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Angular Momentum Coupling Theory

In the last chapter, we calculated (for the special case $s = \frac{1}{2}$) the transformation coefficient $\langle nlm_l sm_s | nlsjm_j\rangle = \langle nlsjm_j | nlm_l sm_s\rangle^*$ from a basis $|nlm_l sm_s\rangle$ in which L_z and S_z are diagonal, which was a good basis for the case in which the external B_0 field was the dominant perturbation, to the basis $|nlsjm_j\rangle$, the proper basis in the limit $B_0 = 0$ in which the $(\vec{L}\cdot\vec{S})$ term is the dominant perturbation and in which the operators $(\vec{J}\cdot\vec{J})$ and J_z are diagonal. This was a special case of an important and common problem, met in many applications of quantum theory.

Given two commuting angular momentum operators, $\vec{J}_1$ and $\vec{J}_2$, each with standard angular momentum commutation relations, i.e., with

$$[\vec{J}_1, \vec{J}_2] = 0, \qquad \text{and}$$
$$[J_0, J_\pm] = \pm J_\pm, \qquad [J_+, J_-] = 2J_0, \qquad \text{for both} \quad \vec{J}_1,\ \vec{J}_2. \tag{1}$$

We construct the coupled angular momentum vector

$$\vec{J} = \vec{J}_1 + \vec{J}_2, \tag{2}$$

which also satisfies the standard angular momentum commutation relations of eq. (1). We will often need to make the transformation from the $|j_1 m_1 j_2 m_2\rangle$ basis, where these are simultaneously eigenvectors of the four commuting operators

$$(\vec{J}_1\cdot\vec{J}_1), \quad (J_1)_z, \quad (\vec{J}_2\cdot\vec{J}_2), \quad (J_2)_z,$$

to the $|j_1 j_2 jm\rangle$ basis, where these are simultaneously eigenvectors of the four commuting operators

$$(\vec{J}_1\cdot\vec{J}_1), \quad (\vec{J}_2\cdot\vec{J}_2), \quad (\vec{J}\cdot\vec{J}), \quad J_z.$$

The possible m values are

$$\begin{aligned} m_1 &= j_1,\ (j_1-1),\ (j_1-2),\ \ldots,\ -j_1, \\ m_2 &= j_2,\ (j_2-1),\ (j_2-2),\ \ldots,\ -j_2, \\ m &= j,\ (j-1),\ (j-2),\ \ldots,\ -j, \end{aligned} \tag{3}$$

where m is an additive quantum number

$$m = m_1 + m_2. \tag{4}$$

First, we need to find the possible j values for a given j_1, j_2. We shall name the j_1, j_2, such that $j_1 \geq j_2$. To find the possible values of j, we simply count the number of occurences for each possible value of m.

The maximum possible m value is $m = j_1 + j_2$, which can be made in only one way, with $m_1 = j_1$ and $m_2 = j_2$. Hence, one j value must exist with $j = j_1 + j_2$.

There are two ways of making $m = (j_1 + j_2 - 1)$; either with $m_1 = j_1, m_2 = (j_2 - 1)$, or with $m_1 = (j_1 - 1), m_2 = j_2$. One linear combination of these two states will be the state with $j = j_1 + j_2$ and $m = (j_1 + j_2 - 1)$. The other linear combination of these two states must be a state with $m = j = (j_1 + j_2 - 1)$. Thus, one j value must exist with $j = (j_1 + j_2 - 1)$.

There are three ways of making states with $m = (j_1 + j_2 - 2)$, viz., with $m_1, m_2 = j_1, (j_2 - 2), (j_1 - 1), (j_2 - 1)$, or $(j_1 - 2), j_2$. One linear combination of these three states is needed to make the state with $j = j_1 + j_2$ and $m = (j_1 + j_2 - 2)$. A second linear combination of these three states is needed to make the state with $j = (j_1 + j_2 - 1)$ and $m = (j_1 + j_2 - 2)$. This leaves one linear combination to make a single state with $m = j = (j_1 + j_2 - 2)$, so one j value exists with $j = (j_1 + j_2 - 2)$.

This process can be continued for $k \leq 2j_2$ (recall we chose $j_1 \geq j_2$), so that there are $(k + 1)$ ways of making states with $m = (j_1 + j_2 - k)$. Of these, k linear combinations are needed to make the states with this m value, but with one of the allowed j values with $j > (j_1 + j_2 - k)$, leaving but a single linear combination of these states with $m = j = (j_1 + j_2 - k)$, so a single j value exists with $(j_1 + j_2 - k)$.

This process quits with $k = 2j_2$. For $k \geq 2j_2$ and $m \geq 0$, there are only $(2j_2 + 1)$ ways of making the m value $m = (j_1 + j_2 - k)$ with $k \geq 2j_2$, and all $(2j_2 + 1)$ independent linear combinations of these states are needed to make the states with $j \geq (j_1 - j_2)$, so no new j values arise, with $j < (j_1 - j_2)$. Finally, symmetry exists between the positive and negative m values.

Thus, the possible j values are

$$(j_1 + j_2),\ (j_1 + j_2 - 1),\ (j_1 + j_2 - 2),\ \ldots,\ |(j_1 - j_2)|,$$

with each j value occuring once only. The total number of states is

$$\begin{aligned} \sum_{|(j_1-j_2)|}^{(j_1+j_2)} (2j+1) &= \sum_{k=0}^{k=2j_2} [2(j_1 + j_2 - k) + 1] \\ &= (2j_2 + 1)(2j_1 + 2j_2 + 1) - 2\frac{(2j_2+1)2j_2}{2} \\ &= (2j_1 + 1)(2j_2 + 1), \end{aligned} \tag{5}$$

as it should be.

A General Properties of Vector Coupling Coefficients

We shall need the transformation coefficients of the unitary transformation

$$|j_1 j_2 jm\rangle = \sum_{m_1,(m_2)} |j_1 m_1 j_2 m_2\rangle\langle j_1 m_1 j_2 m_2 | j_1 j_2 jm\rangle, \tag{6}$$

where $\langle j_1 m_1 j_2 m_2 | j_1 j_2 jm\rangle$ is the unitary transformation matrix, which could be written as,

$$U_{m_1 m_2, jm},$$

where the row label is given by $m_1 m_2$, and the column label is specified by jm. We sum over both m_1 and m_2 in eq. (6), but m is fixed and because $m = m_1 + m_2$, m_2 is determined by m_1 and m, so it gets "dragged along" in the sum. This is why we have put m_2 in parentheses in the summation symbol. Because j_1 and j_2 is common to both bases, the unitary transformation coefficient is often abbreviated by

$$\langle j_1 m_1 j_2 m_2 | jm\rangle.$$

It is known as a "Clebsch–Gordan coefficient," or as a "Wigner coefficient," or as a "vector coupling coefficient." Slightly different notations are used by different people. Other commonly used notations are $\langle j_1 j_2 m_1 m_2 | jm\rangle$ (note the different order of the labels in the left-hand side), or $C^{j_1 j_2 j}_{m_1 m_2 m}$, or several others.

The inverse of the above transformation, eq. (6), is in Dirac notation

$$|j_1 m_1 j_2 m_2\rangle = \sum_j |j_1 j_2 jm\rangle\langle j_1 j_2 jm | j_1 m_1 j_2 m_2\rangle, \tag{7}$$

where the summation is one over j only, because m is fixed by the fixed values of m_1 and m_2 and

$$\begin{aligned}\langle j_1 j_2 jm | j_1 m_1 j_2 m_2\rangle &= (U^{-1})_{jm,m_1 m_2} = (U_{m_1 m_2, jm})^* \\ &= \langle j_1 m_1 j_2 m_2 | j_1 j_2 jm\rangle^* = \langle j_1 m_1 j_2 m_2 | jm\rangle^*.\end{aligned} \tag{8}$$

The Clebsch–Gordan coefficients can all be made real. (This is the "world" standard to which everyone adheres!) Therefore, the complex conjugate sign is not needed for the inverse transformation, and we can write the inverse transformation, in terms of the Clebsch–Gordan coefficient notation, as

$$|j_1 m_1 j_2 m_2\rangle = \sum_j |j_1 j_2 jm\rangle\langle j_1 m_1 j_2 m_2 | jm\rangle. \tag{9}$$

(From the point of view of the Dirac notation, the transformation coefficient appears to have bra and ket inverted. This inversion is because we have made use of the unitary property of this *real* transformation coefficient. We shall always write the Clebsch–Gordan coefficient in the Dirac-like notation, but with the m_1, m_2

labels always on the left!) Using the unitary property of this real transformation coefficient, we get the: Orthogonality relations of the Clebsch–Gordan coefficients:

$$\sum_{m_1,(m_2)} \langle j_1 m_1 j_2 m_2 | jm \rangle \langle j_1 m_1 j_2 m_2 | j' m' \rangle = \delta_{jj'} \delta_{mm'},$$

$$\sum_{j} \langle j_1 m_1 j_2 m_2 | jm \rangle \langle j_1 m_1' j_2 m_2' | jm \rangle = \delta_{m_1 m_1'} \delta_{m_2 m_2'}. \tag{10}$$

B Methods of Calculation

For $j_2 = \frac{1}{2}$, we have already found one method: diagonalize the operator $(\vec{J}_1 \cdot \vec{J}_2)$ in the $|j_1 m_1 j_2 m_2\rangle$ basis. For $j_2 \geq 1$, however, this method would lead to a diagonalization of 3×3, $4 \times 4, \ldots,$ matrices. Hence, we shall look for better methods. One of these methods involves recursion formulae for the Clebsch–Gordan coefficients. We shall derive a recursion formula for the Clebsch–Gordan coefficients by acting on the state vector $|j_1 j_2 jm\rangle$ with the operator,

$$J_+ = (J_1)_+ + (J_2)_+,$$

$$J_+ |j_1 j_2 jm\rangle = \sum_{m_1',(m_2')} \Big((J_1)_+ + (J_2)_+\Big) |j_1 m_1' j_2 m_2'\rangle \langle j_1 m_1' j_2 m_2' | jm\rangle, \tag{11}$$

or

$$\begin{aligned} &\sqrt{(j-m)(j+m+1)}|j_1 j_2 j(m+1)\rangle \\ &= \sum_{m_1',(m_2')} \Big(\sqrt{(j_1 - m_1')(j_1 + m_1' + 1)}|j_1(m_1'+1) j_2 m_2'\rangle \\ &+ \sqrt{(j_2 - m_2')(j_2 + m_2' + 1)}|j_1 m_1' j_2 (m_2'+1)\rangle\Big) \langle j_1 m_1' j_2 m_2' | jm\rangle. \end{aligned} \tag{12}$$

Now, expanding $|j_1 j_2 j(m+1)\rangle$ on the left-hand side of this relation, and renaming the dummy summation indices $m_1', m_2' = (m_1 - 1), m_2$ in the first term of the right-hand side, and making the change $m_1', m_2' = m_1, (m_2 - 1)$ in the second term of the right-hand side, we get

$$\begin{aligned} &\sqrt{(j-m)(j+m+1)} \sum_{m_1,(m_2)} |j_1 m_1 j_2 m_2\rangle \langle j_1 m_1 j_2 m_2 | j(m+1)\rangle \\ &= \sum_{m_1,(m_2)} |j_1 m_1 j_2 m_2\rangle \Big(\sqrt{(j_1 - m_1 + 1)(j_1 + m_1)} \langle j_1 (m_1 - 1) j_2 m_2 | jm\rangle \\ &+ \sqrt{(j_2 - m_2 + 1)(j_2 + m_2)} \langle j_1 m_1 j_2 (m_2 - 1) | jm\rangle \Big). \end{aligned} \tag{13}$$

Now, with left-multiplication by a $\langle j_1 m_1 j_2 m_2|$ with a specific, fixed m_1 and m_2, this equation is converted to the recursion relation, as follows.

Recursion Formula I:

$$\sqrt{(j-m)(j+m+1)} \langle j_1 m_1 j_2 m_2 | j(m+1)\rangle$$

$$= \sqrt{(j_1+m_1)(j_1-m_1+1)}\langle j_1(m_1-1)j_2m_2|jm\rangle + \sqrt{(j_2+m_2)(j_2-m_2+1)}\langle j_1m_1j_2(m_2-1)|jm\rangle. \quad (14)$$

For states with $m = j$, this three-term recursion formula is reduced to a two-term recursion formula, which leads to

$$\frac{\langle j_1(m_1-1)j_2m_2|jj\rangle}{\langle j_1m_1j_2(m_2-1)|jj\rangle} = -\sqrt{\frac{(j_2+m_2)(j_2-m_2+1)}{(j_1+m_1)(j_1-m_1+1)}}. \quad (15)$$

We can use this successively, starting with $m_1 = j_1$, and, hence, $m_2 = j - j_1 + 1$, to relate

$$\langle j_1m_1j_2(m_2 = j - m_1)|jj\rangle \quad \text{to} \quad \langle j_1j_1j_2(j-j_1)|jj\rangle,$$

and, thus, get

$$\frac{\langle j_1m_1j_2(j-m_1)|jj\rangle}{\langle j_1j_1j_2(j-j_1)|jj\rangle} = (-1)^{j_1-m_1}\sqrt{\frac{(j_2+j-j_1+1)(j_2+j-j_1+2)\cdots(j_2+j-m_1)}{2j_1(2j_1-1)\cdots(j_1+m_1+1)}}$$
$$\times \sqrt{\frac{(j_2-j+j_1)(j_2-j+j_1-1)\cdots(j_2-j+m_1+1)}{1\cdot 2\cdots(j_1-m_1)}}$$
$$= (-1)^{j_1-m_1}\sqrt{\frac{(j_2+j-m_1)!}{(j_2+j-j_1)!}\,\frac{(j_2-j+j_1)!}{(j_2-j+m_1)!}\,\frac{(j_1+m_1)!}{2j_1!(j_1-m_1)!}}. \quad (16)$$

Now we can calculate $|\langle j_1j_1j_2(j-j_1)|jj\rangle|$ by using the orthonormality

$$\sum_{m_1}|\langle j_1m_1j_2(j-m_1)|jj\rangle|^2 = 1. \quad (17)$$

To do the sum, we will need an addition theorem for binomial coefficients

$$\sum_{m_1}\frac{(a+m_1)!(b-m_1)!}{(c+m_1)!(d-m_1)!} = \frac{(a+b+1)!(a-c)!(b-d)!}{(c+d)!(a+b-c-d+1)!}. \quad (18)$$

Because this relation will only give us the absolute value of the starting coefficient $\langle j_1j_1j_2(j-j_1)|jj\rangle$, its phase must be chosen. The choice universally accepted, the so-called Condon and Shortley phase convention, is the following: This starting coefficient is chosen to be real and positive. Then,

$$\langle j_1j_1j_2(j-j_1)|jj\rangle = \sqrt{\frac{2j_1!(2j+1)!}{(j_1+j_2+j+1)!(j_1-j_2+j)!}}, \quad (19)$$

and, finally,

$$\langle j_1m_1j_2(j-m_1)|jj\rangle = (-1)^{j_1-m_1}\times$$
$$\sqrt{\frac{(j_1+m_1)!(j_2+j-m_1)!(j_1+j_2-j)!(2j+1)!}{(j_1-m_1)!(j_2-j+m_1)!(j_2-j_1+j)!(j_1-j_2+j)!(j_1+j_2+j+1)!}}. \quad (20)$$

Now we need to calculate coefficients with $m < j$. We can accomplish this by deriving a recursion formula that steps down in m. By repeating the steps of eqs. (11)–(14) by acting on the coupled state $|j_1 j_2 jm\rangle$ with the step-down operator $J_- = (J_1)_- + (J_2)_-$, we arrive at the analogue of eq. (14) as follows.

Recursion Formula II:

$$\begin{aligned}&\sqrt{(j+m)(j-m+1)}\langle j_1 m_1 j_2 m_2 | j(m-1)\rangle\\ &= \sqrt{(j_1-m_1)(j_1+m_1+1)}\langle j_1(m_1+1) j_2 m_2 | jm\rangle\\ &+ \sqrt{(j_2-m_2)(j_2+m_2+1)}\langle j_1 m_1 j_2(m_2+1) | jm\rangle. \qquad (21)\end{aligned}$$

Repeated application of this recursion formula II will give us the coefficients with arbitrary m, starting with the known coefficient with $m = j$. In practice, the most widely used tables are those in which one of the angular momenta is reasonably small, say, $j_2 = \frac{1}{2}, 1, \frac{3}{2}, 2$. (See problem 39.) To calculate some of these it will be useful to first study the symmetries of the Clebsch–Gordan coefficients.