Irreducible half-integer rank unit spherical tensors

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A new class of half-integer rank spherical tensors is introduced. The motivation for investigating this new class of tensors originated from a desire to be able to partition matrices using mixtures of fictitious integer and half-integer spin labels. However, it is shown that they can also be used as annihilation/creation operators for spin-1/2, 3/2, etc., particles. In particular, half-integer rank tensors can be used to add/subtract a spin-1/2 particle from a given ensemble. Thus they can be viewed as the natural generalization of the raising and lowering operators $I_{\pm}$, in that they change both I and M, simultaneously.

The concept of a "universal rotator" is introduced and it is demonstrated that half-integer rank tensors obey the same contractional and rotational properties as their integer counterparts, but with half-integer rank. In addition, it is shown that half-integer rank tensors can be used to factorize the Pauli spin matrices. Finally, an example of the use of half-integer rank tensors in the block-diagonalization of a simple 3×3 matrix is presented and discussed.

1. Introduction

It has been known for many years that integer rank irreducible tensor operators $T^K_Q(I)$ [1] can be used to describe real physical operators on single spin systems. Such tensors possess well documented rotation and commutation properties, and can be represented by spherical harmonics. More recently, it has been shown that Fano's unit spherical tensor operators $\hat{U}^K_Q(I_i, I_j)$ [2,3] can be used to describe coupled nuclear spin systems evolving under various hyperfine interactions. For example, for three coupled spin-1/2 nuclei, the total angular momentum can take on the values of $I = 3/2, 1/2$, and $1/2'$, where the spin states $1/2$ and $1/2'$ differ by virtue of their different coupling schemes. Thus the Hamiltonian for the three-spin-1/2 system and the density matrix can be described in terms of the $\hat{U}^K_Q(I_i, I_j)$, where I_i and I_j can take on the values of $I = 3/2, 1/2$, and $1/2'$. For unit spherical tensors with $I_i = I_j$, it can be shown that $\hat{U}^K_Q(I_i, I_i)$ is identical with the single spin operator $\hat{T}^K_Q(I_i)$. However, when $I_i \neq I_j$, the $\hat{U}^K_Q(I_i, I_j)$ are off-diagonal and non-square if $|I_i| \neq |I_j|$. Such off-diagonal tensors are unobservable, but they play an important role in exchanging information between the various spin states available to the system.

In this paper a new class of half-integer rank tensors is introduced. The motivation behind this work was provided by a desire to (i) generalize Fano's unit spherical tensors $\hat{U}^K_Q(I_i, I_j)$ to half-integer rank tensors, and (ii) address the problem of block-diagonalization, using mixtures of half-integer and integer spin [4]. For example, it should be possible, at least from a mathematical point of view, to block-diagonalize a simple 3×3 matrix into a $2 \times 2 \oplus 1 \times 1$ matrices, using fictitious spins of $I_1 = 1/2$ and $I_2 = 0$, respectively.

In the course of this work it soon became apparent that (i) half-integer rank tensors obey the same multiplication and commutation rules as their integer counterparts, but with K half-integer, and (ii) half-integer rank tensors can be viewed as the generalization of the familiar creation and annihilation operators, $a^\dagger$ and a, for two level spin system, to multi-level spin systems. In essence, half-integer rank tensors can be used to add or subtract spin 1/2 nuclei from a given spin system, thereby changing the total spin I and total projection M, simultaneously.

The structure of this paper is as follows. In the following three sections, the basic properties of half-integer rank tensors are explored. This is followed by a discussion of the creation and annihilation operators for multi-level spin-1/2 spin systems, in the strongly coupled representation. Finally, the problem of block-diagonalizing a simple 3×3 matrix into a $2 \times 2 \oplus 1 \times 1$ matrices is discussed within the framework of both half-integer and integer rank unit spherical tensors.

2. Half integer rank unit spherical tensors

Unit spherical tensors of integer rank K were first used by [5,6], in the theory of radioactive decay. However, since unit spherical tensors form an orthonormal set, they can be used to describe any matrix. For the purposes of this paper, the unit spherical tensors are defined via

$$\langle I_i M_i | \hat{U}^K_Q(I_i, I_j) | I_j M_j \rangle = (-1)^{I_j - M_i} \sqrt{2K+1} \begin{pmatrix} I_i & K & I_j \\ -M_i & Q & M_j \end{pmatrix}, \tag{1}$$

or alternatively

$$\langle I_i M_i | \hat{U}^K_Q(I_i, I_j) | I_j M_j \rangle = (-1)^{I_i + M_i - K} \sqrt{2K+1} \begin{pmatrix} I_i & I_j & K \\ -M_i & M_j & Q \end{pmatrix}, \tag{2}$$

a form which is useful in proving the orthogonality of the unit spherical spherical tensors (see below). The reader should note that eq. (2) differs from that of ref. [6] (eq. (12.42)) by a phase-factor $(-1)^{-K}$. With the phase convention used in this paper, the unit spherical operators reduce to the single spin irreducible tensor operators $\hat{T}^K_Q(I)$ of Buckmaster [1] for $I_i = I_j = I$. Further, for integer K all the unit spherical tensors are real, whereas for half-integer K, all the unit spherical tensors are pure imaginary.

Following [6], but with a change in phase, the Hermitian transpose is defined via

$$\langle I_j M_j | \hat{U}^K_Q(I_i, I_j)^\dagger | I_i M_i \rangle = \langle I_i M_i | \hat{U}^K_Q(I_i, I_j) | I_j M_j \rangle^* . \tag{3}$$

Using (3), together with the symmetry properties of the Wigner 3j coefficient, it can be shown that

$$\hat{U}^K_Q(I_i, I_j)^\dagger = (-1)^{I_i - I_j + Q + 2K} \hat{U}^K_{-Q}(I_j, I_i) , \tag{4}$$

Note that this transpose differs from that for integer rank tensors by an extra phase factor $(-1)^{2K}$. For integer rank tensors this phase factor is unimportant.

Given equations (2) and (4) it is easily shown that the unit spherical tensors form an orthonormal set. Explicitly,

$$\begin{aligned}
&\mathrm{Tr}\left[\hat{U}^K_Q(I_i, I_j)^\dagger \hat{U}^{K'}_{Q'}(I_i, I_j)\right] \\
&= \sum_{M_i, M_j} \langle I_j M_j | \hat{U}^K_Q(I_i, I_j)^\dagger | I_i M_i \rangle \langle I_i M_i | \hat{U}^{K'}_{Q'}(I_i, I_j) | I_j M_j \rangle \\
&= \sum_{M_i, M_j} \left\{ (-1)^{I_i - I_j + Q + 2K} (-1)^{I_j + M_j - K} \sqrt{2K+1} \begin{pmatrix} I_j & I_i & K \\ -M_j & M_i & -Q \end{pmatrix} \right\} \\
&\quad \times \left\{ (-1)^{I_i + M_i - K'} \sqrt{2K'+1} \begin{pmatrix} I_i & I_j & K' \\ -M_i & M_j & Q' \end{pmatrix} \right\} \\
&= (-1)^{K-K'} \sqrt{(2K+1)(2K'+1)} \sum_{M_i, M_j} \begin{pmatrix} I_i & I_j & K \\ -M_i & M_j & Q \end{pmatrix} \begin{pmatrix} I_i & I_j & K' \\ -M_i & M_j & Q' \end{pmatrix} \\
&= \delta_{KK'} \delta_{QQ'} ,
\end{aligned} \tag{5}$$

where we have used the orthonormal and symmetry properties of the Wigner 3j coefficients [7].

As with integer rank tensors, it is possible to project out the half-integer components in the usual way, i.e.

$$\rho^K_Q(I_i, I_j) = \mathrm{Tr}\left[\hat{U}^K_Q(I_i, I_j)^\dagger M\right] , \tag{6}$$

where M is an arbitrary matrix, and $\rho^K_Q(I_i, I_j)$ is the magnitude of the unit spherical tensor $\hat{U}^K_Q(I_i, I_j)$ appearing in M. Thus any matrix can be reduced to a sum of integer and half-integer rank unit spherical tensors, multiplied by their appropriate coefficients $\rho^K_Q(I_i, I_j)$. It should be noted that half-integer rank unit spherical tensors are always "non-square". The matrix dimensions of half-integer rank tensors must differ by an odd number.

As an example of half-integer unit spherical tensors, consider the case of the 3×3 matrix mentioned earlier. This matrix can now be partitioned using the spin labels $I_i = 1/2$ and $I_j = 0$, giving rise to block diagonal 2×2 and 1×1 matrices and two non block-diagonal 2×1 and 1×2 matrices. The block diagonal 2×2 matrices spanned by the $I = 1/2$ manifold have already been given (see for example

Table 1
The half-integer unit spherical operators $\hat{U}^{1/2}_{\pm 1/2}(\frac{1}{2},0)$ and $\hat{U}^{1/2}_{\pm 1/2}(0,\frac{1}{2})$.

$\hat{U}^{1/2}_{1/2}(\frac{1}{2},0)=\begin{pmatrix} \mathrm{i} \\ 0 \end{pmatrix}$	$\hat{U}^{1/2}_{-1/2}(\frac{1}{2},0)=\begin{pmatrix} 0 \\ \mathrm{i} \end{pmatrix}$
$\hat{U}^{1/2}_{1/2}(0,\frac{1}{2})=\begin{pmatrix} 0 & \mathrm{i} \end{pmatrix}$	$\hat{U}^{1/2}_{-1/2}(0,\frac{1}{2})=\begin{pmatrix} -\mathrm{i} & 0 \end{pmatrix}$

table 1(b) of ref. [3]). The off-block diagonal matrices can be seen in table 1. In a similar fashion, a 5×5 matrix can be partitioned using the spin labels $I = 1$ and $1/2$. the off block-diagonal matrices for this case are shown in table 2.

3. Factorization of integer rank tensors

It is of some interest to examine the products of half-integer rank tensors. For the irreducible tensors of rank $1/2$, we find

$$\hat{U}^{1/2}_{1/2}(\tfrac{1}{2},0)\,\hat{U}^{1/2}_{1/2}(0,\tfrac{1}{2}) = \begin{bmatrix} 0 & -1 \\ 0 & 0 \end{bmatrix} = \hat{U}^{1}_{1}(\tfrac{1}{2},\tfrac{1}{2}),$$

Table 2
The half-integer unit spherical operators $\hat{U}^{1/2}_{\pm Q}(1,\frac{1}{2})$, $\hat{U}^{3/2}_{\pm Q}(1,\frac{1}{2})$, $\hat{U}^{1/2}_{\pm Q}(\frac{1}{2},1)$ and $\hat{U}^{3/2}_{\pm Q}(\frac{1}{2},1)$.

$\hat{U}^{1/2}_{1/2}(1,\frac{1}{2})=\frac{\mathrm{i}}{\sqrt{3}}\begin{pmatrix} \sqrt{2} & 0 \\ 0 & 1 \\ 0 & 0 \end{pmatrix}$	$\hat{U}^{1/2}_{-1/2}(1,\frac{1}{2})=\frac{\mathrm{i}}{\sqrt{3}}\begin{pmatrix} 0 & 0 \\ 1 & 0 \\ 0 & \sqrt{2} \end{pmatrix}$
$\hat{U}^{1/2}_{1/2}(\frac{1}{2},1)=\frac{\mathrm{i}}{\sqrt{3}}\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & \sqrt{2} \end{pmatrix}$	$\hat{U}^{1/2}_{-1/2}(\frac{1}{2},1)=-\frac{\mathrm{i}}{\sqrt{3}}\begin{pmatrix} \sqrt{2} & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$
$\hat{U}^{3/2}_{3/2}(1,\frac{1}{2})=\begin{pmatrix} 0 & -\mathrm{i} \\ 0 & 0 \\ 0 & 0 \end{pmatrix}$	$\hat{U}^{3/2}_{-3/2}(1,\frac{1}{2})=\begin{pmatrix} 0 & 0 \\ 0 & 0 \\ \mathrm{i} & 0 \end{pmatrix}$
$\hat{U}^{3/2}_{1/2}(1,\frac{1}{2})=\frac{\mathrm{i}}{\sqrt{3}}\begin{pmatrix} 1 & 0 \\ 0 & -\sqrt{2} \\ 0 & 0 \end{pmatrix}$	$\hat{U}^{3/2}_{-1/2}(1,\frac{1}{2})=\frac{\mathrm{i}}{\sqrt{3}}\begin{pmatrix} 0 & 0 \\ \sqrt{2} & 0 \\ 0 & -1 \end{pmatrix}$
$\hat{U}^{3/2}_{3/2}(\frac{1}{2},1)=\begin{pmatrix} 0 & 0 & -\mathrm{i} \\ 0 & 0 & 0 \end{pmatrix}$	$\hat{U}^{3/2}_{-3/2}(\frac{1}{2},1)=\begin{pmatrix} 0 & 0 & 0 \\ -\mathrm{i} & 0 & 0 \end{pmatrix}$
$\hat{U}^{3/2}_{1/2}(\frac{1}{2},1)=\frac{\mathrm{i}}{\sqrt{3}}\begin{pmatrix} 0 & \sqrt{2} & 0 \\ 0 & 0 & -1 \end{pmatrix}$	$\hat{U}^{3/2}_{-1/2}(\frac{1}{2},1)=\frac{\mathrm{i}}{\sqrt{3}}\begin{pmatrix} -1 & 0 & 0 \\ 0 & \sqrt{2} & 0 \end{pmatrix}$

$$\hat{U}^{1/2}_{-1/2}(\tfrac{1}{2},0)\,\hat{U}^{1/2}_{-1/2}(0,\tfrac{1}{2}) = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} = \hat{U}^{1}_{-1}(\tfrac{1}{2},\tfrac{1}{2}),$$

$$\hat{U}^{1/2}_{1/2}(\tfrac{1}{2},0)\,\hat{U}^{1/2}_{-1/2}(0,\tfrac{1}{2}) + \hat{U}^{1/2}_{-1/2}(\tfrac{1}{2},0)\,\hat{U}^{1/2}_{1/2}(0,\tfrac{1}{2}) = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = \sqrt{2}\,\hat{U}^{1}_{0}(\tfrac{1}{2},\tfrac{1}{2}),$$

$$\hat{U}^{1/2}_{1/2}(\tfrac{1}{2},0)\,\hat{U}^{1/2}_{-1/2}(0,\tfrac{1}{2}) - \hat{U}^{1/2}_{-1/2}(\tfrac{1}{2},0)\,\hat{U}^{1/2}_{1/2}(0,\tfrac{1}{2}) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \sqrt{2}\,\hat{U}^{0}_{0}(\tfrac{1}{2},\tfrac{1}{2}). \quad (7)$$

Thus the $K = 1/2$ rank irreducible tensors can be used to "factorize" the Pauli spin matrices. However these are not unique. For example using table 2, for spins $1/2$ and 1, it can be shown that

$$\hat{U}^{3/2}_{1/2}(\tfrac{1}{2},1)\,\hat{U}^{3/2}_{1/2}(1,\tfrac{1}{2}) = \tfrac{2}{3}\begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} = -\tfrac{2}{3}\hat{U}^{1}_{1}(\tfrac{1}{2},\tfrac{1}{2}),$$

$$\hat{U}^{3/2}_{-1/2}(\tfrac{1}{2},1)\,\hat{U}^{3/2}_{-1/2}(1,\tfrac{1}{2}) = -\tfrac{2}{3}\begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} = -\tfrac{2}{3}\hat{U}^{1}_{-1}(\tfrac{1}{2},\tfrac{1}{2}),$$

$$\hat{U}^{3/2}_{1/2}(\tfrac{1}{2},1)\,\hat{U}^{3/2}_{-1/2}(1,\tfrac{1}{2}) + \hat{U}^{3/2}_{-1/2}(\tfrac{1}{2},1)\,\hat{U}^{3/2}_{1/2}(1,\tfrac{1}{2}) = -\tfrac{1}{3}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = -\frac{\sqrt{2}}{3}\hat{U}^{1}_{0}(\tfrac{1}{2},\tfrac{1}{2}),$$

$$\hat{U}^{3/2}_{1/2}(\tfrac{1}{2},1)\,\hat{U}^{3/2}_{-1/2}(1,\tfrac{1}{2}) - \hat{U}^{3/2}_{-1/2}(\tfrac{1}{2},1)\,\hat{U}^{3/2}_{1/2}(1,\tfrac{1}{2}) = -\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = -\sqrt{2}\,\hat{U}^{0}_{0}(\tfrac{1}{2},\tfrac{1}{2}). \quad (8)$$

These results can be generalized to unit spherical tensors characterized by spins $I_1 = 1/2$ and $I_2 = I$, where I is general.

4. Commutation and rotational relationships

Following [2], it is a relatively straightforward matter to show that the multiplication of two unit spherical tensors is given by

$$\hat{U}^{K}_{Q}(I_i,I_k)\,\hat{U}^{K'}_{Q'}(I_k,I_j) = \sum_{\mathcal{K},\Omega} B(K,K',\mathcal{K},I_i,I_j,I_k)\langle KQK'Q'|\mathcal{K}\Omega\rangle\,\hat{U}^{\mathcal{K}}_{\Omega}(I_i,I_j), \quad (9)$$

where the constant $B(K,K',\mathcal{K},I_i,I_j,I_k)$ is given by

$$B(K,K',\mathcal{K},I_i,I_j,I_k) = (-1)^{I_i+I_j+\mathcal{K}}\sqrt{(2K+1)(2K'+1)}\begin{Bmatrix} K & K' & \mathcal{K} \\ I_j & I_i & I_k \end{Bmatrix}. \quad (10)$$

These relationships hold for both integer and half-integer rank tensors. A proof of this result is given in appendix A.

Using eqs. (9) and (10), it is possible to generate the commutation relationships

$$\left[\mathfrak{J}_z, \hat{U}_Q^K(I_i, I_k)\right]_- = Q\hat{U}_Q^K(I_i, I_k),$$

$$\left[\mathfrak{J}_\pm, \hat{U}_Q^K(I_i, I_k)\right]_- = \sqrt{(K \mp Q)(K \pm Q + 1)}\,\hat{U}_{Q\pm1}^K(I_i, I_k), \tag{11}$$

where $\mathfrak{J}_z$ and $\mathfrak{J}_\pm$ are given by

$$\mathfrak{J}_z = \sum_i I_z(i),$$

$$\mathfrak{J}_\pm = \sum_i I_\pm(i). \tag{12}$$

Note that the $I_z(i)$ are all in non-unit form, and the sum over i runs over all the spin states (fictitious or otherwise) available to the spin system. These operations hold for both integer and half-integer operators. A proof is given in appendix B.

For single spins, the wave functions $|Im\rangle$ transform according to

$$|Im\rangle \to \sum_{m'} \mathcal{D}^I_{m'm}(\alpha, \beta, \gamma)|Im'\rangle, \tag{13}$$

where

$$\mathcal{D}^I_{m'm}(\alpha, \beta, \gamma) = \langle Im'|D(\alpha, \beta, \gamma)|Im\rangle$$
$$= \langle Im'|\exp i\gamma I_z \exp i\beta I_y \exp i\alpha I_z|Im\rangle. \tag{14}$$

Here the $\mathcal{D}^I_{m'm}(\alpha, \beta, \gamma)$ are the well known rotation matrices, for passive rotations of the co-ordinate system, see for example [8].

We now generalize equations (13) and (14) to the case of multiple connected spins. In ref. [2], it was shown that the unit spherical tensors $\hat{U}_Q^K(I_i, I_j)$ for arbitrary I_i and I_j transform according to

$$D(\alpha, \beta, \gamma)\hat{U}_Q^K(I_i, I_j)D(\alpha, \beta, \gamma)^\dagger = \sum_{Q'} \hat{U}_{Q'}^K(I_i, I_j)\mathcal{D}^K_{Q'Q}(\alpha, \beta, \gamma). \tag{15}$$

Thus following a rotation through the Euler angles (α, β, γ), the unit spherical tensors rotate within the manifold spanned by I_i and I_j, independent of the other tensors in different blocks. This result can be also generalized to half-integer rank tensors [9]. Indeed, the Racah like commutation relationships of eq. (11), which hold for both integer and half-integer rank tensors, are equivalent to the statement that under rotation from one co-ordinate system to another the unit spherical tensors transform according to eq. (15), for K both integer and half-integer. Thus the half-integer spherical tensors obey the same rotation properties as spinors, a not entirely unexpected result.

Next we observe that the results embodied in eqs. (11), (12) and (15) can be used to define a "universal spin operator":

$$D_{\text{uni}}(\alpha, \beta, \gamma) = \exp i\gamma\mathfrak{J}_z \exp i\beta\mathfrak{J}_y \exp i\alpha\mathfrak{J}_z, \tag{16}$$

which holds for both single and multiple connected spin systems. Note that the exponential operators appearing in eq. (16) are block-diagonal and cannot link differing spins. The link between differing spins is effected solely by the unit spherical tensors appearing on the LHS of eq. (15).

Finally, we state without proof that non-unit spherical tensors can be constructed from their unit counterparts, using the "normalization factor" given by [2].

5. Creation and annihilation operators

The raising and lowering operators

$$I_{\pm}|I,m\rangle = \sqrt{(I\mp m)(I\pm m+1)}\,|I,m\pm 1\rangle \tag{17}$$

play an important role, in the theory of angular momentum. Here the action of the operators $I_{\pm}$ is to change the state of the azimuthal quantum number m, whist leaving the spin I unchanged. In this section it is shown that half-integer (integer) rank spherical tensors can be used to (i) create spinor (boson) fields, respectively, and (ii) change both I and m simultaneously.

We commence by examining the simplest operator $\hat{U}^{1/2}_{1/2}(\frac{1}{2},0)$ which creates a spin 1/2 particle in the $m=+1/2$ state, starting from the spin zero state. In full 3×3 matrix form

$$\hat{U}^{1/2}_{1/2}(\tfrac{1}{2},0)\begin{pmatrix}0\\0\\-\\1\end{pmatrix} = \begin{pmatrix}0&0&\mathrm{i}\\0&0&0\\0&0&0\end{pmatrix}\begin{pmatrix}0\\0\\-\\1\end{pmatrix} = \mathrm{i}\begin{pmatrix}1\\0\\-\\0\end{pmatrix}. \tag{18}$$

Here the horizontal line in the column vector is a guide to the eye. The first two upper levels represent the spin up and the spin down states of the spin 1/2 particle, respectively, whereas the last entry represents the $|00\rangle$ spin $I=0$ state.

The annihilation operator which returns the $|\frac{1}{2},\frac{1}{2}\rangle$ state to the spin zero state $|00\rangle$ is the transpose of the creation operator. This is easily verified by noting that (i)

$$\mathrm{Tr}\left[\hat{U}^{1/2}_{1/2}(\tfrac{1}{2},0)^{\dagger}\,\hat{U}^{1/2}_{1/2}(\tfrac{1}{2},0)\right] = 1\,, \tag{19}$$

and (ii) since the operator product inside the trace is a 1×1 matrix, the action of the transpose is to reverse the creation of the $|I=\frac{1}{2},m=\frac{1}{2}\rangle$ spinor state. Clearly, these arguments can be generalized to any spin I. The creation and annihilation operators for a spin I in the $|I,m\rangle$ state are given by $\hat{U}^{I}_{m}(I,0)$ and $\hat{U}^{I}_{m}(I,0)^{\dagger}$, respectively.

The situation for products of half-integer spinors is a little more complicated. We begin by examining the products listed below:

$$\hat{U}^{1/2}_{1/2}(1,\tfrac{1}{2})\hat{U}^{1/2}_{1/2}(\tfrac{1}{2},0) = \frac{\mathrm{i}}{\sqrt{3}}\begin{pmatrix}\sqrt{2} & 0\\ 0 & 1\\ 0 & 0\end{pmatrix}\mathrm{i}\begin{pmatrix}1\\0\end{pmatrix} = -\frac{1}{\sqrt{3}}\begin{pmatrix}\sqrt{2}\\0\\0\end{pmatrix},$$

$$\hat{U}^{1/2}_{-1/2}(1,\tfrac{1}{2})\hat{U}^{1/2}_{1/2}(\tfrac{1}{2},0) = \frac{\mathrm{i}}{\sqrt{3}}\begin{pmatrix}0 & 0\\ 1 & 0\\ 0 & \sqrt{2}\end{pmatrix}\mathrm{i}\begin{pmatrix}1\\0\end{pmatrix} = -\frac{1}{\sqrt{3}}\begin{pmatrix}0\\1\\0\end{pmatrix},$$

$$\hat{U}^{1/2}_{1/2}(1,\tfrac{1}{2})\hat{U}^{1/2}_{-1/2}(\tfrac{1}{2},0) = \frac{\mathrm{i}}{\sqrt{3}}\begin{pmatrix}\sqrt{2} & 0\\ 0 & 1\\ 0 & 0\end{pmatrix}\mathrm{i}\begin{pmatrix}0\\1\end{pmatrix} = -\frac{1}{\sqrt{3}}\begin{pmatrix}0\\1\\0\end{pmatrix},$$

$$\hat{U}^{1/2}_{-1/2}(1,\tfrac{1}{2})\hat{U}^{1/2}_{-1/2}(\tfrac{1}{2},0) = \frac{\mathrm{i}}{\sqrt{3}}\begin{pmatrix}0 & 0\\ 1 & 0\\ 0 & \sqrt{2}\end{pmatrix}\mathrm{i}\begin{pmatrix}0\\1\end{pmatrix} = -\frac{1}{\sqrt{3}}\begin{pmatrix}0\\0\\\sqrt{2}\end{pmatrix}. \tag{20}$$

From an examination of the above equations, it is clear that the products of two half-integer rank tensors creates a spin $I = 1$ state, with the expected azimuthal quantum number m. However, their amplitudes are rather puzzling. For example, the product of two $K = \frac{1}{2}$ rank tensors, both with order $Q = Q' = \frac{1}{2}$, should create a $|I = 1, m = 1\rangle$ state with amplitude 1 rather than $\sqrt{\frac{2}{3}}$. Moreover, these difficulties cannot be circumvented simply by replacing the unit tensors by their non-unit counterparts.

However, these problems can be resolved by defining creation and annihilation operators via

$$\mathbf{C}^K_Q(I, I-\tfrac{1}{2})^\dagger = (-1)^{-K}\sqrt{\frac{2I+1}{2K+1}}\hat{U}^K_Q(I, I-\tfrac{1}{2}),$$

$$\mathbf{C}^K_Q(I-\tfrac{1}{2}, I) = (-1)^{+K}\sqrt{\frac{2I+1}{2K+1}}\hat{U}^K_Q(I, I-\tfrac{1}{2})^\dagger, \tag{21}$$

respectively, where $K = \frac{1}{2}$. Note that when $K = \frac{1}{2}$ and $I = \frac{1}{2}$, the numerical constant appearing in eq. (21) is unity. Thus eq. (18) is retained but with (i) the spherical operator now replaced by the appropriate creation operator, and (ii) a change in phase.

With this simple change, eq. (20) can be rewritten in the form:

$$\mathbf{C}^{1/2}_{1/2}(1,\tfrac{1}{2})^\dagger\mathbf{C}^{1/2}_{1/2}(\tfrac{1}{2},0)^\dagger = \begin{pmatrix}1 & 0\\ 0 & \frac{1}{\sqrt{2}}\\ 0 & 0\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = \begin{pmatrix}1\\0\\0\end{pmatrix},$$

$$\mathbf{C}^{1/2}_{-1/2}(1,\tfrac{1}{2})^{\dagger}\mathbf{C}^{1/2}_{1/2}(\tfrac{1}{2},0)^{\dagger} = \begin{pmatrix} 0 & 0 \\ \frac{1}{\sqrt{2}} & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix},$$

$$\mathbf{C}^{1/2}_{1/2}(1,\tfrac{1}{2})^{\dagger}\mathbf{C}^{1/2}_{-1/2}(\tfrac{1}{2},0)^{\dagger} = \begin{pmatrix} 1 & 0 \\ 0 & \frac{1}{\sqrt{2}} \\ 0 & 0 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix},$$

$$\mathbf{C}^{1/2}_{-1/2}(1,\tfrac{1}{2})^{\dagger}\mathbf{C}^{1/2}_{-1/2}(\tfrac{1}{2},0)^{\dagger} = \begin{pmatrix} 0 & 0 \\ \frac{1}{\sqrt{2}} & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \tag{22}$$

Note that the coefficients of the final column vectors are now in accord with expectations.

When a third spin-1/2 particle is added to the two spin-1/2 spin system, the following possibilities occur:

$$\mathbf{C}^{1/2}_{1/2}(\tfrac{3}{2},1)^{\dagger}\mathbf{C}^{1/2}_{1/2}(1,\tfrac{1}{2})^{\dagger}\mathbf{C}^{1/2}_{1/2}(\tfrac{1}{2},0)^{\dagger} = |\tfrac{3}{2}\,\tfrac{3}{2}\rangle,$$

$$\mathbf{C}^{1/2}_{1/2}(\tfrac{3}{2},1)^{\dagger}\mathbf{C}^{1/2}_{-1/2}(1,\tfrac{1}{2})^{\dagger}\mathbf{C}^{1/2}_{1/2}(\tfrac{1}{2},0)^{\dagger} = \frac{1}{\sqrt{3}}|\tfrac{3}{2}\,\tfrac{1}{2}\rangle,$$

$$\mathbf{C}^{1/2}_{1/2}(\tfrac{3}{2},1)^{\dagger}\mathbf{C}^{1/2}_{1/2}(1,\tfrac{1}{2})^{\dagger}\mathbf{C}^{1/2}_{-1/2}(\tfrac{1}{2},0)^{\dagger} = \frac{1}{\sqrt{3}}|\tfrac{3}{2}\,\tfrac{1}{2}\rangle,$$

$$\mathbf{C}^{1/2}_{-1/2}(\tfrac{3}{2},1)^{\dagger}\mathbf{C}^{1/2}_{1/2}(1,\tfrac{1}{2})^{\dagger}\mathbf{C}^{1/2}_{1/2}(\tfrac{1}{2},0)^{\dagger} = \frac{1}{\sqrt{3}}|\tfrac{3}{2}\,\tfrac{1}{2}\rangle. \tag{23}$$

with a similar set of results for the $M = -1/2$ and $-3/2$ state. Thus viewed in the light of creation and annihilation operators the reason for the half-integer rank tensors is now clear. They can be used to create/annihilate spinor states with half-integer spin.

In a similar fashion creation operators can be defined for spin 1 bosons, using

$$\mathbf{C}^{1}_{Q}(I,I-1)^{\dagger} = -\sqrt{\frac{2I+1}{3}}\hat{U}^{1}_{Q}(I,I-1), \tag{24}$$

where K has now been set equal to unity. Further, in general, it can be shown that

$$\mathbf{C}^{K}_{Q}(I,I-K)^{\dagger} = (-1)^{-K}\sqrt{\frac{2I+1}{2K+1}}\hat{U}^{K}_{Q}(I,I-K). \tag{25}$$

A proof of this result can be found in appendix C, for both integer and half-integer K.

Finally, we remark that the framework developed above for half-integer spins bears a strong resemblance to the spinor eigenvectors:

$$|j,m\rangle = \frac{\chi_+^{j+m}\chi_-^{j-m}}{\sqrt{(j+m)!(j-m)!}}, \tag{26}$$

where

$$\chi_+ = |\tfrac{1}{2},\tfrac{1}{2}\rangle,$$

$$\chi_- = |\tfrac{1}{2},-\tfrac{1}{2}\rangle, \tag{27}$$

(see, for example, Edmonds [7]). The difference between the two representations is simply that the monomials of eq. (26) are expressed in the decoupled representation, with no spin labelling. However, the unit spherical tensors developed in this paper are the appropriate choice for strongly coupled spin systems, where spin labelling is paramount. For single spin-1/2 systems of course, both representations are identical.

6. Block diagonalization using half-integer rank tensors

In a previous paper [4], the problem of block-diagonalizing Hamiltonian matrices was examined using Fano's unit spherical operators $\hat{U}_Q^K(I_i, I_j)$ together with an exponential unitary transform due to Slichter [10]. In particular, it was shown that any matrix could be re-labelled in terms of fictitious spins, enabling a wide variety of differing unit spherical tensors to be used in the diagonalization process. But it was noted that mixtures of non-integer and integer spins could not be used. For example, a 3×3 matrix could not be partitioned using spin labels 1/2 and 0, because unit spherical tensors with integer rank cannot 'link' integer and half-integer spins, by virtue of the vector coupling rule. Similarly, 5×5 matrices cannot be partitioned using spins labels 1 and 1/2. However, this impasse can be overcome by the use of half-integer rank unit spherical tensor operators.

As an example of the use of half-integer rank tensors in the block-diagonalization process, consider the simple example of an $I = 1$ nuclear ensemble evolving in the presence of a Zeeman offset, an axially symmetric quadrupole interaction, and an rf field applied along the x-axis in the rotating frame (see [11]). Thus the Hamiltonian takes the form

$$\mathcal{H}/\hbar = \Delta\omega T_0^1 + \sqrt{\tfrac{2}{3}}\omega_Q T_0^2 - \omega_1 T_1^1(a), \tag{28}$$

or, alternatively, in matrix form

$$I_z = \quad 1 \qquad 0 \qquad -1$$

$$\mathcal{H}/\hbar = \begin{vmatrix} \Delta\omega + \frac{\omega_Q}{3} & \frac{\omega_1}{\sqrt{2}} & 0 \\ \frac{\omega_1}{\sqrt{2}} & -\frac{2\omega_Q}{3} & \frac{\omega_1}{\sqrt{2}} \\ 0 & \frac{\omega_1}{\sqrt{2}} & -\Delta\omega + \frac{\omega_Q}{3} \end{vmatrix}, \tag{29}$$

where the symbols possess their usual meanings. The eigenvalues of this matrix can, of course, be found using standard techniques. However, for the purposes of this paper, we shall attempt to block-diagonalize this simple matrix into $2 \times 2 \oplus 1 \times 1$ matrices, using an admixture of integer and half-integer rank tensors.

Firstly, to simplify the mathematics, we shift the energy reference from zero to $-\omega_Q/3$. Secondly, we re-label the Hamiltonian according to

$$I_z = \quad 1 \quad -1 \quad 0$$

$$\mathcal{H}'/\hbar = \begin{vmatrix} \Delta\omega & 0 & \frac{\omega_1}{\sqrt{2}} \\ 0 & -\Delta\omega & \frac{\omega_1}{\sqrt{2}} \\ \frac{\omega_1}{\sqrt{2}} & \frac{\omega_1}{\sqrt{2}} & -\omega_Q \end{vmatrix}. \tag{30}$$

Finally, we re-label this matrix in terms of two fictitious spins $I_1 = \frac{1}{2}$, and 0. Thus the Hamiltonian matrix of eq. (30) can be partitioned into a diagonal and off-diagonal matrices

$$\mathcal{H}' = \mathcal{H}'_\mathrm{D} + \mathcal{H}'_\mathrm{OD}, \tag{31}$$

where

$$I_z = \quad \tfrac{1}{2} \quad -\tfrac{1}{2} \quad 0$$

$$\mathcal{H}'_\mathrm{D}/\hbar = \begin{vmatrix} \Delta\omega & 0 & 0 \\ 0 & -\Delta\omega & 0 \\ 0 & 0 & -\omega_Q \end{vmatrix} \tag{32}$$

and

$$I_z = \quad \tfrac{1}{2} \quad -\tfrac{1}{2} \quad 0$$

$$\mathcal{H}'_\mathrm{OD}/\hbar = \begin{vmatrix} 0 & 0 & \frac{\omega_1}{\sqrt{2}} \\ 0 & 0 & \frac{\omega_1}{\sqrt{2}} \\ \frac{\omega_1}{\sqrt{2}} & \frac{\omega_1}{\sqrt{2}} & 0 \end{vmatrix}. \tag{33}$$

Alternatively, in unit spherical form

$$\mathcal{H}'_{\mathrm{D}}/\hbar = \sqrt{2}\Delta\omega \hat{U}_0^1(\tfrac{1}{2},\tfrac{1}{2}) - \omega_Q \hat{U}_0^0(0,0) \tag{34}$$

and

$$\mathcal{H}'_{\mathrm{OD}}/\hbar = -\mathrm{i}\omega_1 \hat{U}_{1/2}^{1/2}(\tfrac{1}{2},0,a) - \mathrm{i}\omega_1 \hat{U}_{1/2}^{1/2}(0,\tfrac{1}{2},s)\,. \tag{35}$$

Our strategy should now be clear. We hope to block-diagonalize $\mathcal{H}'$ into a 2×2 and a 1×1 matrix, spanned by the two fictitious spins $I=\frac{1}{2}$ and 0.

If the strength of the rf field ω_1 is small, the prescription advocated by Bowden and Prandolini [4] can be used. Specifically, we seek a transformation S such that

$$[S,\mathcal{H}'_{\mathrm{D}}]_- = \mathcal{H}'_{\mathrm{OD}}\,. \tag{36}$$

If this can be done then the Hamiltonian reduces to

$$\mathcal{H}' = \mathcal{H}_{\mathrm{D}} - \tfrac{1}{2}[S,\mathcal{H}_{\mathrm{OD}}]_-\,, \tag{37}$$

which is block-diagonal to second order in S. After some manipulation it is easily shown that a suitable transformation is given by

$$S = \alpha \hat{U}_{1/2}^{1/2}(\tfrac{1}{2},0,s) + \beta \hat{U}_{1/2}^{1/2}(0,\tfrac{1}{2},a)\,, \tag{38}$$

where

$$\alpha = \frac{\mathrm{i}\omega_1}{\Delta\omega+\omega_Q}\,, \quad \beta = \frac{\mathrm{i}\omega_1}{\Delta\omega-\omega_Q}\,. \tag{39}$$

Note that if we are "on resonance", i.e. $\Delta\omega = \pm\omega_Q$, this transformation must fail because even if ω_1 is weak one or either of the two denominators in eq. (39) must go to zero. For the purposes of this section therefore we shall assume that we are sufficiently far "off resonance" for this not to be a problem. With this assumption it is easily shown that eq. (37) reduces to

$$\mathcal{H}' = \begin{vmatrix} \Delta\omega & 0 & 0 \\ 0 & -\Delta\omega & 0 \\ 0 & 0 & -\omega_Q \end{vmatrix} + \begin{vmatrix} \dfrac{\omega_1^2}{2(\Delta\omega+\omega_Q)} & \dfrac{-\omega_1^2\omega_Q}{2(\Delta\omega^2-\omega_Q^2)} & 0 \\ \dfrac{-\omega_1^2\omega_Q}{2(\Delta\omega^2-\omega_Q^2)} & \dfrac{-\omega_1^2}{2(\Delta\omega-\omega_Q)} & 0 \\ 0 & 0 & \dfrac{\omega_1^2\omega_Q}{\Delta\omega^2-\omega_Q^2} \end{vmatrix}, \tag{40}$$

which is clearly block-diagonal, correct to S^2. We are now in a position to make contact with normal second order perturbation theory. Using standard techniques, it is easily shown that the energy eigenvalues, correct to ω_1^2, are given by the diagonal entries in eq. (40).

To make further progress, it is necessary to evaluate the transformation

$$\mathcal{H}'' = e^{-\lambda S}\mathcal{H}' e^{+\lambda S}\,, \tag{41}$$

where λ is an adjustable parameter. Given the eigenvalues and eigenfunctions of S, the precise form of eq. (41) can be easily found using projection techniques. The eigenvalues of S are

$$\Lambda_1 = 0; \quad \Lambda_2 = -r/\sqrt{2}; \quad \Lambda_3 = r/\sqrt{2};$$

$$r = \sqrt{\alpha^2+\beta^2}\,, \tag{42}$$

with eigenvectors

$$\psi_1 = \frac{\beta}{r}|\tfrac{1}{2},\tfrac{1}{2}\rangle + \frac{\alpha}{r}|\tfrac{1}{2},-\tfrac{1}{2}\rangle\,,$$

$$\psi_2 = \frac{-i\alpha}{\sqrt{2}r}|\tfrac{1}{2},\tfrac{1}{2}\rangle + \frac{i\beta}{\sqrt{2}r}|\tfrac{1}{2},-\tfrac{1}{2}\rangle + \frac{1}{\sqrt{2}}|0,0\rangle\,,$$

$$\psi_3 = \frac{i\alpha}{\sqrt{2}r}|\tfrac{1}{2},\tfrac{1}{2}\rangle - \frac{i\beta}{\sqrt{2}r}|\tfrac{1}{2},-\tfrac{1}{2}\rangle + \frac{1}{\sqrt{2}}|0,0\rangle\,. \tag{43}$$

Using Mathematica we find that the transformed Hamiltonian can be re-written in the block diagonal form

$$\mathcal{H}'' = \mathcal{H}''_{\mathrm{D}} + \mathcal{H}''_{\mathrm{OD}} \tag{44}$$

where (i)

$$\mathcal{H}''_{\mathrm{D}} = \rho_0^1(\tfrac{1}{2},\tfrac{1}{2})\hat{U}_0^1(\tfrac{1}{2},\tfrac{1}{2}) + \rho_0^0(\tfrac{1}{2},\tfrac{1}{2})\hat{U}_0^0(\tfrac{1}{2},\tfrac{1}{2}) + \rho_1^1(\tfrac{1}{2},\tfrac{1}{2},a)\hat{U}_1^1(\tfrac{1}{2},\tfrac{1}{2},a) + \rho_0^0(0,0)\hat{U}_0^0(0,0) \tag{45}$$

and (ii)

$$\mathcal{H}''_{\mathrm{OD}} = \rho_{1/2}^{1/2}(\tfrac{1}{2},0,a)\hat{U}_{1/2}^{1/2}(\tfrac{1}{2},0,a) + \rho_{1/2}^{1/2}(0,\tfrac{1}{2},s)\hat{U}_{1/2}^{1/2}(0,\tfrac{1}{2},s)\,. \tag{46}$$

Our task therefore is to find values of α, β, and λ which will simultaneously reduce the coefficients of the two half-integer rank tensors appearing in eq. (46) to zero.

The precise algebraic forms of the two off-diagonal Fano coefficients appearing in eq. (46) are

$$\rho_{1/2}^{1/2}(\tfrac{1}{2},0,a) = \frac{2\sqrt{2}\Delta\omega\alpha\beta^2\sinh\theta}{r^3} + \frac{\alpha}{\sqrt{2}r^3}\left(\Delta\omega(\alpha^2-\beta^2)+r^2\omega_Q\right)\sinh 2\theta - \frac{i\beta\omega_1(\alpha+\beta)\cosh\theta}{r^2} - \frac{i\alpha\omega_1(\alpha-\beta)\cosh 2\theta}{r^2}\,,$$

$$\rho_{1/2}^{1/2}(0,\tfrac{1}{2},s) = \frac{2\sqrt{2}\Delta\omega\alpha^2\beta\sinh\theta}{r^3} - \frac{\beta}{\sqrt{2}r^3}\left(\Delta\omega(\alpha^2-\beta^2)+r^2\omega_Q\right)\sinh 2\theta - \frac{i\alpha\omega_1(\alpha+\beta)\cosh\theta}{r^2} + \frac{i\beta\omega_1(\alpha-\beta)\cosh 2\theta}{r^2}\,, \tag{47}$$

where

$$\theta = \frac{\lambda r}{\sqrt{2}} \,. \tag{48}$$

In general, it is difficult to find values of α, β, and λ which will reduce the two Fano coefficients to zero, simultaneously. We have therefore considered a few special cases.

If the resonant offset $\Delta\omega$ is zero, a solution can be found by (i) dropping the restrictions given in eq. (39), (ii) setting $\alpha = -\beta$ and (iii) substituting $\lambda = \lambda' \mathrm{i}$. With these changes it can be shown that the off diagonal coefficients $\rho^{1/2}_{1/2}(\frac{1}{2}, 0, a)$ and $\rho^{1/2}_{1/2}(0, \frac{1}{2}, s)$ can be made to vanish by setting

$$\theta = \lambda'\alpha = \tfrac{1}{2}\tan^{-1}\left(\frac{2\omega_1}{\omega_Q}\right) . \tag{49}$$

With this transformation it is easily shown that

$$\mathcal{H} = \begin{vmatrix} \frac{\omega_Q}{12} + \frac{\sqrt{\omega_Q^2 + 4\omega_1^2}}{4} & -\frac{\omega_Q}{4} + \frac{\sqrt{\omega_Q^2 + 4\omega_1^2}}{4} & 0 \\ -\frac{\omega_Q}{4} + \frac{\sqrt{\omega_Q^2 + 4\omega_1^2}}{4} & \frac{\omega_Q}{12} + \frac{\sqrt{\omega_Q^2 + 4\omega_1^2}}{4} & 0 \\ 0 & 0 & \frac{-\omega_Q}{6} - \frac{\sqrt{\omega_Q^2 + 4\omega_1^2}}{2} \end{vmatrix} , \tag{50}$$

where we have reshifted the energy reference back to its original value. Thus we have successfully used half-integer rank tensors to effect block-diagonalization. However, it should be acknowledged that for the simple case of $\Delta\omega = 0$, the characteristic equation can be factorized according to

$$\tfrac{1}{27}\Big[(\omega_Q - 3\Lambda)(9\Lambda^2 + 3\Lambda\omega_Q - 2\omega_Q^2 - 9\omega_1^2)\Big] = 0 \,, \tag{51}$$

thereby indicating that block-diagonalization is possible.

In an attempt to make further progress, in the general case, we have substituted the explicit values of α and β (eq. (39)) into our two expressions for the off diagonal Fano coefficients (eq. (47)). After some manipulation we find

$$\rho^{1/2}_{1/2}(\tfrac{1}{2}, 0, a) = + \frac{\mathrm{i}\Delta\omega\omega_1(\Delta\omega + \omega_Q)}{\Delta\omega^2 + \omega_Q^2}\left(\frac{\sqrt{2}\sinh\theta}{r} - \cosh\theta\right)$$
$$- \frac{\mathrm{i}\omega_Q\omega_1(\Delta\omega - \omega_Q)}{\Delta\omega^2 + \omega_Q^2}\left(\frac{\sinh 2\theta}{\sqrt{2}r} - \cosh 2\theta\right) ,$$

$$\rho^{1/2}_{1/2}(0,\tfrac{1}{2},s) = +\frac{\mathrm{i}\Delta\omega\omega_1(\Delta\omega-\omega_Q)}{\Delta\omega^2+\omega_Q^2}\left(\frac{\sqrt{2}\sinh\theta}{r}-\cosh\theta\right) + \frac{\mathrm{i}\omega_Q\omega_1(\Delta\omega+\omega_Q)}{\Delta\omega^2+\omega_Q^2}\left(\frac{\sinh 2\theta}{\sqrt{2}r}-\cosh 2\theta\right). \quad (52)$$

From an examination of these equations it is evident that, in general, we cannot choose a value of θ which will reduce both the off-diagonal Fano coefficients to zero, simultaneously, because of the change in sign of the last terms in the two coefficients. The best one could do is to choose a value of θ which minimises the magnitudes of the two coefficients in question. However, if we could choose a value of θ such that

$$\tanh\theta = \tanh(|r|/\sqrt{2}) = |r|/\sqrt{2},$$

$$\tanh 2\theta = \tanh(\sqrt{2}|r|) = \sqrt{2}|r|, \quad (53)$$

then all four terms vanish identically. In fact, both these equations can be satisfied provided (i) r is small and (ii) we set λ equal to unity. But this, of course, corresponds to case of perturbation theory considered earlier.

In summary therefore, although we have demonstrated the use of half-integer rank tensors in the diagonalization process, it would appear that "force" block-diagonalization can only be achieved using an iterative procedure.

7. Conclusion

In this paper, a new class of half-integer rank tensors has been introduced. These tensors are a natural extension of the non-square integer rank tensors developed by [2,3]. In particular, it has been demonstrated that (i) half-integer rank tensors can be used to factorize the Pauli spin matrices, (ii) the multiplication rule for half-integer and integer rank tensors is identical, (iii) the Racah commutation relationships $[\mathcal{I}_z, \hat{U}^K_Q(I_i, I_j)]_-$ still hold for half-integer rank tensors, and (iv) under rotation of the co-ordinate system through the Euler angles (α, β, γ), half-integer rank tensors obey the same rotational properties as their integer counterparts, but with K half-integer.

In addition, two applications for half-integer rank tensors have been discussed. In the first place it has been shown that such tensors can be used to create/annihilate spinor eigenvectors, in the strongly coupled representation. In essence, they represent the generalization of the creation and annihilation operators $a^\dagger$, a, respectively, for two level systems. Secondly, the problem of block-diagonalizing a single 3×3 Hamiltonian into $2\times 2 \oplus 1\times 1$ matrices has been examined in some detail. In particular, it was shown that results obtained using the unit spherical tensor approach are in agreement with those obtained using standard perturbation theory. However, an attempt to "force" block-diagonalization in a single step was unsuccessful, except in special circumstances.

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Appendix A

CONTRACTION OF UNIT SPHERICAL TENSORS

Consider the matrix element

$$M = \langle I_i m_i | \hat{U}^K_Q(I_i, I_k)\,\hat{U}^{K'}_{Q'}(I_k, I_j) | I_j m_j \rangle\,. \tag{A.1}$$

Using sum over closure, together with eq. (1), and the symmetry properties of the 3j coefficients, it can be shown that

$$M = [(2K+1)(2K'+1)]^{1/2}(-1)^{I_k+I_j-2m_i+Q} \times \sum_{m_k} \begin{pmatrix} I_i & K & I_k \\ -m_i & Q & m_k \end{pmatrix} \begin{pmatrix} K' & I_j & I_k \\ Q' & m_j & -m_k \end{pmatrix}. \tag{A.2}$$

Using an identity given by Landolt and Börnstein [12], the summation over the two 3j coefficients appearing in (A.2) can be re-expressed in the form

$$\begin{aligned} \sum_{m_k} \begin{pmatrix} I_i & K & I_k \\ -m_i & Q & m_k \end{pmatrix} \begin{pmatrix} K' & I_j & I_k \\ Q' & m_j & -m_k \end{pmatrix} &= \sum_{\mathcal{K},\Omega} (-1)^{I_k+\mathcal{K}-m_i+Q'}(2\mathcal{K}+1) \\ &\quad\times \begin{Bmatrix} I_i & K & I_k \\ K' & I_j & \mathcal{K} \end{Bmatrix} \begin{pmatrix} K' & K & \mathcal{K} \\ Q' & Q & \Omega \end{pmatrix} \begin{pmatrix} I_i & I_j & \mathcal{K} \\ -m_i & m_j & -\Omega \end{pmatrix} \\ &= \sum_{\mathcal{K},\Omega} (-1)^{I_k+\mathcal{K}-m_i+Q'}(-1)^{K+K'+\mathcal{K}}(2\mathcal{K}+1) \\ &\quad\times \begin{Bmatrix} I_i & K & I_k \\ K' & I_j & \mathcal{K} \end{Bmatrix} \begin{pmatrix} K & K' & \mathcal{K} \\ Q & Q' & -\Omega \end{pmatrix} \begin{pmatrix} I_i & I_j & \mathcal{K} \\ -m_i & m_j & \Omega \end{pmatrix}, \end{aligned} \tag{A.3}$$

where we have reversed the summation over Ω in obtaining the last line of (A.3). On substituting (A.3) into (A.2) therefore

$$M = [(2K+1)(2K'+1)]^{1/2} \sum_{\mathcal{K},Q} (-1)^{2I_k+I_j-3m_i+\Omega+K+K'+2\mathcal{K}} (2\mathcal{K}+1) \times \begin{Bmatrix} I_i & K & I_k \\ K' & I_j & \mathcal{K} \end{Bmatrix} \begin{pmatrix} K & K' & \mathcal{K} \\ Q & Q' & -\Omega \end{pmatrix} \begin{pmatrix} I_i & I_j & \mathcal{K} \\ -m_i & m_j & \Omega \end{pmatrix}, \tag{A.4}$$

where we have made use of $\Omega = Q + Q'$.

Next we observe that

$$\langle I_i m_i | \hat{U}^{\mathcal{K}}_{\Omega}(I_i, I_j) | I_j m_j \rangle = (2\mathcal{K}+1)^{1/2} (-1)^{I_j - m_i} \begin{pmatrix} I_i & \mathcal{K} & I_j \\ -m_i & \Omega & m_j \end{pmatrix}$$
$$= (2\mathcal{K}+1)^{1/2} (-1)^{I_j - m_i} (-1)^{I_i + I_j + \mathcal{K}} \begin{pmatrix} I_i & I_j & \mathcal{K} \\ -m_i & m_j & \Omega \end{pmatrix}. \tag{A.5}$$

Consequently, on combining (A.4) and (A.5)

$$M = [(2K+1)(2K'+1)]^{1/2} \sum_{\mathcal{K},\Omega} (-1)^{2(I_k - m_i + K) + 2(\mathcal{K}+\Omega)} (-1)^{-I_i - I_j - \mathcal{K}} \times \begin{Bmatrix} K & K' & \mathcal{K} \\ I_j & I_i & I_k \end{Bmatrix} \langle KQK'Q' | \mathcal{K}\Omega \rangle \langle I_i m_i | \hat{U}^{\mathcal{K}}_{\Omega}(I_i, I_j) | I_j m_j \rangle, \tag{A.6}$$

where (i) use has been made of the symmetry properties of the 6j coefficient, and (ii) the 3j coefficient involving K, K', and $\mathcal{K}$, has been replaced by a Clebsch–Gordan coefficient. Finally, we observe that (i) for all values of $\mathcal{K}$, both integer or half-integer, $2(\mathcal{K}+\Omega)$ is even, (ii) for all allowed values of I_k, m_i and K, $2(I_k - m_i + K)$ is even, and (iii) for all allowed values of I_i, I_j and $\mathcal{K}$, $(I_i + I_j + \mathcal{K})$ is an integer. Consequently, we may write

$$\hat{U}^{K}_{Q}(I_i, I_k) \hat{U}^{K'}_{Q'}(I_k, I_j) = \sum_{\mathcal{K},\Omega} B(K, K', \mathcal{K}, I_i, I_j, I_k) \langle KQK'Q' | \mathcal{K}\Omega \rangle \hat{U}^{\mathcal{K}}_{\Omega}(I_i, I_j), \tag{A.7}$$

where the constant $B(K, K', \mathcal{K}, I_i, I_j, I_k)$ is given by

$$B(K, K', \mathcal{K}, I_i, I_j, I_k) = (-1)^{I_i + I_j + \mathcal{K}} [(2K+1)(2K'+1)]^{1/2} \begin{Bmatrix} K & K' & \mathcal{K} \\ I_j & I_i & I_k \end{Bmatrix}, \tag{A.8}$$

which holds for all K, K', and $\mathcal{K}$, integer or half-integer.

Appendix B

RACAH LIKE COMMUTATION RELATIONS

We commence by examining the commutation relationship

$$\left[\mathcal{I}_z, \hat{U}^K_Q(I_i, I_j)\right]_- = I_z(i)\hat{U}^K_Q(I_i, I_j) - \hat{U}^K_Q(I_i, I_j)I_z(j)\,. \tag{B.1}$$

To apply the multiplication rule for unit spherical tensors derived in appendix A, it is necessary to convert the non-unit operators $I_z(i)$ into unit form. Using the normalization factor given by [11] we find

$$I_z(i) = T^1_0(i) = \left[\frac{(2I_i+2)!}{12(2I_i-1)!}\right]^{1/2} \hat{I}_z(i) = N(I_i)\hat{U}^1_0(I_i, I_i)\,, \tag{B.2}$$

where the normalization constant is given by

$$N(I_i) = \left[\frac{(2I_i+2)!}{12(2I_i-1)!}\right]^{1/2}. \tag{B.3}$$

Thus

$$\left[\mathcal{I}_z, \hat{U}^K_Q(I_i, I_j)\right]_- = N(I_i)\hat{U}^1_0(I_i, I_i)\hat{U}^K_Q(I_i, I_j) - N(I_j)\hat{U}^K_Q(I_i, I_j)\hat{U}^1_0(I_j, I_j)\,. \tag{B.4}$$

Using the multiplication rule for unit spherical operators, we find

$$\begin{aligned}
&\left[\mathcal{I}_z, \hat{U}^K_Q(I_i, I_j)\right]_- \\
&= \Bigg[\sqrt{3}\sqrt{2K+1}\sum_{\mathcal{K}} N(I_i)(-1)^{I_i+I_j+\mathcal{K}}\begin{Bmatrix} 1 & K & \mathcal{K} \\ I_j & I_i & I_i \end{Bmatrix}\langle 10KQ|\mathcal{K}Q\rangle \hat{U}^{\mathcal{K}}_Q(I_i, I_j)_{me} \\
&\quad -\sqrt{3}\sqrt{2K+1}\sum_{\mathcal{K}} N(I_j)(-1)^{I_i+I_j+\mathcal{K}}\begin{Bmatrix} K & 1 & \mathcal{K} \\ I_j & I_i & I_j \end{Bmatrix}\langle KQ10|\mathcal{K}Q\rangle \hat{U}^{\mathcal{K}}_Q(I_i, I_j)\Bigg] \\
&= \sqrt{3}\sqrt{2K+1}(-1)^{I_i+I_j}\sum_{\mathcal{K}}(-1)^{\mathcal{K}}\langle 10KQ|\mathcal{K}Q\rangle \hat{U}^{\mathcal{K}}_Q(I_i, I_j)C[I_i, I_j, K, \mathcal{K}]\,,
\end{aligned} \tag{B.5}$$

where the coefficient $C[I_i, I_j, K, \mathcal{K}]$ is given by

$$C[I_i, I_j, K, \mathcal{K}] = N(I_i)\begin{Bmatrix} 1 & K & \mathcal{K} \\ I_j & I_i & I_i \end{Bmatrix} - (-1)^{\mathcal{K}-K-1}N(I_j)\begin{Bmatrix} 1 & K & \mathcal{K} \\ I_i & I_j & I_j \end{Bmatrix}. \tag{B.6}$$

In arriving at (B.5), use has been made of the symmetry properties of both the 3j and 6j coefficients.

Because of the vector coupling rule for the 6j coefficients appearing in (B.5) and (B.6), $\mathcal{K}$ can only take on the values $K-1, K, K+1$. Thus there are three cases to be considered. If we set $\mathcal{K} = K+1$ then

$$C[I_i, I_j, K, \mathcal{K}] = N(I_i)\begin{Bmatrix} 1 & K & K+1 \\ I_j & I_i & I_i \end{Bmatrix} - N(I_j)\begin{Bmatrix} 1 & K & K+1 \\ I_i & I_j & I_j \end{Bmatrix}. \tag{B.7}$$

Using an identity given by [13] (eq. (6.3.1)) it can be shown that

$$\begin{Bmatrix} 1 & K & K+1 \\ I_j & I_i & I_i \end{Bmatrix} = \begin{Bmatrix} I_j & I_i & K+1 \\ 1 & K & I_i \end{Bmatrix}$$

$$= (-1)^{I_i+I_j+K+1} \left[\frac{2(2K)!(2I_i - 1)!}{(2K+3)!(2I_i+2)!} \right]^{1/2} G(I_i, I_j, K) , \quad \text{(B.8)}$$

where

$$G(I_i, I_j, K) = \big[(I_i + I_j + K + 2)(I_j - I_i + K + 1) \times (I_i - I_j + K + 1)(I_i + I_j - K) \big]^{1/2} , \quad \text{(B.9)}$$

which is symmetric in I_i and I_j. Using (B.8) it is easily shown that

$$\begin{Bmatrix} 1 & K & K+1 \\ I_j & I_i & I_i \end{Bmatrix} \Big/ \begin{Bmatrix} 1 & K & K+1 \\ I_i & I_j & I_j \end{Bmatrix} = N(I_j)/N(I_i) . \quad \text{(B.10)}$$

Thus the coefficient $C[I_i, I_j, K, K+1]$ of (B.7) vanishes identically. In a similar fashion it can be shown that $C[I_i, I_j, K, K-1] = 0$. So the sum over in (B.5) reduces to just one term $= K$.

Using another 6j identity, (see ref. [7, table 5]), formulae for the 6j symbol, it can be shown that

$$\begin{Bmatrix} 1 & K & K \\ I_i & I_j & I_j \end{Bmatrix} = (-1)^{I_i+I_j+K+1} \times \frac{2[I_j(I_j+1) + K(K+1) - I_i(I_i+1)]}{N(I_j)\sqrt{24K(2K+1)(2K+2)}} , \quad \text{(B.11)}$$

thus

$$C[I_i, I_j, K, K] = (-1)^{I_i+I_j+K+1} \frac{4K(K+1)}{\sqrt{24K(2K+1)(2K+2)}} . \quad \text{(B.12)}$$

On substituting (B.12) into (B.5) therefore, with

$$\langle 10KQ|KQ\rangle = -\frac{Q}{\sqrt{K(K+1)}} , \quad \text{(B.13)}$$

we find

$$\left[{}_z, \hat{U}^K_Q(I_i, I_j) \right]_- = (-1)^{2(I_i+I_j+K)} Q \hat{U}^K_Q(I_i, I_j) , \quad \text{(B.14)}$$

which holds for all K, integer or half-integer. Finally, since $(I_i + I_j + K)$ is an integer for all possible values of I_i, I_j, and K by virtue of the vector coupling rule, we may conclude that

$$\left[{}_z, \hat{U}^K_Q(I_i, I_j) \right]_- = Q \hat{U}^K_Q(I_i, I_j) \quad \text{(B.15)}$$

as asserted in the text.

Commutation relationships involving $_\pm$ are readily obtained by a modest adaptation of the above treatment.

Appendix C

NORMALIZED CREATION AND ANNIHILATION OPERATORS

It is evident from an examination of the 3×2 matrices in eq. (20), that the magnitudes of all the entries must be less than 1, otherwise the spherical tensors would be unnormalized. Thus it is impossible to generate fully stretched wave functions $|I, M = \pm I\rangle$ with unit amplitude. We seek therefore that a general coefficient which can be used to circumvent this difficulty.

By definition, the unit spherical tensor is given by

$$\langle I_1 M_1 | \hat{U}_Q^K(I_1, I_2) | I_2 M_2 \rangle = (-1)^{I_2 - M_1} \sqrt{2K+1} \begin{pmatrix} I_1 & K & I_2 \\ -M_1 & Q & M_2 \end{pmatrix} . \tag{C.1}$$

For the fully "stretched case", $Q = K, M_1 = I_1$ therefore

$$\langle I_1 I_1 | \hat{U}_K^K(I_1, I_1 - K) | I_1 - K I_1 - K \rangle = (-1)^{-K} \sqrt{2K+1} \begin{pmatrix} I_1 & K & I_1 - K \\ -I_1 & K & I_1 - K \end{pmatrix} . \tag{C.2}$$

It can be shown, using eq. (3.7.10) of Edmonds, that the Wigner 3j coefficient appearing in (C.2) reduces to:

$$\begin{pmatrix} I_1 & K & I_1 - K \\ -I_1 & K & I_1 - K \end{pmatrix} = (-1)^{2K} \frac{1}{\sqrt{2I_1 + 1}} . \tag{C.3}$$

Consequently,

$$\langle I_1 I_1 | \hat{U}_K^K(I_1, I_1 - K) | I_1 - K I_1 - K \rangle = (-1)^{+K} \sqrt{\frac{2K+1}{2I_1 + 1}} . \tag{C.4}$$

Thus if we define the creation operator

$$\mathbf{C}_K^K(I_1, I_1 - K)^\dagger = (-1)^{-K} \sqrt{\frac{2I_1 + 1}{2K+1}} \hat{U}_K^K(I_1, I_1 - K) , \tag{C.5}$$

then

$$\langle I_1 I_1 | \mathbf{C}_K^K(I_1, I_1 - K)^\dagger | I_1 - K I_1 - K \rangle = 1 , \tag{C.6}$$

as required.

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