

Note

On mixed vs. exclusively-bosonic
 $\{[\tilde{\lambda}] : p \leq 2^2\}(\text{SU}2 \times \mathcal{S}_n)$ irrep sets over $\{\tilde{\mathbb{H}}_v\}$ carrier
 subspaces, in the structure of $(\text{SU}2 \times \mathcal{S}_n \otimes (\text{SU}2 \times \mathcal{S}_n)^\dagger)$ -
 derived Liouville space of NMR spin dynamics

F.P. Temme

Department of Chemistry, Queen's University, Kingston K7L 3N6, Canada

Received 13 June 1995

The $\text{SU}2 \times \mathcal{S}_n$ dual group algebra underlying Liouville NMR formalisms, which applies to extended spin cage-clusters $[A]_n$ of $[AX]_n$ NMR spin systems, is briefly presented in terms of its mapping and superbosonic properties over the $\{\tilde{\mathbb{H}}_v\}$ specialised carrier subspaces. By considering further both the origins of Liouville space as an augmented space based on inner tensor products of simple Hilbert space, and also the λ_{SA} -self-associate forms in terms of the contrasting structural aspects of the $8, 12, 16 \leq n$ and $17, 20 \leq n$ \mathcal{S}_n groups, it is shown that mixed boson/fermion sets of component irreps should only exist up to $n \leq 16$. This property is traced to the need for the symmetric group irreps to span a set of $\{[\tilde{\lambda}] : p \leq 2^2\}(\mathcal{S}_n)$ irreps corresponding to $\text{SU}2$ branching over the augmented $\text{SU}2 \times \mathcal{S}_n$ spin space. Parallels are drawn with the more general quonic algebras over simple Hilbert space.

1. Introduction

In the context of present interest [1,2] in quon(ic) algebras from the work of Greenberg [2], it is pertinent to bring to wider attention the existence of a further algebra in which fermion and boson aspects co-exist at least for some range of symmetric groups amenable to $\mathbb{Z}(\mathcal{S}_n)$ tabulation, namely that for $n \leq 16, 17$. One is referring to the $\{D^k(\tilde{U}) \times \tilde{F}^{[\lambda]}(v)\}$ irreps associated with dual $\text{SU}2 \times \mathcal{S}_n$ tensors [3,4], as bases implicit in the spin dynamical evolution [5] of NMR spin clusters. These span a $\{[\tilde{\lambda}]\}(\mathcal{S}_n; p \leq 2^2)$ set within a dual group algebra [6], as a consequence of the inner tensor product (ITP) structure of Liouville space. In this context, the $\text{SU}2$ -simple reducibility over the carrier space(s) derives from the distinctness of the explicit $\text{SU}2$ v -recoupling aspects, now within the democracy imparted by the dual groups. The latter aspect derives from an extension of the fundamental boson

mapping concepts of ref. [7] from the original simple Hilbert space into the (further) realm of Liouville space over tensorial bases [8].

In contrast to quonic algebras over simple Hilbert spaces [1,2], for these $\{[\tilde{\lambda}]\}(\mathcal{S}_n)$ sets the co-existence of boson and fermion components is a function of the n -degree of the symmetric group which defines the spin cluster NMR problem. Hence, it is convenient to refer to these algebras as being ‘pseudo-quonic’ in form over a limited n -degree range of the augmented spin space.

2. An outline of the origin of Liouville space properties

From the mapping properties under $SU2 \times \mathcal{S}_n$ of Liouville forms of carrier space [8], $\{\tilde{\mathbb{H}}_v\}$, utilizing the rotation and projection operators pertinent to such a formalism, one obtains

$$\tilde{\mathbb{U}} \times \mathcal{P}(\tilde{\Gamma}) : \tilde{\mathbb{H}} \rightarrow \tilde{\mathbb{H}}\{D^k(\tilde{\mathbb{U}}) \times \tilde{\Gamma}^{|\lambda]}(v) | \tilde{\mathbb{U}} \in SU2; \mathcal{P}(\tilde{\Gamma}) \in \mathcal{S}_n\} \quad (1)$$

for which it may be shown [6,8] that sets of distinct $\{\tilde{\mathbb{H}}_v\}$ carrier subspaces exist, on account of the uniqueness of the fully explicit v -recoupling aspect in the expansion:

$$\tilde{\mathbb{H}} \equiv \sum_v \tilde{\mathbb{H}}_v. \quad (2)$$

It is these aspects which both differ from the simple Hilbert space formalism of ref. [7] and which now ensure that the $SU2 \times \mathcal{S}_n$ algebras over Liouville space retain the property of simple-reducibility. A further general consequence of the mapping concept, applied over the augmented carrier subspaces, leads one to the conclusion that there exists an appropriate set of ladder (super)operators over a superboson space [9] defined on the additional augmented Heisenberg generator,

$$[(\tilde{j}_i^2), (\tilde{j}_j^2)]_- = 2\delta_{ij}, \quad (3)$$

as derived from the right-derivation property, i.e., on expanding this from a $[\hat{\mathbf{a}}\hat{\mathbf{b}}, \mathbf{cd}]_-$ commutator, whose superoperators, defined by $\hat{\mathbf{a}}\mathbf{C} = [A, C]_-$, imply that $\hat{\mathbf{a}}\mathbf{1} \equiv 0$. A brief indication of the nature of superboson algebras is given below to clarify the context and nature of these remarks.

Underlying the natural structure of NMR cluster Liouville space is the intra-cluster- $\{J_{ij}\}$ automorphic spin symmetry [10,11] of NMR cluster problems, in the higher \mathcal{S}_n limit in which NMR magnetic-equivalence is totally absent and with it any implication of reconstructive higher exclusively-unitary group aspects. Hence the Latin-square constructions derived from ITP processes [6b], utilising the simple Hilbert space properties that define the specific n -fold $[A]_n$ spin cluster of the $[AX]_n$ NMR system, yield the following general set with the upper bounds for the $(SU2 \times \mathcal{S}_n) \otimes (SU2 \times \mathcal{S}_n)^\dagger$ direct product dual spin space being:

$$\{[\tilde{\lambda}]\}(\mathcal{S}_n : 1 \leq p \leq 2^2). \tag{4}$$

Here, p is associated with the $\lambda \vdash n$ partition structure and its (unitary) branching, as derived under standard $\not\leq$ dominance sequence ordering [12]. This equally applies to irrep branching. Here, it serves to define the persistence of these “pseudo-quonic” properties by affording a comparison with the structure of the self-associate forms for specific \mathcal{S}_n groups.

The mathematical texts on combinatorial \mathcal{S}_n -algorithms, such as Sagan [12], or ref. [13], should be consulted for a fuller background to the properties of $\lambda \vdash n$ partitions, \mathcal{S}_n -modules and the $\{A_{\lambda|\lambda'}\}$ Kostka coefficients associated with decompositions of the latter. Their application to NMR dual group spin algebras [14] and its more general $SU(m) \times \mathcal{S}_n$ associated models for $\mathcal{S}_n \supset \mathcal{G}$ subgroup natural embedding are topics discussed in related papers [15,16].

3. The ladder-superoperators algebra of Liouville spin space

The superboson $(\begin{smallmatrix} j & 2 \\ j & 1 \end{smallmatrix})$ -algebra associated with superoperators \mathcal{I}_μ , defined over $\{|kqv\rangle\rangle\}$ bases of Liouville space, arises from mappings over $\{\tilde{\mathbb{H}}_\nu\}$ carrier subspaces [8,9], taking *all* upper(lower) components respectively throughout the following expressions, which constitute a consistent set of ladder superoperator properties for the augmented spin space:

$$\begin{aligned} & \begin{pmatrix} j & 1 & j & 2 \end{pmatrix} \\ [\mathcal{I}_\pm, \begin{pmatrix} j & 2 \\ j & 1 \end{pmatrix}]_- &= \begin{pmatrix} j & 2 & j & 1 \end{pmatrix}, \\ & \begin{pmatrix} j & 2 \\ j & 1 \end{pmatrix} \\ [\mathcal{I}_\pm, \begin{pmatrix} j & 1 & j & 2 \end{pmatrix}]_- &= \begin{pmatrix} j & 2 \\ j & 1 \end{pmatrix}; \end{aligned} \tag{5}$$

$$\begin{aligned} & \begin{pmatrix} \bar{j} & 1 & \bar{j} & 2 \end{pmatrix} \\ [\mathcal{I}_\mp, \begin{pmatrix} \bar{j} & 2 \\ \bar{j} & 1 \end{pmatrix}]_- &= \begin{pmatrix} \bar{j} & 2 & \bar{j} & 1 \end{pmatrix}, \\ & \begin{pmatrix} \bar{j} & 2 \\ \bar{j} & 1 \end{pmatrix} \\ [\mathcal{I}_\pm, \begin{pmatrix} \bar{j} & 1 & \bar{j} & 2 \end{pmatrix}]_- &= \begin{pmatrix} \bar{j} & 2 \\ \bar{j} & 1 \end{pmatrix} \end{aligned} \tag{6}$$

with any cross terms in (5a, 6a) vanishing, whereas

$$[\mathcal{I}_0, \begin{pmatrix} j & 2 \\ j & 1 \end{pmatrix}]_- = \pm \begin{pmatrix} j & 2 \\ j & 1 \end{pmatrix}; \quad [\mathcal{I}_0, \begin{pmatrix} \bar{j} & 2 \\ \bar{j} & 1 \end{pmatrix}] = \mp \begin{pmatrix} \bar{j} & 2 \\ \bar{j} & 1 \end{pmatrix} \tag{7}$$

lead to mappings between the superbosons and the fundamental Wigner (super)-operators characterizing the structure of the carrier space, $\{\mathbb{H}_v\}$. This is seen in the forms

$$\begin{aligned} \{(\jmath_1^2), (\jmath_1 \jmath_2), (\jmath_2^2)\} &\rightarrow \left\{ \ll 2_{1+Q}^2 0 \gg \right\}, \\ \{(\bar{\jmath}_1^2), -(\bar{\jmath}_2 \bar{\jmath}_1), -(\bar{\jmath}_2^2)\} &\rightarrow \left\{ \ll 2_{1-Q}^0 0 \gg^\dagger \right\}, \quad \text{as } 1 \geq Q \geq -1. \end{aligned} \tag{8}$$

The standard realizations of $\{\mathcal{I}_+, \mathcal{I}_0, \mathcal{I}_-\}$ is retained in the sense that

$$\{\mathcal{I}_+, \mathcal{I}_0, \mathcal{I}_-\} \equiv \{\jmath_1 \bar{\jmath}_2, (\bar{\jmath}_1 \jmath_1 - \bar{\jmath}_2 \jmath_2)/2, \jmath_2 \bar{\jmath}_1\}. \tag{9}$$

4. Conclusions

On realizing these self-associate irreps for contrasting $n \leq 20$ S_n groups as

$$\begin{aligned} \{[\lambda_{SA}]\}(S_{20}) &\quad \{[5^2 4^2 2], \dots\}, \\ (S_{18}) &\equiv \{[5 4^3 1], \dots\}, \\ (S_{17}) &\quad \{[5 5 4 3 2], \dots\} \end{aligned} \tag{10a}$$

compared to the lower subset $n \leq 16$,

$$\begin{aligned} &\quad \{[4^4], [6 5 2^3 1], \dots\}(S_{16}) \\ &\quad \{[4^2 2^2], [5 3 2 1^2], \dots\}(S_{12}) \\ \{[\lambda_{SA}]\}(S_n) &\equiv \{[3^3], [5 1^4]\}(S_9) \\ &\quad \{[3^2 2], [4 2 1^2]\}(S_8) \\ &\quad \{[3 2 1]\}(S_6) \end{aligned} \tag{10b}$$

in which one notes the occurrence of $p \leq 4$ part $\lambda \vdash n$ structure is limited to the latter subset. This observation serves to define the extent of the ‘pseudo-quonic properties’. For all S_n above S_{16} , the $SU2 \times S_n$ algebra over Liouville space reverts to an exclusively bosonic form, typical of the initial mapping of eq. (1).

Hence, the distinction and resemblance of the above Liouville space algebra to more general quonic algebras [1,2] over simple Hilbert space has been clarified by finding the bounds to the ‘pseudo-quonic’ S_n (Liouvillian) algebras from the nature of S_n self-associate irrep structures.

The $\mathbb{Z}(S_n)$ structures of these higher S_n algebras for $12 \leq n \leq 18$ may be found in the work of Ziauddin [17] and others [18], whilst the principal character of S_n has a rather general realization for all n , based on a combinatorial construction, i.e. the hooklength.

Finally, applications of S_n modules, and similarly derived models for $S_n \downarrow \mathcal{G}$ subduced spin algebras, to NMR spin cluster problems has been stressed in several recent works [15,16].

References

- [1] S. Meljanac and A. Perica, *J. Phys.* A27 (1994) 4737.
- [2] O.W. Greenberg, *Physica* A180 (1992) 419.
- [3] F.P. Temme, *Math. Comp. Modelling* (special issue on Role of S_n Group in Physics: MSS II/III) to be published.
- [4] For a corresponding single SU_2 group presentation, see: J.A.R. Coope and R.F. Snider, *J. Math. Phys.* 11 (1970) 1003; J.A.R. Coope, *ibid.*, p. 1591.
- [5] B.C. Sanctuary and T.K. Halstead, *Adv. Magn. Opt. Reson.* 15 (1991) 97.
- [6] F.P. Temme, *Z. Phys.* B88 (1992) 83;
F.P. Temme and J.P. Colpa, *Z. Phys.* B89 (1992) 335;
F.P. Temme, *J. Math. Chem.* 13 (1992) 153; *J. Math. Phys.* 32 (1991) 1638.
- [7] L.C. Biedenharn and J.D. Louck, *Angular Momentum in Quantum Physics*, Vols. 8, (9), in: *Encyclopedia of Mathematics* series (Addison-Wesley/Cambridge Univ. Press, Cambridge, UK, 1985 reprinting).
- [8] F.P. Temme, *Physica* A166 (1990) 676.
- [9] F.P. Temme, *Physica* A198 (1993) 245.
- [10] P.L. Corio, *The Structure of High Resolution NMR Spectra* (Academic Press, New York, 1966).
- [11] K. Balasubramanian, *J. Chem. Phys.* 78 (1983) 6369;
K. Balasubramanian, *Chem. Rev.* 88 (1985) 559; *J. Magn. Reson.* 112 (1995) 182; et loc cit.
- [12] B.E. Sagan, *The Symmetric Group, its Representations, Combinatorial Algorithms and Symmetric Functions* (Wadsworth Math. Publ., CA, 1991).
- [13] J.D. James and A. Kerber, *Representation of the S_n Group* (Addison-Wesley, MA, 1985).
- [14] F.P. Temme, *Chem. Phys. Lett.*, to be published;
F.P. Temme, C.E.J. Mitchell and M.S. Krishnan, *Molec. Phys.* 79 (1993) 953.
- [15] F.P. Temme, *Math. Comp. Modelling* (special issue: Papers I, III) to be published;
F.P. Temme, *Molec. Phys.* (1995) (Papers I/II) in press.
- [16] F.P. Temme, *Physica* A202 (1994) 595; A210 (1994) 435; *Co-ord. Chem. Rev.* 143 (1995) in press.
- [17] M. Ziauddin, *Proc. Lond. Math. Soc.* 42 (1936) 340.
- [18] X. Liu and K. Balasubramanian, *J. Comp. Chem.* 10 (1989) 417;
see also the bibliography cited in an appendix of: G. de B. Robinson, *Representation Theory of the Symmetric Group* (University of Toronto Press, Ontario, 1961).