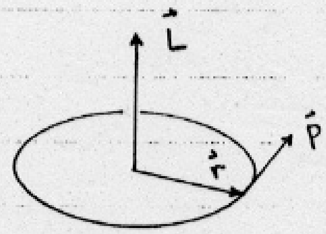
Angular Momentum

Classical definition:



$$\vec{L} = \vec{r} \times \vec{p} \qquad \text{dimensions: } \hbar$$

$$\vec{r} = x\,\hat{e}_x + y\,\hat{e}_y + z\,\hat{e}_z$$
$$\vec{p} = p_x\,\hat{e}_x + p_y\,\hat{e}_y + p_z\,\hat{e}_z$$

$$\vec{L} = \begin{vmatrix} \hat{e}_x & \hat{e}_y & \hat{e}_z \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix}$$

$$L_x = y p_z - z p_y$$
$$L_y = z p_x - x p_z$$
$$L_z = x p_y - y p_x$$

Quantum mechanics:

$$\hat{\vec{L}} = \hat{\vec{r}} \times \hat{\vec{p}}$$

Commutation relations:

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

We cannot specify more than one component of the angular momentum of a system precisely.

But $[\hat{L}^2, \hat{L}_z] = 0$.

Raising and lowering operators :

Define $\boxed{\hat{L}_+ \equiv \hat{L}_x + i\hat{L}_y}$, $\boxed{\hat{L}_- \equiv \hat{L}_x - i\hat{L}_y}$

Commutation relations:

$$\boxed{[\hat{L}_+, \hat{L}_z] = -\hbar\hat{L}_+} \qquad \boxed{[\hat{L}_-, \hat{L}_z] = \hbar\hat{L}_-} \qquad \boxed{[\hat{L}_+, \hat{L}_-] = 2\hbar\hat{L}_z}$$

$$\boxed{[\hat{L}^2, \hat{L}_+] = [\hat{L}^2, \hat{L}_-] = 0} \qquad [\hat{L}^2, L_z] = 0$$

Denote the simultaneous eigenstates of $\hat{L}^2$ and $\hat{L}_z$ by $|nm\rangle$:

$$\hat{L}_z |nm\rangle = \underset{\substack{\uparrow \\ \text{dimensionless} \\ \text{real number}}}{m}\hbar\, |nm\rangle$$

Then $\hat{L}^2 |nm\rangle = \hbar^2 f(n,m)\, |nm\rangle$

$$f(n,m) = \frac{1}{\hbar^2} \langle nm| \hat{L}^2 |nm\rangle = \frac{1}{\hbar^2} \langle \Phi_{nm} | \Phi_{nm}\rangle \geq 0$$

where $|\Phi_{nm}\rangle \equiv \hat{\vec{L}}\, |nm\rangle$.

$$(\hat{L}^2 - \hat{L}_z^2)\, |nm\rangle = \hbar^2 (f - m^2)\, |nm\rangle \quad \text{and}$$

$$\langle nm| \hat{L}^2 - \hat{L}_z^2 |nm\rangle = \hbar^2 [f(n,m) - m^2]$$

But $\quad \hat{L}^2 - \hat{L}_z^2 = \hat{L}_x^2 + \hat{L}_y^2 \quad$ and

$$\langle nm | \hat{L}^2 - \hat{L}_z^2 | nm \rangle = \langle nm | \hat{L}_x^2 | nm \rangle + \langle nm | \hat{L}_y^2 | nm \rangle \geq 0 .$$

Therefore $\quad f(n,m) \geq m^2 .$

Next, notice that

$$\hat{L}^2 \, \hat{L}_+ \, | nm \rangle = \hat{L}_+ \, \hat{L}^2 \, | nm \rangle = \hat{L}_+ \, f(n,m) \hbar^2 \, | nm \rangle \quad \Rightarrow$$

$\hat{L}_+ | nm \rangle$ is an eigenstate of $\hat{L}^2$ with eigenvalue $\hbar^2 f(n,m)$.

So application of $\hat{L}_+$ on $|nm\rangle$ does not change the magnitude of the total angular momentum.

Now, let's examine the result of applying $\hat{L}_z$ on $\hat{L}_+ |nm\rangle$:

$$\hat{L}_z \hat{L}_+ | nm \rangle = \left(\hbar \hat{L}_+ + \hat{L}_+ \hat{L}_z \right) | nm \rangle = \left(\hbar \, \hat{L}_+ + \hbar m \, \hat{L}_+ \right) | nm \rangle \quad \Rightarrow$$

$$\boxed{\hat{L}_z \; \hat{L}_+ | nm \rangle = (m+1) \hbar \; \hat{L}_+ | nm \rangle}$$

Therefore $\hat{L}_+ |nm\rangle$ is an eigenstate of $\hat{L}_z$ with eigenvalue $(m+1)\hbar$.

Similarly, $\quad \boxed{\hat{L}_z \; \hat{L}_- | nm \rangle = (m-1) \hbar \; \hat{L}_- | nm \rangle}$

$$\boxed{\hat{L}_+ | nm \rangle = \hbar \, c^+_{nm} \, | n, m+1 \rangle} \qquad \boxed{\hat{L}_- | nm \rangle = \hbar \, c^-_{nm} \, | n, m-1 \rangle}$$

By operating with $\hat{L}_+$ on $|nm\rangle$ repeatedly, we will eventually reach an eigenvalue larger than $\sqrt{f(n,m)}$. Since this cannot happen, there must be a state $|n, m_{max}\rangle$ that terminates the process:

$$\hat{L}_+ |n, m_{max}\rangle = 0$$

Let's find the value of m_{max}:

$$\hat{L}_- \hat{L}_+ |n, m_{max}\rangle = 0 = (\hat{L}_x - i\hat{L}_y)(\hat{L}_x + i\hat{L}_y)|n, m_{max}\rangle$$

But $\hat{L}_-\hat{L}_+ = \hat{L}_x^2 + \hat{L}_y^2 + i(\hat{L}_x\hat{L}_y - \hat{L}_y\hat{L}_x) = \hat{L}^2 - \hat{L}_z^2 - \hbar\hat{L}_z$.

Thus,

$$(\hat{L}^2 - \hat{L}_z^2 - \hbar\hat{L}_z)|n, m_{max}\rangle = 0 \quad \Rightarrow$$

$$\hat{L}^2 |n, m_{max}\rangle = (\hat{L}_z^2 + \hbar\hat{L}_z)|n, m_{max}\rangle$$

$$= (\hbar^2 m_{max}^2 + \hbar^2 m_{max})|n, m_{max}\rangle$$

$$= m_{max}(m_{max}+1)\hbar^2 |n, m_{max}\rangle \quad \Rightarrow$$

$$f(n, m_{max}) = m_{max}(m_{max}+1)$$

So we have

$$\hat{L}^2 |n, m_{max}\rangle = \hbar^2 m_{max}(m_{max}+1)|n, m_{max}\rangle$$

We have shown that when $\hat{L}_-$ operates on $|n, m\rangle$ it doesn't change the eigenvalue of $\hat{L}^2$. Therefore

$$\hat{L}^2 \, |nm\rangle = \hbar^2 \, m_{max} \, (m_{max} + 1) \, |n, m\rangle$$

Call $\boxed{m_{max} \equiv l}$.

Thus, the only quantity that specifies the particular eigenstate of $\hat{L}^2$ is l, so let's denote this by setting $n = l$:

$$\boxed{\hat{L}^2 \, |lm\rangle = \hbar^2 \, l(l+1) \, |lm\rangle}, \qquad m = l, \, l-1, \, \ldots$$

Now focus on $\hat{L}_- |lm\rangle$. Operating repeatedly we will reach an eigenvalue lower than $-\sqrt{f(n,m)} = -\sqrt{l(l+1)}$. Therefore, there must be a state $|l, m_{min}\rangle$ that terminates the process:

$$\hat{L}_- |l, m_{min}\rangle = 0 .$$

Let's find the value of m_{min}:

$$\hat{L}_+ \hat{L}_- |l, m_{min}\rangle = 0 = (\hat{L}_x + i\hat{L}_y)(\hat{L}_x - i\hat{L}_y) \, |l, m_{min}\rangle$$

But $\hat{L}_+ \hat{L}_- = \hat{L}_x^2 + \hat{L}_y^2 - i(\hat{L}_x \hat{L}_y - \hat{L}_y \hat{L}_x) = \hat{L}^2 - \hat{L}_z^2 + \hbar \hat{L}_z \Rightarrow$

$$(\hat{L}^2 - \hat{L}_z^2 + \hbar \hat{L}_z) |l, m_{min}\rangle = 0 \Rightarrow [\hbar^2 l(l+1) - \hbar^2 m_{min}^2 + \hbar \cdot \hbar \, m_{min}] \, |l, m_{min}\rangle = 0$$

$$\Rightarrow m_{min}(m_{min} - 1) = l(l+1) \Rightarrow \boxed{m_{min} = -l}$$

Therefore,

$$m_{max} - m_{min} = 2\ell = \text{integer}$$

(because we reach the $|\ell, m_{min}\rangle$ level by operating on $|\ell, m_{max}\rangle$ a number of times.)

$$\Rightarrow \quad \boxed{\ell = \text{integer or half-integer}}$$

Finally, let's determine the coefficients $c^{+}_{\ell m}$ and $c^{-}_{\ell m}$.

$$\hat{L}_{-}\hat{L}_{+}|\ell m\rangle = (\hat{L}^2 - \hat{L}_z^2 - \hbar\hat{L}_z)|\ell m\rangle = \hbar^2(\ell(\ell+1) - m(m+1))|\ell m\rangle$$

$$\Rightarrow \langle \ell m|\hat{L}_{-}\hat{L}_{+}|\ell m\rangle = \hbar^2[\ell(\ell+1) - m(m+1)]$$

Because $\hat{L}_{-} = \hat{L}_{+}^{\dagger}$,

$$\langle \ell m|\hat{L}_{-}\hat{L}_{+}|\ell m\rangle = \langle \ell, m+1|\ell, m+1\rangle \cdot (\hbar c^{+}_{\ell m})^{*}(\hbar c^{+}_{\ell m}) \Rightarrow$$

$$\hbar^2|c^{+}_{\ell m}|^2 = \hbar^2[\ell(\ell+1) - m(m+1)] \Rightarrow$$

$$c^{+}_{\ell m} = [\ell(\ell+1) - m(m+1)]^{1/2}$$

$$\boxed{\hat{L}_{+}|\ell m\rangle = \hbar[\ell(\ell+1) - m(m+1)]^{1/2}|\ell, m+1\rangle}$$

$$\boxed{\hat{L}_{-}|\ell m\rangle = \hbar[\ell(\ell+1) - m(m-1)]^{1/2}|\ell, m-1\rangle}$$

<u>Orbital angular momentum:</u>

Solve $\hat{L}_+ |l, l\rangle = 0$ to find the eigenfunctions.

Spherical polar coordinates:

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

$y = r \sin\theta \sin\varphi$

$z = r \cos\theta$

$$\hat{L}_x = i\hbar \left[\sin\varphi \frac{\partial}{\partial\theta} + \cot\theta \cos\varphi \frac{\partial}{\partial\varphi} \right]$$

$$\hat{L}_y = -i\hbar \left[\cos\varphi \frac{\partial}{\partial\theta} - \cot\theta \sin\varphi \frac{\partial}{\partial\varphi} \right]$$

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

Spherical harmonics $\quad Y_{lm}(\theta, \varphi) \equiv \langle\theta\varphi | lm\rangle$

$$\boxed{\hat{L}_\pm = \pm\hbar e^{\pm i\varphi} \left(\frac{\partial}{\partial\theta} \pm i\cot\theta \frac{\partial}{\partial\varphi} \right)}$$

Find the explicit form of Y_{lm}:

$$\hat{L}_z Y_{lm}(\theta, \varphi) = m\hbar Y_{lm}(\theta, \varphi)$$

With $\hat{L}_z = -i\hbar \frac{\partial}{\partial\varphi}$ we have

$$-i\hbar \frac{\partial}{\partial\varphi} Y_{\ell m}(\theta,\varphi) = m\hbar\, Y_{\ell m}(\theta,\varphi) \Rightarrow$$

$$\boxed{Y_{\ell m}(\theta,\varphi) = y_{\ell m}(\theta)\, e^{im\varphi}}$$

Next, use $\hat{L}_\pm Y_{\ell,\pm\ell}(\theta,\varphi) = 0$.

$$\left.\begin{aligned} \frac{\partial}{\partial\theta} Y_{\ell m} &= e^{im\varphi} \frac{d}{d\theta} y_{\ell m}(\theta) \\ \frac{\partial}{\partial\varphi} Y_{\ell m} &= y_{\ell m}(\theta)\, im\, e^{im\varphi} \end{aligned}\right\} \text{apply with } m = \pm\ell :$$

$$e^{\pm i\ell\varphi}\left[\frac{d}{d\theta} y_{\ell,\pm\ell}(\theta) \pm i\cot\theta \cdot i(\pm\ell)\, y_{\ell,\pm\ell}(\theta)\right] = 0 \Rightarrow$$

$$\left(\frac{d}{d\theta} - \ell\cot\theta\right) y_{\ell,\pm\ell}(\theta) = 0 \Rightarrow \boxed{y_{\ell,\pm\ell}(\theta) = \alpha_\ell^\pm \sin^\ell(\theta)}$$

Can ℓ be a half-integer? Let's try $\ell = 1/2$. Then

$$Y_{\frac{1}{2}\,\pm\frac{1}{2}}(\theta,\varphi) = \alpha_{1/2}^\pm \sqrt{\sin\theta}\, e^{\pm i\varphi/2}.$$

Apply $\hat{L}_-$:

$$\hat{L}_- Y_{\frac{1}{2}\,\frac{1}{2}}(\theta,\varphi) = -\hbar e^{-i\varphi}\left[\frac{\partial}{\partial\theta} - i\cot\theta \frac{\partial}{\partial\varphi}\right] \alpha_{\frac{1}{2}}^{+} \sqrt{\sin\theta}\, e^{i\varphi/2}$$

$$= -\hbar e^{-i\varphi}\left[\alpha_{1/2}^{+}\frac{\cos\theta}{2\sqrt{\sin\theta}}\,e^{i\varphi/2} - i\,\frac{\cos\theta}{\sin\theta}\,\alpha_{1/2}^{+}\sqrt{\sin\theta}\,\frac{i}{2}\,e^{i\varphi/2}\right]$$

$$= -\hbar\,\alpha_{1/2}^{+}\,e^{-i\varphi/2}\,\frac{\cos\theta}{\sqrt{\sin\theta}} \quad \underline{\underline{\text{not}}} \text{ proportional to } Y_{\frac{1}{2}\,-\frac{1}{2}}(\theta,\varphi)!$$

We conclude that only integer l values are allowed

This follows physically from the requirement that the wfn be single-valued, i.e., does not change if we rotate φ by 2π (as we saw for the particle on a ring) $\Rightarrow$ m must be integer.

Finally, find $Y_{lm}(\theta,\varphi)$:

$$\hat{L}_{\pm} Y_{lm}(\theta,\varphi) = \hbar\left[l(l+1) - m(m\pm1)\right]^{1/2} Y_{l,m\pm1}(\theta,\varphi) \Rightarrow$$

$$\hat{L}_{-} Y_{ll} = \hbar\left[l(l+1) - l(l-1)\right]^{1/2} Y_{l,l-1} = \sqrt{2l}\,\hbar\,Y_{l,l-1} \Rightarrow$$

$$Y_{l,l-1}(\theta,\varphi) = \frac{1}{\sqrt{2l}\,\hbar}\,\hat{L}_{-} Y_{ll}(\theta,\varphi)$$

$$\hat{L}_{-} Y_{l,l-1} = \hbar\left[l(l+1) - (l-1)(l-2)\right]^{1/2} Y_{l,l-2} = \sqrt{4l-2}\,\hbar\,Y_{l,l-2} \Rightarrow$$

$$Y_{l,l-2}(\theta,\varphi) = \hbar^{-1}\left[2(2l-1)\right]^{-1/2}\hat{L}_{-} Y_{l,l-1} = \hbar^{-2}\left[2(2l)(2l-1)\right]^{-1/2}\hat{L}_{-}^{2} Y_{ll}$$

etc

Therefore, $$Y_{\ell m}(\theta,\varphi) = \sqrt{\frac{(\ell+m)!}{(2\ell)!\,(\ell-m)!}}\left(\frac{1}{\hbar}\hat{L}_-\right)^{\ell-m} Y_{\ell\ell}(\theta,\varphi)$$

After some algebra one finds

$$Y_{\ell m}(\theta,\varphi) = \frac{(-1)^\ell}{2^\ell \ell!}\sqrt{\frac{2\ell+1}{4\pi}}\sqrt{\frac{(\ell+m)!}{(\ell-m)!}}\; e^{im\varphi}\sin^{-m}\theta\left(\frac{d}{d\cos\theta}\right)^{\ell-m}\sin^{2\ell}\theta$$

With $m=0$, $$Y_{\ell 0}(\theta,\varphi) = \sqrt{\frac{2\ell+1}{4\pi}}\; P_\ell(\cos\theta)$$

Spherical harmonics from solving the diff equation

In spherical polar coordinates,

$$\frac{1}{\hbar^2}\hat{L}^2 = -\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} - \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}$$

Differential equation : $\hat{L}^2\, Y_{\ell m}(\theta,\varphi) = \hbar^2\ell(\ell+1)\, Y_{\ell m}(\theta,\varphi)$

Write $Y_{\ell m}(\theta,\varphi) = \Theta(\theta)\cdot\Phi(\varphi)$

$$\Phi(\varphi)\cdot\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}\Theta(\theta) + \frac{1}{\sin^2\theta}\Theta(\theta)\frac{\partial^2}{\partial\varphi^2}\Phi(\varphi)$$

$$+\ \ell(\ell+1)\,\Theta(\theta)\,\Phi(\varphi) = 0$$

Dividing by $\Theta(\theta)\,\Phi(\varphi)/\sin^2\theta$,

$$\sin\theta\,\frac{1}{\Theta(\theta)}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}\Theta(\theta) + \ell(\ell+1)\sin^2\theta + \underbrace{\frac{1}{\Phi(\varphi)}\frac{\partial^2}{\partial\varphi^2}\Phi(\varphi)}_{-m^2} = 0$$

Therefore,

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) + \left(\ell(\ell+1) - \frac{m^2}{\sin^2\theta}\right)\Theta(\theta) = 0$$

This is equivalent to the Legendre equation ; the solutions are

$$\Theta(\theta) \sim \sin^m\theta \; P_\ell^m(\cos\theta)$$

$\uparrow$

associated Legendre polynomials

For example, for $m=0$,

$$P_0(\cos\theta) = 1, \qquad P_1(\cos\theta) = \cos\theta, \qquad P_2(\cos\theta) = \frac{1}{2}(3\cos^2\theta - 1)$$

Finally, the equation for φ gives

$$\Phi(\varphi) \sim e^{\pm im\varphi}$$

Requiring periodicity at 2π implies that m must be an integer.

The hydrogen atom

$$H = -\frac{\hbar^2}{2\mu}\nabla^2 - \frac{e^2}{4\pi\varepsilon_0}\frac{1}{r}$$

$$\begin{cases} \mu: \text{ reduced mass,} \qquad \mu = \dfrac{m_e m_p}{m_e + m_p} \\ \varepsilon_0: \text{ permittivity of free space} \end{cases}$$

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} - \frac{\hat{L}^2}{r^2\hbar^2}$$

$$-\frac{\hbar^2}{2\mu}\frac{1}{r^2}\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r}\Psi(r,\theta,\varphi) + \frac{1}{2\mu r^2} L^2 \Psi(r,\theta,\varphi)$$

$$- \frac{e^2}{4\pi\varepsilon_0 r}\Psi(r,\theta,\varphi) = E\,\Psi(r,\theta,\varphi)$$

The angular dependence should be given by spherical harmonics, so try the factorization

$$\Psi(r,\theta,\varphi) = R(r)\,Y(\theta,\varphi)$$

This gives, using $L^2 Y = \hbar^2 \ell(\ell+1) Y$,

$$\frac{1}{r}\frac{\partial^2}{\partial r^2} rRY - \frac{1}{r^2}\ell(\ell+1) RY + \frac{\mu e^2}{2\pi\varepsilon_0 \hbar^2 r} RY = -\frac{2\mu E}{\hbar^2} RY$$

Equation for $R(r)$:

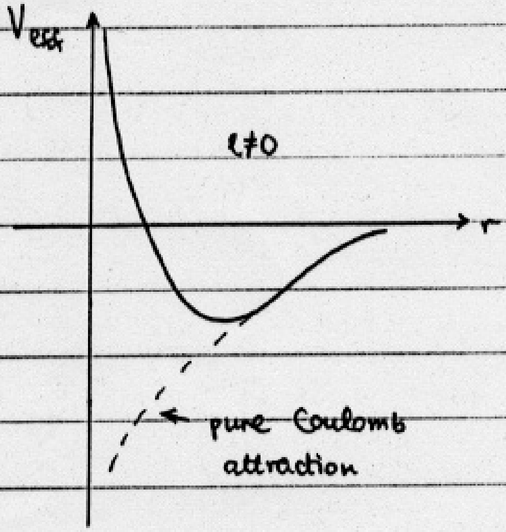
$$\frac{1}{r}\frac{d^2}{dr^2} rR + \left[\frac{\mu e^2}{2\pi\varepsilon_0\hbar^2 r} - \ell(\ell+1)\frac{1}{r^2}\right] R = -\frac{2\mu E}{\hbar^2} R$$

Writing $\qquad P(r) \equiv r R(r)$,

$$\frac{d^2P}{dr^2} + \frac{2\mu}{\hbar^2}\left[\frac{e^2}{4\pi\varepsilon_0 r} - \ell(\ell+1)\frac{\hbar^2}{2\mu r^2}\right] P = -\frac{2\mu E}{\hbar^2} P .$$

Looks like 1-dim. Schrödinger eqn. for effective potential

$$V_{eff}(r) = -\frac{e^2}{4\pi\varepsilon_0 r} + \frac{\ell(\ell+1)\hbar^2}{2\mu r^2}$$



Radial solutions: Laguerre polynomials
(two quantum numbers, n and ℓ)

Energy eigenvalues: $\boxed{E_n = -\frac{\mu e^4}{32\pi^2\varepsilon_0^2\hbar^2}\frac{1}{n^2}}$, $\quad n = 1, 2, \ldots$