Multipole operators for an arbitrary number of spins*

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Basis states and operators composed of n, in general, different nuclear spins of integer or half-integer values are explicitly constructed. Various coupling schemes are discussed, and transformations between them derived. Following this, a complete set of irreducible tensor operators $T^{(k)}_{\{V\}}$ is constructed which can be used as a basis for expanding operators which depend on n nuclear spins. It is further shown that decomposition of the tensor's components $T^{(k)q}_{\{V\}}$ into a sum of products of two irreducible tensor components involves transformation matrices between different coupling schemes. Various properties and commutation relations of the $T^{(k)q}_{\{V\}}$'s are given along with a discussion of their reduced matrix elements.

I. INTRODUCTION

The purpose of this paper is to construct and discuss irreducible tensor operators which depend on n different, integer or half-integer spins. Such operators can be used in multipole expansions. For example, if ϕ is a scalar operator on the n spins, then it can be written

$$\phi = \sum_{k\{V\}} \phi^{(k)}_{\{V\}} \odot^k T^{(k)}_{\{V\}} , \qquad (1)$$

where the $T^{(k)}_{\{V\}}$'s are irreducible tensors of rank k. $T^{(k)}_{\{V\}}$ has $2k+1$ components, $T^{(k)q}_{\{V\}}$, which form a basis for the irreducible representation $D^{(k)}$ of the rotation group (SO_3). In addition, the set of labels $\{V\}$ allow a specification of a complete set of basis states for the n spins. In Eq. (1) the $\phi^{(k)}_{\{V\}}$ are kth rank tensor coefficients and the notation $\odot^k$ indicates a kth order contraction of the two tensors.

In part, the motivation for this work lies in the fact that rotational invariance can be exploited when the expansion Eq. (1) is used, but not when the expansion

$$\phi = \sum_{\alpha\beta} |\alpha\rangle\langle\alpha|\phi|\beta\rangle\langle\beta| \qquad (2)$$

is employed. Here the basis states $|\alpha\rangle$ form a complete set (say the product state of the n spins). For example, in studying nuclear magnetic hyperfine spectra via the Redfield equations, the expansion (2) is usually used for the spin part of the density operator. Even for the simplest problems[1,2] involving only a few spins, the treatment is quite involved. This is partly because the whole series Eq. (2) must be used. In contrast, use of the expansion Eq. (1) can often lead to considerable simplification since only the first few terms in the k expansion need be retained in many situations of physical interest. This is because nuclear magnetization is, to an excellent approximation, proportional to the dipolar polarization of the spins only ($k=1$). In all cases the tensor rank of the spin part of the spin–lattice coupling Hamiltonian is low thus allowing couplings between $k=1$ and only a few terms in the multipole expansion. Thus the expansion Eq. (1) can be truncated. For a treatment of hyperfine NMR from an operator viewpoint, see Pyper[3] and Banwell and Primas.[4]

Pyper[3] discusses a basis set of irreducible tensor operators for systems containing several nuclear spins and evaluates supermatrix elements of Liouville operators for some special cases. He stresses that explicit construction of the irreducible operators for each spin is not necessary and that sufficient information is contained by knowing only the tensor rank, the component and the spin magnitude. For several spins, the coupling scheme must also be specified. Evaluation of matrix elements is greatly simplified by the exploitation of rotational invariance (the Wigner–Eckart theorem). This paper follows in the same spirit with emphasis also being placed on rotational invariance. In addition, some general statements concerning the importance of the choice of the coupling scheme are made. Also, for completeness, the single nucleus multipole operators, here denoted by $\mathcal{Y}^{(k)q}(I_n)$ [Pyper uses $T^{(k)}_{qn}$ which differ by a phase (see Sec. III)] are given explicitly for any tensor rank and spin magnitude. These are not given by Pyper nor does he obtain an expansion for the operator $\Pi_n |I_n m_n\rangle\langle I_n m_n'|$ in a multipole series. This is given here, and leads to the construction of tensor operators for n spins, $T^{(k)q}_{\{V\}}$. It is these operators and their properties which are studied with special attention being given to the commutation relations and their reduced matrix elements.

In Sec. II, Dirac spin states for n spins are defined. Both the product state and various coupled states are considered along with the transformations between them. Section III is concerned with the construction of the tensors $T^{(k)q}_{\{V\}}$ where the labels $\{V\}$ are explicitly specified. The $\{V\}$ labels do not affect the transformation properties of the $T^{(k)q}_{\{V\}}$'s under the rotation group, these being determined by k and q alone. They do, however, depend upon the coupling scheme employed. Also in Sec. III $T^{(k)q}_{\{V\}}$ is decomposed into a sum of products of two tensor components $T^{(k_a)q_a}_{\{V_a\}}$, $T^{(k_b)q_b}_{\{V_b\}}$. This has the general form

$$T^{(k)q}_{\{V\}} = \sum_{\substack{k_a\{V_a\}q_a \\ k_b\{V_b\}q_b}} (-1)^{k_a-k_b+k}(k)^{1/2}(-1)^{k-q} \times \begin{pmatrix} k & k_a & k_b \\ -q & q_a & q_b \end{pmatrix} T^{(k_a)q_a}_{\{V_a\}} T^{(k_b)q_b}_{\{V_b\}} \mathbf{A}^{ab} . \qquad (3)$$

Here $\mathbf{A}^{ab}$ is a (q, q_a, q_b)-independent matrix which accounts for a necessary transformation when decomposing $T^{(k)}_{\{V\}}$. A particular choice of coupling scheme is shown to make $\mathbf{A}^{ab}$ the identity. The orthonormal properties of the $T^{(k)q}_{\{V\}}$ and their adjointness are also given

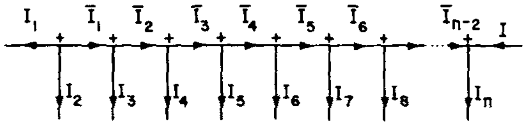

FIG. 1. Diagram α which shows the coupling scheme Z_{n0}.

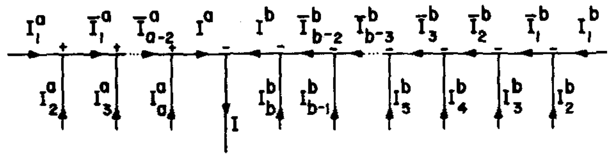

FIG. 2. Coupling scheme Z_{ab}.

in Sec. III. In Sec. IV, the commutation relation of the $T^{(k)q}_{\{V\}}$'s are given. Section V presents some reduced matrix and supermatrix elements of the $T^{(k)q}_{\{V\}}$'s. Some of the expressions used throughout the paper are given by Yutsis[5] diagrams as well as in terms of nj symbols. Finally, the results are summarized and compared with the work of Pyper.[3]

II. SETS OF BASIS STATES FOR n SPINS

In this section, various sets of states $|\alpha\rangle$ for an n-spin system are given. These are required in order to establish the notation and introduce definitions which are used for the expansion of operators of the form $|\alpha\rangle\langle\beta|$ in Sec. III. In particular, various coupling schemes are discussed along with the transformations between them. The specific formulas presented follow from the general treatment of Yutsis.[5]

All n spins can in general be different and they can have integer or half-integer magnitudes. Necessarily these n spin magnitudes are fixed having a value I_i ($i=1,n$). A possible state of the n-spin system is the simple product,

$$|I_1m_1I_2m_2\cdots I_nm_n\rangle=|I_1m_1\rangle|I_2m_2\rangle\cdots|I_nm_n\rangle\ . \tag{4}$$

Another possible choice of basis state is that obtained by coupling the spins to a given total resultant I and M value. For n spins, a complete specification of the state requires $n-2$ parameters in addition to I and M. These may be chosen to be intermediate angular momentum. Such a set is denoted by $\{\bar I\}=(\bar I_1,\bar I_2,\ldots,\bar I_{n-2})$ and depends upon the way in which the coupling is constructed. An example of such a state is written,

$$|(I_1\ldots I_n)^{Z_{n0}}\{\bar I\}IM\rangle\ , \tag{5}$$

where Z_{n0} denotes the coupling scheme. Clearly complete sets formed from either Eqs. (4) or (5) can be used to describe the spin system. The relationship between Eqs. (4) and (5) is given in terms of generalized Clebsch–Gordan coefficients

$$|(I_1\ldots I_n)^{Z_{n0}}\{\bar I\}IM\rangle=\sum_{\substack{m_i\\ i=1,n}}\langle I_1m_1\cdots I_nm_n|(I_1\cdots I_n)^{Z_{n0}}\{\bar I\}IM\rangle|I_1m_1\cdots I_nm_n\rangle\ . \tag{6}$$

The chosen coupling scheme Z_{n0} is defined to be the consecutive coupling of spin $\mathbf{I}_i$ to the resultant of the previous $i-1$ couplings. This is illustrated by means of a Yutsis diagram in Fig. 1. The generalized Clebsch–Gordan coefficients are related to $n\,j\,m$ coefficients by [see Yutsis,[5] Eq. (10.1)],

$$\langle I_1m_1\cdots I_nm_n|(I_1\cdots I_n)^{Z_{n0}}\{\bar I\}IM\rangle=(-1)^{I_1-I_2-I_3\cdots-I_n+I}[(\bar I_1)\cdots(\bar I_{n-2})]^{1/2}(-1)^{I-M}\times(I)^{1/2}\begin{pmatrix}I_1\cdots I_n & I\\ m_1\cdots m_n & -M\end{pmatrix}^{Z_{n0}}_{\{\bar I\}}, \tag{7}$$

where $(I)=2I+1$. The $n\,j\,m$ coefficients are generalized Wigner coefficients and, for the coupling scheme Z_{n0}, are given by,

$$\begin{pmatrix}I_1\cdots I_n & I\\ m_1\cdots m_n & -M\end{pmatrix}^{Z_{n0}}_{\{\bar I\}}=\boldsymbol{\alpha}\ . \tag{8}$$

The diagram $\boldsymbol{\alpha}$ is given in Fig. 1. This form, Eq. (8), satisfies the orthogonality relations of Yutsis[5] [Eqs. (10.8a) and (10.8b)].

An alternative coupling scheme is shown in Fig. 2. Here the first "a" spins are coupled to $\mathbf{I}^a$ by scheme Z_{a0}. The next "b" spins are coupled to $\mathbf{I}^b$ by scheme Z_{b0}. Finally, the $\mathbf{I}^a$ and $\mathbf{I}^b$ are coupled together to resultant $\mathbf{I}$. The overall coupling scheme is denoted by Z_{ab}, where $a+b=n$. Within this scheme, the basis states are denoted by [cf. Eq. (19)]

$$|(I_1\cdots I_n)^{Z_{ab}}\{\bar I^a\}\{\bar I^b\}I^aI^bIM\rangle\ . \tag{9}$$

The simplest case is, of course, when two spins are coupled together. In this case, scheme Z_{11} is equivalent to Z_{20}. This state is related to the product state by a Clebsch–Gordan coefficient or, in terms of a $3-j$ coefficient, by

$$|I_1I_2IM\rangle=\sum_{m_1m_2}(-1)^{I_1-I_2+I}(I)^{1/2}\times(-1)^{I-M}\begin{pmatrix}I & I_1 & I_2\\ -M & m_1 & m_2\end{pmatrix}|I_1m_1I_2m_2\rangle\ . \tag{10}$$

The situation is also simple when two spins are coupled to a resultant and the resultant to a third spin. The state $|(I_1I_2I_3)^{Z_{30}}\bar I_1IM\rangle$ is related to the product $|I_1I_2\bar I_1\bar m_1\rangle|I_3m_3\rangle$ by

$$|(I_1I_2I_3)^{Z_{30}}\bar I_1IM\rangle=\sum_{\bar m_1m_3}(-1)^{\bar I_1-I_3+I}(I)^{1/2}\,(-1)^{I-M}\begin{pmatrix}I & \bar I_1 & I_3\\ -M & \bar m_1 & m_3\end{pmatrix}|I_1I_2\bar I_1\bar m_1\rangle|I_3m_3\rangle. \tag{11}$$

In general, the coupling scheme Z_{n0} is related to the scheme whereby the *last* spin is separated in the same way as in Eq. (11), viz

$$|(I_1\cdots I_aI_{a+1})^{Z_{n0}}\{\bar I\}IM\rangle=\sum_{\bar m_{a-2},m_{a+1}}(-1)^{\bar I_{a-2}-I_{a+1}+I}(I)^{1/2}(-1)^{I-M}\begin{pmatrix}I & \bar I_{a-2} & I_{a+1}\\ -M & \bar m_{a-2} & m_{a+1}\end{pmatrix}|(I_1\cdots I_a)^{Z_{a0}}\{\bar I'\}\bar I_{a-2}\bar m_{a-2}\rangle|I_{a+1}m_{a+1}\rangle . \tag{12}$$

Here $\{\bar I'\}=(\bar I_1\cdots\bar I_{n-3})$ are the intermediate values which arise in the coupling of the first a spins via Z_{a0}. Equation (12) merely shows that schemes Z_{n0} and Z_{a1} are identical $(a+1=n)$.

The situation is different when scheme Z_{n0} is related to Z_{ab} where $b>1$. The transformation from Z_{n0} to Z_{a2} involves one $6-j$ coefficient while that from Z_{n0} to Z_{ab} involves $b-1$ $6-j$ coefficients. The case of four spins has the transformation,

$$|(I_1^aI_2^aI_1^bI_2^b)^{Z_{40}}\{\bar I_1\bar I_2\}IM\rangle=\sum_{I^a,I^b}(-1)^{I_1^b+I_2^b+I^a+I}[(I^b)(\bar I_2)]^{1/2}\begin{Bmatrix}I & I^b & I^a\\ I_1^b & \bar I_2 & I_2^b\end{Bmatrix}\delta(\bar I_1I^a)|(I_1^aI_2^aI_1^bI_2^b)^{Z_{22}}I^aI^bIM\rangle , \tag{13}$$

where

$$|(I_1^aI_2^aI_1^bI_2^b)^{Z_{22}}I^aI^bIM\rangle=\sum_{m_a,m_b}(-1)^{I^a-I^b+I}(I)^{1/2}(-1)^{I-M}\begin{pmatrix}I & I^a & I^b\\ -M & m^a & m^b\end{pmatrix}|I_1^aI_2^aI^am^a\rangle|I_1^bI_2^bI^bm^b\rangle . \tag{14}$$

The general transformation between Z_{n0} and Z_{ab} is given by

$$|(I_1^a\cdots I_a^aI_1^b\cdots I_b^b)^{Z_{n0}}\{\bar I\}IM\rangle=\sum_{\substack{I_a\{\bar I^a\}\\ I_b\{\bar I^b\}}}\langle(I_1^a\cdots I_a^aI_1^b\cdots I_b^b)^{Z_{ab}}\{\bar I^a\}\{\bar I^b\}I^aI^bIM|(I_1^a\cdots I_a^aI_1^b\cdots I_b^b)^{Z_{n0}}\{\bar I\}IM\rangle$$
$$\times|(I_1^a\cdots I_a^aI_1^b\cdots I_b^b)^{Z_{ab}}\{\bar I^a\}\{\bar I^b\}I^aI^bIM\rangle , \tag{15}$$

where the transformation is independent of M and is given by

$$\langle(I_1^a\cdots I_a^aI_1^b\cdots I_b^b)^{Z_{ab}}\{\bar I^a\}\{\bar I^b\}I^aI^bIM|(I_1^a\cdots I_a^aI_1^b\cdots I_b^b)^{Z_{n0}}\{\bar I\}IM\rangle$$
$$=(-1)^{2\Sigma_{i=1}^aI_i^a+2\Sigma_{i=1}^bI_i^b+2I_1^b+2I^a}[(I^a)(I^b)(\bar I_{a-1})(\bar I_a)]^{1/2}[(\bar I_1^a)\cdots(\bar I_{a-2}^a)]^{1/2}[(\bar I_1^b)\cdots(\bar I_{b-2}^b)]^{1/2}[(\bar I_1)\cdots(\bar I_{a-2})]^{1/2}[(\bar I_{a+1})\cdots(\bar I_{a+b-2})]^{1/2}\gamma . \tag{16}$$

The diagram γ is given in Fig. 3 and it is seen to arise from the total contraction of the two coupling schemes illustrated in Figs. 1 and 2. The diagram γ is reduced[5] to give

$$\gamma^{ab}=(-1)^{\Phi_\gamma}\delta(I_1^aI_2^a\bar I_1)\delta(\bar I_1I_3\bar I_2)\cdots\delta(\bar I_{a-2}I_a^aI^a)[(\bar I_1)\cdots(\bar I_{a-2})]^{-1}$$
$$\times\prod_{i=1}^{a-2}\{\delta(\bar I_i,\bar I_i^a)\}\delta(\bar I_{a-1},I^a)(I^a)^{-1}\begin{Bmatrix}I_1^b & I_2^b & \bar I_1^b\\ \bar I_{a+1} & I^a & \bar I_a\end{Bmatrix}\begin{Bmatrix}\bar I_1^b & I_3^b & \bar I_2^b\\ \bar I_{a+2} & I^a & \bar I_{a+1}\end{Bmatrix}\cdots\begin{Bmatrix}\bar I_{b-3}^b & I_{b-1}^b & \bar I_{b-2}^b\\ \bar I_{a+b-2} & I^a & \bar I_{a+b-3}\end{Bmatrix}\begin{Bmatrix}I^a & I^b & I\\ I_b^b & \bar I_{a+b-2} & \bar I_{b-2}^b\end{Bmatrix} , \tag{17}$$

with phase

$$\Phi_\gamma=(b-1)I^a+2I^b+I+\sum_{i=1}^bI_i^b-\{\bar I^b\}+2\bar I_a-\bar I_{a+1}-\bar I_{a+2}-\cdots-\bar I_{a+b-2} . \tag{18}$$

Here the notation $(-1)^{\{\bar I^b\}}$ has the meaning $(-1)^{\bar I_1^b+\bar I_2^b+\bar I_3^b+\cdots+\bar I_{b-2}^b}$. Further, the dots between two quantities indicate that all intermediate values must be inserted. Finally in Eq. (15), the Z_{ab} state is defined analogously to Eq. (10), as

$$|(I_1^a\cdots I_a^aI_1^b\cdots I_b^b)^{Z_{ab}}\{\bar I^a\}\{\bar I^b\}I^aI^bIM\rangle=\sum_{m^am^b}(-1)^{I^a-I^b+I}(I)^{1/2}(-1)^{I-M}\begin{pmatrix}I & I^a & I^b\\ -M & m^a & m^b\end{pmatrix}$$
$$\times|(I_1^a\cdots I_a^a)^{Z_{a0}}\{\bar I^a\}I^am^a\rangle|(I_1^b\cdots I_b^b)^{Z_{b0}}\{\bar I^b\}I^bm^b\rangle . \tag{19}$$

Thus the coupling schemes Z_{ab} are simply related to a product of two states in schemes Z_{a0} and Z_{b0}. This has the advantage of avoiding a transformation such as arises in Eq. (15). The Z_{n0} scheme is related to a product of two states in schemes Z_{a0} and Z_{b0} by

$$|(I_1^a\cdots I_a^aI_1^b\cdots I_b^b)^{Z_{n0}}\{\bar I\}IM\rangle=\sum_{\substack{I^a\{\bar I^a\}m^a\\ I^b\{\bar I^b\}m^b}}\langle(I_1^a\cdots I_a^aI_1^b\cdots I_b^b)^{Z_{ab}}\{\bar I^a\}\{\bar I^b\}I^aI^bIM|(I_1^a\cdots I_a^aI_1^b\cdots I_b^b)^{Z_{n0}}\{\bar I\}IM\rangle$$
$$\times\langle I^am^aI^bm^b|II^aI^bM\rangle|(I_1^a\cdots I_a^a)^{Z_{a0}}\{\bar I^a\}I^am^a\rangle|(I_1^b\cdots I_b^b)^{Z_{b0}}\{\bar I^b\}I^bm^b\rangle , \tag{20}$$

where the transformation matrix between schemes Z_{n0} and Z_{ab} [Eq. (16)] must be used.

By repeated application of the transformation between Z_{n0}, and Z_{ab}, the states in Eq. (15) can be further decomposed and any coupling scheme devised.

III. IRREDUCIBLE TENSOR OPERATORS FOR n SPINS

In this section, operators of the type $|\alpha\rangle\langle\beta|$ are expanded in a multipole series and the general component $T_{\{V\}}^{(k)q}$ of the multipole expansion tensor $T_{\{V\}}^{(k)}$ are defined.

For one spin, the operator $|I_i m_i\rangle\langle I_i m_i'|$ can be expanded in a complete set of tensors composed of operator I_{ix}, I_{iy}, and I_{iz} of $\mathbf{I}_i$. The maximum tensor rank which can occur in the expansion is $k_i = 2I_i$. These tensors are chosen to be irreducible cartesian symmetric traceless tensor operators[6] and are denoted by $[\mathbf{I}_i]^{(k_i)}$. Explicitly these tensors are scaled according to[7]

$$\mathcal{Y}^{(k_i)}(\mathbf{I}_i) \equiv (k_i)^{1/2}\{[\mathbf{I}_i]^{(k_i)} \odot^{k_i}[\mathbf{I}_i]^{(k_i)}\}^{-1/2}[\mathbf{I}_i]^{(k_i)} , \tag{21}$$

so that complete tensorial contraction of $\mathcal{Y}^{(k_i)}$ with itself gives the dimensionality

$$\mathcal{Y}^{(k_i)}(\mathbf{I}_i)\odot^{k_i}\mathcal{Y}^{(k_i)}(\mathbf{I}_i) = (k_i) \equiv 2k_i+1 , \tag{22}$$

of the irreducible representation of the rotation group SO(3), to which $\mathcal{Y}^{(k_i)}$ belongs. The $2k_i+1$ components of $\mathcal{Y}^{(k_i)}(\mathbf{I}_i)$ can be written with respect to a spherical basis $e^{(k_i)q_i}$. This basis is defined in Ref. 6 and, in particular, the complex conjugate of $e^{(k_i)q_i}$ is

$$e^{(k_i)q_i^*} = (-1)^{k_i-q_i}e^{(k_i)-q_i} . \tag{23}$$

Thus, the spherical components of $\mathcal{Y}^{(k_i)}(\mathbf{I}_i)$, which are defined by

$$\mathcal{Y}^{(k_i)q_i}(\mathbf{I}_i) = \mathcal{Y}^{(k_i)}(\mathbf{I}_i)\odot^{k_i}e^{(k_i)q_i} \tag{24}$$

obey an analogous relation, namely

$$\mathcal{Y}^{(k_i)q_i}(\mathbf{I}_i)^\dagger = (-1)^{k_i-q_i}\mathcal{Y}^{(k_i)-q_i}(\mathbf{I}_i) . \tag{25}$$

The † denotes the ordinary operator adjoint. It follows that the quantum trace of two $\mathcal{Y}$'s gives,

$$\mathrm{Tr}[\mathcal{Y}^{(k_i)q_i}(\mathbf{I}_i)]^\dagger\mathcal{Y}^{(k_i')q_i'}(\mathbf{I}_i) = (I_i)\delta(k_ik_i')\delta(q_iq_i') . \tag{26}$$

TABLE I. Explicit formulas for $\mathcal{Y}^{(k)q}(\mathbf{I})$ up to $k=3$.

k	q	$\mathcal{Y}^{(k)q}(\mathbf{I})$
0	0	1
1	0	$\{3/I(I+1)\}^{1/2}i(I_Z)$
1	±1	$\{3/I(I+1)\}^{1/2}(\mp i/\sqrt{2})(I_\pm)$
2	0	$\{5/[\mathbf{I}]^{(2)}:[\mathbf{I}]^{(2)}\}^{1/2}(1/\sqrt{6})(I^2-3I_Z^2)$
2	±1	$\{5/[\mathbf{I}]^{(2)}:[\mathbf{I}]^{(2)}\}^{1/2}(\pm\frac{1}{2})(I_ZI_\pm+I_\pm I_Z)$
2	±2	$\{5/[\mathbf{I}]^{(2)}:[\mathbf{I}]^{(2)}\}^{1/2}(-\frac{1}{2})(I_\pm I_\pm)$
3	0	$\{7/[\mathbf{I}]^{(3)}:[\mathbf{I}]^{(3)}\}^{1/2}(i/\sqrt{10})(3I^2-5I_Z^2-1)I_Z$
3	±1	$\{7/[\mathbf{I}]^{(3)}:[\mathbf{I}]^{(3)}\}^{1/2}[(\pm i\sqrt{3/10})/4]\{I_\pm(I^2-5I_Z+\frac{1}{2})$ $+(I^2-5I_Z+\frac{1}{2})I_\pm\}$
3	±2	$\{7/[\mathbf{I}]^{(3)}:[\mathbf{I}]^{(3)}\}^{1/2}(-i\sqrt{3/2})(I_\pm I_ZI_\pm)$
3	±3	$\{7/[\mathbf{I}]^{(3)}:[\mathbf{I}]^{(3)}\}^{1/2}(\pm i/2\sqrt{2})I_\pm I_\pm I_\pm$

These $\mathcal{Y}$'s obey the standard commutation relations, [see Yutsis[5] Eqs. (31.4a) and (31.4b)]. Table I gives the explicit forms for the $\mathcal{Y}^{(k)q}$'s up to $k=3$. Higher values may be obtained by constructing the $e^{(k)q}$'s; using Eq. (24), and the formula[6]

$$[\mathbf{I}]^{(k)}\odot^k[\mathbf{I}]^{(k)} = \frac{(k!)^2(2I+k+1)!}{2^k(2I+1)(2k)!(2I-k)!} . \tag{27}$$

The $\mathcal{Y}^{(k)q}(\mathbf{I})$'s here differ from the basis operators of Rose[6] T_{kq} (also used by Pyper[3]) by a phase. The phase differs because the basis $e^{(k)q}$ is constructed starting from $e^{(1)0} = i\hat{z}$, $e^{(1)\pm1} = \mp i/\sqrt{2}(x\pm iy)$, whereas that of Ref. 8 starts with $e_R^{(1)0} \equiv \hat{z}$, $e_R^{(1)\pm1} = \mp 1/\sqrt{2}(x\pm iy)$. This has the consequence that $e_R^{(k)q*} = (-1)^q e_R^{(k)-q}$ in contrast to Eq. (23).

An alternate procedure by which the $\mathcal{Y}$'s, (and Table I), can be constructed is to start with the standard vector coupling relation of Rose, Eq. (15.2), after each application of which the resulting tensor component is normalized. Equations (21), (24), and (27) summarize the results of such a procedure.

Turning now to the multipole expansion, it can be shown that the operator $|I_im_i\rangle\langle I_im_i'|$ can be expanded in terms of $\mathcal{Y}^{(k_i)q_i}(\mathbf{I}_i)$'s. The expression is

$$|I_im_i\rangle\langle I_im_i'| = (I_i)^{-1/2}(-1)^{I_i-m_i}\sum_{k_i=0}^{2I_i}\sum_{q_i=-k_i}^{k_i}(k_i)^{1/2} \times(-i)^{k_i}\begin{pmatrix} I_i & k_i & I_i \\ -m_i & q_i & m_i' \end{pmatrix}\mathcal{Y}^{(k_i)q_i}(\mathbf{I}_i) , \tag{28}$$

while inverse relation is

$$\mathcal{Y}^{(k_i)q_i}(\mathbf{I}_i) = (i)^{k_i}[(I_i)(k_i)]^{1/2}\sum_{m_im_i'}(-1)^{I_i-m_i}\begin{pmatrix} I_i & k_i & I_i \\ -m_i & q_i & m_i' \end{pmatrix} \times|I_im_i\rangle\langle I_im_i'| . \tag{29}$$

These follow from the Wigner–Eckart theorem and the reduced matrix elements of $\mathcal{Y}^{(k_i)q_i}$ namely

$$\langle I_i||\mathcal{Y}^{(k_i)}(\mathbf{I}_i)||I_i'\rangle = (i)^{k_i}[(I_i)(k_i)]^{1/2}\delta(I_iI_i') . \tag{30}$$

The expansion of operators of two spins coupled together to form a resultant I is

$$|I_1I_2IM\rangle\langle I_1I_2I'M'| = \sum_{k_1,k_2}\sum_{kq}(i)^{k_1+k_2}[(I')(k)(k_1)(k_2)]^{1/2}\begin{Bmatrix} I_1 & I_2 & I \\ k_1 & k_2 & k \\ I_1 & I_2 & I' \end{Bmatrix}(-1)^{k-I'+I} \times(I)^{1/2}(-1)^{I-M}\begin{pmatrix} I & k & I' \\ -M & q & M' \end{pmatrix}T^{(k)q}(k_1k_2) . \tag{31}$$

Here the tensor component in the expansion is constructed from the $\mathcal{Y}$'s as follows,

$$T^{(k)q}(k_1k_2) = [(I_1)(I_2)]^{-1/2}\sum_{q_1q_2}(-1)^{k_1-k_2+k}(k)^{1/2} \times(-1)^{k-q}\begin{pmatrix} k & k_1 & k_2 \\ -q & q_1 & q_2 \end{pmatrix}\mathcal{Y}^{(k_1)q_1}(\mathbf{I}_1)\mathcal{Y}^{(k_2)q_2}(\mathbf{I}_2) . \tag{32}$$

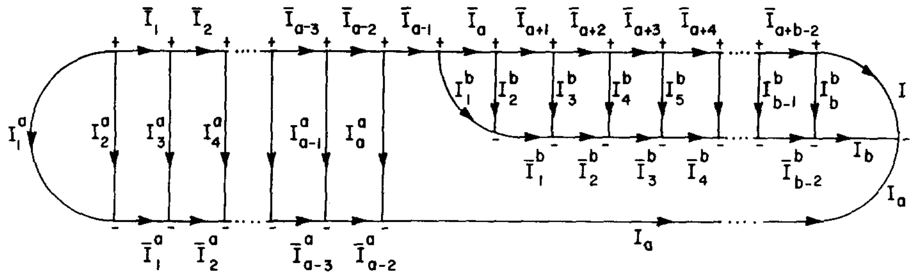

FIG. 3. Diagram γ^{ab}.

These quantities are the desired operators in the expansion with the additional required labels k_1k_2 specified. In Eq. (32), and future $T^{(k)q}_{\{V\}}$'s, the spin magnitudes I_1I_2 are surpressed.

The expansion, Eq. (31), can be obtained by expanding $|I_1I_1IM\rangle\langle I_1I_1I'M'|$ in the product basis; namely, $\sum_{m_1m_2m_1'm_2'}|I_1m_1I_2m_2\rangle\langle I_1m_1'I_2m_2'|$ and using the expansion Eq. (28) twice. The recoupling leads to the $9-j$ coefficient in Eq. (31). By use of the same procedure on n spins, a general expansion of operators composed of the ket–bra's of Eq. (4) can be obtained. This needs the n fold application of the expansion Eq. (28) which can be written in terms of n $3-j$ coefficients

$$|I_1m_1I_2m_2\cdots I_nm_n\rangle\langle I_1m_1'I_2m_2'\cdots I_nm_n'| = (-1)^{\sum_i(I_i-m_i)}\sum_{\substack{k_iq_i\\ i=1,n}}^{2I_i}[(k_1)\cdots(k_n)]^{1/2}(-i)^{\sum_ik_i}$$
$$\times\left\{\begin{pmatrix} I_1 & k_1 & I_1\\ -m_1 & q_1 & m_1'\end{pmatrix}\begin{pmatrix} I_2 & k_2 & I_2\\ -m_2 & q_2 & m_2'\end{pmatrix}\cdots\begin{pmatrix} I_n & k_n & I_n\\ -m_n & q_n & m_n'\end{pmatrix}\right.$$
$$\times\sum_{k\{\overline{K}\}q}T^{(k)q}_{\{\overline{K}\}}(k_1k_2\cdots k_n)^Z\langle(k_1k_2\cdots k_n)^Z\{\overline{K}\}kq\,|\,k_1q_1k_2q_2\cdots k_nq_n\rangle\ . \tag{33}$$

Here the $T^{(k)q}$'s are defined by

$$T^{(k)q}_{\{\overline{K}\}}(k_1k_2\cdots k_n)^Z \equiv\left[\prod_{i=1}^n(I_i)^{-1/2}\right]\sum_{\substack{q_i\\ i=1,n}}\langle k_1q_1k_2q_2\cdots k_nq_n\,|\,(k_1k_2\cdots k_n)^Z\{\overline{K}\}kq\rangle$$
$$\times\,\mathcal{Y}^{(k_1)q_1}(\mathbf{I}_1)\mathcal{Y}^{(k_2)q_2}(\mathbf{I}_2)\cdots\mathcal{Y}^{(k_n)q_n}(\mathbf{I}_n)\ . \tag{34}$$

[See Yutsis, Eqs. (32.8) and (32.9).] These are the irreducible operator components $T^{(k)q}_{\{V\}}$ with the set of $\{\overline{K}\}=\overline{K}_1,\overline{K}_2,\ldots,\overline{K}_{n-2}$ intermediate values and the values of $k_1k_2\cdots k_n$ along with the coupling scheme Z, being the explicit labels which replace $\{V\}$. These operators are related to their adjoint by

$$T^{(k)q}_{\{\overline{K}\}}(k_1k_2\cdots k_n)^{Z\,\dagger}=(-1)^{k-q}T^{(k)-q}_{\{\overline{K}\}}(k_1k_2\cdots k_n)^Z \tag{35}$$

and are orthonormalized in the sense that,

$$\mathrm{Tr}[T^{(k)q}_{\{\overline{K}\}}(k_1k_2\cdots k_n)^Z]^\dagger T^{(k')q'}_{\{\overline{K}'\}}(k_1'k_2'\cdots k_n')^Z$$
$$=\delta(kk')\delta(qq')\delta(\{\overline{K}\}\{\overline{K}'\})\prod_{i=1}^n\delta(k_i,k_i')\ , \tag{36}$$

where $\delta(\{\overline{K}\}\{\overline{K}'\})\equiv\delta(\overline{K}_1,\overline{K}_1')\delta(\overline{K}_2,\overline{K}_2')\cdots\delta(\overline{K}_n,\overline{K}_n')$. Clearly $T^{(k)q}(k_1k_2)$, Eq. (32) is a special case of Eq. (34).

In the above definitions, the k's all have integer values since in the $3-j$ coefficients of Eq. (33), $2I_i+k_i$ must be an integer. Also, the simple phase relation between $T^{(k)q}$ and its adjoint in Eq. (35) is a consequence of the property given in Eq. (23). Had the basis been defined so that the complex conjugate is $e_R^{(k)q*}=(-1)^q e_R^{(k)-q}$, the phase in Eq. (35) would be changed to $(-1)^{\sum_ik_i+k-q}$ which seems less desirable.

The coupling scheme Z in the above definitions of the $T^{(k)q}$'s is arbitrary. In the remainder of this section, specific schemes are used. The coupling scheme Z_{n0} is shown in Fig. 1 with $I_1\cdots I_n$, $\overline{I}_1\cdots\overline{I}_{n-2}$, and I replaced by $k_1\cdots k_n$, $\overline{K}_1\cdots\overline{K}_n$, and k, respectively.

The expansion of $|(I_1\cdots I_n)^{Z_{n0}}\{\overline{I}\}IM\rangle\langle(I_1\cdots I_n)^{Z_{n0}}$

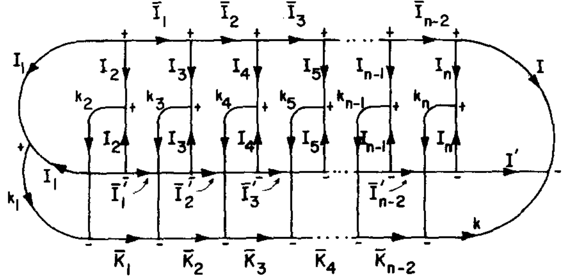

FIG. 4. The closed diagram is Δ.

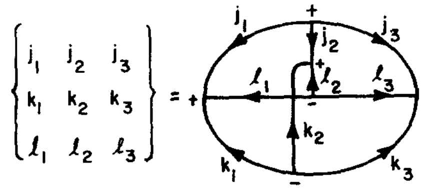

FIG. 5. A 9-j coefficient of the first kind.

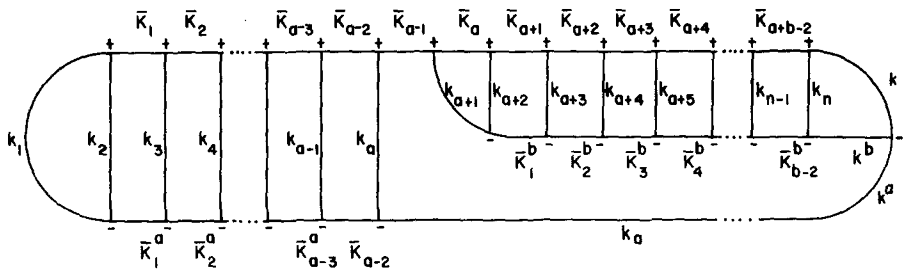

FIG. 6. Diagrammatic representation of the transformation matrix between coupling schemes Z_{n0} and Z_{ab}. The diagram is equivalent to γ^{ab} in Fig. 3.

$\times\{\bar{I}'\}I'M'|$ in terms of the $T^{(k)q}$'s may be obtained by the same procedure as for two spins in Eq. (31). First the operator is resolved by use of $\Pi_n|I_n m_n\rangle\langle I_n m_n'|$. Following this, via Eq. (33), the expansion is written in terms of the $T^{(k)q}$'s. The sum over $m_1\cdots m_n$, $m_1'\cdots m_n'$ can then be explicitly performed which leads to the closed diagram Δ in Fig. 4. This is decomposed into $n-1$ $9-j$ coefficients. [A diagram for the $9-j$ coefficient (of the first kind) is given in Fig. 5.] The expression for Δ is

$$\Delta=(-1)^{2(\bar{I})+2(\bar{I}')}\begin{Bmatrix} I_1 & I_2 & \bar{I}_1\\ k_1 & k_2 & \bar{K}_1\\ I_1 & I_2 & \bar{I}_1'\end{Bmatrix}\begin{Bmatrix} \bar{I}_1 & I_3 & \bar{I}_2\\ \bar{K}_1 & k_3 & \bar{K}_2\\ \bar{I}_1' & I_3 & \bar{I}_2'\end{Bmatrix}\begin{Bmatrix} \bar{I}_2 & I_4 & \bar{I}_3\\ \bar{K}_2 & k_4 & \bar{K}_3\\ \bar{I}_2' & I_4 & \bar{I}_3'\end{Bmatrix}\cdots\begin{Bmatrix} \bar{I}_{n-3} & I_{n-1} & \bar{I}_{n-2}\\ \bar{K}_{n-3} & k_{n-1} & \bar{K}_{n-2}\\ \bar{I}_{n-3}' & I_{n-1} & \bar{I}_{n-2}'\end{Bmatrix}\begin{Bmatrix} \bar{I}_{n-2} & I_n & I\\ \bar{K}_{n-2} & k_n & k\\ \bar{I}_{n-2}' & I_n & I'\end{Bmatrix}. \tag{37}$$

Thus, the expansion of spin operators coupled via Z_{n0} is given in terms of $T^{(k)q}$ with the Δ's being the expansion coefficients, viz.

$$|(I_1\cdots I_n)^{Z_{n0}}\{\bar{I}\}IM\rangle\langle(I_1\cdots I_n)^{Z_{n0}}\{\bar{I}'\}I'M'|$$
$$=\sum_{\substack{k_i\\ i=1,n}}\sum_{k\{\bar{K}\}q}(i)^{\Sigma_i^n k_i}[(I')(k)(k_1)\cdots(k_n)]^{1/2}[(\bar{I}_1)\cdots(\bar{I}_{n-2})]^{1/2}[(\bar{I}_1')\cdots(\bar{I}_{n-2}')]^{1/2}[(\bar{K}_1)\cdots(\bar{K}_{n-2})]^{1/2}$$
$$\times\Delta(-1)^{k-I'+I}(I)^{1/2}(-1)^{I-M}\begin{pmatrix} k & I' & I\\ q & M' & -M\end{pmatrix}T^{(k)q}_{\{\bar{K}\}}(k_1\cdots k_n)^{Z_{n0}}. \tag{38}$$

This is the obvious generalization of the expansion of $|I_1I_2IM\rangle\langle I_1I_2I'M'|$ as given in Eq. (31).

In practical situations, many of the n spins in a system are of the same type or species. It is therefore useful to consider the relationship between an operator $T^{(k)q}_{\{\bar{K}\}}(k_1\cdots k_n)^{Z}$, and products of the type $T^{(k^a)q^a}_{\{\bar{K}^a\}}(k_1\cdots k_a)^{Z'}$ and $T^{(k^b)q^b}_{\{\bar{K}^b\}}(k_{a+1}\cdots k_{a+b})^{Z''}$. This is studied in the case where the first a spins are coupled via scheme Z_{a0}; the remaining b spins are coupled via scheme Z_{b0}, and the product related to two different coupling schemes namely Z_{a+b0} and Z_{ab}. The procedure and results are the operator analogue of the state vector case which is presented in Sec. II.

The simplest situation is for two spins only which is given by Eq. (32). For more than two spins, consider the relationship between coupling schemes Z_{n0}, and schemes Z_{a0} and Z_{b0} $(a+b=n)$. In decomposing $T^{(k)q}_{\{\bar{K}\}}(k_1\cdots k_n)^{Z_{n0}}$ into a product of operators in schemes Z_{a0} and Z_{b0}, a change in coupling schemes, and hence a transformation matrix, must be employed. This is shown in Fig. 6, and is completely analogous to Fig. 3. The transformation is found to be

$$T^{(k)q}_{\{\bar{K}\}}(k_1\cdots k_n)^{Z_{n0}}=\sum_{\substack{k^aq^a\{\bar{K}^a\}\\ k^bq^b\{\bar{K}^b\}}}(-1)^{k^a-k^b+k}(k)^{1/2}(-1)^{k-q}\begin{pmatrix} k & k^a & k^b\\ -q & q^a & q^b\end{pmatrix}T^{(k^a)q^a}_{\{\bar{K}^a\}}(k_1\cdots k_a)^{Z_{a0}}T^{(k^b)q^b}_{\{\bar{K}^b\}}(k_{a+1}\cdots k_{a+b})^{Z_{b0}}\mathbf{A}^{ab}, \tag{39}$$

where $\mathbf{A}^{ab}$ is related to the reducible closed diagram in Fig. 6, γ^{ab}, by

$$\mathbf{A}^{ab}=[(\bar{K}_1^a)\cdots(\bar{K}_{a-2}^a)]^{1/2}[(\bar{K}_1^b)\cdots(\bar{K}_{b-2}^b)]^{1/2}[(\bar{K}_1)\cdots(\bar{K}_{a-2})]^{1/2}[(\bar{K}_{a+1})\cdots(\bar{K}_{n-2})]^{1/2}[(k^a)(k^b)(\bar{K}_{a-1})(\bar{K}_a)]^{1/2}\gamma^{ab}, \tag{40}$$

while γ^{ab} is [cf. Eq. (17)]

$$\gamma^{ab}=(-1)^{\phi_\gamma}\delta(k_1k_2\bar{K}_1)\delta(\bar{K}_1k_3\bar{K}_2)\cdots\delta(\bar{K}_{a-2}k_ak^a)[(\bar{K}_1)\cdots(\bar{K}_{a-2})]^{-1}\prod_{i=1}^{a-2}\{(\bar{K}_i,\bar{K}_i^a)\}\delta(\bar{K}_{a-1},k^a)$$
$$\times(k^a)^{-1}\begin{Bmatrix} k_{a+1} & k_{a+2} & \bar{K}_1^b\\ \bar{K}_{a+1} & k^a & \bar{K}_a\end{Bmatrix}\begin{Bmatrix} \bar{K}_1^b & k_{a+3} & \bar{K}_2^b\\ \bar{K}_{a+2} & k^a & \bar{K}_{a+1}\end{Bmatrix}\cdots\begin{Bmatrix} \bar{K}_{b-3}^b & k_{a+b-1} & \bar{K}_{b-2}^b\\ \bar{K}_{a+b-3} & k^a & \bar{K}_{a+b-2}\end{Bmatrix}\begin{Bmatrix} \bar{K}_{b-2}^b & k_{a+b} & k^b\\ k & k^a & \bar{K}_{a+b-2}\end{Bmatrix} \tag{41}$$

and

$$\phi_\gamma = (b-1)k^a + k + \sum_{i=1}^{b} k_{a+i} + \{\bar{K}^b\} + \bar{K}_{a+1} \cdots \bar{K}_{a+b-2} \; . \tag{42}$$

From the above discussion, it is evident that the relation between the n vectors coupled by scheme Z_{n0} to the Z_{a0} and Z_{b0} schemes is complicated by the matrix $\mathbf{A}^{ab}$. However, $\mathbf{A}^{ab}$ becomes the identity if the scheme Z_{n0} is replaced by Z_{ab} [cf. Eq. (19)],

$$T^{(k)q}_{\{\bar{K}\}}(k_1 \cdots k_n)^{Z_{ab}} = \sum_{q^a q^b} (-1)^{k^a-k^b+k}(k)^{1/2}(-1)^{k-q} \begin{pmatrix} k & k^a & k^b \\ -q & q^a & q^b \end{pmatrix} T^{(k^a)q^a}_{\{\bar{K}^a\}}(k_1 \cdots k_a)^{Z_{a0}} T^{(k^b)q^b}_{\{\bar{K}^b\}}(k_{a+1} \cdots k_{a+b})^{Z_{b0}} , \tag{43}$$

where $\{\bar{K}\} = \{\{\bar{K}^a\}\{\bar{K}^b\}k^a k^b\}$.

The decomposition of tensor operators into products of more than two operators follows by repeated application of Eq. (39) or (43).

IV. COMMUTATION RELATIONS

In this section, the commutation relations between $\mathcal{Y}^{(l)m}(\mathbf{I}_i)$ and $T^{(k)q}_{\{\bar{K}\}}(k_1 \cdots k_i \cdots k_n)^Z$ are given. First the commutator of two $\mathcal{Y}^{(l)m}$'s is derived before some general results are presented.

A commutator is the difference between the product of two operators and the product in opposite order. This can be calculated by working out the product $\mathcal{Y}^{(l)m}(\mathbf{I}_i)\mathcal{Y}^{(k_i)q_i}(\mathbf{I}_i)$ first and then relating this to the product in the reverse order, namely $\mathcal{Y}^{(k_i)q_i}(\mathbf{I}_i)\mathcal{Y}^{(l)m}(\mathbf{I}_i)$. To this end, such a product is written as a linear combination of $\mathcal{Y}^{(k_i')q_i'}(\mathbf{I}_i)$'s

$$\mathcal{Y}^{(l)m}(\mathbf{I}_i)\mathcal{Y}^{(k_i)q_i}(\mathbf{I}_i) = \sum_{k_i' q_i'} a^{lk_ik_i'}_{I_i}(-1)^{l-k_i+k_i'}(k_i')^{1/2}(-1)^{k_i'-q_i'} \begin{pmatrix} l & k_i & k_i' \\ m & q_i & -q_i' \end{pmatrix} \mathcal{Y}^{(k_i')q_i'}(\mathbf{I}_i) , \tag{44}$$

where $a^{lk_ik_i'}_{I_i}$ is found to be

$$a^{lk_ik_i'}_{I_i} = (i)^{k_i'+l+k_i}[(l)(k_i)(I_i)]^{1/2}(-1)^{2I_i} \begin{Bmatrix} k_i' & l & k_i \\ I_i & I_i & I_i \end{Bmatrix} . \tag{45}$$

Notice that $a^{lk_ik_i'}_{I_i}$ is symmetric to the interchange of l and k_i. Hence the only difference between Eq. (44) and that of the product in the reverse order, namely $\mathcal{Y}^{(k_i)q_i}(\mathbf{I}_i)\mathcal{Y}^{(l)m}(\mathbf{I}_i)$, appears in the 3-$j$ coefficient, thereby introducing the phase $(-1)^{k_i+l+k_i'}$. Consequently, the commutator is given by

$$\begin{aligned}[\mathcal{Y}^{(l)m}(\mathbf{I}_i), \mathcal{Y}^{(k_i)q_i}(\mathbf{I}_i)]_- = 2 \sum_{k_i'q_i'} \Phi(l, k_i k_i')(i)^{k_i'+l+k_i}[(l)(k_i)(\mathbf{I}_i)]^{1/2} \\ \times(-1)^{2I_i} \begin{Bmatrix} k_i' & l & k_i \\ I_i & I_i & I_i \end{Bmatrix} (-1)^{l-k_i+k_i'}(k_i')^{1/2}(-1)^{k_i'-q_i'} \begin{pmatrix} l & k_i & k_i' \\ m & q_i & -q_i' \end{pmatrix} \mathcal{Y}^{(k_i')q_i'}(\mathbf{I}_i) ,\end{aligned} \tag{46}$$

where[3] $\Phi(l, k_i, k_i') = 1$, if $l + k_i + k_i'$ is odd and zero otherwise. Clearly, for the anticommutator, $\Phi(l, k_i, k_i')$ is replaced by $\Phi(l, k_i, k_i'+1)$.

The commutator of $\mathcal{Y}^{(l)m}(\mathbf{I}_i)$, with $T^{(k)q}(k_1k_2)$, is obtained by decomposing $T^{(k)q}(k_1k_2)$ via Eq. (32) into a product of two $\mathcal{Y}$'s, and then applying Eq. (46). The result is then recoupled back to a $T^{(k')q'}(k_1'k_2)$ to give

$$[\mathcal{Y}^{(l)m}(I_1), T^{(k)q}(k_1k_2)]_\mp = 2 \sum_{k_1' k'q'} (-1)^{l+k_1+k_2+k'} a^{lk_1k_1'}_{I_1\mp} [(k)(k_1)]^{1/2} \begin{Bmatrix} k_1 & k_1' & l \\ k' & k & k_2 \end{Bmatrix} (-1)^{l-k+k'}(k')^{1/2}(-1)^{k'-q'} \begin{pmatrix} l & k & k' \\ m & q & -q' \end{pmatrix} T^{(k')q'}(k_1'k_2) , \tag{47}$$

where

$$a^{lk_ik_i'}_{I_i\mp} = \Phi(l, k_i, k'^{+0}_{i+1}) a^{k_ik_i'}_{I_i} \; . \tag{48}$$

The commutator for $\mathcal{Y}^{(l)m}(\mathbf{I}_2)$ with $T^{(k)q}(k_1k_2)$ is obtained from Eq. (47) by interchanging the labels 1 and 2 and replacing $T^{(k')q'}(k_1'k_2)$ by $T^{(k')q'}(k_1k_2')$. The commutators and anticommutators of $\mathcal{Y}^{(l)m}$ with the $T^{(k)q}$'s, which involve three nuclei, are found in the same way. These are given by

$$\begin{aligned}[\mathcal{Y}^{(l)m}(\mathbf{I}_1), T^{(k)q}_{\bar{K}_1}(k_1k_2k_3)]_\mp = 2 \sum_{k_1'k'q'\bar{K}_1'} a^{lk_1k_1'}_{I_1\mp}[(k)(k_1')(\bar{K}_1)(\bar{K}_1')]^{1/2} \\ \times(-1)^{k_1+k_2+k_3+\bar{K}_1+\bar{K}_1'+k'} \begin{Bmatrix} k_1 & k_1' & l \\ \bar{K}_1' & \bar{K}_1 & k_2 \end{Bmatrix} \begin{Bmatrix} \bar{K}_1 & \bar{K}_1' & l \\ k' & k & k_3 \end{Bmatrix} (-1)^{l-k+k'}(k')^{1/2}(-1)^{k'-q'} \begin{pmatrix} l & k & k' \\ m & q & -q' \end{pmatrix} T^{(k')q'}_{\bar{K}_1'}(k_1'k_2k_3) ,\end{aligned} \tag{49}$$

$$[\mathcal{Y}^{(l)m}(\mathbf{I}_2), T^{(k)q}_{\bar{K}_1}(k_1k_2k_3)]_\mp = 2 \sum_{k_2'k'q'\bar{K}_1'} a^{lk_2k_2'}_{I_2\mp}[(k)(k_2')(\bar{K}_1)(\bar{K}_1')]^{1/2}$$

$$\times(-1)^{k_1+k_2'+k_3+k'}\begin{Bmatrix} k_2 & k_2' & l \\ \bar{K}_1' & \bar{K}_1 & k_1 \end{Bmatrix}\begin{Bmatrix} \bar{K}_1 & \bar{K}_1' & l \\ k' & k & k_3 \end{Bmatrix}(-1)^{l-k+k'}(k')^{1/2}(-1)^{k'-q'}\begin{pmatrix} l & k & k' \\ m & q & -q' \end{pmatrix} T_{\bar{K}_1'}^{(k')q'}(k_1k_2'k_3)\ , \tag{50}$$

and

$$[\mathcal{Y}^{(l)m}(\mathbf{I}_3), T_{\bar{K}_1}^{(k)q}(k_1k_2k_3)]_{\mp} = 2\sum_{k_3'k'q'} a_{I_3\mp}^{lk_3k_3'}[(k)(k_3')]^{1/2}(-1)^{k+l+\bar{K}_1+k_3'}\begin{Bmatrix} k_3 & k_3' & l \\ k' & k & \bar{K}_1 \end{Bmatrix}(-1)^{l-k+k'}(k')^{1/2}(-1)^{k'-q'}\begin{pmatrix} l & k & k' \\ m & q-q' \end{pmatrix} T_{\bar{K}_1}^{(k')q'}(k_1k_2k_3')\ . \tag{51}$$

The commutation relations of operators composed of a higher number of spins can be given in general. In particular, the commutator of $\mathcal{Y}^{(l)m}(\mathbf{I}_n)$ on the last spin will always involve a transformation similar to Eq. (51). In fact the commutator $[\mathcal{Y}^{(l)m}(I_n), T_{\{\bar{K}\}}^{(k)q}(k_1\cdots k_n)^Z]_-$ can be obtained from Eq. (51) simply by replacing the label 3 by n; $\bar{K}_1$ by $\bar{K}_{n-2}$ and $T_{\bar{K}}^{(k')q'}(k_1k_2k_3')$ by $T_{\{\bar{K}_1\}}^{(k')q'}(k_1\cdots k_n')$. Other cases involve $(n-i+1)$ 6-j's. The result for coupling scheme Z_{n0} is

$$[\mathcal{Y}^{(l)m}(\mathbf{I}_i), T_{\{\bar{K}\}}^{(k)q}(k_1\cdots k_i\cdots k_n)^{Zn0}]_{\mp} = \sum_{\substack{k_i'k'q' \\ \{\bar{K}'\}}} \phi_{\mp}^{lk_i'}(k,k',\{\bar{K}\},\{\bar{K}'\},k_i\cdots k_n)^{Zn0}(-1)^{k'-q'}\begin{pmatrix} k' & l & k \\ -q' & m & q \end{pmatrix} T_{\{\bar{K}'\}}^{(k')q'}(k_1\cdots k_i'\cdots k_n)^{Zn0}\ , \tag{52}$$

where

$$\phi_{\mp}^{lk_i'}(k,k',\{\bar{K}\},\{\bar{K}'\},k_i\cdots k_n)^{Zn0} = 2(-1)^{l+k+k'}a_{I_i\mp}^{lk_ik_i'}[(k)(k_i')(k')]^{1/2}[(\bar{K}_{i-1})\cdots(\bar{K}_{n-2})]^{1/2}[(\bar{K}_{i-1}')\cdots(\bar{K}_{n-2}')]^{1/2}\prod_{j=1}^{n-2}\{\delta(\bar{K}_j\bar{K}_j')\}\mathbf{D}\ . \tag{53}$$

The diagram **D** is the closed reducible diagram in Fig. 7 explicitly given by

$$\mathbf{D} = (-1)^{\phi_D}\begin{Bmatrix} k_i & k_i' & l \\ \bar{K}_{i-1}' & \bar{K}_{i-1} & \bar{K}_{i-2} \end{Bmatrix}\begin{Bmatrix} \bar{K}_{i-1} & \bar{K}_{i-1}' & l \\ \bar{K}_i' & \bar{K}_i & k_{i+1} \end{Bmatrix}\cdots\begin{Bmatrix} \bar{K}_{n-2} & \bar{K}_{n-2}' & l \\ k' & k & k_n \end{Bmatrix}\ , \tag{54}$$

where

$$\phi_D = (n-i+1)l + k_i' + k_{i+1} + \cdots + k_n + \bar{K}_i + \cdots + \bar{K}_{n-2} + \bar{K}_i' + \cdots + \bar{K}_{n-2}' + k' + \bar{K}_{i-2}\ . \tag{55}$$

Some confusion might arise in the use of Eq. (54) for the case when $n \le 3$, and for cases when $i = 1, 2,$ or n, for any n. The commutation relations for $n = 1, 2, 3$ are given by Eqs. (46), (47), and (49)–(51). The expression for $i = n$ is discussed after Eq. (51). For $n > 3$ and $i = 1$ or 2, Eqs. (52) and (54) can still be used, but with the following modifications. For $i = 1$, $\bar{K}_{i-2}$ must be replaced by k_2, and ϕ_D by $(n-1)l + k_1 + k_2 + \cdots + k_n + \bar{K}_1 + \cdots + \bar{K}_{n-2} + \bar{K}_1' + \cdots + \bar{K}_{n-1}' + k'$, while for $i = 2$, $\bar{K}_{i-2}$ must be replaced by k_1 and ϕ_D by $(n-1)l + k_1 + k_2' + k_3 + \cdots + k_n + \bar{K}_2 + \cdots + \bar{K}_{n-2} + \bar{K}_2' + \cdots + \bar{K}_{n-2}' + k'$.

V. REDUCED MATRIX ELEMENTS

The results from the preceeding sections are now used to evaluate reduced matrix elements in any coupling scheme. These are defined in the usual manner,[9] namely,

$$\langle\gamma IM|\, T_{\{\bar{K}\}}^{(k)q}(k_1\cdots k_n)\,|\gamma'I'M'\rangle = (-1)^{I-M}\begin{pmatrix} I & k & I' \\ -M & q & M' \end{pmatrix}\langle\gamma I||\, T_{\{\bar{K}\}}^{(k)q}(k_1\cdots k_n)||\gamma'I'\rangle\ . \tag{56}$$

As a consequence of Eq. (23), the following relation holds

$$\langle\gamma'I'||\, T_{\{\bar{K}\}}^{(k)}(k_1\cdots k_n)||\gamma I\rangle = (-1)^{I+k-I'}\langle\gamma I||\, T_{\{\bar{K}\}}^{(k)}(k_1\cdots k_n)||\gamma'I'\rangle^*\ , \tag{57}$$

where the * indicates the complex conjugate. The reduced matrix elements in the coupling scheme Z_{n0} are,

$$\langle (I_1\cdots I_n)^{Zn0}\{\bar{I}'\}I'||\, T_{\{\bar{K}\}}^{(k)}(k_1\cdots k_n)^{Zn0}||(I_1\cdots I_n)^{Zn0}\{\bar{I}\}I\rangle = (i)^{\Sigma_1^n k_i}[(I)(I')(k)]^{1/2}[(k_1)\cdots(k_n)]^{1/2}[(\bar{K}_1)\cdots(\bar{K}_{n-2})]^{1/2}[(\bar{I}_1)\cdots(\bar{I}_{n-2})]^{1/2}[(\bar{I}_1')\cdots(\bar{I}_{n-2}')]^{1/2}\Delta\ , \tag{58}$$

where Δ is given by Eq. (37).

By use of Eq. (43), the reduced matrix elements of $T^{(k)q}$ in the Z_{ab} scheme can be obtained, viz.[9,5]

$$\langle\gamma I||\, T_{\{\bar{K}\}}^{(k)}(k_1\cdots k_n)^{Zab}||\gamma'I'\rangle = (k)^{1/2}(-1)^{I+I'+k}\sum_{\gamma''I''}\begin{Bmatrix} k^a & k^b & k \\ I' & I & I'' \end{Bmatrix} \times\langle\gamma I||\, T_{\{\bar{K}^a\}}^{(k^a)}(k_1\cdots k_n)^{Za0}||\gamma''I''\rangle\langle\gamma''I''||\, T_{\{\bar{K}^b\}}^{(k^b)}(k_{a+1}\cdots k_{a+b})^{Zb0}||\gamma'I'\rangle\ . \tag{59}$$

The reduced matrix elements on the RHS of Eq. (59) depend upon the coupling scheme used. If $||\gamma I\rangle$ in Eq. (59) are the states in the Z_{n0} coupling scheme, see Eq. (7), then the reduced matrix elements are,

$$\langle (I_1\cdots I_n)^{Zn0}\{\bar{I}\}I||\, T_{\{\bar{K}^a\}}^{(k^a)}(k_1\cdots k_a)^{Za0}||(I_1\cdots I_n)^{Zn0}\{\bar{I}'\}I'\rangle$$

$$= \sum_{\substack{\{\bar{I}^a\}\{\bar{I}^{a'}\} \\ \{\bar{I}^b\} I^a I^{a'} I^b}} \langle (I_1 \cdots I_n)^{Z_{n0}} \{\bar{I}\} IM | (I_1 \cdots I_n)^{Z_{ab}} \{\bar{I}^a\}\{\bar{I}^b\} I^a I^b IM \rangle \langle (I_1 \cdots I_n)^{Z_{n0}} \{\bar{I}'\} I'M' | (I_1 \cdots I_n)^{Z_{ab}} \{\bar{I}^{a'}\}\{\bar{I}^b\} I^{a'} I^b I'M' \rangle$$

$$\times (-1)^{I^a + I^b + I' + k^a} [(I)(I')]^{1/2} \begin{Bmatrix} I^a & I' & I^b \\ I & I^{a'} & k^a \end{Bmatrix} \langle (I_1 \cdots I_a)^{Z_{a0}} \{\bar{I}^a\} I^a || T^{(k^a)}_{\{\bar{K}^a\}}(k_1 \cdots k_a)^{Z_{a0}} || (I_1 \cdots I_n)^{Z_{a0}} \{\bar{I}^{a'}\} I^{a'} \rangle , \qquad (60)$$

which is a more explicit form of Edmonds,[9] (7.1.7). The two (M independent) transformation matrices are given in Eq. (16). Again, if the scheme Z_{ab} is used, instead of Z_{n0}, the transformation matrices become identities.

Consider now matrix elements of superoperators. For spin operators, an inner product is defined,

$$\langle\langle A | B \rangle\rangle \equiv \mathrm{Tr}(A^\dagger B) , \qquad (61)$$

where the trace is over all spin states. A reduced matrix element of the superoperator $\mathcal{L}^{lm}$ are then defined as

$$\langle\langle T^{(k')q'}_{\{V'\}} | \mathcal{L}^{lm} | T^{(k)q}_{\{V\}} \rangle\rangle = (-1)^{k'-q'} \begin{pmatrix} k' & l & k \\ -q' & m & q \end{pmatrix} \langle\langle T^{(k')}_{\{V'\}} || \mathcal{L}^l || T^{(k)}_{\{V\}} \rangle\rangle . \qquad (62)$$

Here $\mathcal{L}^{lm}$ is to be a superoperator of tensor rank l and spherical component m. These reduced matrix elements differ from those of Pyper[3] who uses the definition in Rose's[8] book which are in terms of Clebsch–Gordan coefficients rather than $3-j$ coefficients.

In many situations of interest, $\mathcal{L}^{lm}$ may depend on several different spins. Moreover, $\mathcal{L}^{lm}$ usually is a product of commutators of $\mathcal{Y}^{(l)q}(\mathbf{I}_i)$'s. With the understanding that this is the case a superoperator for several spins acting on some operator A is

$$\mathcal{L}^{lm}_{\{\bar{L}\}}(l_i l_j \cdots l_k) A = \sum_{\substack{m_\nu \\ \nu = ij \cdots k}} \langle (l_i l_j \cdots l_k)^{Z_{n0}} \{\bar{L}\} lm | l_i m_i l_j m_j \cdots l_k m_k \rangle [\mathcal{Y}^{(l_i)m_i}(\mathbf{I}_i), [\mathcal{Y}^{(l_j)m_j}(\mathbf{I}_j), \ldots, [\mathcal{Y}^{(l_k)m_k}(\mathbf{I}_k), A]_-, \ldots]_-]_- . \qquad (63)$$

It is then a simple matter to obtain reduced matrix elements for any special case. A few examples illustrate this. If $\mathcal{L}^{lm}(i) \equiv [\mathcal{Y}^{lm}(\mathbf{I}_i),]_-$ then from Eq. (53)

$$\langle\langle T^{(k')}_{\{\bar{K}'\}}(k_1 \cdots k_i' \cdots k_n)^{Z_{n0}} || \mathcal{L}^{lm}(i) || T^{(k)}_{\{\bar{K}\}}(k_1 \cdots k_i \cdots k_n)^{Z_{n0}} \rangle\rangle = \phi_-^{lk_i'}(k, k', \{\bar{K}\}\{\bar{K}'\}, k_i \cdots k_n) . \qquad (64)$$

For $\mathcal{L}^{lm}_{\bar{L}}({}^l i\, {}^l j\, {}^l k)$ depending upon spins i, j, and k, the reduced matrix element is

$$\langle\langle T^{(k''')}_{\{\bar{K}'''\}}(k_1 \cdots k_i' \cdots k_j' \cdots k_k' \cdots k_n)^{Z_{n0}} || \mathcal{L}^l_{\bar{L}}(l_i l_j l_k) || T^{(k)}_{\{\bar{K}\}}(k_1 \cdots k_i \cdots k_j \cdots k_k \cdots k_n)^{Z_{n0}} \rangle\rangle$$

$$= \sum_{\substack{k' k'' \\ \{\bar{K}'\}\{\bar{K}''\}}} \phi^{l_k k_k'}(kk'\{\bar{K}\}\{\bar{K}'\} k_k \cdots k_n) \phi_-^{l_j k_j'}(k'k''\{\bar{K}'\}\{\bar{K}''\} k_j \cdots k_k' \cdots k_n)$$

$$\times \phi_-^{l_i k_i'}(k''k'''\{\bar{K}''\}\{\bar{K}'''\} k_i \cdots k_j' \cdots k_k' \cdots k_n) [(\bar{L})(l)]^{1/2} (-1)^{k+k'+l+\bar{L}} \begin{Bmatrix} l_i & k'' & k''' \\ k' & \bar{L} & l_j \end{Bmatrix} \begin{Bmatrix} \bar{L} & k' & k''' \\ k & l & l_k \end{Bmatrix} . \qquad (65)$$

If n is taken as 3, the reduced matrix element of

$$\mathcal{L}^{(l)}_{(2)} \odot^l \mathcal{L}^{(l)}_{(3)} \equiv \sum_m (-1)^{l-m} \mathcal{L}^{(l)-m}_{(2)} \mathcal{L}^{(l)m}_{(3)}$$

is

$$\langle\langle T^{(k')}_{\bar{K}'}(k_1 k_2' k_3')^{Z_{n0}} || \mathcal{L}^{(l)}_{(2)} \odot_l \mathcal{L}^{(l)}_{(3)} || T^{(k)}_{\bar{K}}(k_1 k_2 k_3)^{Z_{n0}} \rangle\rangle$$

$$= \delta_{kk'} 4 \alpha^{lk_2k_2'}_{I_2-} \alpha^{lk_3k_3'}_{I_3-} [(k_2')(k_3')(\bar{K}_1)(\bar{K}_1')]^{1/2} (-1)^{k_1+k_2'+k_3+k} \begin{Bmatrix} k_2 & l & k_2' \\ \bar{K}_1' & k_1 & \bar{K}_1 \end{Bmatrix} \begin{Bmatrix} k_3 & l & k_3' \\ \bar{K}_1' & k & \bar{K}_1 \end{Bmatrix} \qquad (66)$$

These few examples show that with only a minimum of recoupling, the reduced super matrix elements of $\mathcal{L}^{lm}$ can be obtained for any case. They are given, however, for coupling scheme Z_{n0}. The reduced matrix elements in coupling schemes other than Z_{n0} can be obtained by first transforming to coupling scheme Z_{n0} (see Sec. III). Some special cases of reduced matrix elements (up to $n=5$) are given for useful forms of $\mathcal{L}^{lm}$ by Pyper.[3]

VI. DISCUSSION

The object of this paper is to construct a set of operators, $T^{(k)}_{\{\bar{K}\}}(k_1 \cdots k_n)^Z$, which form a complete set of basis operators for a system of n spins which are coupled via some scheme Z. Moreover, the properties of these T's are discussed and general formulas derived for transformations between different coupling schemes. In particular it is shown that in decomposing a T into a product of two operators which are constructed from distinct parts of spin space, a particular choice of coupling scheme greatly simplifies the formulas. That is, if the n spins are

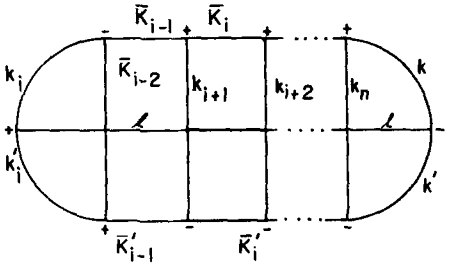

FIG. 7. Diagrammatic representation of commutation at the ith position. The closed diagram is D.

coupled via scheme Z_{n0}, then a complicated transformation matrix arises if the resultant decomposed operators are required to be in the *same* coupling scheme, namely Z_{a0} and Z_{b0} $[a+b=n$, see Eq. (39)]. However, the transformation matrix is the identity if the n spins are coupled via scheme Z_{ab} rather than scheme Z_{n0}. The same is true for the n-spin basis states as shown in Sec. II.

The T's for multiple spins are composed of tensor operators for individual spins, namely $\mathcal{Y}^{(l)m}(\mathbf{I}_i)$'s. The explicit form of the $\mathcal{Y}$'s is given for $l=0-3$, in Table I while for $l>3$, they can be obtained from Eqs. (21), (24), and (27) (see also Ref. 8). Knowing the $\mathcal{Y}$'s explicitly facilitates the writing of scalar operators (say a spin Hamiltonian) in terms of the $\mathcal{Y}$'s. This leads to matrix and super matrix elements of the spin part of the Hamiltonian being given in terms of products of $\mathcal{Y}$'s or products of commutators of $\mathcal{Y}$'s. Evaluation of these, however, does not depend on the explicit form of the $\mathcal{Y}$'s or T's, but follows from arguments of rotational invariance. In many cases, this requires a great deal of tedious recoupling of the tensors. To circumvent this problem, the commutation relations are given between the $\mathcal{Y}$'s and T's for any number of spins. The coupling scheme used is Z_{n0}, with other schemes being related to the Z_{n0} commutation relations by transformation matrices. A consequence of giving the commutation relations is a great reduction in the amount of recoupling needed to arrive at the reduced matrix elements. In general, evaluation of Eq. (62) with $\mathcal{L}^{lm}$ depending on i spins requires recoupling which results in $i-1$ additional $6-j$ coefficients. In most situations an i of 1 to 4 is common. The evaluation of reduced matrix elements is consequently simplified. Moreover, the generality of the expressions which are valid for arbitrary n is a new and hopefully useful part of this work.

A further aspect of this work which appears to be new is the explicit expansion of multispin operators of the form $|\alpha\rangle\langle\beta|$ in a multipole series [Eq. (38)]. With this expansion, the relation between equations such as (1) and (2) is established.

In conclusion, some remarks are made regarding Pyper's[3] work, which in many aspects is close to this. As mentioned above, the formulas here are more general than Pyper's in that here they are given for an arbitrary number of spins. Moreover, the forms of the multispin multipole operators $T^{(k)q}_{\{V\}}$, with emphasis on different coupling schemes and general transformation matrices between them, are given here as well as explicit multipole expansions of spin operators. Pyper emphasizes that explicit construction of the single spin operators, here denoted $\mathcal{Y}^{(l)m}(\mathbf{I})$, it not necessary in order to evaluate reduced matrix elements. This is true, yet before evaluation of reduced matrix elements is undertaken, it is necessary to re-express a given spin operator in terms of the $\mathcal{Y}^{(l)m}$'s. Thus the explicit form is required, and for this reason they are given here. In doing so, however, a restriction to this particular set of single spin operators is made. More general angular momentum operators, such as those with off-diagonalities in I_i, namely $|I_i m_i\rangle\langle I_i' m_i'|$, are not treated.

Finally Pyper discusses a symmetry operation which he calls spin inversion to which the symbol $\mathcal{S}$ is given here. This is defined by $\mathcal{S}=\mathcal{T}R_y(\pi)$. $R_y(\pi)$ rotates an operator about the space fixed y axis by π and $\mathcal{T}$ is a conjugation operation: $\mathcal{T}|a\rangle\langle b|=|b\rangle\langle a|$. In fact the operation $\mathcal{T}$ was introduced by Ben Reuven[10] and called Liouville conjugation (and given the symbol C_L). $\mathcal{S}$ is a superoperator, and from Eq. (29) it follows that

$$\mathcal{S}\mathcal{Y}^{(k)q}(\mathbf{I}_i)=\mathcal{Y}^{(k)q}(\mathbf{I}_i)\ . \tag{67}$$

This is in contrast to the property of Pyper's $T^{(k)}_{qi}$ which has eigenvalue $(-1)^k$ under the $\mathcal{S}$ operation. The difference lies in the phase difference of $(i)^k$ between T and $\mathcal{Y}$.

It therefore follows the $\mathcal{S}$ is not a useful symmetry operation for the operators defined here. The equivalent statement to Pyper's symmetry operation $\mathcal{S}$ for the super matrix elements of the commutator (or anticommutator) type is that it vanishes unless k_i+l+k_i' is odd (even). [See Eq. (46).]

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