Unitary-group approach to the theory of nuclear magnetic resonance of higher-spin nuclei. II

Pardu S. Ponnapalli and M. Schlesinger
Department of Physics, University of Windsor, Windsor, Ontario N9B 3P4

R. D. Kent
School of Computer Science, University of Windsor, Windsor, Ontario N9B 3P4 Canada
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NMR spectra of A_3 systems with nuclei of spin-1 are treated two different ways. One is the unitary-group approach (UGA), the other is the more conventional spin-product-basis method. This is done to illustrate the efficiency of UGA compared to other methods and to clarify some ambiguities in a recent publication of ours on the subject. An extension of UGA to the case of more than three particles of spin higher than 1 is straightforward.

I. INTRODUCTION

In a series of papers[1,2] Siddall and Flurry (SF) have discussed the use of many-spin basis sets in evaluating matrix elements of the nuclear-magnetic-resonance (NMR) Hamiltonian. Recently, we presented[3] the description of the unitary-group approach (UGA) to the treatment of NMR spectra of A_n systems with nuclei of higher than spin $\frac{1}{2}$. We outlined the use of the UGA to symmetry-adapted basis states of pure σ^N configurations where for an N-particle system σ is the single-particle spin.

Note that the Weyl basis is not an orthogonal one for $U(n)$ (where $n>2$). Matrix elements that we calculate using formulas of Ref. 4 (jawbone) are done so by implicitly assuming that the bases have been orthonormalized using, say, Gram-Schmidt orthogonalization procedures, or using Gelfand bases instead of Weyl's.

In the present work we first make clear the relation between the tensor operators employed in Refs. 1 and 2 on the one hand and Ref. 3 (KS) on the other (Sec. II). Next, we work out a nontrivial example of a three-particle spin-1 system employing the methods of both Refs. 1 and 3 (Sec. III). Finally, we discuss the consequences of the comparison and comment about the merits of the two methods (Sec. IV). As such, this paper should be considered as an extension of Ref. 3.

II. GENERAL THEORY

We begin with the definition of a many-particle operator in terms of single-particle operators

$$I_q^k=\sum_{w=1}^{N} I_q^k(w) , \tag{1}$$

which, in the unitary group approach, has the explicit form

$$I_q^k=\sum_{m,m'=-\sigma}^{\sigma} (-1)^{\sigma-m'}\begin{pmatrix} \sigma & k & \sigma \\ -m & q & m' \end{pmatrix} E_{ij} , \tag{2}$$

where

$$j=\sigma+1-m' ,$$

$$i=\sigma+1-m .$$

The NMR coupling Hamiltonian is defined as

$$H_{\rm NMR}=-\sum_{k=1}^{2\sigma} T^k I^k\cdot I^k , \tag{3}$$

where the T^k are tensor-operator coupling constants.

The scalar product of the unit tensor operators is written

$$\begin{aligned} I^k\cdot I^k &= \sum_{q=-k}^{k} (-1)^q I_q^k I_{-q}^k \\ &= \sum_{w<w'=1}^{N} \sum_{q=-k}^{k} (-1)^q I_q^k(w) I_{-q}^k(w') + \sum_{w>w'=1}^{N} \sum_{q=-k}^{k} (-1)^q I_q^k(w) I_{-q}^k(w') + \sum_{w=1}^{N} \sum_{q=-k}^{k} (-1)^q I_q^k(w) I_{-q}^k(w) . \end{aligned} \tag{4}$$

The first two terms on the right-hand side of Eq. (4) constitute Siddall's operator as defined in Ref. 1, Eq. (4). The third is the self-interaction term and can be shown[5] to be equal to $N/(2\sigma+1)$. The expression is equal to our operator definition in Ref. 3, Eq. (2.3). Note, however, that in order to calculate the matrix elements given in Eqs. (3.2) and (3.3) in that reference, we employed Siddall's operator, since those values were derived for purposes of comparison with his results. The matrix elements for the case of A_4 with spin equal to $\frac{3}{2}$ were calculated using "our" operator[3] since no comparison was intended. In summary, we observe that

$$[I^k \cdot I^k]_{\mathrm{KS}} = 2[I^k \cdot I^k]_{\mathrm{SF}} + \frac{N}{2\sigma+1}\ , \tag{5}$$

where KS indicates Ref. 3 and SF Ref. 1.

III. THREE-PARTICLE SPIN-1 SYSTEM

In this section we treat the case of a three-particle spin-1 system—A_3. The state labeling is based in this case on the group chain $U(3) \supset U(2) \supset U(1)$.

First, we list the tableau basis states in Table I. Next, we list the nonzero matrix elements of the corresponding E_{ij} operators in Table II. These were calculated using the formulas given in Ref. 4.

For the sake of clarity, we give explicit forms for the $I^k \cdot I^k$ operators for the $\sigma = 1$ case:

$$[I' \cdot I']_{\mathrm{KS}} = \tfrac{1}{6}[(E_{11}-E_{33})^2 + (E_{11}-E_{33}) + 2(E_{32}E_{23} + E_{21}E_{12} + E_{12}E_{32} + E_{23}E_{21})]\ , \tag{6}$$

$$[I^2 \cdot I^2]_{\mathrm{KS}} = \tfrac{1}{30}[(E_{11} - 2E_{22} + E_{33})^2] + \tfrac{1}{10}[E_{11} - E_{33} + 2(E_{23}E_{32} + E_{12}E_{21} - E_{32}E_{12} - E_{21}E_{23}) + 2(E_{31}E_{13})]\ . \tag{7}$$

In Table III we list the matrix (elements) of the $[I' \cdot I']_{\mathrm{SF}}$ operator, while in Table IV we list the same for the $[I^2 \cdot I^2]_{\mathrm{SF}}$ operator in the A_3 case. For the partition $[\lambda] = [1^3]$, we have the values

$$\left\langle\begin{smallmatrix}1\\2\\3\end{smallmatrix}\right| [I' \cdot I']_{\mathrm{SF}} \left|\begin{smallmatrix}1\\2\\3\end{smallmatrix}\right\rangle = \left\langle\begin{smallmatrix}1\\2\\3\end{smallmatrix}\right| [I^2 \cdot I^2]_{\mathrm{SF}} \left|\begin{smallmatrix}1\\2\\3\end{smallmatrix}\right\rangle = -\tfrac{1}{2}\ . \tag{8}$$

TABLE I. Tableau states of $\sigma^{[\lambda]}$ for $\sigma = 1$, including correlation with $R(3)$.

$[\lambda]$	M	Tableau states	ΔQ_M	$R(3)$ correlation
[3]	3	$\lvert 111\rangle$	1	F
	2	$\lvert 112\rangle$	0	F
	1	$\lvert 113\rangle$, $\lvert 122\rangle$	1	P,F
	0	$\lvert 123\rangle$, $\lvert 222\rangle$	0	P,F
	-1	$\lvert 133\rangle$, $\lvert 223\rangle$	1	P,F
	-2	$\lvert 233\rangle$	0	F
	-3	$\lvert 333\rangle$	1	F
[21]	2	$\left\lvert\begin{smallmatrix}1&1\\2\end{smallmatrix}\right\rangle$	1	D
	1	$\left\lvert\begin{smallmatrix}1&1\\3\end{smallmatrix}\right\rangle$, $\left\lvert\begin{smallmatrix}1&2\\3\end{smallmatrix}\right\rangle$	1	D,P
	0	$\left\lvert\begin{smallmatrix}1&2\\3\end{smallmatrix}\right\rangle$, $\left\lvert\begin{smallmatrix}1&3\\2\end{smallmatrix}\right\rangle$	0	D,P
	-1	$\left\lvert\begin{smallmatrix}1&3\\3\end{smallmatrix}\right\rangle$, $\left\lvert\begin{smallmatrix}2&2\\3\end{smallmatrix}\right\rangle$	1	D,P
	-2	$\left\lvert\begin{smallmatrix}2&3\\3\end{smallmatrix}\right\rangle$	1	D
$[1^3]$	0	$\left\lvert\begin{smallmatrix}1\\2\\3\end{smallmatrix}\right\rangle$	1	S

In these tables the dots represent a zero-value matrix element.

The results can be compared with values obtained by us using methods of Ref. 1 in the following fashion. First we transform from tableau states to states of definite total spin $\lvert[\lambda]SM\rangle$. For the partition [3], we find

$$\begin{aligned}
&\lvert[3]33\rangle = \lvert 111\rangle\ ,\\
&\lvert[3]32\rangle = \lvert 112\rangle\ ,\\
&\lvert[3]31\rangle = 1/\sqrt{5}\,\lvert 113\rangle + 2/\sqrt{5}\,\lvert 122\rangle\ ,\\
&\lvert[3]30\rangle = \sqrt{3/5}\,\lvert 123\rangle + \sqrt{2/5}\,\lvert 222\rangle\ ,\\
&\lvert[3]3-1\rangle = \sqrt{1/5}\,\lvert 133 + \sqrt{4/5}\,\lvert 223\rangle\ ,
\end{aligned} \tag{9}$$

TABLE II. One-body operator matrix elements for E_{ij} for $i = j + q$.

1	1	2
$\langle 112\lvert E_{21}\rvert 111\rangle = \sqrt{3}$	$\left\langle\begin{smallmatrix}1&1\\3\end{smallmatrix}\right\rvert E_{32} \left\lvert\begin{smallmatrix}1&1\\2\end{smallmatrix}\right\rangle = 1$	$\langle 113\lvert E_{31}\rvert 111\rangle = \sqrt{3}$
$\langle 122\lvert E_{21}\rvert 112\rangle = 2$	$\left\langle\begin{smallmatrix}1&2\\2\end{smallmatrix}\right\rvert E_{21} \left\lvert\begin{smallmatrix}1&1\\2\end{smallmatrix}\right\rangle = 1$	$\langle 123\lvert E_{31}\rvert 112\rangle = \sqrt{2}$
$\langle 113\lvert E_{32}\rvert 112\rangle = 1$	$\left\langle\begin{smallmatrix}1&2\\3\end{smallmatrix}\right\rvert E_{32} \left\lvert\begin{smallmatrix}1&2\\2\end{smallmatrix}\right\rangle = 1/\sqrt{2}$	$\langle 133\lvert E_{31}\rvert 11\rangle = 2$
$\langle 123\lvert E_{21}\rvert 113\rangle = \sqrt{2}$	$\left\langle\begin{smallmatrix}1&3\\2\end{smallmatrix}\right\rvert E_{32} \left\lvert\begin{smallmatrix}1&2\\2\end{smallmatrix}\right\rangle = \sqrt{3/2}$	$\langle 233\lvert E_{31}\rvert 122\rangle = 1$
$\langle 222\lvert E_{21}\rvert 122\rangle = \sqrt{3}$	$\left\langle\begin{smallmatrix}1&2\\3\end{smallmatrix}\right\rvert E_{21} \left\lvert\begin{smallmatrix}1&1\\3\end{smallmatrix}\right\rangle = \sqrt{2}$	$\langle 233\lvert E_{31}\rvert 123\rangle = \sqrt{2}$
$\langle 123\lvert E_{32}\rvert 122\rangle = 2$	$\left\langle\begin{smallmatrix}2&2\\3\end{smallmatrix}\right\rvert E_{21} \left\lvert\begin{smallmatrix}1&2\\3\end{smallmatrix}\right\rangle = \sqrt{2}$	$\left\langle\begin{smallmatrix}1&2\\3\end{smallmatrix}\right\rvert E_{31} \left\lvert\begin{smallmatrix}1&1\\2\end{smallmatrix}\right\rangle = -1/\sqrt{2}$
$\langle 133\lvert E_{32}\rvert 123\rangle = 2$	$\left\langle\begin{smallmatrix}1&3\\3\end{smallmatrix}\right\rvert E_{32} \left\lvert\begin{smallmatrix}1&2\\3\end{smallmatrix}\right\rangle = 1/\sqrt{2}$	$\left\langle\begin{smallmatrix}1&3\\2\end{smallmatrix}\right\rvert E_{31} \left\lvert\begin{smallmatrix}1&1\\2\end{smallmatrix}\right\rangle = \sqrt{3/2}$
$\langle 223\lvert E_{21}\rvert 123\rangle = 2$	$\left\langle\begin{smallmatrix}1&3\\3\end{smallmatrix}\right\rvert E_{32} \left\lvert\begin{smallmatrix}1&3\\2\end{smallmatrix}\right\rangle = \sqrt{3/2}$	$\left\langle\begin{smallmatrix}1&3\\3\end{smallmatrix}\right\rvert E_{31} \left\lvert\begin{smallmatrix}1&1\\3\end{smallmatrix}\right\rangle = 1$
$\langle 223\lvert E_{32}\rvert 222\rangle = 3$	$\left\langle\begin{smallmatrix}2&3\\3\end{smallmatrix}\right\rvert E_{21} \left\lvert\begin{smallmatrix}1&3\\3\end{smallmatrix}\right\rangle = 1$	$\left\langle\begin{smallmatrix}2&2\\3\end{smallmatrix}\right\rvert E_{31} \left\lvert\begin{smallmatrix}1&2\\2\end{smallmatrix}\right\rangle = -1$
$\langle 233\lvert E_{21}\rvert 133\rangle = 1$	$\left\langle\begin{smallmatrix}2&3\\3\end{smallmatrix}\right\rvert E_{32} \left\lvert\begin{smallmatrix}2&2\\3\end{smallmatrix}\right\rangle = 1$	$\left\langle\begin{smallmatrix}2&3\\3\end{smallmatrix}\right\rvert E_{31} \left\lvert\begin{smallmatrix}1&2\\3\end{smallmatrix}\right\rangle = 1/\sqrt{2}$
$\langle 233\lvert E_{32}\rvert 223\rangle = 2$	$\left\langle\begin{smallmatrix}1\\2\\3\end{smallmatrix}\right\rvert E_{ij} \left\lvert\begin{smallmatrix}1\\2\\3\end{smallmatrix}\right\rangle \equiv 0$	$\left\langle\begin{smallmatrix}2&3\\3\end{smallmatrix}\right\rvert E_{31} \left\lvert\begin{smallmatrix}1&3\\2\end{smallmatrix}\right\rangle = -\sqrt{3/2}$
$\langle 333\lvert E_{32}\rvert 233\rangle = 3$		

TABLE III. Matrix (element) of $[I'\cdot I']_{\mathrm{SF}}$. (a) Operator for $[\lambda]=[3]$. (b) Operator for $[\lambda]=[21]$.

(a)

$\vert 111\rangle$	$\vert 122\rangle$	$\vert 113\rangle$	$\vert 122\rangle$	$\vert 123\rangle$	$\vert 222\rangle$	$\vert 133\rangle$	$\vert 223\rangle$	$\vert 233\rangle$	$\vert 333\rangle$
$\frac{1}{2}$	.	.	.	.	.	.	.	.	.
	$\frac{1}{2}$	.	.	.	.	.	.	.	.
		$-\frac{1}{6}$	$\frac{1}{3}$	.	.	.	.	.	.
			$\frac{1}{3}$	.	.	.	.	.	.
				$\frac{1}{6}$	$1/\sqrt{6}$	.	.	.	.
					.	.	.	.	.
						$-\frac{1}{6}$	$\frac{1}{3}$	.	.
							$\frac{1}{3}$	.	.
								$\frac{1}{2}$	.
									$\frac{1}{2}$

(b)

$\vert {}^{11}_{2}\rangle$	$\vert {}^{11}_{3}\rangle$	$\vert {}^{12}_{2}\rangle$	$\vert {}^{12}_{3}\rangle$	$\vert {}^{13}_{2}\rangle$	$\vert {}^{13}_{3}\rangle$	$\vert {}^{22}_{3}\rangle$	$\vert {}^{23}_{3}\rangle$
.	.	.	.	.	.	.	.
	$-\frac{1}{6}$	$\frac{1}{6}$	.	.	.	.	.
		$-\frac{1}{6}$	.	.	.	.	.
			$-\frac{1}{12}$	$1/4\sqrt{3}$	.	.	.
				$-\frac{1}{4}$	.	.	.
					$-\frac{1}{6}$	$\frac{1}{6}$	.
						$-\frac{1}{6}$	.
							0

$$|[3]3-2\rangle = |233\rangle\,,$$
$$|[3]3-3\rangle = |333\rangle\,,$$
$$|[3]11\rangle = 2/\sqrt{5}\,|113\rangle - 1/\sqrt{5}\,|122\rangle\,,$$
$$|[3]10\rangle = \sqrt{2/5}\,|123\rangle - \sqrt{3/5}\,|222\rangle\,,$$
$$|[3]1-1\rangle = 2/\sqrt{5}\,|133\rangle - 1/\sqrt{5}\,|223\rangle\,.$$

These lead to the following matrix elements:

$$\langle [3]3M\,|\,[I'\cdot I']_{\mathrm{SF}}\,|\,[3]3M\rangle = \tfrac{1}{2}\,,$$
$$\langle [3]3M\,|\,[I^2\cdot I^2]_{\mathrm{SF}}\,|\,[3]3M\rangle = \tfrac{1}{10}\,, \tag{10}$$

where $-3\leq M\leq 3$; and

$$\langle [3]1M\,|\,[I'\cdot I']_{\mathrm{SF}}\,|\,[3]1M\rangle = -\tfrac{1}{3}\,,$$
$$\langle [3]\,|\,M\,|\,[I^2\cdot I^2]_{\mathrm{SF}}\,|\,[3]1M = \tfrac{3}{5}\,,$$

where $-1\leq M\leq 1$.

Now, for the partition [21], we find similarly the transformation coefficients:

$$|[21]22\rangle = |{}^{11}_{2}\rangle\,,$$
$$|[21]21\rangle = 1/\sqrt{2}\,|{}^{11}_{3}\rangle + 1/\sqrt{2}\,|{}^{12}_{2}\rangle\,,$$
$$|[21]20\rangle = \sqrt{3/2}\,|{}^{12}_{3}\rangle + 1/2\,|{}^{13}_{2}\rangle\,,$$
$$|[21]2-1\rangle = 1/\sqrt{2}\,|{}^{13}_{3}\rangle + 1/\sqrt{2}\,|{}^{22}_{3}\rangle\,,$$
$$|[21]2-2\rangle = |{}^{23}_{3}\rangle\,, \tag{11}$$
$$|[21]11\rangle = 1/\sqrt{2}\,|{}^{11}_{3}\rangle - 1/\sqrt{2}\,|{}^{12}_{2}\rangle\,,$$
$$|[21]10\rangle = 1/2\,|{}^{12}_{3}\rangle - \sqrt{3/4}\,|{}^{13}_{2}\rangle\,,$$
$$|[21]1-1\rangle = -1/\sqrt{2}\,|{}^{13}_{3}\rangle + 1/\sqrt{2}\,|{}^{22}_{3}\rangle\,.$$

These lead to the following matrix elements:

$$\langle [21]2M\,|\,[I'\cdot I']_{\mathrm{SF}}\,|\,[21]2M\rangle \equiv 0\,,$$
$$\langle [21]2M\,|\,[I^2\cdot I^2]_{\mathrm{SF}}\,|\,[21]2M\rangle = -\tfrac{1}{5}\,,$$

where $-2\leq M\leq 2$; and (11′)

$$\langle [21]1M\,|\,[I'\cdot I']_{\mathrm{SF}}\,|\,[21]1M\rangle = -\tfrac{1}{3}\,,$$
$$\langle [21]1M\,|\,[I^2\cdot I^2]_{\mathrm{SF}}\,|\,[21]1M\rangle = 0\,,$$

where $-1\leq M\leq 1$.

TABLE IV. Matrix (elements) of $[I^2 \cdot I^2]_{\mathrm{SF}}$. (a) Operator for $[\lambda]=[3]$. (b) Operator for $[\lambda]=[21]$.

(a)

$\|111\rangle$	$\|112\rangle$	$\|113\rangle$	$\|122\rangle$	$\|123\rangle$	$\|222\rangle$	$\|133\rangle$	$\|223\rangle$	$\|233\rangle$	$\|333\rangle$
$\frac{1}{10}$	.	.	.	.	.	.	.	.	.
	$\frac{1}{10}$	.	.	.	.	.	.	.	.
		$\frac{1}{2}$	$-\frac{1}{5}$	.	.	.	.	.	.
			$\frac{1}{5}$	.	.	.	.	.	.
				$\frac{3}{10}$	$-\sqrt{6/100}$	.	.	.	.
					$\frac{2}{5}$	.	.	.	.
						$\frac{1}{2}$	$-\frac{1}{5}$	.	.
							$\frac{1}{5}$	.	.
								$\frac{1}{10}$	.
									$\frac{1}{10}$

(b)

$\|{}^{11}_{2}\rangle$	$\|{}^{11}_{3}\rangle$	$\|{}^{12}_{2}\rangle$	$\|{}^{12}_{3}\rangle$	$\|{}^{13}_{2}\rangle$	$\|{}^{13}_{3}\rangle$	$\|{}^{22}_{3}\rangle$	$\|{}^{23}_{3}\rangle$
$-\frac{1}{5}$	.	.	.	.	.	.	.
	$-\frac{1}{10}$	$-\frac{1}{10}$	.	.	.	.	.
		$-\frac{1}{10}$	.	.	.	.	.
			$-\frac{3}{20}$	$-\sqrt{3/20}$	.	.	.
				$-\frac{1}{20}$	.	.	.
					$-\frac{1}{10}$	$-\frac{1}{10}$	.
						$-\frac{1}{10}$	.
							$-\frac{1}{5}$

IV. THREE-PARTICLE SPIN-1 SYSTEM, AN ALTERNATIVE APPROACH

In this section we wish to verify the results of the preceding section using the "spin-product basis" approach as outlined in Ref. 1.

Here we express the states in terms of eigenvectors of the form $|\sigma m_1;\sigma m_2;\sigma m_3\rangle$, where m_i is the spin magnetic quantum number of the ith particle. This we do in order to compare with the method of Ref. 1, using also the definition of the $I^k \cdot I^k$ operators in that reference. These basis states are referred to in Siddall's work as spin product bases.

Now, Weyl basis states will be expressed as linear combination of the spin product bases:

$$\begin{aligned}|[3]i_1i_2i_3\rangle = \tfrac{1}{6}(\,&|m_1m_2m_3\rangle + |m_3m_1m_2\rangle + |m_2m_1m_3\rangle \\ &+ |m_2m_3m_1\rangle + |m_3m_2m_1\rangle \\ &+ |m_1m_3m_2\rangle)\,, \end{aligned} \tag{12}$$

where $1 \le i_1 i_2 i_3 \le 3$ and $i_\alpha = \sigma + 1 - m_\alpha$.

These states happen to be already orthogonal. In order to normalize them we write

$$\begin{aligned}
|[3]111\rangle &= |111\rangle\,,\\
|[3]112\rangle &= \frac{1}{\sqrt{3}}(|110\rangle + |011\rangle + |101\rangle)\,,\\
|[3]113 &= \frac{1}{\sqrt{3}}(|11-1\rangle + |1-11\rangle + |-111\rangle)\,,\\
|[3]122\rangle &= \frac{1}{\sqrt{3}}(|100\rangle + |010\rangle + |001\rangle)\,,\\
|[3]123\rangle &= \frac{1}{\sqrt{6}}(|10-1\rangle + |-110\rangle + |01-1\rangle\\
&\qquad + |0-11\rangle + |-101\rangle + |1-10\rangle)\,,\\
|[3]222\rangle &= |000\rangle\,,\\
|[3]133\rangle &= \frac{1}{\sqrt{3}}(|-1-11\rangle + |-11-1\rangle + |1-1-1\rangle)\,,\\
|[3]223\rangle &= \frac{1}{\sqrt{3}}(|-100\rangle + |00-1\rangle + |0-10\rangle)\,,\\
|[3]233\rangle &= \frac{1}{\sqrt{3}}(|-1-10\rangle + |0-1-1\rangle + |-10-1\rangle)\,,\\
|[3]333\rangle &= |-1-1-1\rangle\,.
\end{aligned} \tag{13}$$

For the partition [21] we have two sets of basis functions corresponding to two different irreducible representations of $S^{[21]}_{2\sigma+1}$ but belonging to the same irreducible representation $\Gamma^{[21]}_{2\sigma+1}$ of $U(2\sigma+1)$. These are

$$
\begin{aligned}
|{}^{i_1 i_2}_{i_3}\rangle^{(1)} &= \tfrac{1}{3}(|i_1 i_2 i_3\rangle - |i_3 i_2 i_1\rangle + |i_2 i_1 i_3\rangle - |i_3 i_1 i_2\rangle)\,,\\
|{}^{i_1 i_2}_{i_3}\rangle^{(2)} &= \tfrac{1}{3}(|i_1 i_2 i_3\rangle - |i_2 i_1 i_3\rangle + |i_3 i_2 i_1\rangle - |i_2 i_3 i_1\rangle)\,.
\end{aligned}
\tag{14}
$$

We choose the first set as our basis states and obtain upon normalization

$$
\begin{aligned}
|{}^{11}_{2}\rangle &= \frac{1}{\sqrt{2}}(|110\rangle - |011\rangle)\,,\\
|{}^{11}_{3}\rangle &= \frac{1}{\sqrt{2}}(|11-1\rangle - |-111\rangle)\,,\\
|{}^{12}_{2}\rangle &= \frac{1}{\sqrt{2}}(|100\rangle - |001\rangle)\,,\\
|{}^{12}_{3}\rangle^* &= \tfrac{1}{2}(|10-1\rangle - |-101\rangle + |01-1\rangle - |-110\rangle)\,,\\
|{}^{13}_{2}\rangle^* &= \tfrac{1}{2}(|1-10\rangle + |-110\rangle - |0-11\rangle - |01-1\rangle)\,,\\
|{}^{13}_{3}\rangle &= \frac{1}{\sqrt{2}}(|1-1-1\rangle - |-1-11\rangle)\,,\\
|{}^{22}_{3}\rangle &= \frac{1}{\sqrt{2}}(|00-1\rangle - |-100\rangle)\,,\\
|{}^{23}_{3}\rangle &= \frac{1}{\sqrt{2}}(|01-1\rangle - |-1-10\rangle)\,.
\end{aligned}
\tag{15}
$$

We have labeled $|{}^{12}_{3}\rangle^*$ and $|{}^{13}_{2}\rangle^*$ with an asterisk. This is done in order to illustrate the fact that the Weyl bases are not in general orthogonal. We set $|{}^{12}_{3}\rangle^* = |{}^{12}_{3}\rangle$ and orthogonalize $|{}^{13}_{2}\rangle^*$ using the Gram-Schmidt procedure. We then have

$$
\begin{aligned}
|{}^{12}_{3}\rangle = |{}^{12}_{3}\rangle^* &= \tfrac{1}{2}(|10-1\rangle - |-101\rangle\\
&\quad + |01-1\rangle - |-110\rangle)\,,\\
|{}^{13}_{2}\rangle &= \frac{1}{\sqrt{8}}(|-110\rangle - |01-1\rangle + 2|0-11\rangle\\
&\quad + |10-1\rangle - |-101\rangle)\,.
\end{aligned}
\tag{16}
$$

Finally, we have for the partition $[1^3]$,

$$
\begin{aligned}
|[1^3]\begin{smallmatrix}1\\2\\3\end{smallmatrix}\rangle &= \frac{1}{\sqrt{6}}(|10-1\rangle + |-110\rangle - |1-10\rangle - |01-1\rangle\\
&\quad + |0-11\rangle - |-101\rangle)\,,
\end{aligned}
\tag{17}
$$

We substitute into Eqs. (9) and (11) and noting

$$
|[1^3]00\rangle = |[1^3]\begin{smallmatrix}1\\2\\3\end{smallmatrix}\rangle
$$

we obtain, for $S=3$,

$$
\begin{aligned}
|[3]33\rangle &= |111\rangle\,,\\
|[3]32\rangle &= \frac{1}{\sqrt{3}}(|110\rangle + |011\rangle + |101\rangle)\,,\\
|[3]31\rangle &= \frac{1}{\sqrt{15}}(|11-1\rangle + |1-11\rangle + |-111\rangle + 2|100\rangle\\
&\quad + 2|010\rangle + 2|001\rangle)\,,\\
|[3]30\rangle &= \frac{1}{\sqrt{10}}(2|000\rangle + |10-1\rangle + |-110\rangle + |01-1\rangle\\
&\quad + |0-11\rangle + |-101\rangle + |1-10\rangle)\,.
\end{aligned}
\tag{18}
$$

One obtains similar expressions for negative M values. For $S=1$ we have

$$
\begin{aligned}
|[3]11\rangle &= \frac{1}{\sqrt{15}}(2|11-1\rangle + 2|1-11\rangle + 2|-111\rangle\\
&\quad - |100\rangle - |010\rangle - |001\rangle)\,,\\
|[3]10\rangle &= \frac{1}{\sqrt{15}}(|10-1\rangle + |-110\rangle + |01-1\rangle\\
&\quad + |0-11\rangle + |-101\rangle\\
&\quad + |1-10\rangle - 3|000\rangle)\,.
\end{aligned}
\tag{19}
$$

For the [21] partition and $S=2$ we have again, for positive M only,

$$
\begin{aligned}
|[21]22\rangle &= \frac{1}{\sqrt{2}}(|110\rangle - |011\rangle)\,,\\
|[21]21\rangle &= \tfrac{1}{2}(|11-1\rangle - |-111\rangle + |100\rangle - |001\rangle)\,,\\
|[21]20\rangle &= \frac{1}{\sqrt{12}}(2|10-1\rangle - 2|-101\rangle + |01-1\rangle\\
&\quad - |-110\rangle + |1-10\rangle - |0-11\rangle)\,.
\end{aligned}
\tag{20}
$$

For $S=1$ we write

$$
\begin{aligned}
|[21]11\rangle &= \tfrac{1}{2}(|11-1\rangle - |-111\rangle - |100\rangle + |001\rangle)\,,\\
|[21]10\rangle &= \tfrac{1}{2}(|01-1\rangle - |-110\rangle\\
&\quad + |1-10\rangle - |0-11\rangle)\,.
\end{aligned}
\tag{21}
$$

For the partition $[1^3]$ there is the one expression,

$$
\begin{aligned}
|[1^3]00\rangle &= \frac{1}{\sqrt{6}}(|10-1\rangle - |1-10\rangle - |01-1\rangle\\
&\quad + |0-11\rangle + |-110\rangle - |-101\rangle)\,.
\end{aligned}
\tag{22}
$$

Following Eq. (5) of Ref. 1, we write for the matrix elements of the $I^k \cdot I^k$ operators

$$\langle \sigma m_1;\sigma m_2;\sigma m_3 \,|\, I^k\cdot I^k \,|\, \sigma m_1';\sigma m_2';\sigma m_3' \rangle = \sum_{i<j=1}^{3} \sum_{q=-k}^{k} (-1)^q (-1)^{2\sigma-m_i-m_j} \begin{pmatrix} \sigma & k & \sigma \\ -m_i & q & m_i' \end{pmatrix} \begin{pmatrix} \sigma & k & \sigma \\ -m_j & -q & m_j' \end{pmatrix} . \tag{23}$$

We have calculated[5] the matrix elements of these operators for $k=1$ and $k=2$ using the above basis functions and found full agreement with the results of Sec. III A. A few sample calculations are as follows.

For the partition $[1^3]$ we have

$$\begin{aligned} \langle [1^3]00 \,|\, I'\cdot I' \,|\, [1^3]00 \rangle = \tfrac{1}{6}(& \langle 10-1 | I'\cdot I' | 10-1 \rangle + \langle 1-10 | I'\cdot I' | 1-10 \rangle + \langle 01-1 | I'\cdot I' | 01-1 \rangle \\ & + \langle 0-11 | I'\cdot I' | 0-11 \rangle + \langle -110 | I'\cdot I' | -110 \rangle + \langle -101 | I'\cdot I' | -101 \rangle \\ & - 2\langle 10-1 | I'\cdot I' | 1-10 \rangle - 2\langle 10-1 | I'\cdot I' | 01-1 \rangle + 2\langle 10-1 | I'\cdot I' | -110 \rangle \\ & - 2\langle 10-1 | I'\cdot I' | -101 \rangle + 2\langle 1-10 | I'\cdot I' | 01-1 \rangle - 2\langle 1-10 | I'\cdot I' | 0-11 \rangle \\ & - 2\langle 1-10 | I'\cdot I' | -110 \rangle + 2\langle 1-10 | I'\cdot I' | -101 \rangle - 2\langle 01-1 | I'\cdot I' | 0-11 \rangle \\ & - 2\langle 01-1 | I'\cdot I' | -110 \rangle - 2\langle -110 | I'\cdot I' | -101 \rangle - 2\langle 0-11 | I'\cdot I' | -101 \rangle) \\ = 6(\tfrac{1}{6})(-\tfrac{1}{6}) & - \tfrac{1}{18} - \tfrac{1}{18} - \tfrac{1}{18} - \tfrac{1}{18} - \tfrac{1}{18} - \tfrac{1}{18} = -\tfrac{1}{2} , \end{aligned} \tag{24}$$

in agreement with expression (8) above.

For the partition [3] we have

$$\begin{aligned} \langle [3]32 \,|\, I'\cdot I' \,|\, [3]32 \rangle = \tfrac{1}{3}(& \langle 110 | I'\cdot I' | 110 \rangle + \langle 011 | I'\cdot I' | 011 \rangle + \langle 101 | I'\cdot I' | 101 \rangle \\ & + 2\langle 110 | I'\cdot I' | 011 \rangle + 2\langle 110 | I'\cdot I' | 101 \rangle + 2\langle 011 | I'\cdot I' | 101 \rangle) \\ = 3\tfrac{1}{3}(\tfrac{1}{6}) + 3\tfrac{2}{3}(\tfrac{1}{6}) & = \tfrac{1}{2} , \end{aligned} \tag{25}$$

in agreement with expression (10) above.

For the partition [21] we have

$$\begin{aligned} \langle [21]21 \,|\, I^2\cdot I^2 \,|\, [21]21 \rangle = \tfrac{1}{4}(& \langle 11-1 | I^2\cdot I^2 | 11-1 \rangle + \langle -111 | I^2\cdot I^2 | -111 \rangle + \langle 100 | I^2\cdot I^2 | 100 \rangle + \langle 001 | I^2\cdot I^2 | 001 \rangle \\ & + 2\langle 11-1 | I^2\cdot I^2 | 100 \rangle - 2\langle 11-1 | I^2\cdot I^2 | -111 \rangle - 2\langle 11-1 | I^2\cdot I^2 | 001 \rangle \\ & - 2\langle -111 | I^2\cdot I^2 | 100 \rangle + 2\langle -111 | I^2\cdot I^2 | 001 \rangle - 2\langle 100 | I^2\cdot I^2 | 001 \rangle) \\ = \tfrac{1}{4}[\tfrac{1}{10} + \tfrac{1}{10} - \tfrac{2}{10} & - \tfrac{4}{10} - \tfrac{2}{10} - \tfrac{2}{10}] = -\tfrac{1}{5} , \end{aligned} \tag{26}$$

in agreement with Eq. (11′) above.

V. CONCLUSION

We have treated the case of a three-particle spin-1 system using two different procedures. In one procedure we employed the UGA. The other procedure was based on one of the methods advocated in Refs. 1 and 2. It is clear that even though the former method still lacks a closed-form expression for the evaluation of other than one-step one-body operators it is much more efficient than the latter approach. As a matter of fact, any of the approaches of Refs. 1 and 2 become much more cumbersome than the UGA when applied to three particles or more. In addition, it is known[3] that UGA is particularly apt for computer implementation.

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