Chapter 4

Tensor operators

4.1 Introduction

Irreducible tensor operators are central to the theory of angular momentum. This was first emphasized by Racah in his four classic papers, Phys. Rev. **61**, 186 (1942); **62**, 438 (1942); **63**, 367 (1943); and **76**, 1352 (1949). In the second of these papers Racah defined the tensor operator, actually a rather natural extension of the work presented by Condon & Shortley [4] on vector operators. The fractional parentage coefficients were introduced in the third paper and in the last work in the series, Racah derived term energies for a system of equivalent f-electrons using the theory of continuous groups. We will return to the content of Racahs' papers II, III and IV later in the course.

4.2 Definitions

We start by defining the Cartesian tensor of rank N. A Cartesian tensor of rank N is in the 3-dimensional Cartesian space defined as an entity with 3^N components $T_{ijk\ldots}$ (the rank is the number of indexes) that transform under an orthogonal transformation (*c.f.* rotation) of coordinates as

$$T_{ijk\ldots} = \sum_{i'j'k'\ldots} a_{ii'} a_{jj'} a_{kk'} \ldots T_{i'j'k'\ldots} \tag{4.1}$$

Note that a tensor is not dependent on the choice of coordinate system, after all, we use them to describe physics! It follows that a tensor of rank zero has one component that is invariant under rotations, *i.e.* a scalar. A Cartesian tensor of rank one has three components and is similar to a vector in three dimensions. A tensor of rank two is not equivalent to the square matrix formed of its nine components because the tensor is defined <u>only</u> in terms of its transformation properties. (The matrix is not restricted in the types of transformations it may undergo and this is also true for a vector).

We now turn our attention to vector operators. In classical physics we know that a vector is a quantity with three components that transform under rotation as $V_i =$

$\sum_j R_{ij}V_j$ (see above). In quantum mechanics we assume that the expectation value of a vector operator V transforms like the classical vector V under rotation. The operator equation describing this can be found by noting that the ket $|\alpha\rangle$ transforms under a rotation according to

$$|\alpha\rangle \to D(R)|\alpha\rangle \tag{4.2}$$

and forming the expectation value

$$\langle\alpha|V_i|\alpha\rangle \to \langle\alpha|D^\dagger(R)V_iD(R)|\alpha\rangle = \sum_j R_{ij}\langle\alpha|V_j|\alpha\rangle \tag{4.3}$$

which is in accordance with our assumption. Because Eq. (4.3) is true for any $|\alpha\rangle$ we have

$$D^\dagger(R)V_iD(R) = \sum_j R_{ij}V_j \tag{4.4}$$

which is our operator equation. R_{ij} is the matrix corresponding to the rotation R. Now consider an infinitesimal rotation described by

$$D(R) = 1 - \frac{i\epsilon J\cdot\hat{n}}{\hbar} \tag{4.5}$$

Eq. (4.5) in Eq. (4.4) gives

$$V_i - i\epsilon/\hbar[V_i, J\cdot\hat{n}] = \sum_j R_{ij}V_j \tag{4.6}$$

For $\hat{n} = \hat{z}$ we have

$$R(\hat{z},\epsilon) = \begin{pmatrix} 1 & -\epsilon & 0 \\ \epsilon & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{4.7}$$

Eqs. (4.6) and (4.7) now gives

$$\left.\begin{array}{rcl} V_x + \epsilon/(i\hbar)[V_x, J_z] & = & V_x - \epsilon V_y \\ V_y + \epsilon/(i\hbar)[V_y, J_z] & = & \epsilon V_x + V_y \\ V_z + \epsilon/(i\hbar)[V_z, J_z] & = & V_z \end{array}\right\} \tag{4.8}$$

Thus,

$$[V_i, V_j] = i\epsilon_{ijk}\hbar V_k \tag{4.9}$$

Eq. (4.9) is usually used as the definition of a vector operator.

The definition of a N-th rank Cartesian tensor was given in Eq. (4.1). Using the idea that lead to the definition of a vector operator, Eq. (4.9), we will now define the spherical tensor operator. First a few words on why irreducible spherical tensors operators are superior to reducible Cartesian tensors operators. We do this by looking at the simplest Cartesian tensor of rank 2, the dyadic

$$T_{ij} = a_ib_j \tag{4.10}$$

This Cartesian tensor have nine components and it obviously transforms according to Eq. (4.1) under rotation. By rewriting the tensor $a_i b_j$ as

$$a_i b_j = \frac{a \cdot b}{3}\delta_{ij} + \frac{a_i b_j - a_j b_i}{2} + \left(\frac{a_i b_j + a_j b_i}{2} - \frac{a \cdot b}{3}\delta_{ij}\right) \tag{4.11}$$

we see that the first term is a scalar, the second (an antisymmetric tensor) can be rewritten as $\epsilon_{ijk}(a \times b)_k$ and have three independent components. The third term is a 3×3 symmetric traceless tensor with 6-1=5 independent components. We also note that the total number of independent components is the same, *i.e.* $3 \times 3 = 1 + 3 + 5$. Recalling that the number of components for the spherical harmonics was $2l + 1$ we see that Eq. (4.10) has been transformed into tensors that transform like spherical harmonics with $l = 0$, $l = 1$ and $l = 2$, *i.e.* the Cartesian tensor $a_i b_j$ has been reduced into irreducible spherical tensors. The very fact that spherical tensors are irreducible, just as the spherical harmonics, make them better to work with than the reducible Cartesian tensors.

It is obvious that the spherical harmonics are important when discussing spherical tensors, so let us look at how Y_l^m transforms under a rotation. First define the rotated eigenket $|n'\rangle$ as

$$|n\rangle \to D(R)|n\rangle = |n'\rangle \tag{4.12}$$

The problem we now want to solve is how $Y_l^m(\hat{n}')$ look in terms of $Y_l^m(\hat{n})$.

$$\begin{aligned} Y_l^m(\hat{n}') &= \langle \hat{n}'|lm\rangle = \langle \hat{n}|D(R^{-1})|lm\rangle = \sum_{m'} \langle \hat{n}|lm'\rangle\langle lm'|D(R^{-1})|lm\rangle \\ &= \sum_{m'} Y_l^{m'}(\hat{n}) D^{(l)}_{m'm}(R^{-1}) = \sum_{m'} Y_l^{m'}(\hat{n}) D^{*(l)}_{m'm}(R) \end{aligned} \tag{4.13}$$

In analogy with our previous vector operator case it is reasonable to demand that the expectation value of a spherical tensor operator transforms like a spherical harmonic under rotation, *i.e.* like Eq. (4.13). We get

$$\langle \alpha|Y_l^m(\hat{n})|\alpha\rangle \to \langle \alpha|D^\dagger(R) Y_l^m(\hat{n}) D(R)|\alpha\rangle = \sum_{m'} \langle \alpha|Y_l^{m'}(\hat{n})|\alpha\rangle D^{*(l)}_{m'm}(R) \tag{4.14}$$

and because this must be true for any $|\alpha\rangle$we have for the operator $Y_l^m(\hat{n})$ under rotation

$$D^\dagger(R) Y_l^m(\hat{n}) D(R) = \sum_{m'} Y_l^{m'}(\hat{n}) D^{*(l)}_{mm'}(R) \tag{4.15}$$

We now define a spherical tensor operator of rank k with $2k + 1$ components as

$$D(R) T_q^{(k)} D^\dagger(R) = \sum_{q'=-k}^{k} D^{(k)}_{q'q}(R) T_{q'}^{(k)} \tag{4.16}$$

Once again in analogy with the vector operator case we look at the infinitesimal rotation

$$(1 + iJ \cdot \hat{n}\epsilon/\hbar) T_q^{(k)} (1 - iJ \cdot \hat{n}\epsilon/\hbar) = \sum_{q'=-k}^{k} T_{q'}^{(k)} \langle kq'|(1 + iJ \cdot \hat{n}\epsilon/\hbar)|kq\rangle \tag{4.17}$$

with $\hat{n} = \hat{z}$ and $\hat{x} \pm i\hat{y}$ we finally get using the equivalent of Eq. (4.17)

$$[J \cdot \hat{n}, T_q^{(k)}] = \sum_{q'} T_{q'}^{(k)} \langle kq' | J \cdot \hat{n} | kq \rangle \tag{4.18}$$

$$[J_z, T_q^{(k)}] = \hbar q T_q^{(k)} \tag{4.19}$$

$$[J_\pm, T_q^{(k)}] = \hbar \sqrt{(k \mp q)(k \pm q + 1)} T_{q\pm 1}^{(k)} \tag{4.20}$$

Eqs. (4.19) and (4.20) are the definitions Racah used for irreducible spherical tensor operators.

4.3 The product of two tensor operators

When previously discussing the reducibility of the dyadic Cartesian tensor $T_{ij} = a_i b_j$ we formed T_{ij} by multiplying together a_i and b_j thus arriving at the nine components of T_{ij} rank 2 Cartesian tensor. It is now natural to investigate how to form a product of irreducible spherical tensors. We will show that

$$X_Q^{(K)} = \left(T^{(k_1)} U^{(k_2)}\right)_Q^{(K)} = \sum_{q_1 q_2} T_{q_1}^{(k_1)} U_{q_2}^{(k_2)} \langle k_1 k_2 q_1 q_2 | k_1 k_2 K Q \rangle \tag{4.21}$$

is a irreducible spherical tensor. $T_{q_1}^{(k_1)}$ and $U_{q_2}^{(k_2)}$ are irreducible spherical tensors of rank k_1 and k_2, respectively. Note the obvious similarities between Eq. (4.21) and Eq. (2.7) which describe the re-coupling of two angular momenta. In proving Eq. (4.21) we will see that $X_Q^{(K)}$ transforms according to $D^{(K)}(R)$ under rotation, thus the representation $D^{(k_1)}(R) \times D^{(k_2)}(R)$ has been reduced to $D^{(K)}$, *i.e.* we have obtained block-diagonal form.

To show that $X_Q^{(K)}$ is a spherical irreducible tensor operator we want to show that $X_Q^{(K)}$ transforms according to Eq. (4.16) under rotation.

$$\begin{aligned}
D^\dagger(R) X_Q^{(K)} D(R) &= \sum_{q_1 q_2} \langle k_1 k_2 q_1 q_2 | k_1 k_2 K Q \rangle D^\dagger(R) T_{q_1}^{(k_1)} D(R) D^\dagger(R) U_{q_2}^{(k_2)} D(R) \\
&= (\text{Eq.}(4.16)) = \sum_{q_1 q_2 q_1' q_2'} \langle k_1 k_2 q_1 q_2 | k_1 k_2 K Q \rangle D_{q_1 q_1'}^{*(k_1)}(R) T_{q_1'}^{(k_1)} D_{q_2 q_2'}^{*(k_2)}(R) U_{q_2'}^{(k_2)} \\
&= \sum_{q_1 q_2 q_1' q_2'} \langle k_1 k_2 q_1 q_2 | k_1 k_2 K Q \rangle \langle k_1 k_2 q_1 q_2 | D^\dagger(R) | k_1 k_2 q_1' q_2' \rangle T_{q_1'}^{(k_1)} U_{q_2'}^{(k_2)} \\
&= \sum_{q_1 q_2 q_1' q_2' K' Q' K'' Q''} \langle k_1 k_2 q_1 q_2 | k_1 k_2 K Q \rangle \langle k_1 k_2 q_1 q_2 | k_1 k_2 K' Q' \rangle \times \\
&\times \underbrace{\langle k_1 k_2 K' Q' | D^\dagger(R) | k_1 k_2 K'' Q'' \rangle}_{D_{Q'Q''}^{*(K'')} \delta_{K'K''}} \langle k_1 k_2 K'' Q'' | k_1 k_2 q_1' q_2' \rangle T_{q_1'}^{(k_1)} U_{q_2'}^{(k_2)} \\
&= \sum_{q_1 q_2 q_1' q_2' Q' K'' Q''} \langle k_1 k_2 q_1 q_2 | k_1 k_2 K Q \rangle \langle k_1 k_2 q_1 q_2 | k_1 k_2 K'' Q' \rangle D_{Q'Q''}^{*(K'')}(R)
\end{aligned}$$

$$
\begin{aligned}
&\times\langle k_1k_2K''Q''|k_1k_2q_1'q_2'\rangle T^{(k_1)}_{q_1'}U^{(k_2)}_{q_2'} = (\text{Eq.}(2.12)) = \\
&= \sum_{q_1'q_2'Q'K''Q''} \delta_{KK''}\delta_{QQ'} D^{*(K'')}_{Q'Q''}(R)\langle k_1k_2K''Q''|k_1k_2q_1'q_2'\rangle T^{(k_1)}_{q_1'}U^{(k_2)}_{q_2'} \\
&= \sum_{Q''} D^{*(K'')}_{QQ''}(R)\langle k_1k_2KQ''|k_1k_2q_1'q_2'\rangle T^{(k_1)}_{q_1'}U^{(k_2)}_{q_2'} = (Eq.(4.21)) = \\
&= \sum_{Q''} D^{*(K'')}_{QQ''}(R)X^{(K)}_{Q''} \qquad (4.22)
\end{aligned}
$$

Proved! The definition of $X^{(K)}_Q$ through Eq. (4.22) is of course equivalent to specify the commutators such as Eqs. (4.19) and (4.20). Once again the similarities between Eqs. (4.21) and (2.7) should be stressed, the operator defined in Eq. (4.21) can thus be decoupled.

4.3.1 Scalar product of two tensor operators

From the triangular condition Eq. (2.14) we note that $K = |k_1 - k_2|, \ldots, k_1 + k_2$. This condition also tell us that if we have two tensors of the same rank, it is possible to construct a scalar (rank 0),

$$X^{(0)}_0 = \sum_q T^{(k)}_q U^{(k)}_{-q}\langle kkq - q|kk00\rangle \qquad (4.23)$$

The scalar product between two tensor operators is defined as

$$S = (T^{(k)} \cdot U^{(k)}) = \sum_q (-1)^q T^{(k)}_q U^{(k)}_{-q} \qquad (4.24)$$

Eqs. (4.23) and (4.24) differ only by a constant term and we will now show that Eq. (4.24) lead to the "usual" scalar product for vectors when applied to vector operators. Eq. (4.24) with $k = 1$ give

$$S = -T^{(1)}_{-1}U^{(1)}_1 + T^{(1)}_0U^{(1)}_0 - T^{(1)}_1U^{(1)}_{-1},$$

$$\left.\begin{array}{l} V_0 = V_z \\ V_\pm = \mp\frac{1}{\sqrt{2}}(V_x \pm iV_y) \end{array}\right\} c.f.\ Y^{(1)}_m \text{ on cartesian form.} \qquad (4.25)$$

and this give for S

$$S = T_xU_x + T_yU_y + T_zU_z \qquad (4.26)$$

which is recognized as the "standard" scalar product between two vectors.

4.4 The product of three and four tensor operators

We previously showed that an operator defined by multiplying together two irreducible tensor operators according to Eq. (4.21) also is an irreducible spherical tensor operator. The obvious similarities between the definition Eq. (4.21) and re-coupling of two angular momenta Eq. (2.7) lead us to the following definition, where $T^{(k_1)}$, $U^{(k_2)}$ and $V^{(k_3)}$ are tensor operators,

$$\begin{aligned}(T^{(k_1)}(U^{(k_2)}V^{(k_3)})^{(k_{23})})^{(K)}_Q &= \sum_{q_1q_2q_3q_{23}} T^{(k_1)}U^{(k_2)}V^{(k_3)}\langle k_2k_3q_2q_3|k_2k_3k_{23}q_{23}\rangle \\ &\times \langle k_1k_{23}q_1q_{23}|k_1k_{23}KQ\rangle \end{aligned} \tag{4.27}$$

and we have used Eq. (2.38), describing the decoupling of $|j_2(j_2j_3)j_{23}JM\rangle$. This is in complete analogy with the re-coupling of three angular momenta. We could of course have chosen another scheme, *e.g.*

$$\begin{aligned}((T^{(k_1)}U^{(k_2)})^{(k_{12})}V^{(k_3)})^{(K)}_Q &= \sum_{q_1q_2q_3q_{12}} T^{(k_1)}U^{(k_2)}V^{(k_3)}\langle k_1k_2q_1q_2|k_1k_2k_{12}q_{12}\rangle \\ &\times \langle k_{12}k_3q_{12}q_3|k_{12}k_3KQ\rangle \end{aligned} \tag{4.28}$$

By changing representation one can go from Eq. (4.27) to Eq. (4.28), *c.f.* Eq. (2.32).

$$\begin{aligned}&(T^{(k_1)}(U^{(k_2)}V^{(k_3)})^{(k_{23})})^{(K)}_Q = \\ &\sum_{k_{12}}((T^{(k_1)}U^{(k_2)})^{(k_{12})}V^{(k_3)})^{(K)}_Q\langle(k_1k_2)k_{12}k_3K|k_1(k_2k_3)k_{23}K\rangle \end{aligned} \tag{4.29}$$

The overlap element on the right hand side of Eq. (4.29) is proportional to the $6j$-symbol. Now, once at it, we can go ahead and define a tensor operator built from four other tensor operators $T^{(k_1)}$, $U^{(k_2)}$, $V^{(k_3)}$ and $W^{(k_4)}$. Eq. (2.65) and (2.66) describe the decoupling of $|(j_1j_2)j_{12}(j_3j_4)j_{34}JM\rangle$ and $|(j_1j_3)j_{13}(j_2j_4)j_{24}JM\rangle$, respectively. We therefore obtain

$$\begin{aligned}&((T^{(k_1)}U^{(k_2)})^{(k_{12})}(V^{(k_3)}W^{(k_4)})^{(k_{34})})^{(K)}_Q = \sum_{q_1q_2q_3q_4q_{12}q_{34}} T^{(k_1)}U^{(k_2)}V^{(k_3)}W^{(k_4)} \times \\ &\langle k_1k_2q_1q_2|k_1k_2k_{12}q_{12}\rangle\langle k_3k_4q_3q_4|k_3k_4k_{34}q_{34}\rangle\langle k_{12}k_{34}q_{12}q_{34}|k_{12}k_{34}KQ\rangle \end{aligned} \tag{4.30}$$

and

$$\begin{aligned}&((T^{(k_1)}V^{(k_3)})^{(k_{13})}(U^{(k_2)}W^{(k_4)})^{(k_{24})})^{(K)}_Q = \sum_{q_1q_2q_3q_4q_{13}q_{24}} T^{(k_1)}U^{(k_2)}V^{(k_3)}W^{(k_4)} \times \\ &\langle k_1k_3q_1q_3|k_1k_3k_{13}q_{13}\rangle\langle k_2k_4q_2q_4|k_2k_4k_{24}q_{24}\rangle\langle k_{13}k_{24}q_{13}q_{24}|k_{13}k_{24}KQ\rangle \end{aligned} \tag{4.31}$$

which again is in complete analogy with re-coupling of four angular momenta. Changing representation, *i.e.* getting from Eq. (4.30) to (4.31) will involve a $9j$-symbol, *c.f.* Eq. (2.67).

Defining a tensor operator involving five other tensor operators is of course straight forward. However, we leave this to the curious reader. For the case of the product of two tensor operators we showed that $X^{(K)}_Q$, defined by Eq. (4.22), transformed

according the Eq. (4.16) under rotation (Eq. (4.22)). This can be done also for the Eqs. (4.27), (4.28), (4.30) and (4.31), but is rather tedious. We save this for homework and/or an examination problem :)

This section is concluded by noting that tensor operators of the form in Eqs. (4.27) and (4.28) appears, for example, when defining tensor operators for magnetic hyperfine interaction and those used when treating configuration interaction in $l^{(N)}$ systems, *c.f.* $4f^{(N)}$ systems, (particularly the core excitation $l'^{4l'+1}l^{N+1}$ and the excitation $l^{N-1}l'$). If time permits we will return to these interactions.