1.3 Angular Momentum of a One –Particle System

It is found previously that the eigenfunction and eigenvalues for the linear –momentum operator $\hat{p}_x$. In this section we consider the same problem for the angular momentum of a particle. Angular momentum is important in the quantum mechanics of atomic structure. Now we will discuss the classical mechanics of angular momentum.

Classical Mechanics of One -Particle Angular Momentum: Consider a moving particle of mass m. It is necessary to set up a Cartesian coordinate system that is fixed in space. Let **r** be the vector from the origin to the instantaneous position of the particle. We have

$$\mathbf{r} = \mathbf{i}x + \mathbf{j}y + \mathbf{k}z \qquad \text{..................................(32)}$$

where x, y and z are the particle's coordinates at a given instant. These coordinates are function of time, and defining the velocity vector **v** as the time derivation of the position vector (**section 1.2**)

$$v \equiv \frac{dr}{dt} = i\frac{dx}{dt} + j\frac{dy}{dt} + k\frac{dz}{dt} \qquad \text{.................................. (33)}$$

$v_x = dx/dt, \quad v_y = dy/dt, \quad v_z = dz/dt$

We defined the particle's **linear momentum** vector **p** by

$$p \equiv mv \qquad \text{........................... (34)}$$

$$p_x = mv_x,\ p_y = mv_y,\ m_z = mv_z \qquad \text{.................................(35)}$$

The particle's **angular momentum L** with respect to the coordinate origin is defined in classical mechanics as

$$\mathbf{L} \equiv \mathbf{r} \times \mathbf{p} \qquad \text{....................... .... (36)}$$

$$\mathbf{L} = \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix} \qquad \text{.................................... (37)}$$

$$L_x = yp_z - zp_y,\ L_y = zp_x - xp_z,\ L_z = xp_y - yp_x \qquad \text{.................................. (38)}$$

where (Eq.28) was used. L_x, L_y and L_z are the components of **L** along the x, y and z axes. The angular- momentum vector **L** is perpendicular to the plane defined by the particle's position vector r and its velocity v (**figure 5**)

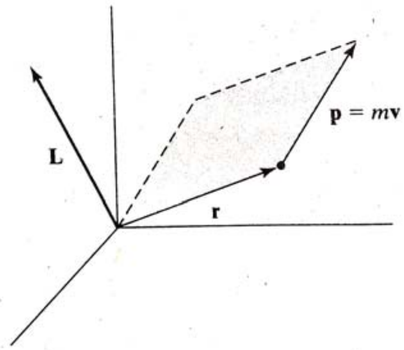

Figure 5: L= rX p

The torque **τ** acting on a particle is defined as the cross product of **r** and the force **F** acting on the particle : **τ ≡ r x F.** It is readily shown that **τ=dL/dt .**When there is no torque acting on the particle, the rate of change of its angular momentum is zero; that is its angular momentum is constant (or conserved). For a planet orbiting the sun, the gravitational force is radially directed. Since the cross product of two parallel vectors is zero, there is no torque on the planet and its angular momentum is conserved.

One –Particle Orbital –Angular Momentum Operator (Quantum Mechanical Treatment):

In quantum mechanics, there are two kinds of angular momenta : **Orbital angular momentum** results from the motion of a particle through space , and is the analog of the classical –mechanical quantity **L** ; **spin angular momentum** is an intrinsic property of many microscopic particles and has no classical –mechanical analog. We are now considering only orbital angular momentum.

$$\hat{L}_x = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right) \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (39)$$

$$\hat{L}_y = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right) \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (40)$$

$$\hat{L}_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (41)$$

(Since $\hat{y}\hat{p}_z = \hat{p}_z\hat{y}$, and so on , we do not run into any problem of noncommutativity in constructing these operators) Using

$$\hat{L}^2 = |\hat{L}|^2 = \hat{L}.\hat{L} = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2 \qquad \text{……………………… (42)}$$

The operator are constructed for the square of the angular –momentum magnitude from the operators in (Eqn.39 – Eqn.41).

Since the commutation relations determine which physical quantities can be simultaneously assigned definite values, we investigate these relations for angular momentum. Operating on some function f(x, y, z) with $\hat{L}_y$, we have

$$\hat{L}_y f = -i\hbar\left(z\frac{\partial f}{\partial x} - x\frac{\partial f}{\partial z}\right)$$

Opearting on this last equation with L_x, we get

$$\hat{L}_x\hat{L}_y f = -\hbar^2\left(y\frac{\partial f}{\partial x} + yz\frac{\partial^2 f}{\partial z\,\partial x} - yx\frac{\partial^2 f}{\partial z^2} - z^2\frac{\partial^2 f}{\partial y\,\partial x} + zx\frac{\partial^2 f}{\partial y\,\partial z}\right) \qquad \text{................(43)}$$

Similarly ,

$$\hat{L}_x f = -i\hbar\left(y\frac{\partial f}{\partial z} - z\frac{\partial f}{\partial y}\right)$$

$$\hat{L}_y\hat{L}_x f = -\hbar^2\left(zy\frac{\partial^2 f}{\partial x\,\partial z} - z^2\frac{\partial^2 f}{\partial x\,\partial y} - xy\frac{\partial^2 f}{\partial z^2} + x\frac{\partial f}{\partial y} + xz\frac{\partial^2 f}{\partial z\,\partial y}\right) \qquad \text{……………….(44)}$$

Subtracting (44) from (43) , we have

$$\hat{L}_x\hat{L}_y f - \hat{L}_y\hat{L}_x f = -\hbar^2\left(y\frac{\partial f}{\partial x} - x\frac{\partial f}{\partial y}\right)$$

$$[\hat{L}_x, \hat{L}_y] = i\hbar\hat{L}_z \qquad \text{…………………………… (45)}$$

Where we used relations such as

$$\frac{\partial^2 f}{\partial z\,\partial x} = \frac{\partial^2 f}{\partial x\,\partial z} \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (46)$$

Which are true for well- behaved functions. We could use the same procedure to find $[\hat{L}_y, \hat{L}_z]$ and $[\hat{L}_z, \hat{L}_x]$, but we can save time by noting a certain kind of symmetry in (eq. 39 to Eqn.41). By a cyclic permutation of x, y and z, we mean replacing x by y, replacing y by z, and replacing z by x. If we carry out a cycle permutation in $\hat{L}_x$, we get $\hat{L}_y$; a cyclic permutation in $\hat{L}_y$ gives $\hat{L}_z$; $\hat{L}_z$ is transformed into $\hat{L}_x$ by cyclic permutation. Hence, by carrying out two successive cyclic permutation on (Eq. 45), we get

$$[\hat{L}_y, \hat{L}_z] = i\hbar\hat{L}_x \; , \; [\hat{L}_z, \hat{L}_x] = i\hbar\hat{L}_y \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (47)$$

Now we evaluate the commutators of $\hat{L}^2$ with each of its components, using commutator identities of section 1.1.

$$\begin{aligned}
[\hat{L}^2, \hat{L}_x] &= [\hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2, \hat{L}_x] \\
&= [\hat{L}_x^2, \hat{L}_x] + [\hat{L}_y^2, \hat{L}_x] + [\hat{L}_z^2, \hat{L}_x] \\
&= [\hat{L}_y^2, \hat{L}_x] + [\hat{L}_z^2, \hat{L}_x] \\
&= [\hat{L}_y, \hat{L}_x]\hat{L}_y + \hat{L}_y[\hat{L}_y, \hat{L}_x] + [\hat{L}_z, \hat{L}_x]\hat{L}_z + \hat{L}_z[\hat{L}_z, \hat{L}_x] \\
&= -i\hbar\hat{L}_z\hat{L}_y - i\hbar\hat{L}_y\hat{L}_z + i\hbar\hat{L}_y\hat{L}_z + i\hbar\hat{L}_z\hat{L}_y \\
[\hat{L}^2, \hat{L}_x] &= 0
\end{aligned}$$

$$\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (48)$$

Since a cyclic permutation of x,y and z leaves $\hat{L}^2 = \hat{L}^2_x + \hat{L}^2_y + \hat{L}^2_z$ unchanged, if we carry out two such permutation on (Eq. 48), we get

$$[\hat{L}^2, \hat{L}_y] = 0 \, , \qquad [\hat{L}^2, \hat{L}_z] = 0 \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (49)$$

To which of the quantities $\hat{L}^2, \hat{L}_x, \hat{L}_y, \hat{L}_z$ can we assign definite values simultaneously ? Because $\hat{L}^2$ commutes with each of its components, we can specify an exact value for $\hat{L}^2$ and any one component. However, no two components of $\hat{L}$ commute with each other, so we cannot specify more than one component simultaneously. It is traditional to take $\hat{L}_z$ as the component of angular momentum that will be specified along with $\hat{L}^2$. Note that in specifying $L^2 = |\mathbf{L}|^2$ we are not specifying the vector **L,** only its magnitude. A complete specification of **L** requires simultaneous specification of each of its three components, which we usually cannot do. In classical mechanics when angular momentum is conserved, only its magnitude and one of its components are possible.

We could now try to find the eigenvalues and common eigenfunctions of $\hat{L}^2$ and $\hat{L}_z$ by using the forms for these operators in Cartesian Coordinates. However, we would find that the partial differential equations obtained would not be separable. For this reason we carry out a transformation to **spherical coordinates** (Figure 6).

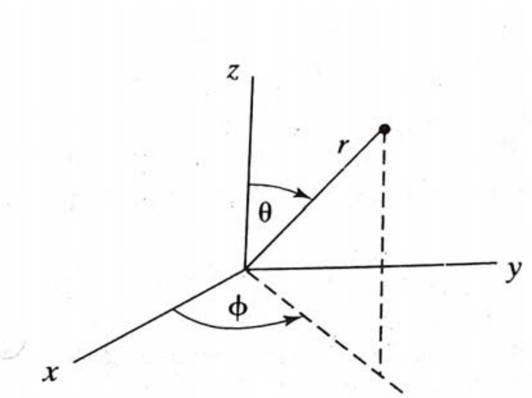

Figure 6: Spherical Coerdinates

The coordinate r is the distance from the origin to point (x,y,z). The angle θ is the angle the vector **r** makes with the positive z axis. The angle that the projection of **r** in the xy plane makes with the positive x axis is φ.

A little trigonometry gives

$$x = r\sin\theta\cos\phi\,, \qquad y = r\sin\theta\sin\phi\,, \qquad z = r\cos\theta \qquad \text{….. (50)}$$

$$r^2 = x^2 + y^2 + z^2. \qquad \cos\theta = \frac{z}{(x^2+y^2+z^2)^{1/2}}, \qquad \tan\phi = y/x \qquad \text{…………..(51)}$$

To transform the angular-momentum operators to spherical coordinates, we must transform ∂/∂x, ∂/∂y and ∂/∂z into these coordinates.

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To perform this transformation, we use the chain rule. Suppose we have a function of r,θ, and φ: f(r,θ, φ). If we change the independent variables by substituting

r= r(x,y,z) , θ= θ(x,y,z) ,φ=φ (x,y,z)

into f, we transform it into a function of x,y and z:

f[r(x,y,z) ,θ(x,y,z) ,φ (x,y,z)]=g(x,y,z)

The chain rule tells us how the partial derivative of g(x,y,z) are related to those of f(r,θ, φ). In fact,

$$\left(\frac{\partial g}{\partial x}\right)_{y,z} = \left(\frac{\partial f}{\partial r}\right)_{\theta,\phi}\left(\frac{\partial r}{\partial x}\right)_{y,z} + \left(\frac{\partial f}{\partial \theta}\right)_{r,\phi}\left(\frac{\partial \theta}{\partial x}\right)_{y,z} + \left(\frac{\partial f}{\partial \phi}\right)_{r,\theta}\left(\frac{\partial \phi}{\partial x}\right)_{y,z} \quad \text{............ (52)}$$

$$\left(\frac{\partial g}{\partial y}\right)_{x,z} = \left(\frac{\partial f}{\partial r}\right)_{\theta,\phi}\left(\frac{\partial r}{\partial y}\right)_{x,z} + \left(\frac{\partial f}{\partial \theta}\right)_{r,\phi}\left(\frac{\partial \theta}{\partial y}\right)_{x,z} + \left(\frac{\partial f}{\partial \phi}\right)_{r,\theta}\left(\frac{\partial \phi}{\partial y}\right)_{x,z} \quad \text{.....................(53)}$$

$$\left(\frac{\partial g}{\partial z}\right)_{x,y} = \left(\frac{\partial f}{\partial r}\right)_{\theta,\phi}\left(\frac{\partial r}{\partial z}\right)_{x,y} + \left(\frac{\partial f}{\partial \theta}\right)_{r,\phi}\left(\frac{\partial \theta}{\partial z}\right)_{x,y} + \left(\frac{\partial f}{\partial \phi}\right)_{r,\theta}\left(\frac{\partial \phi}{\partial z}\right)_{x,y} \quad \text{..................... (54)}$$

To convert these equation to operator equations, we delete f and g to give

$$\frac{\partial}{\partial x} = \left(\frac{\partial r}{\partial x}\right)_{y,z}\frac{\partial}{\partial r} + \left(\frac{\partial \theta}{\partial x}\right)_{y,z}\frac{\partial}{\partial \theta} + \left(\frac{\partial \phi}{\partial x}\right)_{y,z}\frac{\partial}{\partial \phi} \quad \text{.............................(55)}$$

With similar equations for ∂/∂y and ∂/∂z. The task now to evaluate the partial derivatives such as $(\partial r/\partial x)_{y,z}$. Taking the partial derivative of the first equation in (Eq.51) with respect to x at constant y and z, we have

$$2r\left(\frac{\partial r}{\partial x}\right)_{y,z} = 2x = 2r\sin\theta\cos\phi$$

$$\left(\frac{\partial r}{\partial x}\right)_{y,z} = \sin\theta\cos\phi \quad \text{...................................(56)}$$

Differentiating $r^2 = x^2 + y^2 + z^2$ with respect to y and with respect to z, we find

$$\left(\frac{\partial r}{\partial y}\right)_{x,z} = \sin\theta \sin\phi, \quad \left(\frac{\partial r}{\partial z}\right)_{x,y} = \cos\theta \qquad \text{.....................(57)}$$

From the second equation in (51), we find

$$-\sin\theta\left(\frac{\partial \theta}{\partial x}\right)_{y,z} = -\frac{xz}{r^3}$$

$$\left(\frac{\partial \theta}{\partial x}\right)_{y,z} = \frac{\cos\theta\cos\phi}{r} \qquad (58)$$

Also,

$$\left(\frac{\partial \theta}{\partial y}\right)_{x,z} = \frac{\cos\theta\sin\phi}{r}, \quad \left(\frac{\partial \theta}{\partial z}\right)_{x,y} = -\frac{\sin\theta}{r} \qquad (59)$$

From $\tan\phi = y/x$, we find

$$\left(\frac{\partial \phi}{\partial x}\right)_{y,z} = -\frac{\sin\phi}{r\sin\theta}, \quad \left(\frac{\partial \phi}{\partial y}\right)_{x,z} = \frac{\cos\phi}{r\sin\theta}, \quad \left(\frac{\partial \phi}{\partial z}\right)_{x,y} = 0 \qquad (60)$$

Substituting (56), (58), and (60) into (55), we find

$$\frac{\partial}{\partial x} = \sin\theta\cos\phi\frac{\partial}{\partial r} + \frac{\cos\theta\cos\phi}{r}\frac{\partial}{\partial \theta} - \frac{\sin\phi}{r\sin\theta}\frac{\partial}{\partial \phi} \qquad (61)$$

Similarly,

$$\frac{\partial}{\partial y} = \sin\theta\sin\phi\frac{\partial}{\partial r} + \frac{\cos\theta\sin\phi}{r}\frac{\partial}{\partial \theta} + \frac{\cos\phi}{r\sin\theta}\frac{\partial}{\partial \phi} \qquad (62)$$

$$\frac{\partial}{\partial z} = \cos\theta\frac{\partial}{\partial r} - \frac{\sin\theta}{r}\frac{\partial}{\partial \theta} \qquad (63)$$

At last we are ready to express the angular –momentum components in spherical coordinates

Substituting (Eq.50), (Eq.62), and (Eq.63) into (Eq.39), we have

$$\hat{L}_x = -i\hbar\left[r\sin\theta\sin\phi\left(\cos\theta\frac{\partial}{\partial r} - \frac{\sin\theta}{r}\frac{\partial}{\partial \theta}\right) - r\cos\theta\left(\sin\theta\sin\phi\frac{\partial}{\partial r} + \frac{\cos\theta\sin\phi}{r}\frac{\partial}{\partial \theta} + \frac{\cos\phi}{r\sin\theta}\frac{\partial}{\partial \phi}\right)\right]$$

$$\hat{L}_x = i\hbar\left(\sin\phi\frac{\partial}{\partial \theta} + \cot\theta\cos\phi\frac{\partial}{\partial \phi}\right) \qquad \text{.........(64)}$$

Also , we find

$$\hat{L}_y = -i\hbar\left(\cos\phi\frac{\partial}{\partial\theta} - \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right) \quad \text{............ (65)}$$

$$\hat{L}_z = -i\hbar\frac{\partial}{\partial\phi} \quad \text{............................ (66)}$$

By squaring each of $\hat{L}_x$, $\hat{L}_y$, and $\hat{L}_z$ and then adding their squares, we can construct $\hat{L}^2$ (Eqn.42). The result is

$$\hat{L}^2 = -\hbar^2\left(\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right) \quad \text{............ (67)}$$

Although the angular –momentum operators depend on all three Cartesian coordinates , x,y and z, they involve only the two spherical coordinates θ and φ.