Complete set of commuting operators for N spins s with rotational and permutational symmetry

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Complete set of commuting operators for N spins s with rotational and permutational symmetry

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Abstract. We consider a system of N spins s with permutational and rotational symmetry. Then the total spin, its z-component and the representation of the permutation group S_N provide good quantum numbers. For $s > \frac{1}{2}$ further operators are needed. The problem can be reduced to a problem of invariants in the enveloping algebra of $SU(2s+1)$ applying a theorem of Weyl. This can be solved explicitly for $s = 1$ using a theory of Judd. For $s = \frac{3}{2}$ two of the four missing operators are determined and for larger s some properties of the additional are shown.

I. Introduction

It is an old problem in quantum mechanics to find a complete set of commuting operators for a given system. In atomic spectroscopy operators which belong to symmetry groups of the system allowed the classification of the electron configurations, the multiplets and terms [1]–[3] (for further references see Wybourne [4]). Later Wigner, Racah [5], Jahn [6], Elliot [7], [8] and others applied group theory to nuclear spectroscopy. In the last fifteen years commuting operators were used to label the basis states of an irreducible representation (IR) of a Lie Group in particle physics [9]–[15].

In this paper we consider the well known system of N spins s with rotational and permutational symmetry. This problem occurs in the framework of nuclear shell models as well as in atomic spectroscopy. It applies directly to small clusters of spins with isotropic and symmetric spin-spin interaction. The problem is that in general the two symmetry groups do not label the states uniquely. The rotation group in the Hilbert space is given by a representation of $SU(2)$. (For integer spin s this is reduced to a representation of $SO(3)$.) In order to use the two symmetry groups (S_N and $SU(2)$), we decompose the representation $\mathscr{D}(S_N \times SU(2), (\mathbb{C}^{2s+1})^{\otimes N})$ of the cartesian product $S_N \times SU(2)$ in the Hilbert space $(\mathbb{C}^{2s+1})^{\otimes N}$ into IR of $S_N \times SU(2)$:

$$\mathscr{D}(S_N \times SU(2), (\mathbb{C}^{2s+1})^{\otimes N}) = \sum_{\mathbf{m},j} \alpha_{\mathbf{m},j}^{(s,N)} P_{\mathbf{m}} \otimes D_j \tag{1}$$

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where $P_{\mathbf{m}}$ is the IR of S_N characterised by the Young's pattern $(m_1, \ldots, m_{2s+1})$, $m_1+\cdots+m_{2s+1}=N$, D_j the $(2s+1)$-dimensional IR of $SU(2)$ and the multiplicity $\alpha_{\mathbf{m},j}^{(s,N)}$ a positive integer. The cases with $\alpha_{\mathbf{m},j}^{(s,N)}<1$ for all $(\mathbf{m}, j)$ are trivial, because a set of permutation operators (see Section II) distinguishes all equivalent IR D_j and S^z labels the states in a IR D_j uniquely. This is the case, as is well known (see Ref [1], chap. v) for $s=\frac{1}{2}$ and arbitrary N:

$$\mathcal{D}(S_N \times SU(2), (\mathbb{C}^2)^{\otimes N}) = \sum_{j=0,\frac{1}{2}}^{N/2} P_{\mathbf{m}} \otimes D_j \tag{2}$$

where $\mathbf{m}=(m_1, m_2)$ with $m_1=(N/2)+j$, $m_2=(N/2)-j$ and j varies in steps of 1.

For $s>\frac{1}{2}$, as we will see the inequality $\alpha_{\mathbf{m},j}^{(s,N)}\leqslant 1$ for all $\mathbf{m}$ and j is generally not true, except for small N, e.g. $N\leqslant 5$ for $s=1$ or $N\leqslant 3$ for $s=\frac{3}{2}$. If $\alpha_{\mathbf{m},j}^{(s,N)}>1$ for at least one $(\mathbf{m}, j)$ then there is a degeneracy.

The numbers $\alpha_{\mathbf{m},j}^{(s,N)}$ are known for $s=1$ and N arbitrary [7] from which follows that for $N\geqslant 6$ there is always a degeneracy. For small $s>1$ and N up to about 10 they are listed in Refs. [6], [16] and [17].

A simple case, where a degeneracy is evident is the system $N=3$, $s\geqslant 2$. Let us consider the decomposition of the tensor product $(D_s)^{\otimes 3}$:

$$D_s^{\otimes 3} = \bigoplus_{j=0,\frac{1}{2}}^{s} (2j+1)\, D_j \bigoplus_{j=s+1}^{3s} (3s+1-j) D_j.$$

Since $\sum \dim (P_{\mathbf{m}})=4$, the $(2s+1)$ IR D_s cannot be distinguished for $s\geqslant 2$. (For the coefficients of the decomposition of $D_s^{\otimes N}$ for arbitrary N, see Ref [18].)

In all the cases with degeneracy the labeling of the states requires further operators, which commute with the representations of S_N and $SU(2)$. Our aim is to construct such operators. Of course the difficulties arise because both, S_N and $SU(2)$ are symmetry groups. If e.g. only $SU(2)$ is a symmetry group, then a complete set of commuting operators is easily found:

$$\vec{S}_{12}^2, \vec{S}_{123}^2, \ldots, \vec{S}_{12\cdots N}^2 \quad \text{and} \quad S_{12\cdots N}^z$$

where

$$\vec{S}_{12\cdots k} := \sum_{i=1}^{k} \vec{S}_i$$

with $\vec{S}_i$ the spin operator at site i.

The problem is first reduced to a problem of invariants in the enveloping algebra [19] of $SU(2s+1)$ applying a theorem of Weyl. Then, using a method of Judd et al. [13], the determination of these invariants is analysed in detail. This allows an explicit solution for $s=1$ and shows some important features for larger s.

II. Reduction of the problem with a theorem of Weyl

Consider the product basis $\{|s, m_1; \ldots ; s, m_N>|\, m_i \in \{-s, \ldots, +s\}\}$ in the Hilbert space $(\mathbb{C}^{2s+1})^{\otimes N}$. Any unitary basis transformation in the Hilbert space $\mathbb{C}^{2s+1}$

of one spin

$$|m'\rangle = \sum_m U_{mm'}\,|m\rangle$$
$$\bar{U}^T U = 1, \qquad \det U = 1$$

induces the N-th Kronecker product representation $\theta_{(1,0\cdots 0)}^{\otimes N}$ of the special unitary group $SU(2s+1)$ in $(\mathbb{C}^{2s+1})^{\otimes N}$

$$|m_1',\ldots,m_N'\rangle = \sum U_{m_1m_1'}\cdots U_{m_Nm_N'}\,|m_1\cdots m_N\rangle. \tag{3}$$

$\theta_{(1,0\cdots 0)}$ is the defining representation of $SU(2s+1)$ by $(2s+1)\times(2s+1)$ matrices.

As before, the representation $\mathscr{D}(S_N\times SU(2s+1),(\mathbb{C}^{2s+1})^{\otimes N})$ of the cartesian product $S_N\times SU(2s+1)$ in the Hilbert space can be decomposed into IR. For this decomposition the fundamental relation of Weyl (ref. [1], chap. v) holds:

$$\mathscr{D}(S_N\times SU(2s+1),(\mathbb{C}^{2s+1})^{\otimes N}) = \sum_{\substack{m_1\geq m_2\geq\cdots\geq m_{2s+1}\geq 0\\ m_1+m_2+\cdots+m_{2s+1}=N}} P_m\otimes\theta_m \tag{4}$$

where $P_{\mathbf{m}}$ and $\theta_{\mathbf{m}}$ are the IR of S_N and $SU(2s+1)$, characterised uniquely by the Young pattern $(m_1,\ldots,m_{2s+1})$.

$$\left(\text{E.g. the dimension of } \theta_{\mathbf{m}} \text{ is: } \dim(\theta_{\mathbf{m}}) = \prod_{i>j}^{2s+1}\frac{(m_j-m_i+i-j)}{(i-j)}.\right)$$

For $s=\frac{1}{2}$, (4) reduces to the well known relation (2).

II.1. *Distinction of the (equivalent) IR θ_m in the Hilbert space*

With the decomposition (4) the role of the group S_N in the labeling problem is clear: It serves to distinguish the ($\dim P_m$ equivalent) IR θ_m of $SU(2s+1)$ uniquely. However S_N cannot label the IR of $SU(2)$ uniquely which is the reason for the degeneracy. There are several possibilities for operators which label the IR $\theta_{\mathbf{m}}$:

(a) The commuting Young operators (ref [1], chap. v, § 13) belonging to the ordered Young tableaus (those in which numbers increase in each line from left to right and in each column from top to bottom). (5a)

(b) The (commuting) projectors on basis states of the IR $P_{\mathbf{m}}$:

$$e_i(\mathbf{m}) = \frac{\dim(P_{\mathbf{m}})}{N!}\sum_{\pi\in S_N}\Gamma_{ii}^{(\mathbf{m})}(\pi^{-1})\cdot\mathscr{D}(\pi) \tag{5b}$$

where $\mathscr{D}$ is an arbitrary representation of S_N and $(\Gamma_{ij}^{(\mathbf{m})})$ are matrix elements of the IR $P_{\mathbf{m}}$. From the orthogonality relations of the matrix elements $\Gamma_{ij}^{(\mathbf{m})}$ follows

$$e_i(\mathbf{m})\,|\mathbf{m}',k\rangle = \delta\mathbf{m},\mathbf{m}'\delta ki\,|\mathbf{m},i\rangle$$

and

$$e(\mathbf{m})\,|\mathbf{m}', k\rangle = \delta\mathbf{m}, \mathbf{m}'\,|\mathbf{m}', k\rangle$$

where $e(\mathbf{m}) = \sum_{i=1}^{\dim P\mathbf{m}} e_i(\mathbf{m})$ and $|\mathbf{m}, i\rangle$ is the i-th basis state in the IR $P_{\mathbf{m}}$. Therefore $e(\mathbf{m})$ and $e_i(\mathbf{m})$ are the projectors on the subspaces of the Hilbert space corresponding to the IR $P_{\mathbf{m}} \otimes \theta_{\mathbf{m}}$ and one of the IR $\theta_{\mathbf{m}}$ respectively.

Example of (b) for $N=3$:

$$e(\,\square\square\square\,) = \tfrac{1}{6}\{\mathbb{1} + P_{12} + P_{13} + P_{23} + P_{12}P_{13} + P_{12}P_{23}\}$$

$$e\left(\begin{array}{c}\square\\\square\\\square\end{array}\right) = \tfrac{1}{6}\{\mathbb{1} - P_{12} - P_{13} - P_{23} + P_{12}P_{13} + P_{12}P_{23}\}$$

$$e\left(\begin{array}{cc}\square&\square\\\square&\end{array}, 1\right) = \tfrac{1}{3}\{\mathbb{1} + \tfrac{1}{2}(P_{12} + P_{13}) - P_{23} - \tfrac{1}{2}(P_{12}P_{13} + P_{12}P_{23})\}$$

$$e\left(\begin{array}{cc}\square&\square\\\square&\end{array}, 2\right) = \tfrac{1}{3}\{\mathbb{1} - \tfrac{1}{2}(P_{12} + P_{13}) + P_{23} - \tfrac{1}{2}(P_{12}P_{13} + P_{12}P_{23})\}$$

where P_{ij} is the representation of the transposition operator for spin i and j.

With the Schrödinger formula [21] for P_{ij}

$$P_{ij} = (-1)^{2s}\left\{\mathbb{1} + \sum_{p=1}^{2s} \frac{(-1)^p}{(p!)^2} \prod_{q=1}^{p} (2(s(s+1) + \vec{s}_i \cdot \vec{s}_j) - q(q-1))\right\}$$

$$= \sum_{n=0}^{2s} A_n(s)(\vec{s}_i \cdot \vec{s}_j)^n \tag{6}$$

the operators (5a) or (5b) can be expressed in terms of spin operators. Examples:

$s = \frac{1}{2}$: $P_{ij} = \frac{1}{2}\mathbb{1} + 2(\vec{s}_i \cdot \vec{s}_j)$,
$s = 1$: $P_{ij} = -\mathbb{1} + (\vec{s}_i \cdot \vec{s}_j) + (\vec{s}_i \cdot \vec{s}_j)^2$,
$s = \frac{3}{2}$: $P_{ij} = -\frac{67}{32}\mathbb{1} - \frac{9}{8}(\vec{s}_i \cdot \vec{s}_j) + \frac{11}{18}(\vec{s}_i \cdot \vec{s}_j)^2 + \frac{2}{9}(\vec{s}_i \cdot \vec{s}_j)^3$.

Let us make two remarks:

(1) For the projectors (5b) the matrices of the IR of S_N are needed in contrast to case (5a).
(2) From (5b) follows that the projectors $e(\mathbf{m}) = \sum_{i=1}^{\dim P_{\mathbf{m}}} e_i(\mathbf{m})$ are linear combinations of the operators $e(\mu) = \sum_{\pi \in (\mu)} \mathcal{D}(\pi)$, where (μ) are the class of S_N. The $e(\mu)$'s commute with all permutations and distinguish inequivalent IR of S_N i.e. they contain the Casimir operators [7] of S_N.

II.2. *Reduced problem*

Restricting $SU(2s+1)$ to the subgroup $SU(2)$, (4) reduces to the decomposition (1):

$$\theta_{\mathbf{m}} = \sum_j \alpha_{\mathbf{m}, j}^{(s, N)} D_j \tag{7}$$

The remaining problem is therefore to find operators, which commute with $\vec{S}^2$, S^z and the operators (5a) or (5b), and which distinguish the IR D_j of $SU(2)$ in the IR $\theta_{\mathbf{m}}$ under $SU(2s+1)|_{SU(2)}$.

It is clear that we can restrict ourselves to operators which are invariant according to S_N and $SU(2)$, i.e. which commute with all permutations and the generators S^x, S^y, S^z of $SU(2)$. Such operators are diagonal in each IR $P_{\mathbf{m}} \otimes D_j$ of $S_N \times SU(2)$, which follows from the Lemma of Schur. Due to a theorem of Weyl (ref [1], chap. v, §1) these (symmetric) operators are elements in the enveloping algebra of the representation of $SU(2s+1)$ in the Hilbert space.

It will be seen that the problem is solved for arbitrary N if a complete set of commuting $SU(2)$-invariant operators in the enveloping algebra of $SU(2s+1)$ is known.

However, for small N, where in (4) only few IR $\theta_{\mathbf{m}}$ appear, a subset may produce enough labels. The reason is that in these cases the further operators of the set are functions of the operators, contained in the subset. E.g. for $N=3$ and $s=2$, as can be seen by inspection, the operator $(\vec{S}_i \cdot \vec{S}_2)^2 + (\vec{S}_2 \cdot \vec{S}_3)^2 + (\vec{S}_1 \cdot \vec{S}_3)^2$ breaks the twofold degeneracy being left in (1), whereas for larger N, 8 operators are needed.

III. $SU(2)$-invariants in the enveloping algebra of $SU(2s+1)$.

Let $H \subset G$ a Lie subgroup of a Lie group G. The problem of finding H-invariant elements in the enveloping algebra of G was analysed in detail and applied to $SO(3) \subset SU(3)$ by Judd et al. [13] and to $SU(2) \times SU(2) \subset SU(4)$ by Quesne [14]. An alternative method was found by Sharp [22] and applied to many cases.

The main result of Judd et al was that an integrity basis [13] for subgroup invariants follows by examining a similar problem in the corresponding polynomial ring. Here an integrity basis may be found by calculating Schur's generating function [13] for the number of independent invariants of a given degree (i.e. the multiplicity of the identity representation). The remaining problem of separating from the integrity basis a complete set of commuting operators has been solved for many cases where there is only one missing operator [13], [22], [23] and for one case only with two missing operators [15].

Peccia and Sharp [24] calculated the number of independent commuting subgroup invariants. In our case their result is:

$$\begin{aligned} n_{\text{comm}} &= \tfrac{1}{2}\{\dim SU(2s+1) - \dim SU(2) + l_{SU(2s+1)} + l_{SU(2)}\} \\ &= 2s^2 + 3s - 1. \end{aligned} \tag{8}$$

l_G is the rank of the group G. This gives $n_{\text{comm}} = 1$ for $s = \tfrac{1}{2}$, 4 for $s = 1$ and 8 for $s = \tfrac{3}{2}$.

From these n_{comm} operators the $2s$ Casimir operators of $SU(2s+1)$ and $\vec{S}^2$, the Casimir operator of $SU(2)$ are known in the canonical basis [9], [10].

Therefore the number of missing operators is:

$$n_{\text{miss}} = \begin{cases} 0 & s = \tfrac{1}{2} \\ 2s^2 + s - 2 & s > \tfrac{1}{2} \end{cases}$$

For $s = 1$ and $s = \tfrac{3}{2}$ this gives 1 and 4 respectively.

Returning to our problem of finding the missing operators for $SU(2) \subset SU(2s+1)$ we follow Judd [13], generalizing to $SU(2s+1)$. The procedure is as follows:

(1) Decompose the adjoint representation of $SU(2s+1)$, restricted to $SU(2)$, into IR of $SU(2)$.
(2) Calculate Schur's generating function to get the number of invariants. The interpretation of the terms leads to the integrity basis.
(3) Find the commutation relations and separate from the integrity basis a set of commuting operators.

(1) The construction of invariants is simplified very much by studying the adjoint representation of $SU(2s+1)$, which is defined as follows:

$$\begin{aligned} Ad_x(x_\mu) &= e^{-i\phi^\alpha x_\alpha} x_\mu \, e^{i\phi^\alpha x_\alpha} \\ &= \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} [(\phi^\alpha x_\alpha), \ldots, [(\phi^\alpha x_\alpha), x_\mu] \cdots] \end{aligned} \tag{10}$$

where $x = e^{-i\phi^\alpha x_\alpha} \in SU(2s+1)$ and x_α's form a basis of the Lie-Algebra $su(2s+1)$.

Ad_x induces in a natural way a representation (also written as Ad) in the enveloping algebra. With (10) it is clear that an element A of this enveloping algebra is

(i) invariant under $SU(2s+1) \Leftrightarrow Ad_x(A) = A$, for all $x \in SU(2s+1)$
(ii) invariant under the subgroup $SU(2) \Leftrightarrow Ad_x(A) = A$, for all $x \in SU(2)$.

In order to obtain $Ad_x(A)$, $x \in SU(2)$ for elements A, which are polynoms in the $X\alpha$'s, it is necessary to study the transformation behavior of the $X\alpha$'s under $Ad|_{SU(2)}$.

Under the restriction $Ad|_{SU(2)}$, $su(2s+1)$ splits into the direct sum [25]–[27]:

$$Ad|_{SU(2)} = D_1 \oplus D_2 \dot{\oplus} \cdots \dot{\oplus} D_{2s}. \tag{11}$$

This follows from (10) which reads in the defining representation of $SU(2s+1)$ as

$$(Ad_{x(\vec{\phi})}(X_\mu))_{ik} = D_{ij}^{(s)}(\vec{\phi}) \cdot \overline{D_{kl}^{(s)}}(\vec{\phi}) \cdot (x_\mu)_{jl}, \qquad x(\vec{\phi}) \in SU(2)$$

where $(D_{ij}^{(s)})$ are the $(2s+1)$-dimensional matrices of the IR D_s.

The corresponding basis elements of (11) are the operator equivalents of the spherical harmonics [25]–[27]. Here we use a cartesian basis, which allows to build invariants very easily. This is not the case for the spherical basis. In the defining representation these elements are:

S^α: usual $(2s+1)x(2s+1)$ spin matrices

$$T^{\alpha\beta} = \tfrac{1}{2}\{S^\alpha S^\beta + S^\beta S^\alpha - \tfrac{2}{3} S^\gamma S^\gamma \delta^{\alpha\beta}\}$$

$$\begin{aligned} Q^{\alpha\beta\gamma} = \frac{1}{3!} \Big\{ & S^\alpha S^\beta S^\gamma + S^\alpha S^\gamma S^\beta + S^\beta S^\alpha S^\gamma + S^\beta S^\gamma S^\alpha + S^\gamma S^\alpha S^\beta + S^\gamma S^\beta S^\alpha \\ & - \frac{2}{5}\left(3 - \frac{1}{s(s+1)}\right)(\delta^{\alpha\beta} S^\gamma + \delta^{\alpha\gamma} S^\beta + \delta^{\beta\gamma} S^\alpha) S^\mu S^\mu \Big\} \end{aligned}$$

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$$V^{\alpha_1 \cdots \alpha_{2s}} = \frac{1}{(2s)!} S^{\alpha_1} \cdots S^{\alpha_{2s}} + \cdots \tag{12}$$

with $V^{\alpha_1\cdots\alpha_k}$ a symmetric homogeneous (traceless) tensor of rank k in the spin operators S^α and $\sum_\alpha V^{\alpha_1\cdots\alpha_{k-2}\alpha\alpha}=0$. $[S^\alpha]$ transforms according to D_1, $[T^{\alpha\beta}]$ according to $D_2,\ldots,$ and the $(2k+1)$-dimensional subspace $[V^{\alpha_1\cdots\alpha_k}]$ according to D_k under $Ad|_{SU(2)}$, since the $V^{\alpha_1\cdots\alpha_k}$'s are the cartesian components of an irreducible tensor operator of rank k under rotations. (Lemma 1 in the appendix)

It is now easy to construct polynomial $SU(2)$-invariants, e.g.: (Lemma 1)

$$S^\alpha T^{\alpha\beta} S^\beta;\ T^{\alpha\beta}T^{\alpha\beta};\ Q^{\alpha\beta\gamma}Q^{\alpha\beta\gamma};\ \varepsilon^{\alpha\beta\gamma}S^\alpha T^{\beta\mu}Q^{\gamma\mu\rho}S^\rho,\ \text{etc.} \tag{13}$$

The problem is furthermore to determine all of them being independent of each other.

Before going to point (2) let us make an application of (12). As shown in the appendix (Lemma 2), it follows from (12):

$$\begin{aligned} S^{\alpha_1}\cdots S^{\alpha_{2s+1}} &= A_{(0)}^{\alpha_1\cdots\alpha_{2s+1}} + A_{(1)}^{\alpha_1\cdots\alpha_{2s+1}\beta_1}S^{\beta_1}+\cdots \\ &\quad + A_{(2s)}^{\alpha_1\cdots\alpha_{2s+1}\beta_1\cdots\beta_{2s}}V^{\beta_1\cdots\beta_{2s}}, \end{aligned} \tag{14}$$

where the $A_{(i)}$'s are invariant tensors under 3-dim. rotations, e.g.:

$$s=1:\ S^\alpha S^\beta S^\gamma = i\varepsilon^{\alpha\gamma\mu}T^{\mu\beta}+\tfrac{1}{2}(\delta^{\alpha\beta}S^\gamma+\delta^{\beta\gamma}S^\alpha)+\frac{i}{3}\,\varepsilon^{\alpha\beta\gamma}1,$$

$$\begin{aligned} s=\tfrac{3}{2}:\ S^\alpha S^\beta S^\gamma S^\delta &= \tfrac{3}{2}i\varepsilon^{\alpha\delta\mu}Q^{\mu\beta\gamma}+\frac{i}{2}\,\varepsilon^{\beta\gamma\mu}Q^{\mu\alpha\delta} \\ &+\tfrac{5}{4}\delta^{\alpha\beta}T^{\gamma\delta}+\tfrac{1}{4}\delta^{\alpha\gamma}T^{\beta\gamma}-\tfrac{3}{4}\delta^{\alpha\delta}T^{\beta\gamma} \\ &+\tfrac{5}{4}\delta^{\gamma\delta}T^{\alpha\beta}+\tfrac{1}{4}\delta^{\beta\delta}T^{\alpha\gamma}+\tfrac{1}{4}\delta^{\beta\gamma}T^{\alpha\delta} \\ &+\tfrac{41}{40}i\varepsilon^{\alpha\beta\mu}\,\delta^{\gamma\delta}S^\mu+\tfrac{7}{40}i\varepsilon^{\alpha\gamma\mu}\,\delta^{\beta\delta}S^\mu \\ &+\tfrac{41}{40}i\varepsilon^{\gamma\delta\mu}\,\delta^{\alpha\beta}S^\mu+\tfrac{7}{40}i\varepsilon^{\beta\delta\mu}\,\delta^{\alpha\gamma}S^\mu \\ &+\tfrac{41}{40}i\varepsilon^{\delta\gamma\mu}\,\delta^{\alpha\delta}S^\mu+\tfrac{7}{40}i\varepsilon^{\delta\alpha\mu}\,\delta^{\beta\gamma}S^\mu \\ &+\tfrac{17}{16}\delta^{\alpha\beta}\,\delta^{\gamma\delta}+\tfrac{7}{16}\delta^{\alpha\gamma}\,\delta^{\beta\delta}+\tfrac{17}{16}\delta^{\alpha\delta}\,\delta^{\beta\gamma}. \end{aligned}$$

(14) generalizes the well known formula

$$\sigma^i\sigma^j=\delta^{ij}+i\varepsilon^{ijk}\sigma^k$$

for the Pauli matrices.

(2) *Generating function.* Generalizing Judds case to $SU(2)\subset SU(2s+1)$ we find for the generating function for the number of independent invariants:

$$\frac{1}{2}\int_0^{2\pi}\sin^2\frac{\theta}{2}F(e^{i\theta};P_1,\ldots,P_{2s})\,d\theta=\sum_{n_i=0}^{\infty}N_{n_1\cdots n_{2s}}(P_1)^{n_1}\cdots(P_{2s})^{n_{2s}} \tag{15}$$

with

$$F(e^{i\theta};P_1,\ldots,P_{2s}) = \frac{1}{(1-e^{i\theta}P_1)(1-P_1)(1-e^{-i\theta}P_1)\cdots(1-e^{i2s\theta}P_{2s})\cdots(1-e^{-i2s\theta}P_{2s})},$$

$N_{n_1\cdots n_{2s}}$ is the number of independent invariants of degrees n_1 in $S^\alpha,\ldots,n_{2s}$ in $V^{\alpha_1\cdots\alpha_{2s}}$.

The evaluation of the integral (15) by residues is easy and gives a sum of

$$\frac{2s(s+1)(2s+1)}{3} \tag{16}$$

rational expressions. But for the interpretation of (15) in terms of an integrity basis [13], (15) must be simplified to only one rational expression [14] or to a sum of rational expressions with positive terms only in the numerator [23]. This can hardly be done for $s>1$ because the number of elements of the integrity basis increases very rapidly with increasing s. Nevertheless, for our problem it is not necessary to know (15) for $s>1$, because a subgroup of $SU(2s+1)$ simplifies the problem.

Remark: From (15) and Judd's theorem mentioned above it follows that all invariants in the enveloping algebra are of the form (13).

(3) *Commutation relations in the basis* (12). As proved in the appendix (Lemma 3, 4) the following holds:

$$[V^{\alpha_1\cdots\alpha_k}, V^{\beta_1\cdots\beta_l}] = i \sum_{j=1}^{\min(2s,\,k+l-1)} A_{(j)}^{\alpha_1\cdots\alpha_k\beta_1\cdots\beta_l\gamma_1\cdots\gamma_j} V^{\gamma_1\cdots\gamma_j} \tag{17}$$

where

(1) the A's are invariant tensors over $\mathbb{R}^3$ under rotations and therefore built from either ε^{ijk} and/or δ^{ij}'s. (18a)

(2) $k+l+j=\text{odd}$, otherwise $A_{(j)}=0$. (18b)

These two properties simplify the explicit determination of the commutation relations and show their striking structure (see Section IV).

A special case of (17) is:

$$[S^\alpha, V^{\beta_1\cdots\beta_l}] = i(\varepsilon^{\alpha\beta_1\gamma}V^{\gamma\beta_2\cdots\beta_l}+\cdots+\varepsilon^{\alpha\beta_l\gamma}V^{\gamma\beta_1\cdots\beta_{l-1}}). \tag{19}$$

(19) follows from

$$e^{-i(\vec{\phi},\vec{S})}V^{\beta_1\cdots\beta_l}e^{i(\vec{\phi},\vec{S})} = R^{-1}_{\beta_1\gamma_1}(\vec{\phi})\cdots R^{-1}_{\beta_l\gamma_l}(\vec{\phi})V^{\gamma_1\cdots\gamma_l} \tag{20}$$

and reflects the fact that the elements $V^{\alpha_1\cdots\alpha_l}$ span the IR D_l. Here $(R_{\alpha\beta}(\vec{\phi}))$ is the 3×3 rotation matrix with axis $\vec{\phi}/|\vec{\phi}|$ and angle ϕ.

Chains: From (18b) follows that the elements $S^\alpha, Q^{\alpha\beta\gamma}, \ldots$ form a sub-Liealgebra of $su(2s+1)$, containing the sub-Liealgebra $su(2)$. The corresponding subgroup is $SO(2s+1)$ for s integer and $Sp(2s+1)$ for s half integer [28]. They form the chains [28]:

$$\begin{array}{ll} SU(2s+1)\supset SO(2s+1)\supset SO(3) & s \text{ integer} \\ SU(2s+1)\supset Sp(2s+1)\supset SU(2) & s \text{ halfinteger} \end{array} \tag{21}$$

Clearly the chains (21) reduce the problem as follows:

1. Find a complete set of commuting operators which are invariant under G in the enveloping algebra of $SU(2s+1)$. Here G is $SO(2s+1)$ for s integer and $Sp(2s+1)$ for s halfinteger.

2. Find a complete set of commuting $SU(2)$ invariant operators in the enveloping algebra of G.

Operators 1 and 2 label uniquely the IR of G in the IR $\theta_{\mathbf{m}}$ of $SU(2s+1)$ and the IR D_j of $SU(2)$ in the IR of G respectively. Of course they commute with each other, because operators 1 commute with all generators of G.

The chains reduce the number of missing operators by the number of Casimir operators of G to:

$$\begin{aligned} SU(2s+1)\supset G:\ n_{\text{miss}} &= \begin{cases} s^2 & s \text{ integer} \\ s^2-s-\frac{3}{4} & s \text{ halfinteger} \end{cases} \\ G\supset SU(2):\ n_{\text{miss}} &= \begin{cases} s^2-2 & s \text{ integer} \\ s^2+s-\frac{7}{4} & s \text{ halfinteger} \end{cases} \end{aligned} \tag{22}$$

which follows similarly as in (9).

Unfortunately this number still increases rapidly with increasing s. In fact even for $s=\frac{3}{2}$ the problem is quite complicated.

So far the general case. Before proceeding to the examples $s=1$ and $s=\frac{3}{2}$ let us outline the application of the results of this chapter to the original system of N spins s.

For the representation of $SU(2s+1)$ in the Hilbert space we obtain as representation of the basis (12) using (3)

$$\begin{aligned} S^\alpha &= \sum_{i=1}^N S_i^\alpha \\ T^{\alpha\beta} &= \sum_{i=1}^N T_i^{\alpha\beta}, \qquad T_i^{\alpha\beta} = \tfrac{1}{2}\{S_i^\alpha S_i^\beta + S_i^\beta S_i^\alpha - \tfrac{2}{3}\delta^{\alpha\beta} S_i^\gamma S_i^\gamma\} \\ &\vdots \\ &\text{etc.} \end{aligned} \tag{23}$$

where S_i^α is the component α of the spin operator at site i. Actually these formulas should be written as:

$$S_{\text{tot}}^\alpha = S^\alpha \otimes \mathbb{1} \otimes \cdots \otimes \mathbb{1} + \mathbb{1} \otimes S^\alpha \otimes \cdots \otimes \mathbb{1} + \cdots + \mathbb{1} \otimes \cdots \otimes \mathbb{1} \otimes S^\alpha$$

etc. In (23) and in the following, for simplicity we omit the extra unit operators.

From (23) we get for the operators of type (13) expressed in spin operators:

$$\begin{aligned} S^\alpha T^{\alpha\beta} S^\beta &= \sum_{i,j,k} (\vec{S}_i \cdot \vec{S}_j)(\vec{S}_j \cdot \vec{S}_k) + \frac{i}{2}(\vec{S}_i \cdot \vec{S}_j \vec{S}_k) - \tfrac{1}{3}\vec{S}_j^2(\vec{S}_i \cdot \vec{S}_k) \\ &= \sum_{i,j,k} (\vec{S}_i \cdot \vec{S}_j)(\vec{S}_j \cdot \vec{S}_k) - \vec{S}^2\{\tfrac{1}{2} + \tfrac{1}{3}Ns(s+1)\}, \\ T^{\alpha\beta} T^{\alpha\beta} &= \sum_{i,j} (\vec{S}_i \cdot \vec{S}_j)^2 + \tfrac{1}{2}\vec{S}^2 - \{\tfrac{1}{3}(s(s+1))^2 + Ns(s+1)\} \cdot \mathbb{1} \\ &\vdots \\ &\text{etc.} \end{aligned} \tag{24}$$

Notice that the degree of invariants in the basis elements (12) is equal to the maximal number of different summation variables on the right hand side of (24).

For the right hand side of (24) the invariance according to $S_N \otimes SU(2)$ is obvious. This suggests a natural way of constructing $S_N \otimes SU(2)$ invariants: Take an invariant of $SU(2)$ (i.e. a polynom in the variables $(\vec{S}_i \cdot \vec{S}_j)$) and make it invariant according to S_N by summation. However it is difficult to obtain an integrity basis on this way. (see Appendix)

IV. Examples

IV.1. $s = 1$ (*1 missing operator*)

This is the case $SO(3) \subset SU(3)$ studied by Judd et al [13]. Let us summarize their results:

The basis (12) is S^α, $T^{\alpha\beta}$ with commutation relation:

$$[S^\alpha, S^\beta] = i\varepsilon^{\alpha\beta\gamma} S^\gamma$$

$$[S^\alpha, T^{\beta\gamma}] = i\{\varepsilon^{\alpha\beta\mu} T^{\mu\gamma} + \varepsilon^{\alpha\gamma\mu} T^{\mu\beta}\}$$

$$[T^{\alpha\beta}, T^{\gamma\delta}] = \frac{i}{4}\{\delta^{\alpha\gamma}\varepsilon^{\beta\delta\mu} + \delta^{\alpha\delta}\varepsilon^{\beta\gamma\mu} + \delta^{\beta\gamma}\varepsilon^{\alpha\delta\mu} + \delta^{\beta\delta}\varepsilon^{\alpha\gamma\mu}\} S^\mu$$

The generating function (15) simplifies to

$$\frac{1 + P_1^3 P_2^3}{(1-P_1^2)(1-P_2^2)(1-P_2^3)(1-P_1^2 P_2)(1-P_1^2 P_2^2)},$$

from which follows as integrity basis:

$$\vec{S}^2,\ T^{\alpha\beta}T^{\alpha\beta},\ T^{\alpha\beta}T^{\beta\gamma}T^{\gamma\alpha},\ X^{(3)} = S^\alpha T^{\alpha\beta} S^\beta,\ X^{(4)} = S^\alpha T^{\alpha\beta} T^{\beta\gamma} S^\gamma,$$

because $\varepsilon^{\alpha\mu\nu} S^\alpha S^\beta S^\gamma T^{\mu\beta} T^{\nu\rho} T^{\rho\gamma} = i/4\,[S^\alpha T^{\alpha\beta} S^\beta, S^\mu T^{\mu\nu} T^{\nu\rho} S^\rho] +$ lower order terms.

The two Casimir operators of $SU(3)$ are

$$C^{(2)} = \vec{S}^2 + 2T^{\alpha\beta}T^{\alpha\beta}$$

$$C^{(3)} = S^\alpha T^{\alpha\beta} S^\beta - \tfrac{4}{3} T^{\alpha\beta} T^{\beta\gamma} T^{\gamma\alpha}.$$

Thus $\vec{S}^2$, $C^{(2)}$, $C^{(3)}$, $X^{(3)}$ or $X^{(4)}$ give a complete set of commuting $SU(2)$-invariants in the enveloping algebra of $SU(3)$.

Applied to the system of N spins $s = 1$, these operators expressed in spin operators are

$$\begin{aligned}
C^{(2)} &= 2\sum_{i,j} P_{ij} - \{\tfrac{16}{3} + 8N - 2N^2\} \cdot \mathbb{1} \\
C^{(3)} &= \tfrac{4}{3} \sum_{i,j,k} P_{ij} P_{jk} + (\text{linear combination of } C^{(2)} \text{ and } \mathbb{1}\,) \\
X^{(3)} &= \sum_{i,j,k} (\vec{S}_i \cdot \vec{S}_j)(\vec{S}_j \cdot \vec{S}_k) - \vec{S}^2\{\tfrac{1}{2} + \tfrac{2}{3}N\} \\
X^{(4)} &= \sum_{i,j,k,l} (\vec{S}_i \cdot \vec{S}_j)(\vec{S}_j \cdot \vec{S}_k)(\vec{S}_k \cdot \vec{S}_l) - X^{(3)}(1 + \tfrac{4}{3}N) - (\tfrac{3}{4} + \tfrac{2}{3}N + \tfrac{4}{9}N^2)\vec{S}^2.
\end{aligned} \tag{25}$$

The Casimir operators of $SU(2s+1)$, which commute with all bases elements of

$SU(2s+1)$ are a generalisation of the Casimir operator $\vec{S}^2$ of $SU(2)$. They distinguish inequivalent IR $\theta_{\mathbf{m}}$ of $SU(2s+1)$ and are unnecessary for the spin system, since operators (5a), (5b) label the IR $\theta_{\mathbf{m}}$ in the Hilbert space uniquely. From (4) follows that they are also Casimir operators of S_N which explains the form of $C^{(2)}$ and $C^{(3)}$ above.

Thus $X^{(3)}$ (or $X^{(4)}$) breaks the degeneracy being left after reduction according to $S_N \otimes SU(2)$ for arbitrary N. The eigenvalues of $X^{(3)}$ or $X^{(4)}$, needed for distinguishing the degenerated IR D_j are listed for many IR $\theta_{\mathbf{m}}$ of $SU(3)$ in ref. [13].

Consider $N=6$, the simplest case of twofold degeneracy. The eigenvalues of $X^{(3)}$ in the subspace $P_{\mathbf{m}} \otimes \theta_{\mathbf{m}}$ for $\mathbf{m}=(4,2,0)$ are

$$\begin{array}{llllll} S: & 4 & 3 & 2 & 2 & 0 \\ X^{(3)}: & 0 & 0 & 3\sqrt{105} & -3\sqrt{105} & 0. \end{array}$$

IV.2. $s=\frac{3}{2}$ (*4 missing operators*)

Here the basis (12) is: S^α, $T^{\alpha\beta}$, $Q^{\alpha\beta\gamma}$. For the commutation relations we obtain:

$$[S^\alpha, S^\beta] = i\varepsilon^{\alpha\beta\gamma} S^\gamma$$

$$[S^\alpha, Q^{\beta_1\beta_2\beta_3}] = i\{\varepsilon^{\alpha\beta_1\gamma} Q^{\gamma\beta_2\beta_3} + \varepsilon^{\alpha\beta_2\gamma} Q^{\gamma\beta_1\beta_3} + \varepsilon^{\alpha\beta_3\gamma} Q^{\gamma\beta_1\beta_2}\},$$

$$[Q^{\alpha_1\alpha_2\alpha_3}, Q^{\beta_1\beta_2\beta_3}] = \left\{\frac{3i}{40} \operatorname{symm}(\delta^{\alpha_2\beta_2}\delta^{\alpha_3\beta_3}\varepsilon^{\alpha_1\beta_1\gamma_1}) - \frac{3i}{200}\operatorname{symm}(\delta^{\alpha_2\alpha_2}\delta^{\beta_2\beta_3}\varepsilon^{\alpha_1\beta_1\gamma_1})\right\} S^{\gamma_1}$$
$$- \left\{\frac{i}{144}\operatorname{symm}(\varepsilon^{\alpha_1\beta_1\gamma_1}\varepsilon^{\alpha_2\beta_2\gamma_2}\varepsilon^{\alpha_3\beta_3\gamma_3}) + \frac{i}{240}\operatorname{symm}(\delta^{\alpha_1\alpha_2}\delta^{\beta_1\gamma_1}\delta^{\beta_2\gamma_2}\varepsilon^{\alpha_3\beta_3\gamma_3})\right.$$
$$\left. + \frac{i}{240}\operatorname{symm}(\delta^{\beta_1\beta_2}\delta^{\alpha_1\gamma_1}\delta^{\alpha_2\gamma_2}\varepsilon^{\alpha_3\beta_3\gamma_3})\right\} Q^{\gamma_1\gamma_2\gamma_3},$$

$$[S^\alpha, T^{\beta_1\beta_2}] = i\{\varepsilon^{\alpha\beta_1\gamma} T^{\gamma\beta_2} + \varepsilon^{\alpha\beta_2\gamma} T^{\gamma\beta_1}\} \tag{26}$$

$$[T^{\alpha_1\alpha_2}, T^{\beta_1\beta_2}] = \tfrac{3}{5} i \operatorname{symm}(\delta^{\alpha_1\beta_1}\varepsilon^{\alpha_2\beta_2\gamma_1}) S^{\gamma_1} + \frac{i}{6}\operatorname{symm}(\delta^{\alpha_2\gamma_2}\delta^{\beta_2\gamma_3}\varepsilon^{\alpha_1\beta_1\gamma_1}) Q^{\gamma_1\gamma_2\gamma_3}$$

$$[T^{\alpha_1\alpha_2}, Q^{\beta_1\beta_2\beta_3}] = \left\{\frac{i}{8}\operatorname{symm}(\delta^{\alpha_1\beta_1}\delta^{\beta_3\gamma_1}\varepsilon^{\alpha_2\beta_2\gamma_2}) - \frac{i}{40}\operatorname{symm}(\delta^{\alpha_1\gamma_1}\delta^{\beta_1\beta_3}\varepsilon^{\alpha_2\beta_2\gamma_2})\right\} T^{\gamma_1\gamma_2},$$

where

$$\operatorname{symm}(A^{\alpha_1\cdots\alpha_k\beta_1\cdots\beta_m\gamma_1\cdots\gamma_n}) := \sum_{\substack{\pi\in S_k\\ \sigma\in S_m\\ \tau\in S_n}} A^{\alpha_{\pi(1)}\cdots\alpha_{\pi(k)}\beta_{\sigma(1)}\cdots\beta_{\sigma(m)}\gamma_{\tau(1)}\cdots\gamma_{\tau(n)}}.$$

Note again the structure explained by (18). For the generating function (15) we obtain

$$\text{Pol (degrees 12 in } P_1,\ 16 \text{ in } P_2 \text{ and 29 in } P_3) \cdot \{1-P_1^2)(1-P_2^2) \cdot (1-P_2^3)(1-P_1^2P_2^2)(1-P_1^2P_2)(1-P_3^2)(1-P_3^4)(1-P_3^6) \times (1-P_3^{10})(1-P_1^3P_3)(1-P_1^2P_3^2)(1-P_1^4P_3^2) \cdot (1-P_2P_3^2)(1-P_2^2P_3^2)(1-P_2^4P_3^2)(1-P_2^3P_3)(1-P_2^3P_3^2)\}^{-1}$$

which shows that the corresponding integrity basis would contain a considerable number of elements. The 10-dimensional Lie-algebra of $Sp(4)$ is generated by the elements S^α and $Q^{\alpha\beta\gamma}$ as is seen from (26).

The first part of the reduced problem is solved easily, because for $SU(4) \supset Sp(4)$, $n_{\text{miss}} = 0$. For the Casimir operators of $SU(4)$ and $Sp(4)$ we obtained:

$$C_{Sp}^2 = \vec{S}^2 + \tfrac{10}{9} Q^{\alpha\beta\gamma} Q^{\alpha\beta\gamma}$$

$$C_{Sp}^4 = \tfrac{33}{20}\widehat{(S^2)}^2 + \widehat{S^\alpha S^\beta S^\gamma Q^{\alpha\beta\gamma}} + \tfrac{35}{18}\widehat{S^2 Q^2} - \tfrac{5}{3}\widehat{S^\alpha S^\beta Q^{\alpha\mu\nu} Q^{\beta\mu\nu}} - \tfrac{25}{9} S^\alpha \widehat{Q^{\alpha\beta\gamma} Q^{\beta\mu\nu} Q^{\gamma\mu\nu}} + \tfrac{125}{27}\widehat{Q^{\alpha\beta\gamma} Q^{\alpha\mu\nu} Q^{\beta\gamma\rho} Q^{\mu\nu\rho}},$$

where $\hat{A}$ is the symmetrized expression, e.g.

$$\widehat{(S^2)}^2 = \tfrac{1}{3}\{S^\alpha S^\alpha S^\beta S^\beta + S^\alpha S^\beta S^\alpha S^\beta + S^\alpha S^\beta S^\beta S^\alpha\},$$

$$\widehat{S^\alpha S^\beta S^\gamma Q^{\alpha\beta\gamma}} = \tfrac{1}{4}\{S^\alpha S^\beta S^\gamma Q^{\alpha\beta\gamma} + S^\alpha S^\beta Q^{\alpha\beta\gamma} S^\gamma + S^\alpha Q^{\alpha\beta\gamma} S^\beta S^\gamma + Q^{\alpha\beta\gamma} S^\alpha S^\beta S^\gamma\}, \text{ etc.};$$

$$C_{SU}^{(2)} = \vec{S}^2 + \tfrac{5}{6} T^{\alpha\beta} T^{\alpha\beta} + \tfrac{10}{9} Q^{\alpha\beta\gamma} Q^{\alpha\beta\gamma}$$

$$C_{SU}^{(3)} = S^\alpha T^{\alpha\beta} S^\beta + \tfrac{5}{3} S^\alpha T^{\beta\gamma} Q^{\alpha\beta\gamma} - \tfrac{25}{9} Q^{\alpha\beta\gamma} T^{\gamma\mu} Q^{\alpha\beta\mu},$$

$$C_{SU}^{(4)} = C_{Sp}^{(4)} + \text{linear combinations of invariants of degree 4 and at least degree 1 in } T.$$

For the second part holds: $n_{\text{miss}} = 2$. Thus, besides $\vec{S}^2$, $C_{Sp}^{(2)}$ and $C_{Sp}^{(4)}$ there exist two independent commuting $SU(2)$ invariants in the enveloping algebra of $Sp(4)$.

The 2 elementary invariants [23] of order 2 and one of order 4 correspond to the Casimir operators of $Sp(4)$ and $SU(2)$. Apart from these no other pair of commuting invariants of fourth order can be built, as can be shown by a direct but tedious computation. Therefore the two operators X_1 and X_2 must be at least of order 4 and 6 respectively.

In conclusion the operators $C_{Sp}^{(2)}$, $C_{Sp}^{(4)}$, $C_{SU}^{(2)}$, $C_{SU}^{(3)}$, $C_{SU}^{(4)}$, $\vec{S}^2$, X_1 and X_2 (these last two still to be found) form a complete set of commuting $SU(2)$ invariants in the enveloping algebra of $SU(4)$.

Note that because $Sp(4) \cong SO(5)$, X_1 and X_2 also solve the second part for $s = 2$.

Expressed in spin operators:

$$C_{SU}^{(2)} = \sum_{i,j} P_{ij} + \text{const} \cdot \mathbb{1},$$

$$C_{SU}^{(3)} = \sum_{i,j,k} P_{ij}P_{jk} + (\text{linear combination of } C_{SU}^{(2)}, \mathbb{1})$$

$$C_{SU}^{(4)} = \sum_{i,j,k,l} P_{ij}P_{jk}P_{kl} + (\text{linear combination of } C_{SU}^{(2)}, (C_{SU}^{(2)})^2, C_{SU}^{(3)}, \mathbb{1})$$

$$C_{Sp}^{(2)} = \tfrac{10}{9}\sum_{i,j} (\vec{S}_i \cdot \vec{S}_j)^3 + \tfrac{20}{9}\sum_{i,j} (\vec{S}_i \cdot \vec{S}_j)^2 - \tfrac{145}{24}\sum_{i,j} (\vec{S}_i \cdot \vec{S}_j) + \text{const}\cdot\mathbb{1}$$

$C_{Sp}^{(4)}$: complicated expression in $(\vec{S}_i \cdot \vec{S}_j)$ similar as $C_{SU}^{(4)}$ (P_{ij} expressed by (6)).

V. Discussion

Applying the theories of Weyl and others, we analysed the problem of finding a complete set of commuting operators for a system of N spins with rotational and permutational symmetry.

The main results are the following:

(1) Besides a set of permutation operators, the operators $\vec{S}^2$ and S^z some commuting $SU(2)$-invariants are used in addition to label the states uniquely. Without their explicit form, which is only feasible for small s, their important features can be seen:

(2) The additional operators are 'scalars' built by the basis elements S^α, $T^{\alpha\beta}, \ldots$ of the Lie algebra $su(2s+1)$ like $T^{\alpha\beta}T^{\alpha\beta}$, $S^\alpha T^{\beta\gamma}Q^{\alpha\beta\gamma}$, etc. Expressed in terms of spin operators they are symmetrized polynoms in the variables $(\vec{S}_i \cdot \vec{S}_j)$. Notice that for $s=\frac{1}{2}$, $(\vec{S}_i \cdot \vec{S}_j) = \{\frac{1}{2}P_{ij} - \frac{1}{4}\cdot\mathbb{1}\}$. Thus, these polynom operators are contained in the operators (5a), (5b).

(3) Physical interpretation: After Fedders and Miles [29] S_i^α, $T_i^{\alpha\beta} \sim S_i^\alpha S_i^\beta, \ldots$ are the components of the dipole moment and quadrupole moment, respectively, of the spin at site i. Thus $S^\alpha = \sum_i S_i^\alpha$, $T^{\alpha\beta} = \sum_i T_i^{\alpha\beta}, \ldots$ are the components of the total dipole moment, total quadrupole moment, ... and the invariants represent the symmetric isotropic interaction of spins via their multipole moments (up to 2^{2s}). With this, the physical meaning of the additional operators is clear. For example, the operator $S^\alpha S^\beta T^{\alpha\beta}$ is the symmetric isotropic dipol-dipol-quadrupol interaction.

(4) For $s=1$ one needs only one additional operator. The one of lowest possible order is:

$$S^\alpha T^{\alpha\beta} S^\beta = \sum_{i,j,k} (\vec{S}_i \cdot \vec{S}_j)(\vec{S}_j \cdot \vec{S}_k) - \vec{S}^2(\tfrac{1}{2} + \tfrac{2}{3}N).$$

for $s=\frac{3}{2}$ two of the 4 additional operators were found.

(5) Finally, the well known formula

$$\sigma^i\sigma^j = \delta^{ij} + i\varepsilon^{ijk}\sigma^k$$

for the Pauli matrices is generalized to spin s. Explicit formulas are given for $s=1$ and $s=\frac{3}{2}$.

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Appendix

Lemma 1. *The subspace* $[V^{\alpha_1\cdots\alpha_k}]$ *of* $su(2s+1)$ *transforms according to* D_k *under* $Ad|_{SU(2)}$.

Proof. (i) From

$$Ad_{x(\vec{\phi})}(S^\alpha)=e^{-i(\vec{\phi},\vec{S})}S^\alpha e^{i(\vec{\phi},\vec{S})}=R^{-1}_{\alpha\beta}(\vec{\phi})S^\beta$$

follows:

$$Ad_{x(\vec{\phi})}(V^{\alpha_1\cdots\alpha_k})=R^{-1}_{\alpha_1\beta_1}(\vec{\phi})\cdots R^{-1}_{\alpha_k\beta_k}(\vec{\phi})V^{\beta_1\cdots\beta_k}$$

with $R(\vec{\phi})$ as in (20). Thus, $[V^{\alpha_1\cdots\alpha_k}]$ is invariant under $Ad|_{SU(2)}$. With the relation above it is also clear that operators (23) are $SU(2)$-invariants.

(ii) The basis transformation from S^x, S^y, S^z to the normal components S^+, S^-, S^0 induces in $[V^{\alpha_1\cdots\alpha_k}]$ the basis transformation from the cartesian components $\{V^{\alpha_1\cdots\alpha_k}\}$ to the normal components $\{V^{++\cdots+},\cdots\}$. E.g.

$$V^{++\cdots+}=A_{+\alpha_1}\cdots A_{+\alpha_k}V^{\alpha_1\cdots\alpha_k}=(S^+)^k$$

with

$$(A_{i\alpha})=\begin{pmatrix}\frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} & 0\\ \frac{1}{\sqrt{2}} & \frac{-i}{\sqrt{2}} & 0\\ 0 & 0 & 1\end{pmatrix},\quad \begin{matrix} i\in\{+,-,0\}\\ \alpha\in\{1,2,3\}\end{matrix}$$

Since $Ad_{x(\phi\vec{e}_z)}(V^{+\cdots+})=e^{-ik\phi}V^{+\cdots+}$ and $\dim[V^{\alpha_1\cdots\alpha_k}]=2k+1$, it follows that $[V^{\alpha_1\cdots\alpha_k}]$ transforms according to D_k under $Ad|_{SU(2)}$ i.e. $\{V^{\alpha_1\cdots\alpha_k}\}$ are the cartesian components of an irreducible tensor operator of rank k.

Lemma 2. *For spin s operators holds*:

$$S^{\alpha_1}S^{\alpha_2}\cdots S^{\alpha_{2s+1}}=\sum_{j=0}^{2s}A_{(j)}^{\alpha_1\cdots\alpha_{2s+1}\beta_1\cdots\beta_j}V^{\beta_1\cdots\beta_j} \tag{A1}$$

where:

(a) $A_{(j)}$ *are symmetric in the* β_i*'s.*

(b) *The $A_{(j)}$'s are invariant tensors with respect to 3-dimensional rotations and therefore built by ε^{ijk} and δ^{ij}'s.*

Proof. (a): Clear.

(b) 1. After (12), the elements $S^{\alpha}, \ldots, V^{\alpha_1 \cdots \alpha_{2s}}$ from a basis of $su(2s+1)$ i.e. the $(2s+1)\times(2s+1)$ hermitian traceless matrices. Thus 1, $S^{\alpha}, \ldots, V^{\alpha_1 \cdots \alpha_{2s}}$ form a basis of the hermitian $(2s+1)\times(2s+1)$ matrices and, equivalently, of the complex $(2s+1)\times(2s+1)$ matrices. In particular the complex matrices $S^{\alpha_1}\cdots S^{\alpha_{2s+1}}$ are linear combinations of these basis elements.

2.

$$e^{-i(\vec{\Phi}\cdot\vec{S})}[s^{\alpha_1}\cdots S^{\alpha_{2s+1}} - \sum_{j=0}^{2s} A_{(j)}^{\alpha_1\cdots\alpha_{2s+1}\beta_1\cdots\beta_j} V^{\beta_1\cdots\beta_j}]e^{i(\vec{\Phi}\cdot\vec{S})} = 0$$

$$= R^{-1}_{\alpha_1\gamma_1}\cdots R^{-1}_{\alpha_{2s+1}\gamma_{2s+1}} S^{\gamma_1}\cdots S^{\gamma_{2s+1}} - \sum_{j=0}^{2s} A_{(j)}^{\alpha_1\cdots\alpha_{2s+1}\beta_1\cdots\beta_j} R^{-1}_{\beta_1\mu_1}\cdots R^{-1}_{\beta_j\mu_j} V^{\mu_1\cdots\mu_j}$$

$$= R^{-1}_{\alpha_1\gamma_1}\cdots R^{-1}_{\alpha_{2s+1}\gamma_{2s+1}} \Big\{ S^{\gamma_1}\cdots S^{\gamma_{2s+1}} - \sum_{j=0}^{2s} R^{-1}_{\rho_1\gamma_1}\cdots R^{-1}_{\rho_{2s+1}\gamma_{2s+1}} R^{-1}_{\beta_1\mu_1}\cdots R^{-1}_{\beta_j\mu_j} \cdot A_{(j)}^{\rho_1\cdots\rho_{2s+1}\beta_1\cdots\beta_j} V^{\mu_1\cdots\mu_j} \Big\}$$

From (A1) for $S^{\gamma_1}\cdots S^{\gamma_{2s+1}}$, property (a) and the fact that $V^{\mu_1\cdots\mu_j}$ form a basis follows:

$$A_{(j)}^{\gamma_1\cdots\gamma_{2s+1}\mu_1\cdots\mu_j} = R_{\gamma_1\rho_1}\cdots R_{\gamma_{2s+1}\rho_{2s+1}} R_{\mu_1\beta_1}\cdots R_{\mu_j\beta_j} A_{(j)}^{\rho_1\cdots\rho_{2s+1}\beta_1\cdots\beta_j}.$$

But each invariant tensor with respect to 3-dimensional rotations is built by ε^{ijk} and δ^{ij}'s. This follows from decomposition (4) with $s=1$ for the tensors of rank N over $\mathbb{C}^3$ and the construction of such tensors using Young tableaus. (Each invariant tensor transforms according to D_0 under $SU(3)|_{SO(3)}$).

(1) Determine

$$\text{symm}\,(S^{\alpha_1}\cdots S^{\alpha_{2s+1}}) = B^{\alpha_1\cdots\alpha_{2s+1}} + B^{\alpha_1\cdots\alpha_{2s+1}\beta_1\beta_2} T^{\beta_1\beta_2} + \cdots$$

where (A2)

$$\text{symm}\,(S^{\alpha_1}\cdots S^{\alpha_k}) = \sum_{\pi\in S_k} S^{\alpha_{\pi(1)}}\cdots S^{\alpha_{\pi(k)}}$$

and the B's are built only by δ's, because the symmetry of the B's does not allow ε-terms.

(2) $S^{\alpha_1}\cdots S^{\alpha_{2s+1}}$ follows from (A2) using the commutation relations.

Lemma 3

$$[V^{\alpha_1\cdots\alpha_k}, V^{\beta_1\cdots\beta_l}] = i\sum_{j=1} A_{(j)}^{\alpha_1\cdots\alpha_k\beta_1\cdots\beta_l\gamma_1\cdots\gamma_j} V^{\gamma_1\cdots\gamma_j} \tag{A3}$$

where:

(a) *$A_{(j)}$'s are symmetric under the exchange of the α's or the β's or the γ's.*

(b) *$A_{(j)}$'s are invariant tensors with respect to 3-dimensional rotations and therefore built by ε^{ijk}'s and δ^{ij}'s.*

Proof:

(a) follows from the symmetry properties of the V's.
(b) follows in exactly the same manner as Lemma 1(b).

Remark. The factor i appears because $[V^\alpha, V^\beta] = -[V^\alpha, V^\beta]$ and the A's are chosen to be real tensors.

Lemma 4.

$k+l+j=$ odd, otherwise $A_{(j)}^{\alpha_1\cdots\alpha_k\beta_1\cdots\beta_l\gamma_1\cdots\gamma_j} = 0$.

Proof. (a) $k=l$: It is clear that the tensors $A_{(j)}$ must be anti-symmetric under $\alpha_i \leftrightarrow \beta_i$ for $i=1,\ldots,k$. From $\sum_\alpha V^{\alpha_1\cdots\alpha_{k-1}\alpha\alpha}=0$ and Lemma 2 it follows that the indices of the factors ε and β of A must belong to different groups of indices α, β or γ. Therefore for $k+l+j=$even the terms $A_{(j)}$ are all of the form:

$$\varepsilon^{\alpha\beta\gamma}\cdots\delta^{\alpha\gamma}\cdots\delta^{\beta\gamma}\cdots\delta^{\alpha\beta}\cdots \tag{A4}$$

with a typical element:

$$\varepsilon^{\alpha_1\beta_1\gamma_1}\cdots\varepsilon^{\alpha_r\beta_r\gamma_r}\delta^{\alpha_{r+1}\gamma_{r+1}}\cdots\delta^{\beta_{r+1}\gamma_l}\cdots\delta^{\alpha_k\beta_k}, \tag{A5}$$

where the number of factors ε is even.

After Lemma 2(a) the corresponding $A_{(j)}$ is obtained by symmetrizing:

$$A = a \sum_{\substack{\text{permutations } \pi,\sigma,\tau \\ \text{of the } \alpha\text{'s} \\ \beta\text{'s and } \gamma\text{'s}}} \varepsilon^{\alpha_{\pi(1)}\beta_{\sigma(1)}\gamma_{\tau(1)}}\cdots\varepsilon^{\alpha_{\pi(\nu)}\beta_{\sigma(\nu)}\gamma_{\tau(\nu)}}\cdots\delta^{\alpha_{\pi(k)}\beta_{\sigma(k)}} \tag{A6}$$

The space of the tensors A, built from tensors of type (A4), is one dimensional (because all tensors of type (A4) appear in A with factors ± 1). But (A6) is symmetric if $\alpha_i \leftrightarrow \beta_i$, because the number of ε's is even. q.e.d.

(b) $k<l$. From (a) follows that the S^α, $Q^{\alpha\beta\gamma},\ldots$ form a sub-Liealgebra of $su(2s+1)$: the sub Liealgebra G, which is $so(2s+1)$ for s integer and $sp(2s+1)$ for s halfinteger. This means that according to $Ad|_G$ the subspace S^α, $Q^{\alpha\beta\gamma},\ldots$ is invariant. Now, Ad and $Ad|_G$ are unitary representations and therefore the complement of an invariant subspace is itself invariant. From (10) it follows that for k odd, l even, on the right side of (12) only $T^{\alpha\beta}$, $V^{\alpha_1\cdots\alpha_4},\ldots$ appear. q.e.d.

Integrity basis for 3 spins s with rotations symmetry. The spin operators S_n^α generate the algebra of the operators in the Hilbert space.

Similar as Judd [13] we consider the corresponding polynomial ring in the indeterminants s_n^α transforming under rotations in the same way as S_n^α. Then, the generating function for $N_{n_1\cdots n_k}$, the number of invariants of degrees n_1 in $s_1^\alpha,\ldots,n_k$ in s_k^α is:

$$\frac{1}{\pi}\int_0^{2\pi} F(e^{i\theta}; A_1,\ldots,A_k)\sin\frac{2\theta}{2}\,d\theta = \sum_{n_i=0}^{\infty} N_{n_1\cdots n_k} A_1^{n_1}\cdots A_k^{n_k}$$

where

$$F(e^{i\theta}; A_1,\ldots,A_k) = \prod_{i=1}^{k}\frac{1}{(1-e^{i\theta}A_i)(1-A_i)(1-e^{-i\theta}A_i)}.$$

For $N=3$ we obtain:

$$\frac{1+A_1A_2A_3}{(1-A_1^2)(1-A_2^2)(1-A_3^2)(1-A_1A_2)(1-A_1A_3)(1-A_2A_3)}$$

From this follows as integrity basis:

$$\vec{s}_1^{\,2}, \vec{s}_2^{\,2}, \vec{s}_3^{\,2}, (\vec{s}_1\cdot\vec{s}_2), (\vec{s}_1\cdot\vec{s}_3), (\vec{s}_2\cdot\vec{s}_3) \quad \text{and} \quad (\vec{s}_1\cdot\vec{s}_2\wedge\vec{s}_3). \tag{A7}$$

For the spins, we have as integrity basis for the $SU(2)$ invariants

$$(\vec{S}_1\cdot\vec{S}_2), (\vec{S}_1\cdot\vec{S}_3) \quad \text{and} \quad (\vec{S}_2\cdot\vec{S}_3), \tag{A8}$$

because

$$\vec{S}_1^{\,2}=s(s+1) \quad \text{and} \quad (\vec{S}_1\cdot\vec{S}_2\wedge\vec{S}_3)=-i[(\vec{S}_1\cdot\vec{S}_3),(\vec{S}_2\cdot\vec{S}_3)]. \tag{A9}$$

Remark For $N>3$, an integrity basis of $SU(2)$ invariants is obtained from (A7) generalizing to $N>3$. It happens to be so because to each $SU(2)$ invariant it corresponds a constant tensor according to rotations. Thus, it follows from (A9) that in the case of the spins, the elements $(\vec{S}_i\cdot\vec{S}_j)$ form an integrity basis of $SU(2)$ invariants.

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