This comes about because a knowledge of the SIs, as part of the auxiliary labelling, is essential to an understanding of the retention of SR in superboson quasiparticle mapping over carrier spaces [9]. Hence, it is the physical attributes of the auxiliary labelling that yields insightful in the analysis of coherence development. In turn, this gives a greater appreciation of the structure of NMR ensemble-based spin systems, than is possible in state space product representation formalisms, where the SIs lack such an explicit quantum role. A penultimate additional theoretical comment is timely before concluding this work, namely that the technique of utilising the cardinality of $(2n + 1)$ *odd*-indexed spin systems of the preceding linearly recoupled *even* $|SI|^{(2n)}$ result by factor of 2 (as advocated by Corio [1] and Weyl [4]) is essentially restricted to linearly recoupled $(\mathbf{I} \cdot \mathbf{I})(\mathbf{I} \cdot \mathbf{I})$ (pair) TRI theory of low-indexed Abelian abstract spin symmetries. Since regular odd indexed vertix point set-based topologies are especially scarce geometric entities, any further consideration of general SI cardinality for *odd* $(2n + 1) \geqslant 11$ indexed spin ensembles (or of odd uniform dual tensors) under DR for now remains an open question. Finally as a modern mathematical view of group invariants—half a centuary beyond Weyl's original $\mathscr{S}_n, \mathscr{GL}_n$ group duality-based monograph on group invariants-, we refer the interested reader to a recent comprehensive text by Goodman and Wallish [36].

8. Dedication and acknowledgement

This paper is dedicated in memoriam to Professor Mik M. Pintar (1934–2003), most recently of the Department of Physics, University of Waterloo, Canada, and one-time director of a long-running series of well-attended NMR Summer Schools. Beyond the depth of physical insight he brought to his own research area and the invaluable guidance he gave to his physics co-workers and graduate students, Mik will be long remembered by all who knew him for his great personal warmth, sense of humour and his generous encouragement of others in their research. He will be greatly missed by both the NMR and wider physics communities.

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Appendix. Appendix notes

To clarify distinctions between $[AX]_n$ NMR systems governed by high permutational, dominant intra-cluster $J_{AA'}, J_{XX'}$-based zeroth order Liouvillians $\hat{\hat{\mathscr{L}}}^{(0)} = [\hat{\mathbf{H}}^{(0)},]_-$ and the analogous bipartite $AA'A''..XX'X''..$ isochronous spin systems, in which the various inter- and intra-cluster J interactions of $\hat{\hat{\mathscr{L}}}^{(0)}$(s) introduce (some specific) $J_{AX} \gg J_{AA}$, or J_{XX}, (or else yielding J_{AX}s of *comparable magnitude* to either $J_{AA'}, or J_{XX'}$), it is instructive to compare a pre-1990 work of ours [11a] with Sanctuary's 1985 treatment on the role of cross-product polarisation in AX spin system [10b]. In the dominant $J_{AA'}[A]_2$ case, the eigenvalues inherent in the rotating-frame description of the spin dynamical are associated with null value entries throughout the $\{.,.,\}^{[2]}$ salient, which is derived from $\phi_q^k(v : [\tilde{2}])$s. The remaining eigenvalues are associated with the various $[\tilde{1}^2]$ polarisations and in contrast take the values, $\pm J_{AA'}$. From Eqs. (18–28) of [11a], one concludes that the $[\tilde{2}]$ sector rotating frame coherences are stationary local properties, in the sense that:

$$\hat{\phi}_q^2(11; [\tilde{2}])[t] = \phi_q^2(11; [\tilde{2}])[0], \quad \text{for } q = \pm 2, \pm 1, \text{ and} \tag{A.1}$$

$$\hat{\phi}_\pm^1([\tilde{2}])[t] = \phi_\pm^1([\tilde{2}])[0], \tag{A.2}$$

with the expression $\hat{\phi}_q^k(..) = \exp(-iq\overline{w}t)\phi_q^k(..)[t]$ defining the rotating frame. The remaining $\hat{\phi}_\pm^1([1^2]), \hat{\phi}_\pm^1(11)$s are coupled by $J_{AA'}$ but remain unobservable, simply because $\phi_q^1([1^2])[0]$ can not be created by any conventional rf-pulse sequence. The contrasting responses of the AX-based dipolar coherences arise from the existence of four distinct eigenvalues and a overall solution of the QL Eq. in a form equivalent to Eq. (7b) above. Specific matrix elements may be found in Table 5 of [10b]. The now distinct $\hat{\phi}_q^1(v)$ s of AX case with $v = 10$, or 01 are shown to be coupled by the (*symmetry breaking*) cross-product polarisation, $\phi_q^1(11)$. Hence, only the $\hat{\phi}_{\pm 2}^2(11)$ quadrupolar coherences, which may be observed indirectly via 2D NMR sequences, are stationary rotating frame entities for the AX spin dynamics model, with solutions:

$$\hat{\phi}_{\pm 2}^2(11)[t] = \phi_{\pm 2}^2[0]. \tag{A.3}$$

Hence, the two distinct $\hat{\hat{\mathscr{L}}}^{(0)}$-based spin systems exhibit strong contrasts in their analytic spin dynamics. These observations also highlight general distinctions between the zeroth order aspects of wider symmetry-based proper cluster spin systems (i.e., corresponding to the $[A]_2$ monopartite spin system above), as compared to the various isochronous (or related) NMR systems, in which one or other of the J_{AX} intercluster $\mathscr{L}^{(0)}$ interactions are either dominant, or else comparable to one of the $J_{AA'}, J_{XX'}$s. The 1965 work of Jones et al. [2] has also stresses the additional value of parity in isochronous systems, with odd-odd parity allowing the different intracluster $J_{AA'}, J_{XX'}$s to be observed independently. In addition to recalling frequently overlooked formal distinctions, the above views present the topic in a modern NMR context, via contrasting tensorial model spin dynamics.

On turning to the question of role of invariants, one notes that it was precisely the concept of topological FG duality, which provided the original proof (Eq. (7.1) of [35]) that SIs are (Lie algebraic) group measures [20] over isomorphic group algebras. Only by examining this point in the specific context of octahedral/cubic topological duality does one recognise SIs as recoupling based group measures with practical impact on bicluster NMR and their independent $|SI|^{(2n)}(\otimes)$s. Para II of Section 7 comments further on the role of FG duality in SI modelling. Additionally, in the topological context of $^{13}C_{60}$ or other regular fullerene-based spin systems, one notes that no correlation exists between *truncated* higher topological forms and their related simple topologies This has a physical consequence for our knowledge of precise $|SI|^{(2n)}$ cardinalities of various multi-invariant DR-based higher uniform spin ensembles. Illustrations of the known topological fact that there is no higher *regular* simple convex hull (geometric solid) beyond the dodecahedron is available. Beyond the truncated solids (mentioned above) with their mixed sets of polygonial faces, this includes (e.g.) the encapped cube derived by imposing the elements of its dual onto a cube. It will be readily seen that the are two quite distinct sets of vertix points now (six of 3^4 (i.e., a vertix of geometric solid included within 4 distinct 3-gons) from the encapped extremities and eight now of 3^6 type). Hence the solid structure is definitely *not a regular* polyhedra [30,31], as one would require in order to treat $[A]_n$ uniform spin ensembles. Similar arguments show that the *encapped dodecahedron* with its 32 vertix points is not a *regular* convex hull [30] in the sense used here. Refs. [10,12] should consulted for details of the transforms between the less physical product bases (as shift bases) and tensorial basis sets, or between products of tensor bases and full $[AX]_{2n}$ tensorial bases, both of which involve suitable $3j$ coefficient sums. Finally, the evaluation of Liouville operator matrix elements (constrained by commutator relationships which occur within the tensorial basis) is set out in Eq. (229) of the 1991 Sanctuary and Halstead review [12].

References

[1] P.L. Corio, J. Magn. Reson. 134 (1998) 131–137.
[2] R.G. Jones, R.C. Hirst, H.J. Bernstein, Canad. J. Chem. 43 (1965) 683–690.
[3] (a) J.M. Lévy-Leblond, M. Lévy-Nahas, J. Math. Phys. 6 (1965) 1372–1380;
(b)(see cf. in) H.W. Galbraith, J. Math. Phys. 12 (1971) 782–794, 2380–2390.
[4] H. Weyl, Representations and Invariants of Classic Groups, Princeton Press, 1946.
[5] K. Balasubramanian, J. Chem. Phys. 78 (1983) 6358–6369, pp. 6369–6376.
[6] R.G. Jones, Princ. Progr. NMR 1 (1967) 97–172.
[7] P.L. Corio, The Structure of High-resolution NMR, Academic, New York, 1966.
[8] L.C. Biedenharn, J.D. Louck, Permutation Group in Physics and Chemistry, Springer, Berlin, 1979.
[9] F.P. Temme, Physica A 198 (1993) 245–261.
[10] (a) B.C. Sanctuary, J. Magn. Reson. 61 (1986) 116–124;
(b) B.C. Sanctuary, Mol. Phys. 55 (1985) 1017–1031;
(c)(also) B.C. Sanctuary, J. Chem. Phys. 64 (1976) 4352–4361.
[11] (a) F.P. Temme, J. Magn. Reson. 83 (1989) 383–387;
(b) F.P. Temme, Chem. Phys. 32 (1989) 9–32;
(c) B.C. Sanctuary, F.P. Temme, Mol. Phys. 55 (1985) 1049–1062, 58 (1986) 659.
[12] (a) B.C. Sanctuary, T.K. Halstead, Adv. Opt. NMR Reson. 15 (1991) 97–161;
G. Campoleti, B.C. Sanctuary, Canad. J. Chem. 65 (1987) 1746.
[13] M. Atiyah, P.M. Sutcliffe, Proc. Roy. Soc.- Lond. A 458 (2002) 1089–1115.
[14] W. Happer, Phys. Rev B:[3] 1 (1970) 2203–2212.
[15] A. Bain, R.M. Lynden-Bell, Mol. Phys. 30 (1975) 325–356;
(also) B. Gestblom, O. Hartmann, J.M. Anderson, J. Magn. Reson. 5 (1971) 174–179.
[16] D.A. Marcus, Combinatorics a problem-oriented approach, Am. Math. Soc., Rhode Is. (1998).
[17] W. Ledermann, Group Characters, second ed., Cambridge University Press, Cambridge, 1987.
[18] M. Quack, Mol. Phys. 34 (1977) 477–488.
[19] G.J. Bowden, J. Math. Chem. 131 (2002) 363–370.
[20] A.A. Kirillov, Elements of Group Representation Theory, [Transl'd: E. Hewitt], Springer, Berlin, 1975, see pps: 32, 38, 83.
[21] P. Erdös, P.M. Grüber, J. Hammer, Lattice Points, Longman-Sci, Harlow, 1989.
[22] I.Ya. Akimova, Engin. Kybernet. 22 (1985) 6–12.
[23] F.P. Temme, J. Mol. Struct. Theochem. 578 (2000) 145–157;
Int. J. Quantum Chem. 78 (2000) 71–82.
[24] F.P. Temme, Eurphys J. B 11 (1999) 177–185.
[25] B.E. Sagan, Symmetric Group: Its Representations, Combinatorial Algorithms and Symmetric Functions, Wadsworth Pacific Gr.-CA. (1991); A. Kerber, A. Kohnert, A. Lascoux, J. Symb. Comput. 3 (1993) 195–204; Symmetrica Pkg., loc.cit.
[26] A. Schrijver, Encyclopedia of Combinatorics, MIT Press/Elsevier, Amsterdam, 2000 [Polyhedral Combinatorics (Chapter 30)].
[27] L.D. Landau, E.M. Lifschitz, Non-relativistic Quantum Mechanics, second ed., Pergamon, Oxford, p. 218.
[28] (a) F.P. Temme, J. Math. Chem., 31 (2002) 281–312;
F.P. Temme, J. Math. Chem., 33 (2004) (Addenda to [28a]);
F.P. Temme, J. Math. Chem., 27 (2000) 111–130; 131–154;
F.P. Temme, Int. J. Quantum Chem., 90 (2002) 155–165, et loc. cit.
[29] R. Maeder, Math. J. 3 (1993) 48, & Illustr. Chart Supplement thereto.
[30] Z. Harv'el, Geom. Dedicata 47 (1993) 57.
[31] F.P. Temme, Z. Phys. B 88 (1991) 83–92.
[32] J. Listerud, S.J. Glaser, J.P. Drobny, Mol. Phys. 78 (1993) 629–658.
[33] R.P. Feynmann, Theory of Fundamental Processes, W.A. Benjamin, Reading-Mass, 1962, esp. Appendix Tables.
[34] A.G. Avent, J. Magn. Reson. 53 (1984) 513–518.
[35] F.P. Temme, AXX (2004) xx (to appear).
[36] R. Goodman, N.R. Wallish, Representations and Invariants of Classic Groups, Cambridge University Press, Cambridge, 1998.