ANGULAR MOMENTUM of a ONE-PARTICLE SYSTEM

Why the angular momentum? It gives information about the rotational motion of a particle around a center (electron around the nucleus or a molecule around its own center of mass). For atoms, the angular momentum can be obtained by measuring the magnetic moment, which is proportional to the angular momentum. So, if we are able to predict the angular momentum then we can also predict the magnetic moment, which can eventually be compared with experiments

Moreover, the solutions of the eigenvalue problems related to the angular momentum are employed to find the wavefunctions of the hydrogen atom

ANGULAR MOMENTUM of a ONE-PARTICLE SYSTEM

In QM, there are two kinds of angular momentum:

Orbital angular momentum results from the motion of a particle through the space, and is the analog of the classical-mechanical quantity $\mathbf{L}$

Spin angular momentum is an intrinsic property of many microscopic particles and has no classical-mechanical analog (we will see later).

We are considering only the orbital angular momentum

ANGULAR MOMENTUM of a ONE-PARTICLE SYSTEM

The aim is to find the possible outcomes of a measurement of the angular momentum of a particle

Consider a moving particle of mass m. We set up a Cartesian coordinate system that is fixed in space. Let $\mathbf{r}$ be the vector from the origin to the instantaneous position of the particle

$$\mathbf{r} = x\,\mathbf{i} + y\,\mathbf{j} + z\,\mathbf{k} \qquad (1)$$

where x, y, and z are the particle's coordinates at a given instant. These coordinates are functions of time. Hence, we can define the velocity vector $\mathbf{v}$, which corresponds to the time derivative of the position vector

$$\mathbf{v} = \frac{d\mathbf{r}}{dt} = \frac{dx}{dt}\mathbf{i} + \frac{dy}{dt}\mathbf{j} + \frac{dz}{dt}\mathbf{k} = v_x\mathbf{i} + v_y\mathbf{j} + v_z\mathbf{k} \qquad (2)$$

ANGULAR MOMENTUM of a ONE-PARTICLE SYSTEM

The particle's linear momentum vector $\mathbf{p}$ is

$$\mathbf{p} = m\mathbf{v} = p_x\mathbf{i} + p_y\mathbf{j} + p_z\mathbf{k} \quad (3)$$

The particle's **angular momentum** $\mathbf{L}$ with respect to the origin is defined in classical mechanics as

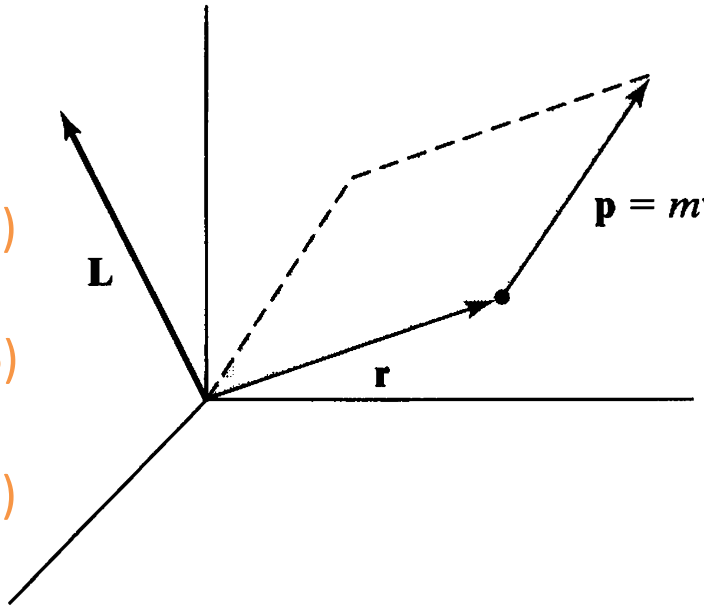
$$\boxed{\mathbf{L} = \mathbf{r} \times \mathbf{p}} \quad (4)$$

Cartesian components of $\mathbf{L}$

$$L_x = y\,p_z - z\,p_y \quad (5)$$

$$L_y = z\,p_x - x\,p_z \quad (6)$$

$$L_z = x\,p_y - y\,p_x \quad (7)$$



ANGULAR MOMENTUM of a ONE-PARTICLE SYSTEM

First step. We get the QM operators for the components of orbital angular momentum of a particle by replacing the coordinates and momenta in the classical equations by their corresponding operators

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

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

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

ANGULAR MOMENTUM of a ONE-PARTICLE SYSTEM

Since the **commutation relations** determine which physical quantities can be simultaneously measured with arbitrary precision (Heisenberg uncertainty principle), we investigate these relations for angular momentum

HEISENBERG UNCERTAINTY PRINCIPLE

$$\sigma_A \sigma_B \geq \frac{1}{2}\left| \int \Psi^* [\hat{A}, \hat{B}] \Psi \, d\tau \right|$$

If 2 operators commutate, then it is possible to measure the corresponding physical quantities simultaneously. Otherwise we cannot do it (only 1 quantity can be measured at a given time)

ANGULAR MOMENTUM COMMUTATION RULES

$$[\hat{L}_x, \hat{L}_y] = i\hbar \hat{L}_z \qquad [\hat{L}_z, \hat{L}_x] = i\hbar \hat{L}_y \qquad [\hat{L}_y, \hat{L}_z] = i\hbar \hat{L}_x$$

ANGULAR MOMENTUM of a ONE-PARTICLE SYSTEM

Since $\mathbf{L}$ is a vector quantity, we cannot determine how it commutates with the single components L_x, L_y and L_z. However $|\mathbf{L}|^2$ is a scalar and we can do that

$$|\mathbf{L}|^2 = \mathbf{L} \cdot \mathbf{L} = L_x^2 + L_y^2 + L_z^2$$

We can transform the quantity $|\mathbf{L}|^2$ in the QM operator exploiting the operators related to the components L_x, L_y and L_z

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

We obtain $\left[\hat{L}^2, \hat{L}_x\right] = 0 \qquad \left[\hat{L}^2, \hat{L}_y\right] = 0 \qquad \left[\hat{L}^2, \hat{L}_z\right] = 0$

We can do a simultaneous measure of $|\mathbf{L}|^2$ and one component of it

ANGULAR MOMENTUM of a ONE-PARTICLE SYSTEM

To which of the quantities L^2, L_x, L_y, 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 L^2 and any one component. However, no two components of $\mathbf{L}$ commute with each other, so we cannot specify more than one component simultaneously

To find L^2 or one component, say L_z, we must find the eigenvalues of $\hat{L}^2$ and $\hat{L}_z$

$$\hat{L}^2 F = b\ F$$

$$\hat{L}_z G = c\ G$$

b and c are the eigenvalues (results of a measure)

It is traditional **to take L_z as the component of angular momentum that will be specified along with L^2**. Note that in specifying L^2 we are not specifying the vector $\mathbf{L}$, only its magnitude

ANGULAR MOMENTUM of a ONE-PARTICLE SYSTEM

In order to deal with partial differential equations separable, we carry out a transformation to **spherical polar coordinates**

$$0 \le r \le \infty \qquad 0 \le \theta \le \pi \qquad 0 \le \phi \le 2\pi$$

$$x = r\sin\theta\cos\phi$$

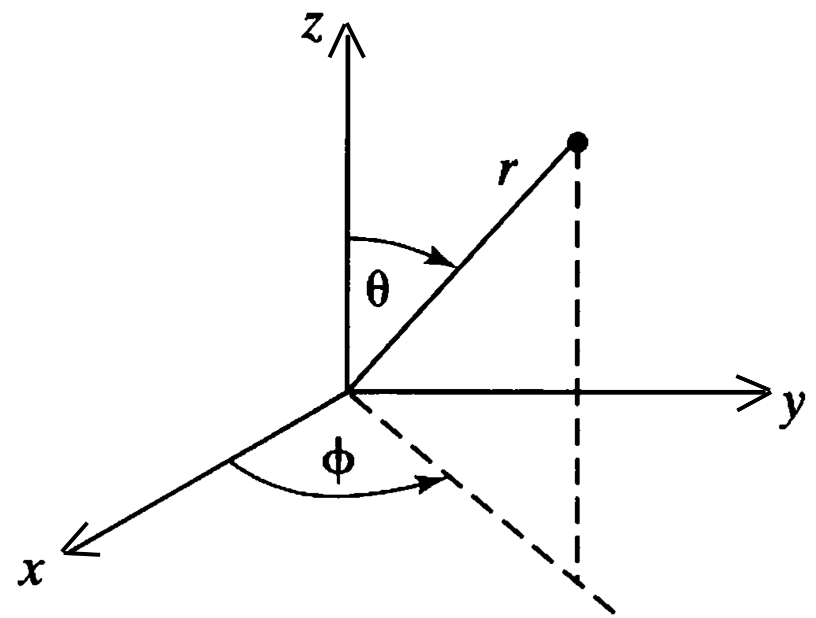
$$y = r\sin\theta\sin\phi$$

$$z = r\cos\theta$$

$$r^2 = x^2 + y^2 + z^2$$

$$\cos\theta = \frac{z}{(x^2 + y^2 + z^2)^{1/2}}$$

$$\tan\phi = \frac{y}{x}$$



Spherical coordinates

ANGULAR MOMENTUM of a ONE-PARTICLE SYSTEM

To transform the angular-momentum operators to spherical coordinates, we must transform $\partial/\partial x$, $\partial/\partial y$, and $\partial/\partial z$ into these coordinates. To perform this transformation, we use the **chain rule**

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

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

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

ANGULAR MOMENTUM of a ONE-PARTICLE SYSTEM

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

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

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

ANGULAR MOMENTUM of a ONE-PARTICLE SYSTEM

After substitutions, we obtain

$$\frac{\partial}{\partial x} = \sin\theta\cos\phi\frac{\partial}{\partial r} + \frac{\cos\theta\cos\phi}{r}\frac{\partial}{\partial\theta} - \frac{\sin\phi}{r\sin\theta}\frac{\partial}{\partial\phi}$$

$$\frac{\partial}{\partial y} = \sin\theta\sin\phi\frac{\partial}{\partial r} + \frac{\cos\theta\sin\phi}{r}\frac{\partial}{\partial\theta} + \frac{\cos\phi}{r\sin\theta}\frac{\partial}{\partial\phi}$$

$$\frac{\partial}{\partial z} = \cos\theta\frac{\partial}{\partial r} - \frac{\sin\theta}{r}\frac{\partial}{\partial\theta}$$

ANGULAR MOMENTUM of a ONE-PARTICLE SYSTEM

Using the previous results for the partial derivatives into the expressions of the angular momentum operators, we have

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

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

$$\hat{L}_z = -i\hbar\frac{\partial}{\partial\phi}$$

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

ANGULAR MOMENTUM of a ONE-PARTICLE SYSTEM

We now find the common eigenfunctions of $\hat{L}^2$ and $\hat{L}_z$ which we denote by Y (this is possible because the operators commutate; we have seen a theorem about). Since these operators involve only θ and ϕ, Y is a function of these two coordinates: $Y = Y(\theta, \phi)$. (Of course, since the operators are linear, we can multiply Y by an arbitrary function of r and still have an eigenfunction of $\hat{L}^2$ and $\hat{L}_z$). We must solve

$$\hat{L}_z Y(\theta, \phi) = b\, Y(\theta, \phi)$$

$$\hat{L}^2 Y(\theta, \phi) = c\, Y(\theta, \phi)$$

where b and c are the eigenvalues of the two operators

ANGULAR MOMENTUM of a ONE-PARTICLE SYSTEM

We now see $\hat{L}_z$

$$-i\hbar \frac{\partial}{\partial\phi} Y(\theta,\phi) = b\, Y(\theta,\phi)$$

Since the operator does not involve θ, we try a separation of variables, writing

$$Y(\theta,\phi) = S(\theta)\, T(\phi)$$

Considering the periodic boundary condition $T(\phi) = T(\phi + 2\pi)$, the solution is

Eigenfunctions $\quad T(\phi) = Ae^{im\phi} \quad m = 0, \pm 1, \pm 2, \ldots$

Eigenvalues $\quad b = m\,\hbar$

ANGULAR MOMENTUM of a ONE-PARTICLE SYSTEM

Normalization in spherical polar coordinates

If the eigenfunction is a function of x, y and z, i.e. $f(x, y, z)$, we know that

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}|f(x,y,z)|^2 \mathrm{d}x\ \mathrm{d}y\ \mathrm{d}z = 1$$

Transforming $f(x, y, z)$ into a function of the spherical polar coordinates, such that $f(x,y,z) = F(r, \theta, \phi)$, the volume element transforms into

$$\mathrm{d}x\ \mathrm{d}y\ \mathrm{d}z = r^2 \sin\theta\ \mathrm{d}r\ \mathrm{d}\theta\ \mathrm{d}\phi$$

Normalization becomes

$$\int_0^{2\pi}\int_0^{\pi}\int_0^{\infty}|F(r,\theta,\phi)|^2\, r^2 \sin\theta\ \mathrm{d}r\ \mathrm{d}\theta\ \mathrm{d}\phi = 1$$

ANGULAR MOMENTUM of a ONE-PARTICLE SYSTEM

If $F(r,\theta,\phi)$ happens to have the form

$$F(r,\theta,\phi) = R(r)\,S(\theta)\,T(\phi)$$

we get $$\int_0^\infty |R(r)|^2\, r^2 \mathrm{d}r \int_0^{2\pi} |T(\phi)|^2 \mathrm{d}\phi \int_0^\pi |S(\theta)|^2 \sin\theta\,\mathrm{d}\theta = 1$$

It is convenient to normalize each factor of $F(r,\theta,\phi)$ separately:

$$\int_0^\infty |R(r)|^2\, r^2 \mathrm{d}r = 1 \qquad \int_0^{2\pi} |T(\phi)|^2 \mathrm{d}\phi = 1 \qquad \int_0^\pi |S(\theta)|^2 \sin\theta\,\mathrm{d}\theta = 1$$

ANGULAR MOMENTUM of a ONE-PARTICLE SYSTEM

The normalized eigenfunctions of $\hat{L}_z$ are

$$T_m(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi} \qquad m = 0, \pm 1, \pm 2, \dots$$

Eigenvalues $\quad b = m\,\hbar$

ANGULAR MOMENTUM of a ONE-PARTICLE SYSTEM

Memo

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

$$\hat{L}^2 Y(\theta,\phi) = c\, Y(\theta,\phi)$$

$$Y(\theta,\phi) = S(\theta)\, T_m(\phi)$$

$$T_m(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi}$$

The above info can be collected in the following equation

$$-\hbar^2 \left(\frac{\partial^2}{\partial \theta^2} + \cot\theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial \phi^2} \right) \left(S(\theta) \frac{1}{\sqrt{2\pi}} e^{im\phi} \right) = c\, S(\theta) \frac{1}{\sqrt{2\pi}} e^{im\phi}$$

ANGULAR MOMENTUM of a ONE-PARTICLE SYSTEM

which leads to …

$$\frac{d^2S}{d\theta^2} + \cot\theta\,\frac{dS}{d\theta} - \frac{m^2}{\sin^2\theta}\,S = -\,\frac{c}{\hbar^2}\,S$$

ANGULAR MOMENTUM of a ONE-PARTICLE SYSTEM

The solution for $S(\theta)$ is

Associated Legendre functions

$$S_{l,m}(\theta) = \sin^{|m|}\theta \sum_{\substack{j=1,3,5,\dots \\ j=0,2,4,\dots}}^{l-|m|} a_j \cos^j\theta$$

Quantum numbers $\begin{cases} l = 0,1,2,3,\dots \\ m = -l, -l+1, \dots, 0, \dots, l-1, l \end{cases}$

where the sum is over even or odd values of j, depending on whether $l - |m|$ is even or odd. The coefficients a_j satisfy the recursion relation

$$a_{j+2} = \frac{(j+|m|)(j+|m|+1) - l(l+1)}{(j+1)(j+2)}\, a_j$$

Eigenvalues $\quad c = l(l+1)\,\hbar^2$

ANGULAR MOMENTUM of a ONE-PARTICLE SYSTEM (summary)

Eigenfunctions of $\hat{L}^2$ and $\hat{L}_z$ are **spherical harmonics**

$$\hat{L}_z Y_l^m(\theta,\phi) = m\,\hbar\, Y_l^m(\theta,\phi)$$

$$\hat{L}^2 Y_l^m(\theta,\phi) = l(l+1)\hbar^2\, Y_l^m(\theta,\phi)$$

$$l = 0,1,2,3,\dots$$

$$m = -l,\dots,0,\dots,l$$

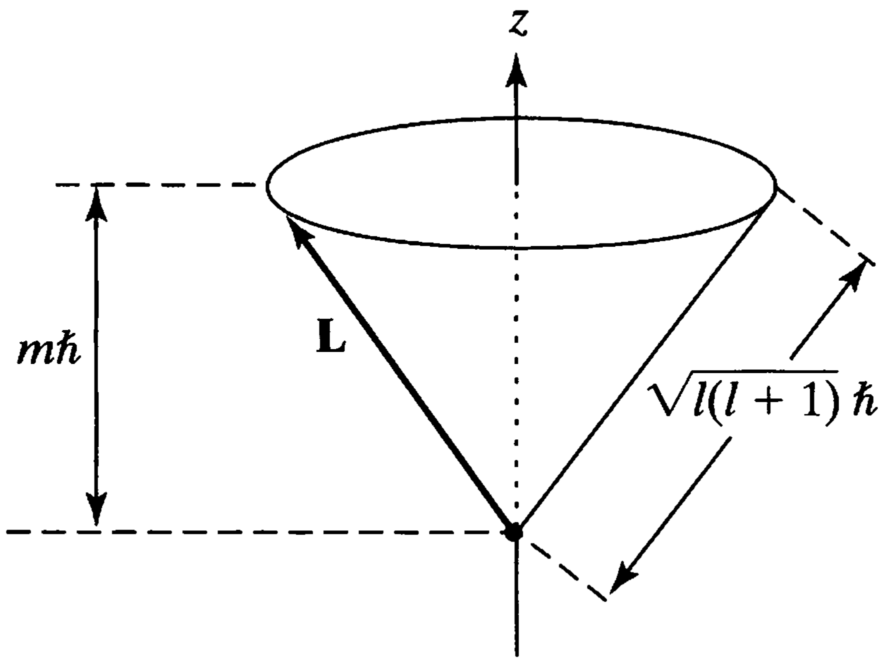
$$Y_l^m(\theta,\phi) = S_{l,m}(\theta)\, T_m(\phi)$$

$$T_m(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi} \qquad S_{l,m}(\theta) = \sin^{|m|}\theta \sum_{\substack{j=1,3,5,\dots \\ j=0,2,4,\dots}}^{l-|m|} a_j \cos^j\theta$$

Recursion relation $$a_{j+2} = \frac{(j+|m|)(j+|m|+1) - l(l+1)}{(j+1)(j+2)}\, a_j$$

ANGULAR MOMENTUM of a ONE-PARTICLE SYSTEM

Since we cannot specify L_x and L_y, the vector $\mathbf{L}$ can lie anywhere on the surface of a cone whose axis is the z axis



The magnitude of the orbital angular momentum of a particle is

$$|\mathbf{L}| = [l(l+1)]^{1/2}\hbar$$

ANGULAR MOMENTUM of a ONE-PARTICLE SYSTEM

The possible orientations of $\mathbf{L}$ with respect to the z axis for the case $l = 1$ are shown in the figure. For each eigenvalue of $\hat{L}^2$, there are $2l + 1$ different eigenfunctions Y, corresponding to the $2l + 1$ values of m. We say that the $\hat{L}^2$ eigenvalues are $(2l + 1)$-fold degenerate