Lecture 13 : Title : Coupling of angular momentum

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In this lecture we will go through the method of coupling of angular momentum.

We will start with the need for this coupling and then develop the method for evaluating coupled state in terms of uncoupled states.

First we will take up the case of coupling of two generalized angular momenta and then utilize this to take the case of three angular momenta.

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In previous lecture, we have seen that the electron-electron repulsion term is responsible for the splitting of energy levels. The reason for this is the one electron quantum numbers are not the good quantum numbers for the total Hamiltonian.

Because,_ $H_1 \equiv \left(\frac{e^2}{r_{ij}}\right)$ does not commute with ℓ_i, but H_1 commutes with L and S where $L = \sum_i \ell_i$; $S = \sum_i S_i$. It is equivalent to saying that H_1 is invariant under a rotation of spatial and spin coordinates.

Proof:

$$[H_1, L] = e^2 \sum_{i<j} \sum_k \frac{1}{r_{ij}} \ell_k - e^2 \sum_{i<j} \sum_{r_{ij}} \ell_k \frac{1}{r_{ij}}$$

$$where,\ \ell_k = -i r_k \times \nabla_k$$

Allowing the operators to act on arbitrary function ψ

$$\begin{bmatrix} \ell_k\left(\frac{1}{r_{ij}}\psi\right) = \frac{1}{r_{ij}}\ell_k\psi + \psi\ell_k\frac{1}{r_{ij}} \\ \ell_k\left(\frac{1}{r_{ij}}\right) = \frac{1}{r_{ij}}\ell_k + \ell_k\frac{1}{r_{ij}} \end{bmatrix}$$

$$= \frac{1}{r_{ij}}\ell_k - i\, r_k \times \nabla_k \left(\frac{1}{r_{ij}}\right)$$

$$So\ [H_1, L] = e^2 \sum_{i<j}\sum_k \frac{1}{r_{ij}}\ell_k - e^2 \sum_{i<j}\sum_k \ell_k \frac{1}{r_{ij}}$$

$$= e^2 \sum_{i<j}\sum_k \frac{1}{r_{ij}}\ell_k - e^2 \sum_{i<j}\sum_k \frac{1}{r_{ij}}\ell_k + i\,e^2 \sum_{i<j}\sum_k r_k \times \nabla_k \left(\frac{1}{r_{ij}}\right)$$

$$Now,\ \sum_k r_k \times \vec{\nabla}_k \left(\frac{1}{r_{ij}}\right) = \sum_k \left[-\vec{r}_k \times \frac{\vec{r}_i - \vec{r}_j}{r_{ij}^3}\delta_{ik} + \vec{r}_k \times \frac{\vec{r}_i - \vec{r}_j}{r_{ij}^3}\delta_{jk} \right]$$

$$= + \frac{r_i \times r_j}{r_{ij}^3} - \frac{r_i \times r_j}{r_{ij}^3} = 0$$

$$So\ [H, L] = 0$$

$$Similarly\ [H, S] = 0$$

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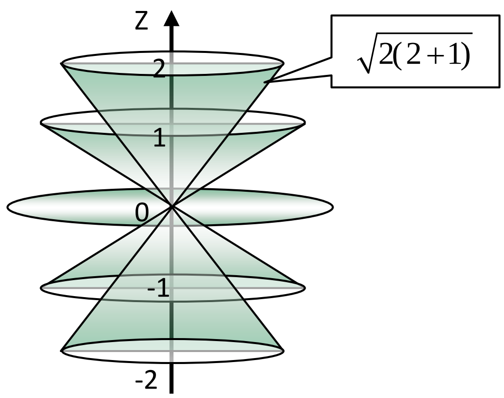
The angular momentum for an atomic electron can be visualized in terms of a vector model where the angular momentum vector is seen as precessing about a direction in space.

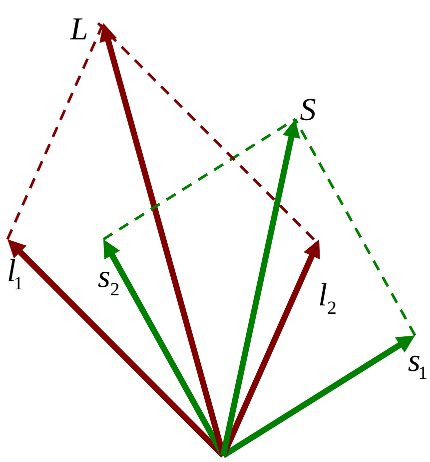
Let us consider the set of states having a common value of the quantum number j. For each of these states the length of the orbital angular momentum vector, $= \sqrt{j(j+1)}$ in units of $\hbar$.

The z-component of this vector is m in units of $\hbar$.

For example if j = 2 then there are five projections as shown in the figure.



In this model, we can understand that, for two electron system, the electron-electron repulsion is responsible to couple l_1 and l_2 to form the resultant vector L .Similarly, s_1 and s_2 to form the resultant vector S



Generalized angular momentum operator $\vec{J}$ is defined as a vector operator with Hermitian components J_x, J_y *and* J_z satisfying $\vec{J}\times\vec{J}=i\vec{J}$

The components are defined as

$$J_+ = -\frac{1}{\sqrt{2}}\left(J_x + iJ_y\right), \qquad J_0 = J_z \quad \text{and} \quad J_+ = \frac{1}{\sqrt{2}}\left(J_x - iJ_y\right)$$

And the inverse relations are

$$J_x = -\frac{1}{\sqrt{2}}\left(J_+ - J_-\right) \text{ and } J_y = \frac{1}{\sqrt{2}}\left(J_+ + J_-\right)$$

The commutation relations between them are

$$\left[J_0, J_+\right] = J_+,\ \left[J_0, J_-\right] = -J_-, \text{ and } \left[J_+, J_-\right] = -J_0$$

Since J_x, J_y *and* J_z are Hermitian, the total angular momentum operator

$$J^2 = J_x^2 + J_y^2 + J_z^2 = -J_+J_- + J_0^2 - J_-J_+$$

Using the Dirac notation, the eigen functions are represented as $\left|j,m\right\rangle$ where m is the projection of *J*, we have

$$J^2 \left| j\, m\right\rangle = j\left(j+1\right)\left| J\, m\right\rangle$$
$$J_z \left| j\, m\right\rangle = m\left| j\, m\right\rangle$$
$$\left\langle j'm' \middle| jm\right\rangle = \delta_{jj'}\delta_{mm'}$$

Similarly we have

$$J_+\left|j,m\right\rangle = -\sqrt{\frac{1}{2}\left[j(j+1)-m(m+1)\right]}\ \left|j,m+1\right\rangle$$

And

$$J_-\left|j,m\right\rangle = \sqrt{\frac{1}{2}\left[j(j+1)-m(m-1)\right]}\ \left|j,m-1\right\rangle$$

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Coupling of Angular Momenta

Two angular momentum operators J_1 and J_2 operate on two different spaces $|\, j_1, m_1\rangle$ and $|\, j_2, m_2\rangle$ such that,

$$\left.\begin{array}{l} J_1^{\,2}\,|\, j_1\, m_1\rangle = j_1\left(j_1+1\right)|\, j_1\, m_1\rangle \\ J_{1z}\,|\, j_1\, m_1\rangle = m_1\,|\, j_1\, m_1\rangle \\ J_2^{\,2}\,|\, j_2\, m_2\rangle = j_2\left(j_2+1\right)|\, j_2\, m_2\rangle \\ J_{2z}\,|\, j_2\, m_2\rangle = m_2\,|\, j_2\, m_2\rangle \end{array}\right\}----(1)$$

Let us define,

$$\vec{J} = \vec{J}_1 + \vec{J}_2$$

With understanding $$\left.\begin{array}{l} J_x = J_{1x} + J_{2x} \\ J_y = J_{1y} + J_{2y} \\ J_z = J_{1z} + J_{2z} \end{array}\right\}----(2)$$

And
$$\begin{aligned} J_t &= J_x + iJ_y \\ &= \left(J_{1x} + J_{2x}\right) + i\left(J_{1y} + J_{2y}\right) \\ &= \left(J_{1x} + iJ_{1y}\right) + \left(J_{2x} + iJ_{2y}\right) \\ \Rightarrow J_t &= J_{1t} + J_{2t} \end{aligned}$$

Now the question is whether $\vec{J}$ will be an angular momentum?

For this it should follow all the commutation relation for generalized angular momentum.

$$\begin{aligned} \left[J_x, J_y\right] &= \left[J_{1x} + J_{2x}, J_{1y} + J_{2y}\right] \\ &= \left[J_{1x}, J_{1y}\right] + \left[J_{1x}, J_{2y}\right] + \left[J_{2x}, J_{1y}\right] + \left[J_{2x}, J_{2y}\right] \\ &\qquad (\because \textit{ for different spaces}) \\ &= \left[J_{1x}, J_{1y}\right] + \left[J_{2x}, J_{2y}\right] \\ &= iJ_{1z} + iJ_{2z} = i\left[J_{1z} + iJ_{2z}\right] = iJ_z \end{aligned}$$

So, $\left[J_x, J_y\right] = iJ_z$

The other relations will also follow. So we can conclude that

$$\vec{J} \times \vec{J} = i\vec{J}$$

And this relation is sufficient to identify $\vec{J}$ as an angular momentum operator.

So the orthonormal Eigen function corresponding to this operator is:

$$| j_1, j_2, j, m\rangle \equiv | j, m\rangle$$

The meaning of this notation is that, the coupled $| j\, m\rangle$ should arise from two uncoupled Eigen function $| j_1\, m_1\rangle$ and $| j_2\, m_2\rangle$.

So,
$$J^2 | j\, m\rangle = j\left(j+1\right) | j_1\, j_2\, j\, m\rangle$$
$$J_z | j\, m\rangle = m | j_1\, j_2\, j\, m\rangle$$

Where, $j = 0, \frac{1}{2}, 1, \frac{3}{2}, ...$

and $m = j, j-1, j-2, ..., -j \quad \left(2J+1\right) values$

Now we have to setup the relationships between coupled Eigen function $| j\, m\rangle$ and uncoupled Eigen functions $| j_1\, m_1\rangle$ and $| j_2\, m_2\rangle$.

Similarly, coupled Eigen values j, m with uncoupled Eigen values j_1, j_2 and m_1, m_2.

Let us construct a product wavefunction,

$$| j_1\, j_2\, m_1\, m_2\rangle \equiv | j_1\, m_1\rangle | j_2\, m_2\rangle$$

As we know that, the products and their linear combinations are also the Eigen functions of J_1^2, J_{1z} and J_2^2, J_{2z}.

$$J_1^2 \,|\, j_1\, j_2\, m_1\, m_2\rangle = J_1^2 \,|\, j_1\, m_1\rangle \,|\, j_2\, m_2\rangle = j_1\left(j_1+1\right) |\, j_1\, m_1\rangle \,|\, j_2\, m_2\rangle = j_1\left(j_1+1\right) |\, j_1\, j_2\, m_1\, m_2\rangle$$
$$J_2^2 \,|\, j_1\, j_2\, m_1\, m_2\rangle = J_2^2 \,|\, j_2\, m_2\rangle \,|\, j_1\, m_1\rangle = j_2\left(j_2+1\right) |\, j_1\, m_1\rangle \,|\, j_2\, m_2\rangle = j_2\left(j_2+1\right) |\, j_1\, j_2\, m_1\, m_2\rangle$$
$$J_{1z} \,|\, j_1\, j_2\, m_1\, m_2\rangle = J_{1z} \,|\, j_1\, m_1\rangle \,|\, j_2\, m_2\rangle = m_1 \,|\, j_1\, m_1\rangle \,|\, j_2\, m_2\rangle = m_1 \,|\, j_1\, j_2\, m_1\, m_2\rangle$$
$$J_{2z} \,|\, j_1\, j_2\, m_1\, m_2\rangle = J_{2z} \,|\, j_2\, m_2\rangle \,|\, j_1\, m_1\rangle = m_2 \,|\, j_1\, m_1\rangle \,|\, j_2\, m_2\rangle = m_2 \,|\, j_1\, j_2\, m_1\, m_2\rangle$$

Now, let us apply J_z on the uncoupled Eigen functions:

$$\begin{aligned} J_z \,|\, j_1\, j_2\, m_1\, m_2\rangle &= \left(J_{1z} + J_{2z}\right) |\, j_1\, j_2\, m_1\, m_2\rangle \\ &= J_{1z} \,|\, j_1\, m_1\rangle \,|\, j_2\, m_2\rangle + J_{2z} \,|\, j_2\, m_2\rangle \,|\, j_1\, m_1\rangle \\ &= \left(m_1 + m_2\right) |\, j_1\, m_1\rangle \,|\, j_2\, m_2\rangle \\ &= m \,|\, j_1\, m_1\rangle \,|\, j_2\, m_2\rangle \end{aligned}$$

If $m = m_1 + m_2$, then $|\, j_1\, j_2\, m_1\, m_2\rangle$ is an Eigen function of J_z.

Since $\quad J^2 = \left(J_1 + J_2\right)^2 = J_1^2 + J_2^2 + 2J_1J_2$

$|\, j_1\, j_2\, m_1\, m_2\rangle$ will not be the Eigen function of J^2.

So, we have to find a common Eigen function of J^2 and J_z.

We construct a linear combination of the uncoupled Eigen function, such that

$$\underbrace{|\, j_1\; j_2\; j\, m\rangle}_{\substack{\text{Eigen function of} \\ J^2 \text{ and } J_z}} = \sum_{m_1, m_2} \underbrace{\langle j_1\; j_2\; m_1\, m_2 \,|\, j_1\; j_2\; j\, m\rangle}_{\substack{\text{Numeric value known as} \\ \text{Vector Addition Coefficients} \\ \text{or,} \\ \text{Clebsch-Gordon Coefficients}}} \underbrace{|\, j_1\; j_2\; m_1\, m_2\rangle}_{\substack{\text{Eigen function of} \\ J_1 \text{ and } J_2}}$$

We have to find out the relationships between the quantum numbers representing the coupled and uncoupled Eigen functions.

First applying J_z on both sides of the equation, we get:

$$m\,|\,j_1\;j_2\;j\,m\rangle = \sum_{m_1,m_2}\left(m_1+m_2\right)\langle j_1\;j_2\;m_1\,m_2\,|\,j_1\;j_2\;j\,m\rangle\,|\,j_1\;j_2\;m_1\,m_2\rangle$$

It suggests that the value of $\langle j_1\;j_2\;m_1\,m_2\,|\,j_1\;j_2\;j\,m\rangle = 0$ if $m \neq m_1+m_2$

We have to find the possible values of j

We know that

$$-j_1 \le m_1 \le j_1 \quad \text{and} \quad -j_2 \le m_2 \le j_2$$

Since $m = m_1 + m_2$

We have $-j_1 \le m - m_2 \le j_1$ and $-j_2 \le m - m_1 \le j_2$

Let m assume its maximum value j, m_1 its maximum value j_1

and m_2 its maximum value j_2 then

$$-j_1 \le j - j_2 \le j_1 \quad \text{and} \quad -j_2 \le j - j_1 \le j_2$$

So $j_2 - j_1 \le j \le j_1 + j_2$ and $j_1 - j_2 \le j \le j_1 + j_2$

Combining these two we get $\left|j_1 - j_2\right| \le j \le j_1 + j_2$

For example if, $j_1 = \frac{1}{2},\; m_1 = \frac{1}{2}, -\frac{1}{2}$ and $j_2 = 1,\; m_2 = 1, 0, -1$, then the possible values of

$j = \frac{1}{2}, m = +\frac{1}{2}, -\frac{1}{2}$ and $j = \frac{3}{2}, m = +\frac{3}{2}, +\frac{1}{2}, -\frac{1}{2}, -\frac{3}{2}$

because

$$\begin{aligned} m &= m_1 + m_2 \\ &= -\frac{1}{2} - 1 = -\frac{3}{2}, \quad = +\frac{1}{2} - 1 = -\frac{1}{2} \\ &= -\frac{1}{2} + 0 = -\frac{1}{2}, \quad = +\frac{1}{2} + 0 = +\frac{1}{2} \\ &= -\frac{1}{2} + 1 = +\frac{1}{2}, \quad = +\frac{1}{2} + 1 = +\frac{3}{2} \end{aligned}$$

It is also important to put the condition that $j_1 + j_2 + j = n$, where n is an integer.

This follows that

$$\left.\begin{array}{r} j_1 + j_2 - j \\ j_1 - j_2 + j \\ -j_1 + j_2 + j \end{array}\right\} \geq 0$$. This is known as triangular conditions.

Considering all these we have, $j = j_1 + j_2, j_1 + j_2 - 1, j_1 + j_2 - 2, \ldots\ldots\ldots, |j_1 - j_2|$

And $m = j, j-1, \ldots\ldots\ldots\ldots, -j$

Coupling of three angular momenta

Let take three angular momenta J_1, J_2 and J_3 such that $\vec{J} = \vec{J}_1 + \vec{J}_2 + \vec{J}_3$

There are three ways to couple these. As an example, $j_1 = \frac{1}{2}, j_2 = \frac{1}{2}, j_3 = 1$

Case -1,

First couple $j_1 = \frac{1}{2}$ and $j_2 = \frac{1}{2}$

This gives $j_1, j_2 \Rightarrow j_{12} = \begin{cases} \frac{1}{2}, \frac{1}{2} \Rightarrow 0 \\ \frac{1}{2}, \frac{1}{2} \Rightarrow 1 \end{cases}$

Now we couple j_{12} with $j_3 = 1$

This gives $j \Rightarrow j_1, j_2(j_{12}), j_3 \Rightarrow j_{12}, j_3 = \begin{cases} \left\{\frac{1}{2}, \frac{1}{2}\right\} \Rightarrow \{0\}, 1 \Rightarrow 1 \\ \left\{\frac{1}{2}, \frac{1}{2}\right\} \Rightarrow \{1\}, 1 \Rightarrow 0 \\ \left\{\frac{1}{2}, \frac{1}{2}\right\} \Rightarrow \{1\}, 1 \Rightarrow 1 \\ \left\{\frac{1}{2}, \frac{1}{2}\right\} \Rightarrow \{1\}, 1 \Rightarrow 2 \end{cases}$

Case-2

First couple $j_1 = \frac{1}{2}$ and $j_3 = 1$

This gives $j_1, j_3 \Rightarrow j_{13} = \begin{cases} \frac{1}{2}, 1 \Rightarrow \frac{1}{2} \\ \frac{1}{2}, 1 \Rightarrow \frac{3}{2} \end{cases}$

Now we couple j_{13} with $j_2 = \frac{1}{2}$

This gives $j \Rightarrow j_1, j_3 (j_{13}), j_2 \Rightarrow j_{13}, j_2 = \begin{cases} \left\{\frac{1}{2}, 1\right\} \Rightarrow \left\{\frac{1}{2}\right\}, \frac{1}{2} \Rightarrow 0 \\ \left\{\frac{1}{2}, 1\right\} \Rightarrow \left\{\frac{1}{2}\right\}, \frac{1}{2} \Rightarrow 1 \\ \left\{\frac{1}{2}, 1\right\} \Rightarrow \left\{\frac{3}{2}\right\}, \frac{1}{2} \Rightarrow 1 \\ \left\{\frac{1}{2}, 1\right\} \Rightarrow \left\{\frac{3}{2}\right\}, \frac{1}{2} \Rightarrow 2 \end{cases}$

Case -3

First couple $j_2 = \frac{1}{2}$ and $j_3 = 1$

This gives $j_2, j_3 \Rightarrow j_{23} = \begin{cases} \frac{1}{2}, 1 \Rightarrow \frac{1}{2} \\ \frac{1}{2}, 1 \Rightarrow \frac{3}{2} \end{cases}$

Now we couple j_{23} with $j_1 = \frac{1}{2}$

This gives $j \Rightarrow j_2, j_3(j_{23}), j_1 \Rightarrow j_{23}, j_1 = \begin{cases} \left\{\frac{1}{2},1\right\} \Rightarrow \left\{\frac{1}{2}\right\},\frac{1}{2} \Rightarrow 0 \\ \left\{\frac{1}{2},1\right\} \Rightarrow \left\{\frac{1}{2}\right\},\frac{1}{2} \Rightarrow 1 \\ \left\{\frac{1}{2},1\right\} \Rightarrow \left\{\frac{3}{2}\right\},\frac{1}{2} \Rightarrow 1 \\ \left\{\frac{1}{2},1\right\} \Rightarrow \left\{\frac{3}{2}\right\},\frac{1}{2} \Rightarrow 2 \end{cases}$

Note: When three angular momentum operators are coupled to form the total angular momentum, the possible values of the total angular momentum will be the same, independent of the method of coupling scheme. However, the coupled wavefunctions (discussed later) will depend on the coupling scheme.

Recap

In this lecture, we have learnt that the two angular momenta get coupled to form new angular momentum.

The reason for coupling of angular momentum is to form a new basis set that will be the eigenfunction of the total Hamiltonian.

In case of three angular momenta, the coupled angular momentum does not depend on the coupling scheme. However, the coupled wavefunction arising from the uncoupled state does depend on the coupling scheme.

We will understand this in the next lectures.