1 Notes on spherical tensors and Wigner-Eckart theorem

(The following is based on Section 3.10 of Sakurai.)

Under a rotation in three-dimensional space, a three-vector transforms according to

$$V_i \quad \to \quad V_i' = \sum_{j=1}^{3} R_{ij} V_j \tag{1.1}$$

where V_i, $i = 1, 2, 3$ stand for the x, y, z components of the vector $\vec{V}$. (Note: this generalizes trivially to rotations in higher dimensional spaces, but we restrict here to three dimensions). Examples, include the position vector $\vec{r}$ with components x_i, the momentum $\vec{p}$ and angular momentum $\vec{L}$.

In quantum mechanics we demand that the expectation value of a vector operator transforms under rotation like a classical vector. This means that when a state $|\alpha\rangle$ transforms under rotation, according to

$$|\alpha\rangle \quad \to \quad \mathcal{D}(R)|\alpha\rangle \tag{1.2}$$

$$\mathcal{D}(R) = \exp(-i \sum_{i=1}^{3} \beta_i J_i/\hbar) \tag{1.3}$$

then the following operator equation must hold

$$\mathcal{D}^\dagger(R) V_i \mathcal{D}(R) = \sum_{j=1}^{3} R_{ij} V_j \tag{1.4}$$

Considering an infinitesimal rotation this conditions becomes

$$[V_i, J_k] = i\epsilon_{ijk}\hbar V_k \tag{1.5}$$

which can also be regarded as the defining property of a vector. It is not difficult to see that this indeed holds for the above mentioned examples of vectors.

Before we go on to generalize the above notion to higher rank tensors (a vector is a rank 1 tensor), let us introduce also the notion of a scalar. A scalar is invariant under rotation

$$s \quad \to \quad s' = s \tag{1.6}$$

Given two vectors $\vec{U}$ and $\vec{V}$, we know that the scalar product $s = \vec{U} \cdot \vec{V}$ is invariant under rotation. This easily follows from (1.1) and the fact that rotations are orthogonal transformations, i.e. satisfying

$$R^T R = 1 \quad , \quad \sum_{k=1}^{3} R_{ik} R_{jk} = \delta_{ij} \tag{1.7}$$

So, in quantum mechanics the property of a scalar is

$$\mathcal{D}^\dagger(R) s \mathcal{D}(R) = s \quad \Leftrightarrow \quad [s, J_k] = 0 \tag{1.8}$$

and using (1.5) it is not difficult to check that this holds for the scalar product of two vectors.

Now we introduce **Cartesian tensors**, generalizing the vectors given in (1.1). A tensor of rank n is an object with n indices transforming under rotations as

$$T_{i_1 i_2 \ldots i_n} \quad \rightarrow \quad T'_{i_1 i_2 \ldots i_n} = \sum_{j_1=1}^{3} \sum_{j_2=1}^{3} \cdots \sum_{j_n=1}^{3} R_{i_1 j_1} R_{i_2 j_2} \cdots R_{i_n j_n} T_{j_1 j_2 \ldots j_n} \tag{1.9}$$

So each index transforms as a vector under the rotation group. The simplest example is that of a Cartesian rank 2 tensor constructed out of two vectors $W_{ij} = U_i V_j$. Because we know that both U and V transform as a vector, it immediately follows that W_{ij} then transforms under rotations according to (1.9) with $n = 2$.

In general these Cartesian tensors are reducible[1].This means that we can decompose them into smaller representations which transform into themselves under rotations. We know from our study of the rotation group in three dimensions that the irreducible representations are classified by the quantum numbers j, and for given j the dimension of the representation is $\dim(T^{(j)}) = 2j+1$, since $m = -j \ldots j$. In particular, we have encountered the spherical harmonics Y_l^m, which transform as irreducible representations under the rotation group. More generally, we define a **spherical tensor** of rank k (which is like l) with $2k + 1$ components labelled by q (which is like m) as

$$\mathcal{D}^\dagger(R) T_q^{(k)} \mathcal{D}(R) = \sum_{q'=-k}^{k} \mathcal{D}_{qq'}^{(k)\star} T_{q'}^{(k)} \tag{1.10}$$

Here the matrix elements $\mathcal{D}_{qq'}^{(k)\star}$ which specify the transformation properties under rotation are identified with the corresponding matrix elements $\mathcal{D}_{mm'}^{(l)\star}$ that enter the transformation properties of the Y_l^m under rotations.

It is illustrative to consider the following example of a spherical tensors

$$T_q^{(k)}(\vec{V}) = Y_{l=k}^{m=q}(\vec{V}) \tag{1.11}$$

[1]Without resorting to a precise mathematical definition, this means that when we act with the rotation group on these tensors, for a given rank n, we get some big $n^2 \times n^2$-dimensional rotation matrix. Being reducible means that it has the property that by making an appropriate basis change, we can block diagonalize this matrix into smaller subsets. These smaller subsets are then called the irreducible components. This is precisely what we have also seen when we add angular momentum (going from the uncoupled basis to the coupled basis where rotations act block diagonally, see also the cover of the Sakurai book !).

where $Y_{l=k}^{m=q}(\vec{V})$ is obtained from $Y_l^m(\theta,\phi)$ by writing it as $Y_l^m(\hat{n})$, with $\hat{n}$ the unit vector characterized by (θ,ϕ) and then replacing $\hat{n}\to\vec{V}$. In particular for the case $k=1$ this gives us

$$T_0^{(1)} = V_z \quad , \quad T_{\pm 1}^{(1)} = \mp\frac{1}{\sqrt{2}}(V_x \pm iV_y) \tag{1.12}$$

(where we have chosen a particular normalization, which is of course unimportant as far as transformation under the rotation group is concerne) Note that, for simplicity of notation, I have dropped the "$(\vec{V})$" in $T_{q=0,\pm1}^{(1)}(\vec{V})$, but is important to realize that this is the particular rank 1 spherical tensor constructed from the given vector $\vec{V}$. This thus shows the (expected) result that a three-vector is really the same as the $l=1$ representation of the rotation group. The relation (1.12) gives us the transformation between the vector in Cartesian basis and when viewed as a spherical tensor of rank 1. The inverse of (1.12) is given by

$$V_x = \frac{1}{\sqrt{2}}(T_{-1}^{(1)} - T_1^{(1)}) \quad , \quad V_y = \frac{i}{\sqrt{2}}(T_{-1}^{(1)} + T_1^{(1)}) \quad , \quad V_z = T_0^{(1)} \tag{1.13}$$

Another important example is the dyadic $W_{ij} = U_iV_j$. This has (for $\vec{U}\neq\vec{V}$) a total of $3\times 3 = 9$ independent components. As we will see below, this representation turns out to be reducible, and we find that the decomposition in terms of irreducible spherical tensors involves the $k=0$ representation of dimension 1 (this is the trivial representation, i.e. a scalar), the $k=1$ representation of dimension 3 (i.e. a vector) and the $k=2$ representation of dimension 5. Indeed this checks with $9=1+3+5$.

Explicitly we can write

$$U_iV_j = \frac{\vec{U}\cdot\vec{V}}{3}\delta_{ij} + \frac{(U_iV_j - U_jV_i)}{2} + \left(\frac{U_iV_j + U_jV_i}{2} - \frac{\vec{U}\cdot\vec{V}}{3}\delta_{ij}\right) \tag{1.14}$$

This way of rewriting incorporates precisely the decomposition into irreducible representations. The first term is the scalar product and hence proportional to the tensor $T_0^{(0)}$, which is the one-dimensional trivial representation. The second term is the antisymmetrized product of two vectors. Clearly this has three independent components (there are three ways to take two unequal indices out of three), and we recognize the components of the cross product of the two vectors $(\vec{U}\times\vec{V})_k = \epsilon_{ijk}U_iV_j = \frac{1}{2}\epsilon_{ijk}(U_iV_j - U_jV_i)$. So this part transforms itself like a vector (the cross product of two vectors is a vector) or, equivalently, as a rank 1 tensor $T^{(1)}$. Finally, the third term is the symmetrized product of two vectors, with the extra condition that it is made traceless. Symmetrizing gives us six components, but making it also traceless leaves five independent components. It can then be shown that this part transforms as a rank 2 spherical tensor $T^{(2)}$.

In further detail we have the useful formulae

$$T_0^{(0)} = -\frac{\vec{U} \cdot \vec{V}}{3} = \frac{U_1 V_{-1} + U_{-1} V_1 - U_0 V_0}{3} \tag{1.15}$$

$$T_q^{(1)} = \frac{(\vec{U} \times \vec{V})_q}{i\sqrt{2}} \quad , \quad q = -1, 0, 1 \tag{1.16}$$

$$T_{\pm 2}^{(2)} = U_{\pm 1} V_{\pm 1} \tag{1.17}$$

$$T_{\pm 1}^{(2)} = \frac{U_{\pm 1} V_0 + U_0 V_{\pm 1}}{\sqrt{2}} \tag{1.18}$$

$$T_0^{(2)} = \frac{U_1 V_{-1} + U_{-1} V_1 + 2 U_0 V_0}{\sqrt{6}} \tag{1.19}$$

where we have used the definitions $U_q \equiv T_q^{(1)}(\vec{U})$, $q = 0, \pm 1$ and the same for V_q, $q = 0, \pm 1$, in terms of the combinations defined in (1.12). Note also that we use here the same type of definition for the components $(\vec{U} \times \vec{V})_q$, $q = 0, \pm 1$.

It is also useful to invert the above 9 relations, expressing the Cartesian products in terms of spherical tensors. After some algebra the result is as given in the maple file posted on Uge 51. (see the last page, where you should read $UV_{i,j} \to U_i V_j$ and $Ts_{kq} \to T_q^{(k)}$). Note that these expressions are valid for the general case $\vec{U} \neq \vec{V}$. For the special case $\vec{U} = \vec{V}$, recall that the rank 1 tensor $T_q^{(1)}$ in (1.16) is zero, so in that case one can use the expressions in the maple file but evaluated with $T_q^{(1)} = 0$.

The theorem in eq.(3.10.27) (Sakurai) is a useful result. It states that when $X_{q_1}^{(k_1)}$ and $Z_{q_2}^{(k_2)}$ are irreducible tensors of rank k_1 and k_2 respectively, then

$$T_q^{(k)} = \sum_{q_1=-k_1}^{k_1} \sum_{q_2=-k_2}^{k_2} \langle k_1 k_2; q_1 q_2 | k_1 k_2; kq \rangle X_{q_1}^{(k_1)} Z_{q_2}^{(k_2)} \tag{1.20}$$

is a spherical (irreducible) tensor of rank k. Here $\langle k_1 k_2; q_1 q_2 | k_1 k_2; kq \rangle$ are nothing but the Clebsch-Gordon coefficients involving the coupling of angular momenta k_1 and k_2 to obtain total angular momentum k. A necessary condition for the Clebsch-Gordon coefficients to be non-zero is

$$\langle k_1 k_2; q_1 q_2 | k_1 k_2; kq \rangle \neq 0 \quad \Rightarrow \quad |k_1 - k_2| \leq k \leq k_1 + k_2 \quad \text{and} \quad q_1 + q_2 = q \tag{1.21}$$

In fact the relations in (1.15)-(1.19) represent an explicit realization of (1.20) for the case of $k_1 = k_2 = 1$. Note in particular that one explicitly sees in each of these expressions the addition rule $q = q_1 + q_2$.

The relation (1.20) shows thus that: *multiplying spherical tensors is exactly the same as addition of angular momentum.* Recall the fact that Clebsch-Gordon coefficients enter when one adds two angular momenta $\vec{J} = \vec{J}_1 + \vec{J}_2$, and are defined via the relation

$$|j_1 j_2; jm\rangle = \sum_{m_1=-l_1}^{m_1} \sum_{m_2=-l_2}^{m_2} \langle j_1 j_2, m_1 m_2 | j_1 j_2; jm\rangle |j_1 j_2, m_1 m_2\rangle \tag{1.22}$$

where the basis kets $|j_1 j_2, m_1 m_2\rangle \equiv |j_1 m_1\rangle |j_2 m_2\rangle$ are in the uncoupled basis, and the kets $|j_1 j_2; jm\rangle$ the coupled basis.

The inverse of the relation (1.20) is

$$X_{q_1}^{(k_1)} Z_{q_2}^{(k_2)} = \sum_{k=|k_1-k_2|}^{k_1+k_2} \sum_{q=-k}^{k} \langle k_1 k_2; kq | k_1 k_2; q_1 q_2\rangle T_q^{(k)} \tag{1.23}$$

This relation, combined with (1.12) (and possibly (1.15)-(1.19)) is useful when one has higher rank Cartesian tensors and wishes to find out how to decompose these into spherical tensors. Also here is it useful to keep in mind that we need to have $q_1 + q_2 = q$.

Given a spherical tensor $T_q^{(k)}$ we can now state the Wigner-Eckart theorem: The matrix elements of tensor operators with respect to angular momentum eigenstates satisfy

$$\langle \alpha', j'm' | T_q^{(k)} | \alpha, jm\rangle = \langle jk; mq | jk; j'm'\rangle \frac{\langle \alpha', j' || T^{(k)} || \alpha, j\rangle}{\sqrt{2j+1}} \tag{1.24}$$

Here $|\alpha, j, m\rangle$ denote the eigenstates of the system under consideration, with the (j, m)-part denoting the usual angular-momentum eigenstates satisfying $J^2|j,m\rangle = \hbar^2 j(j+1)|j,m\rangle$ and $J_z|j,m\rangle|j,m\rangle = \hbar m|j,m\rangle$. The label α stands for all other quantum numbers. In most of our applications the system under consideration is an electron in a central potential, so that the eigenstates take the form $|n,l,m\rangle$, so that $\alpha \sim n$ and $j \sim l$.

In (1.24) we have again that $\langle jk; mq | jk; j'm'\rangle$ denote the Clebsch-Gordon coefficients of the decomposition of angular-momentum j and k into total angular momentum j'. This gives us immediately the m-selection rule that in order for the matrix element on the left of (1.24) to be non-zero we need to have

$$m' = q + m \quad \Leftrightarrow \quad \Delta m \equiv m' - m = q \tag{1.25}$$

Moreover, we see that another necessary condition for this matrix element to be non-zero is that

$$|j-k| \leq j' \leq j+k \quad \Leftrightarrow \quad |\Delta j| \equiv |j' - j| \leq k \tag{1.26}$$

It is also useful to apply the parity selection rule: If the operator $T_q^{(k)}$ has parity $\pi = \pm 1$ then it follows from parity conservation that $(-1)^{|\Delta j|+\pi} = 1$, in other words $|\Delta j| =$ even when $\pi = 1$ and $|\Delta j| =$ odd when $\pi = -1$.

The meaning of $\langle \alpha', j' || T^{(k)} || \alpha, j \rangle$ is that it contains the part of the tensor that does not depend on the angles and the part of the eigenstates that do not depend on the angles. It is best illustrated by thinking again of the example mentioned above, electron in central potential. Suppose $T^{(k)}$ has the radial dependence r^κ, then

$$\langle \alpha', j' || T^{(k)} || \alpha, j \rangle \quad \rightarrow \quad \int_0^\infty R_{n'l'}(r) r^\kappa R_{nl}(r) r^2 dr \tag{1.27}$$

2 A simple application

As a simple application of all this consider the potential

$$V = axy \tag{2.1}$$

We would like to find out the selection rules. To this end we first need to express the potential in terms of spherical tensors. Looking at e.g. the maple notes, we find the general expression

$$U_x V_y = \frac{i}{2}(T_{-2}^{(2)} - T_2^{(2)} + \sqrt{2}\, T_0^{(1)}) \tag{2.2}$$

However, recall that for the potential (2.1) we should also use that we have $\vec{U} = \vec{V} (= \vec{r})$, so that $T_q^{(1)} = 0$, and hence we conclude

$$xy = \frac{i}{2}(T_{-2}^{(2)} - T_2^{(2)}) \tag{2.3}$$

Using (1.24) and the rules (1.25), (1.26), we get the selection rules (for non-zero matrix elements $\langle \alpha', j'm' | V | \alpha, jm \rangle$):

1. from 1st term: $\Delta m = -2$, $|\Delta l| \leq 2$
2. from 2nd term: $\Delta m = 2$, $|\Delta l| \leq 2$

In addition we use parity. The operator xy has even parity, so we need $|\Delta l| = 0, 2, 4, \ldots$. Putting it all together we have

$$|\Delta m| = 2 \quad , \quad |\Delta l| = 0, 2 \tag{2.4}$$