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Production of Courseware

 -Content for Post Graduate Courses

**Paper No. :** Quantum Mechanics-I

**Module :** Angular Momentum-II



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## 1. Learning Outcomes

After studying this module, you shall be able to

- Learn how to derive the matrix representation for the components,  $\hat{J}_x, \hat{J}_y, \hat{J}_z$  and  $\hat{J}^2$  of angular momentum J
- Know the representations of the eigen states as column vectors on which the angular momentum operators for each value of j can operate
- Learn the Pauli spin matrices and their important properties
- Know how to obtain the expressions for the eigen functions in terms of Spherical harmonics for the orbital angular momentum of a particle
- Learn the operation of Parity on Spherical harmonics

## 2. Introduction

The present module is in continuation of the preceding one, wherein starting from the commutation relations of angular momentum operators, we deduced the expressions for the eigen values of the diagonal operators  $\hat{J}^2$  and  $\hat{J}_z$  in the common basis represented by the state  $|jm\rangle$ , where j and m labelling respectively the eigen values of  $\hat{J}^2$  and of  $\hat{J}_z$ . In this module, we shall obtain the matrix representation for the components,  $\hat{J}_x, \hat{J}_y, \hat{J}_z$  and  $\hat{J}^2$  of the angular momentum operator  $\vec{J}$ . Considering a few specific values of the angular momentum, such as  $j=0, \frac{1}{2}$ , and 1, we shall write their matrix representations explicitly. It is remarkable to note that the eigen value spectrum includes not only the integral but also the half-integral values of j. As we already know half integral values of j describe the intrinsic spin of the particle, such as an electron or a proton. We describe the spin matrices for the spin  $\frac{1}{2}$  particles, first introduced by Pauli and briefly mention their important properties. Finally, we illustrate how to obtain the expressions for the eigen functions in terms of the spherical harmonics for the orbital angular momentum of a particle.

## 3. Angular Momentum (continued)

### 3.1 Matrix Representation of the Angular Momentum operator J in the $|jm\rangle$ Basis

The state vectors  $|jm\rangle$ , for  $m = -j$  to  $+j$  constitute the complete orthonormal basis for a  $(2j+1)$  – dimensional subspaces, providing the angular momentum representation in which any function of the angular momentum components will be represented by a matrix having elements  $\langle j'm'|\hat{A}|jm\rangle$ . The rows of the matrix will be labeled by various values of  $j'$  and  $m'$  and the columns by j and m. As we learnt from the preceding module, the basis states are the eigen states of  $\hat{J}^2$  and  $\hat{J}_z$  the matrices of these operators must be diagonal. In fact, just using the Eqs.(12.20a) and (12.40) from the previous module, we can write

$$\langle j'm' | \hat{J}^2 | jm \rangle = j(j+1)\hbar^2 \delta_{jj'} \delta_{mm'} \quad (13.1a)$$

$$\langle j'm' | \hat{J}_z | jm \rangle = m\hbar \delta_{jj'} \delta_{mm'} \quad (13.1b)$$

As far the operators  $\hat{J}_+$  and  $\hat{J}_-$ , taking the scalar product of  $|j'm'\rangle$  with Eqs.(12.32) and (12.33), we write the matrix elements as

$$\langle j'm' | \hat{J}_+ | jm \rangle = c_{jm}^+ \hbar \delta_{jj'} \delta_{m',m+1} \quad (13.2a)$$

$$\langle j'm' | \hat{J}_- | jm \rangle = c_{jm}^- \hbar \delta_{jj'} \delta_{m',m-1} \quad (13.2b)$$

The values of the constants  $c_{jm}^+$  and  $c_{jm}^-$  can be determined by equating the norms of the two sides in each of the Eqs.(12.32) and (12.33). Thus from Eq.(12.32) we get

$$\hat{J}_+ | jm \rangle = c_{jm}^+ \hbar | jm+1 \rangle$$

Note that the bra conjugate to  $\hat{J}_+ | j, m \rangle$  is  $\langle j, m | \hat{J}_-$ , since  $\hat{J}_+^\dagger = \hat{J}_-$ . The left hand side of Eq.(13.2a) can be evaluated by using Eq.(12.28), i.e.,

$$\langle jm | \hat{J}_- \hat{J}_+ | jm \rangle = \langle jm | \hat{J}^2 - \hat{J}_z^2 - \hbar \hat{J}_z | jm \rangle = [j(j+1) - m - m^2] \hbar^2 \quad (13.3)$$

We now equate the right hand sides of Eqs.(13.2a) and (13.3) to get

$$c_{jm}^+ = [(j-m)(j+m+1)]^{1/2} \quad (13.4)$$

In the same way, we can evaluate  $c_{jm}^-$ , using Eq.(13.2b). Here, since from Eq.(12.29)

$$\hat{J}_+ \hat{J}_- | jm \rangle = \hat{J}^2 - \hat{J}_z^2 + \hbar \hat{J}_z | jm \rangle, \text{ we shall find}$$

$$c_{jm}^- = [(j+m)(j-m+1)]^{1/2} \quad (13.5)$$

The matrix elements of  $\hat{J}_+$  and  $\hat{J}_-$  are thus determined completely. Using the relations, Eq.(12.24), one can then express

$$\hat{J}_x = \frac{1}{2}(\hat{J}_+ + \hat{J}_-) \quad \text{and} \quad \hat{J}_y = -\frac{1}{2}i(\hat{J}_+ - \hat{J}_-). \quad (13.6)$$

Let us now recapitulate the important results that we have arrived at:

$$\langle j'm' | \hat{J}^2 | jm \rangle = j(j+1)\hbar^2 \delta_{jj'} \delta_{mm'} \quad (13.1a)$$

$$\langle j'm' | \hat{J}_z | jm \rangle = m\hbar \delta_{jj'} \delta_{mm'} \quad (13.1b)$$

$$\langle j'm' | \hat{J}_+ | jm \rangle = [(j-m)(j+m+1)]^{1/2} \hbar \delta_{jj'} \delta_{m',m+1} \quad (13.7a)$$

$$\langle j'm' | \hat{J}_- | jm \rangle = [(j+m)(j-m+1)]^{1/2} \hbar \delta_{jj'} \delta_{m',m-1} \quad (13.7b)$$

From the above equations, the matrix elements for  $\hat{J}_x$  and  $\hat{J}_y$  are written as

$$\langle j'm'|\hat{J}_x|jm\rangle = \frac{1}{2}\hbar\delta_{jj'}\{[(j-m)(j+m+1)]^{1/2}\delta_{m',m+1} + [(j+m)(j-m+1)]^{1/2}\delta_{m',m-1}\}$$

$$\langle j'm'|\hat{J}_y|jm\rangle = \frac{1}{2i}\hbar\delta_{jj'}\{[(j-m)(j+m+1)]^{1/2}\delta_{m',m+1} - [(j+m)(j-m+1)]^{1/2}\delta_{m',m-1}\}$$

(13.8a, 13.8b)

From the above results, it is clear that the matrices representing the angular momentum operators  $\hat{J}_x, \hat{J}_y, \hat{J}_z, \hat{J}_+, \hat{J}_-,$  and  $\hat{J}^2$  are all diagonal in  $j$  in the basis  $|jm\rangle$ . Thus, for a given value of  $j$  ( $j=0, 1/2, 1, 3/2, 2, \dots$ ) we have an infinite number of representations for these matrices, having  $2j+1$  columns and rows labeled respectively by the values of  $m$  and  $m'$ . One can either consider all these representations together to form a single representation of infinite rank, or consider each of these representations of  $2j+1$  dimensions separately.

Here, for illustration, we just write the first three finite dimensional representations for  $j=0, 1/2, 1$  for the operators  $\hat{J}_x, \hat{J}_y, \hat{J}_z$  and  $\hat{J}^2$ . In writing the explicit matrices the convention is followed of placing the element for  $m'=j$  in the first row,  $m'=j-1$  in the second row etc., and  $m=j$  in the first column,  $m=j-1$  in the second column and so on,.

For the case,  $j=0$ , for which  $m=0$ , we have simply

$$\hat{J}_x = (0), \quad \hat{J}_y = (0), \quad \hat{J}_z = (0), \quad \hat{J}^2 = (0), \quad (13.6)$$

where  $(0)$  is the null matrix of unit rank.

For  $j=1/2$ , we have

$$\begin{aligned} (\hat{J}_x)_{m'=1/2, m=1/2} &= 0 = (\hat{J}_x)_{m'=-1/2, m=-1/2} \\ (\hat{J}_x)_{m'=1/2, m=-1/2} &= 1 = (\hat{J}_x)_{m'=-1/2, m=1/2} \end{aligned}$$

Similarly, the elements for the operators  $\hat{J}_y, \hat{J}_z$  and  $\hat{J}^2$  can also be written. In matrix forms, we have:

$$\begin{aligned} \langle 1/2, m'|\hat{J}_x|1/2, m\rangle &= \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, & \langle 1/2, m'|\hat{J}_y|1/2, m\rangle &= \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \\ \langle 1/2, m'|\hat{J}_z|1/2, m\rangle &= \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, & \langle 1/2, m'|\hat{J}^2|1/2, m\rangle &= \frac{3\hbar^2}{4} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \end{aligned} \quad (13.7)$$

For  $j=1$ , we have the possible values of  $m$  and  $m'=+1, 0, -1$ . As a result we have  $3 \times 3$  matrices.

$$\begin{aligned}
 \langle 1, m' | \hat{J}_x | 1, m \rangle &= \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, & \langle 1, m' | \hat{J}_y | 1, m \rangle &= \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} \\
 \langle 1, m' | \hat{J}_z | 1, m \rangle &= \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, & \langle 1, m' | \hat{J}^2 | 1, m \rangle &= 2\hbar^2 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}
 \end{aligned} \quad (13.8)$$

As to the question regarding the state vectors on which the above matrix representations of the components of angular momentum  $\hat{J}$  are to operate, we know that the representation of an arbitrary state  $|\psi\rangle$  with respect to the  $|jm\rangle$  basis would be a column vector whose elements are given by  $\langle jm|\psi\rangle$ . The dimensionality of the column vector would depend on the values that  $m$  can take for a given  $j$ . For example, for  $j=1/2$ ,  $m$  can take two values,  $+1/2$  and  $-1/2$ ; it has two elements labeled by  $m=+1/2$  and  $m=-1/2$ . The eigen vectors are given by :

$$|\alpha\rangle \equiv |j=1/2, m=+1/2\rangle \quad \text{and} \quad |\beta\rangle \equiv |j=1/2, m=-1/2\rangle.$$

In matrix notation, the eigen vectors are

$$\alpha \equiv \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix}, \quad \text{and} \quad \beta \equiv \begin{pmatrix} \beta_1 \\ \beta_2 \end{pmatrix} \quad (13.9)$$

Since these constitute an ortho-normal set and are also the eigen vectors of the operator  $\hat{J}_z$ , the simplest representation satisfying these conditions would be

$$\alpha \equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \text{and} \quad \beta \equiv \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad (13.10)$$

In a similar way, for  $j=1$ ,  $m$  can take the values  $+1$ ,  $0$ ,  $-1$ , we would have three independent elements. The eigen vectors are given by:

$$|\alpha\rangle = |j=1; m=1\rangle \quad |\beta\rangle = |j=1; m=0\rangle \quad |\gamma\rangle = |j=1; m=-1\rangle \quad (13.11)$$

There will be, in general, three column vectors each of three elements. The simplest representation constituting an orthonormal set of eigen vectors are:

$$\alpha \equiv \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad \beta \equiv \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad \gamma \equiv \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \quad (13.12)$$

### 3.2 Pauli Spin Matrices

You all know that electrons, neutrons and protons, the building blocks of atomic and nuclear physics have intrinsic spin  $1/2$ . The non-relativistic theory of spin  $1/2$  particles was first developed by W. Pauli in 1927. Denoting the spin vector by  $\vec{s}$  which is written as

$$\vec{s} = \frac{\hbar}{2} \vec{\sigma} \quad (13.13)$$

where the vector  $\vec{\sigma}$  has the components  $\sigma_x, \sigma_y, \sigma_z$ , called Pauli spin matrices, are defined as

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (13.14)$$

Compare these matrices with those given for  $j=1/2$  in Eq.(13.7). Following properties of the Pauli spin matrices can be easily verified:

$$[\sigma_i, \sigma_j] = 2i\varepsilon_{ijk}\sigma_k, \quad (13.15a)$$

$$\{\sigma_i, \sigma_j\} = 2\delta_{ij}, \quad (13.15b)$$

$$\sigma_i\sigma_j = \delta_{ij} + i\varepsilon_{ijk}\sigma_k, \quad (13.15c)$$

$$\text{Tr}(\sigma_k) = 0, \text{ and } \det(\sigma_k) = -1 \quad (13.15d, 13.15e)$$

Note that while writing the above relations, we have replaced the x, y, z components of  $\sigma$  by 1,2,3 respectively, denoted by, the indices i, j, or k, each taking the values 1,2,3.

The two basic spin= $1/2$  eigen states  $\alpha$  and  $\beta$ , given by (13.10) correspond to the spin up ( $\uparrow$ ) and spin down ( $\downarrow$ ) states respectively. They satisfy the ortho-normality relations:

$$\langle \alpha | \alpha \rangle = \langle \beta | \beta \rangle = 1; \quad \langle \alpha | \beta \rangle = \langle \beta | \alpha \rangle = 0 \quad (13.16a), (13.16b)$$

### 3.3 Orbital Angular Momentum

It should be emphasized that the commutation relations we have employed are independent of whether J is orbital angular momentum or spin angular momentum or is a sum of both; or whether it is the angular momentum of a single particle or of a system of many particles. If the angular momentum J represents the orbital angular momentum, generally denoted by L, there exists a coordinate representation for the eigen functions. The eigen states are then represented by  $|lm\rangle$ , so that

$$\hat{L}^2 |lm\rangle = \hbar^2 l(l+1) |lm\rangle \quad (13.17a)$$

and

$$\hat{L}_z |lm\rangle = \hbar m |lm\rangle \quad (13.17b)$$

Following the discussion from the preceding module, the coordinate space wave function for a single particle of position vector  $\vec{r}(\theta, \phi)$  may be denoted by  $\langle \theta\phi | lm \rangle$ . In terms of spherical polar co-

ordinates, the components,  $\hat{L}_x, \hat{L}_y$  and  $\hat{L}_z$  are represented by

$$\hat{L}_x = i\hbar \left[ \sin\phi \frac{\partial}{\partial\theta} + \cot\theta \cos\phi \frac{\partial}{\partial\phi} \right], \quad (13.18a)$$

$$\hat{L}_y = i\hbar \left[ -\cos\phi \frac{\partial}{\partial\theta} + \cot\theta \sin\phi \frac{\partial}{\partial\phi} \right], \quad (13.18b)$$

$$\hat{L}_z = -i\hbar \frac{\partial}{\partial\phi}, \quad (13.18c)$$

and



$$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$$

$$= -\hbar^2 \left[ \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] \quad (13.19)$$

You must have already studied that the expression on the right hand side of Eq.(13.19) represents second order differential equation satisfied by

$$\left\{ \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right\} Y_{lm}(\theta, \phi) = -l(l+1) Y_{lm}(\theta, \phi) \quad (13.20)$$

The eigen functions,  $Y_{lm}(\theta, \phi)$ , common to the operators  $\hat{L}^2$  and  $\hat{L}_z$  (see Eq.(13.17a) and (13.17b)) and normalized to unity on the unit sphere are the spherical harmonics, satisfying the orthonormality relations

$$\int Y_{l'm'}^*(\theta, \phi) Y_{lm}(\theta, \phi) d\Omega = \delta_{ll'} \delta_{mm'} \quad (13.21)$$

The standard expression for the spherical harmonics for non-negative values of m are given by

$$Y_{lm}(\theta, \phi) = (-1)^m \left[ \frac{(2l+1)(l-m)!}{4\pi(l+m)!} \right]^{1/2} P_l^m(\cos\theta) \exp(im\phi) \quad (13.22)$$

Recall that the quantum number l can only take the integral values l=0,1,2,... and also for a fixed value of l, the allowed values of m are m=-l, -l+1, ... , l-1, l. For negative values of m, we use the relation

$$Y_{l,m}^*(\theta, \phi) = (-1)^m Y_{l,-m}(\theta, \phi)$$

$$= (-1)^m Y_{l,m}(-\theta, -\phi) \quad (13.23)$$

### 3.3.1 Parity Operation on Spherical harmonics:

The behavior of the spherical harmonics under parity operation, i.e.,  $\vec{r} \rightarrow -\vec{r}$  or in terms of spherical coordinates,  $r \rightarrow r, \theta \rightarrow \pi - \theta$  and  $\phi \rightarrow \phi + \pi$  is of special interest. If  $\hat{P}$  represents the parity operator, then under parity operation

$$\hat{P} Y_{lm}(\theta, \phi) = Y_{l,m}(\pi - \theta, \pi + \phi)$$

Now

$$\exp[im(\pi + \phi)] = \exp(im\pi) \exp(im\phi) = (-1)^m \exp(im\phi)$$

$$\text{and } P_l^m\{\cos(\pi - \theta)\} = P_l^m(-\cos\theta)$$

$$= (-1)^{l+m} P_l^m(\cos\theta)$$

Using these relations, one finds that

$$\hat{P} Y_{lm}(\theta, \phi) = (-1)^{l+m} Y_{l,m}(\theta, \phi) \quad (13.24)$$

It is thus clear that spherical harmonics,  $Y_{lm}(\theta, \phi)$ , have even parity for even  $l$  and odd for odd values of  $l$ . You will find this property to be quite useful in your further studies involving spherical harmonics.

#### 4. Summary

In this module, you have learnt to

- Derive the matrix representation for the components,  $\hat{J}_x, \hat{J}_y, \hat{J}_z$  and  $\hat{J}^2$  of angular momentum  $J$
- Know the representations of the eigen states as column vectors on which the angular momentum operators for each value of  $j$  can operate
  
- Know the Pauli spin matrices and their important properties
- Know how to obtain the expressions for the eigen functions in terms of Spherical harmonics for the orbital angular momentum of a particle
- Know the operation of Parity on Spherical harmonics