Chapter 5: Angular Momentum

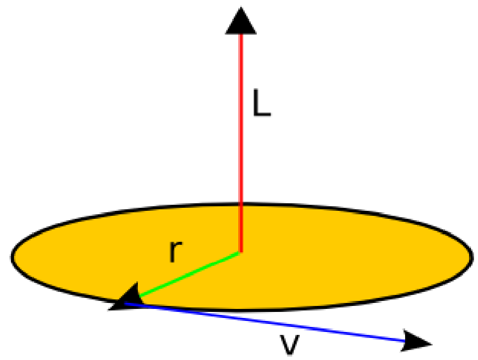
What is angular momentum?

- A quantity used in describing rotating systems.

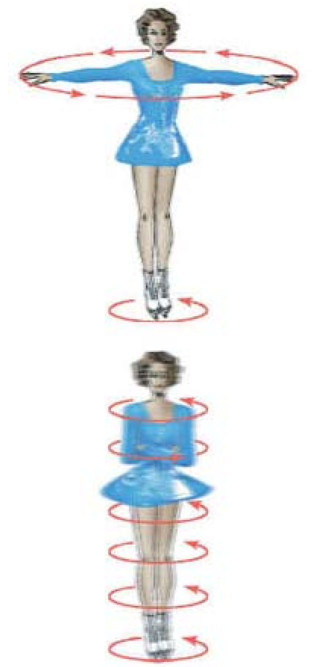
-It is defined as a cross product of linear momentum of the particle (p=mV) and a position vector of a particle (r).

Why do we care about angular momentum?

- To describe the motion of electron around nucleus



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

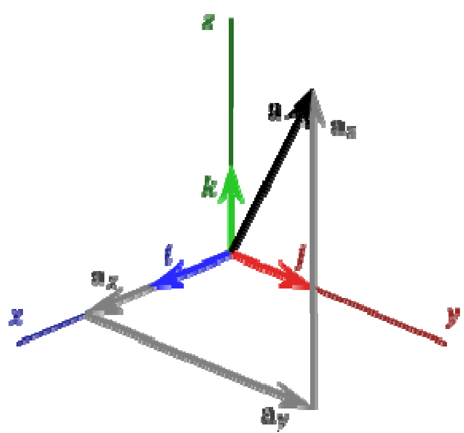


Conservation of angular momentum

Review of vectors

- We use cartesian coordinates to represent vectors:

$$\vec{A} = A_x \cdot \vec{i} + A_y \cdot \vec{j} + A_z \cdot \vec{k}$$



The magnitude of the vector is its length: $\left|\vec{A}\right| = \sqrt{A_x^2 + A_y^2 + A_z^2}$

Sum of two vectors: $\vec{A} + \vec{B} = (A_x + B_x)\,\vec{i} + (A_y + B_y)\,\vec{j} + (A_z + B_z)\,\vec{k}$

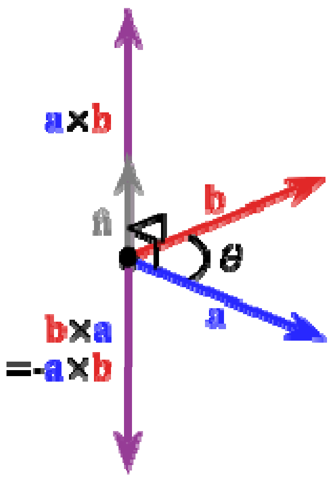
Dot (scalar) product: $\vec{A} \cdot \vec{B} = \left|\vec{A}\right| \cdot \left|\vec{B}\right| \cdot \cos\theta = A_x \cdot B_x + A_y \cdot B_y + A_z \cdot B_z$

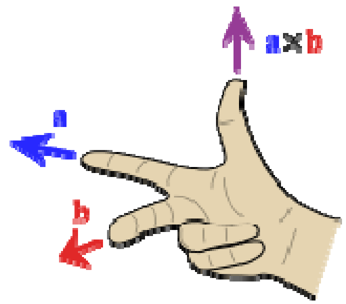
scalar

angle between the vectors

-The cross (vector) product: it is a vector with magnitude: $\left|\vec{A}\times\vec{B}\right| = \left|\vec{A}\right|\cdot\left|\vec{B}\right|\cdot\sin\theta$

Its direction is perpendicular to the plane defined by vectors A and B:





How to calculate vector product:

$$\vec{A}\times\vec{B} = \begin{vmatrix} \vec{i} & \vec{j} & \vec{k} \\ A_x & A_y & A_z \\ B_x & B_y & B_z \end{vmatrix} = \vec{i}\begin{vmatrix} A_y & A_z \\ B_y & B_z \end{vmatrix} - \vec{j}\begin{vmatrix} A_x & A_z \\ B_x & B_z \end{vmatrix} + \vec{k}\begin{vmatrix} A_x & A_y \\ B_x & B_y \end{vmatrix}$$

determinant

-Vector operator del: $\vec{\nabla} = \vec{i}\frac{\partial}{\partial x} + \vec{j}\frac{\partial}{\partial y} + \vec{k}\frac{\partial}{\partial z}$

For example, the linear momentum operator:

$$\vec{\hat{p}} = -i\hbar\vec{\nabla}$$

-Derivative of the vector: $\frac{d\vec{A}}{dt} = \vec{i}\frac{dA_x}{dt} + \vec{j}\frac{dA_y}{dt} + \vec{k}\frac{dA_z}{dt}$

-We can use vector notation to represent particle's coordinates:

$$\Psi(x_1, y_1, z_1, x_2, y_2, z_2) = \Psi\left(\vec{r}_1, \vec{r}_2\right)$$

Example: $\vec{A}(4,-1,3)$

$\vec{B}(-1,2,2)$

$$\left|\vec{A}\right| = ?$$

$$\vec{C} = \vec{A} + \vec{B} = ?$$

$$D = \vec{A} \cdot \vec{B} = ?$$

$$\vec{E} = \vec{A} \times \vec{B} = ?$$

$$\left|\vec{A}\right| = \sqrt{16+1+25} = \sqrt{36} = 6$$

$$\vec{C}(3,1,7)$$

$$D = (-1)\cdot 4 + (-1)\cdot 2 + 3\cdot 2 = -4 - 2 + 6 = 0$$

$$\vec{E} = \begin{vmatrix} \vec{i} & \vec{j} & \vec{k} \\ 4 & -1 & 3 \\ -1 & 2 & 2 \end{vmatrix} = \vec{i}\begin{vmatrix} -1 & 3 \\ 2 & 2 \end{vmatrix} - \vec{j}\begin{vmatrix} 4 & 3 \\ -1 & 2 \end{vmatrix} + \vec{k}\begin{vmatrix} 4 & -1 \\ -1 & 2 \end{vmatrix}$$

$$\vec{E}(-8,-12,7)$$

Back to Angular Momentum

Classical mechanics: $\vec{L} = \vec{r} \times \vec{p}$

$$\vec{r} = x\cdot\vec{i} + y\cdot\vec{j} + z\cdot\vec{k}$$

$$\vec{p} = p_x\cdot\vec{i} + p_y\cdot\vec{j} + p_z\cdot\vec{k}$$

$$\vec{L} = \begin{vmatrix} \vec{i} & \vec{j} & \vec{k} \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix} = \vec{i}\begin{vmatrix} y & z \\ p_y & p_z \end{vmatrix} - \vec{j}\begin{vmatrix} x & z \\ p_x & p_z \end{vmatrix} + \vec{k}\begin{vmatrix} x & y \\ p_x & p_y \end{vmatrix}$$

$$L_x = y\cdot p_z - z\cdot p_y$$

$$L_y = -x\cdot p_z + z\cdot p_x$$

$$L_z = x\cdot p_y - y\cdot p_x$$

Quantum mechanics:

- Operators will be taken from classical physics:

Classical	*Quantum*
$L_x = y\cdot p_z - z\cdot p_y$	$\hat{L}_x = y\cdot\left(-i\hbar\frac{\partial}{\partial z}\right) - z\cdot\left(-i\hbar\frac{\partial}{\partial y}\right) = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$
$L_y = -x\cdot p_z + z\cdot p_x$	$\hat{L}_y = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)$
$L_z = x\cdot p_y - y\cdot p_x$	$\hat{L}_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$

-Can we obtain all three of them simultaneously?
We need to find out if they commute:

$$\left[\hat{L}_x, \hat{L}_y\right] = ?;\ \left[\hat{L}_y, \hat{L}_z\right] = ?;\ \left[\hat{L}_z, \hat{L}_x\right] = ?$$

$$\left[\hat{L}_x, \hat{L}_y\right] = \hat{L}_x\cdot\hat{L}_y - \hat{L}_y\cdot\hat{L}_x$$

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

$$= -\hbar^2\left(y\frac{\partial}{\partial z}\left(z\frac{\partial f}{\partial x}\right) - z\frac{\partial}{\partial y}\left(z\frac{\partial f}{\partial x}\right) - y\frac{\partial}{\partial z}\left(x\frac{\partial f}{\partial z}\right) + z\frac{\partial}{\partial y}\left(x\frac{\partial f}{\partial z}\right)\right) =$$

$$= -\hbar^2\left(y\frac{\partial f}{\partial x} + y\cdot z\frac{\partial}{\partial z}\frac{\partial f}{\partial x} - z^2\frac{\partial}{\partial y}\frac{\partial f}{\partial x} - y\cdot x\frac{\partial^2 f}{\partial z^2} + z\cdot x\frac{\partial}{\partial y}\frac{\partial f}{\partial z}\right)$$

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

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

Similarly:

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

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

Thus, we cannot obtain all three components simultaneously.

What about magnitude?
Let's define magnitude operator as:

$$\hat{L}^2 = \left| \vec{\hat{L}} \right|^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$$

Some useful transformations with operators:

1. $\left[\hat{A}, \hat{B} \right] = -\left[\hat{B}, \hat{A} \right]$
2. $\left[\hat{A}, \hat{B} + \hat{C} \right] = \left[\hat{A}, \hat{B} \right] + \left[\hat{A}, \hat{C} \right]$
3. $\left[\hat{A}, \hat{A}^n \right] = 0$
4. $\left[\hat{A}, \hat{B} \cdot \hat{C} \right] = \left[\hat{A}, \hat{B} \right] \cdot \hat{C} + \hat{B} \cdot \left[\hat{A}, \hat{C} \right]$

Now we need to find if magnitude operator commutes with operators for x,y and z component:

$$\left[\hat{L}^2, \hat{L}_x \right] = ?$$

Rule 1 Rule 3 0

$$\left[\hat{L}^2, \hat{L}_x\right] = \left[\hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2, \hat{L}_x\right] = \left[\hat{L}_x^2, \hat{L}_x\right] + \left[\hat{L}_y^2, \hat{L}_x\right] + \left[\hat{L}_z^2, \hat{L}_x\right] = \left[\hat{L}_y \cdot \hat{L}_y, \hat{L}_x\right] + \left[\hat{L}_z \cdot \hat{L}_z, \hat{L}_x\right]$$

Rule 4

$$= \hat{L}_y \cdot \left[\hat{L}_y, \hat{L}_x\right] + \left[\hat{L}_y, \hat{L}_x\right] \cdot \hat{L}_y + \hat{L}_z \cdot \left[\hat{L}_z, \hat{L}_x\right] + \left[\cdot \hat{L}_z, \hat{L}_x\right] \cdot \hat{L}_z$$

Rule 2

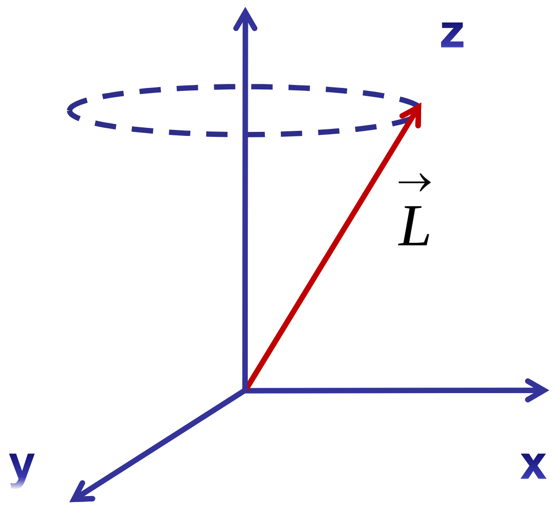
$$= -\hat{L}_y \cdot \left[\hat{L}_x, \hat{L}_y\right] - \left[\hat{L}_x, \hat{L}_y\right] \cdot \hat{L}_y + \hat{L}_z \cdot \left[\hat{L}_z, \hat{L}_x\right] + \left[\cdot \hat{L}_z, \hat{L}_x\right] \cdot \hat{L}_z =$$

$$= i\hbar(-\hat{L}_y \cdot \hat{L}_z - \hat{L}_z \cdot \hat{L}_y + \hat{L}_y \cdot \hat{L}_z + \hat{L}_z \cdot \hat{L}_y = 0$$

Similarly:

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

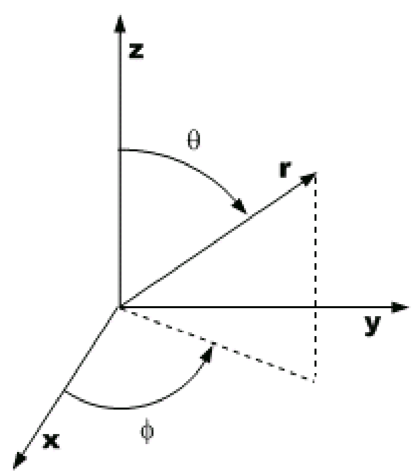
So, we can simultaneously determine the magnitude of orbital angular momentum of the particle and one of the components, say z:



Vector L can lie anywhere on the surface of the cone.

Even though we are using angular orbital momentum derived from classical physics, *__this does NOT mean that the electron is orbiting around nucleus.__*

Thus, we can use eigenvalue problem to obtain L_z and L^2. But, before doing that, we need to move to spherical coordinates in order to make partial derivatives separable).



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

$$y = r\sin\theta\sin\Phi$$

$$z = r\cos\theta$$

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

To convert the operators into spherical coordinates:

cartesian → *spherical*

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

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

Operators depend on three cartesian coordinates (x,y,z) but only two spherical coordinates (θ,Φ).

Now, let's solve the eigenvalue problem: $\hat{L}_z Y(\theta,\Phi) = b\cdot Y(\theta,\Phi)$

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

We try a separation of variables: $Y(\theta,\Phi) = S(\theta)\cdot T(\Phi)$

Applying L_z operator:

$$-i\hbar\frac{\partial}{\partial\Phi}\left[S(\theta)\cdot T(\Phi)\right] = b\cdot S(\theta)\cdot T(\Phi)$$

$$-i\hbar S(\theta)\frac{\partial T(\Phi)}{\partial\Phi} = b\cdot S(\theta)\cdot T(\Phi)$$

$$\frac{dT(\Phi)}{T(\Phi)} = -\frac{b}{i\hbar}d\Phi$$

$$\ln\left(T(\Phi)\right) = \frac{ib\Phi}{\hbar} \Rightarrow T(\Phi) = A\cdot e^{\frac{ib\Phi}{\hbar}}$$

Not a suitable wavefunction, it is not single-valued

For T to be single-valued, we have the restriction:

$$T(\Phi + 2\pi) = T(\Phi)$$

$$A \cdot e^{\frac{ib\Phi}{\hbar}} \cdot e^{\frac{ib2\pi}{\hbar}} = A \cdot e^{\frac{ib\Phi}{\hbar}}$$

$$e^{\frac{ib2\pi}{\hbar}} = 1 \Rightarrow e^{i\alpha} = \cos\alpha + i\sin\alpha = 1$$ → works for α=2πm, where m=0,±1,±2…

$$\frac{b2\pi}{\hbar} = 2\pi m \Rightarrow \boxed{b = m\hbar}$$

$$T(\Phi) = A \cdot e^{im\Phi}$$

$$m = 0, \pm 1, \pm 2 \ldots$$

eigenvalues for L_z are quantized

How do we get A?
By normalization.

$$\int_0^{2\pi} |T(\Phi)|^2 \, d\Phi = 1$$

$$\int_0^{2\pi} \left(A \cdot e^{im\Phi}\right) \cdot \left(A \cdot e^{im\Phi}\right)^* d\Phi = A^2 \int_0^{2\pi} d\Phi = A^2 2\pi$$

$$A = \frac{1}{\sqrt{2\pi}}$$

$$\boxed{T(\Phi) = \sqrt{\frac{1}{2\pi}} \cdot e^{im\Phi}}$$

Derivation of solution for eigenvalues of L^2 operator is more complex, so we will present only the solution:

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

$$S(\theta)=\sin^{|m|}\theta\sum_{j=1,3...}^{l-|m|}a_j\cos^j\theta$$

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

l=0,1,2…

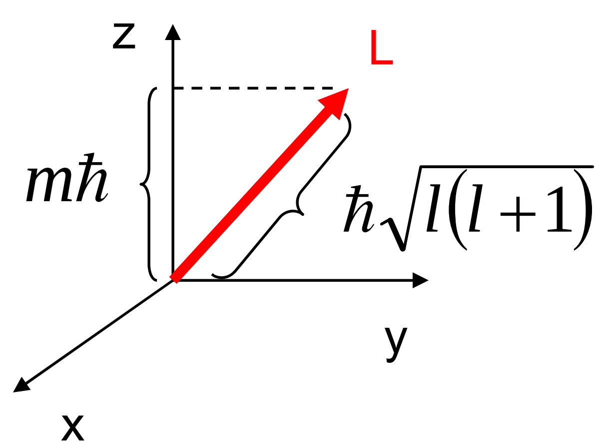
$|m|\leq l$

Possible values for m are:-l, -l+1,…0, 1….l-1, l

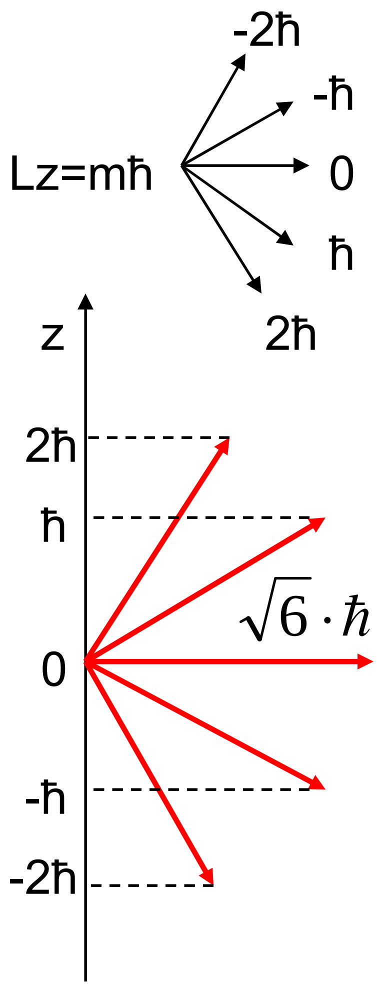
Thus, the final solutions are:

$$\hat{L}^2 Y = l(l+1)\hbar^2 Y \qquad l=0,\ 1,\ 2...$$

$$\hat{L}_z Y = m\hbar Y \qquad m=-l,\ -l+1,\ ...0...l-1,\ l$$



Example: if l=2, how many possible outcomes can we have?



$$|L| = \sqrt{6}\cdot\hbar$$

If ψ is an eigenfunction of L_z and L^2 operators, how many outcomes?

Only one outcome

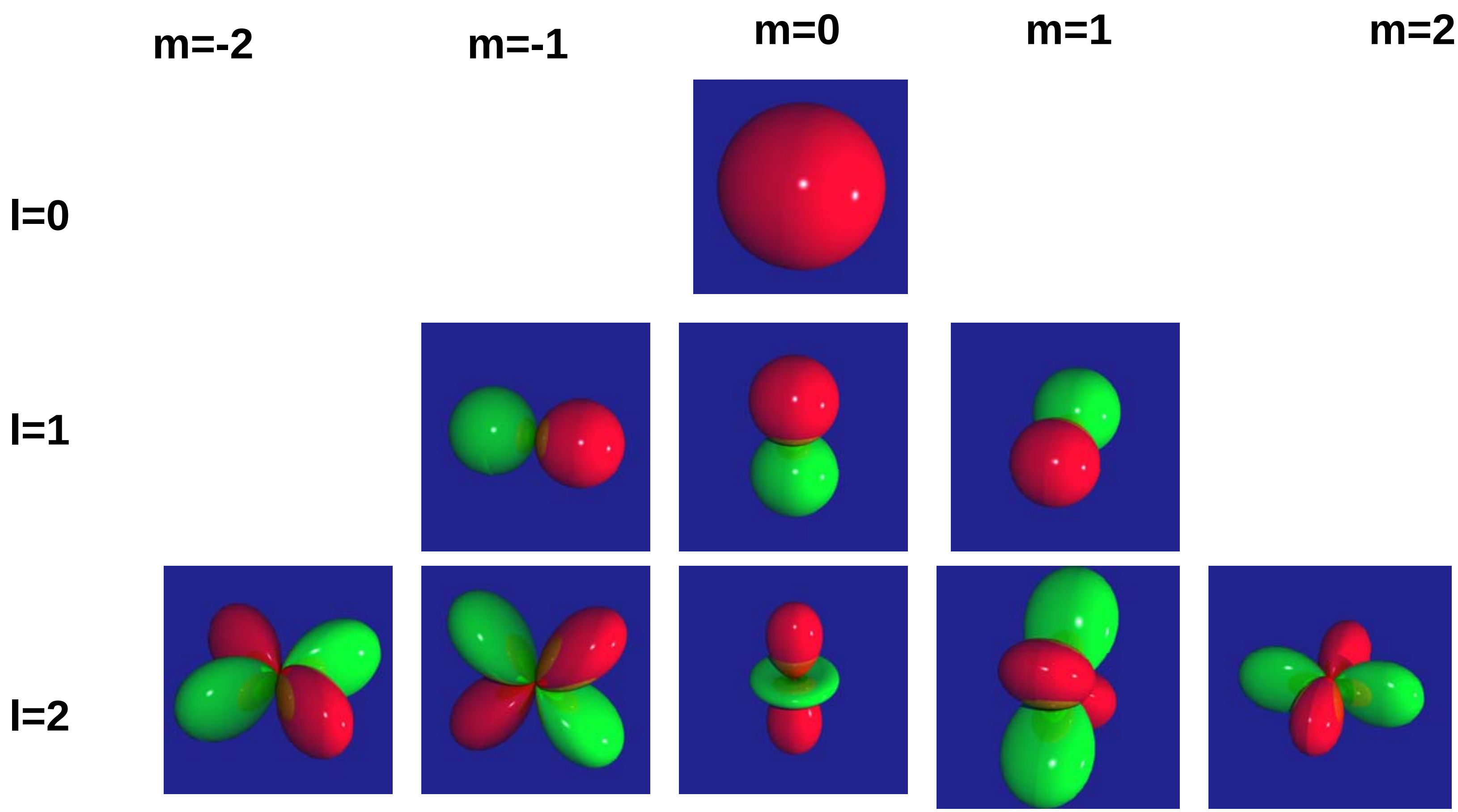
If ψ is not an eigenfunction of L_z and L^2 operators, how many outcomes?

Five outcomes

Eigenfunctions Y are called spherical harmonics. They are complex functions. But, to visualize them, we can use the real combinations of spherical harmonics defined as:

$$S_l^m = \frac{1}{\sqrt{2}}\left(Y_l^m + Y_l^{-m}\right) \qquad S_l^{-m} = \frac{1}{i\sqrt{2}}\left(Y_l^m - Y_l^{-m}\right)$$

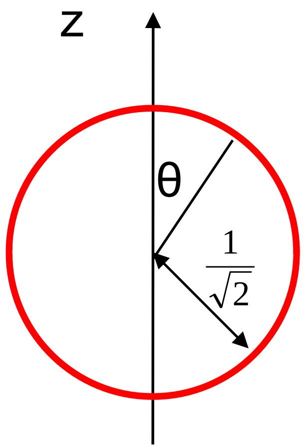
Here is how the combinations look like (the plot is made using *polar coordinates*, where the distance from the origin to a point on the graph is ST):

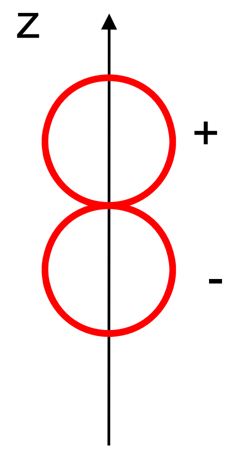


In polar coordinates, variables θ and Φ are expressed as angles with z-axis. For example:

$$S_{00} = \frac{1}{\sqrt{2}}$$

$$S_{10} = \frac{1}{2}\sqrt{6}\cos\theta$$





-The same spherical harmonics are obtained if we solved Schrodinger equation for a particle rotating on a sphere.

-To describe H-atom, we also treat it as a particle rotating on a sphere. The only difference is that the solution we obtained in this chapter involves a particle on a fixed distance r from the center, while in the case of H-atom, the distance between electron and a nucleus is not fixed. It is determined by Coulombic interactions between electron and a nucleus (attractive force that decays as 1/r). Thus, the final wavefunction ψ for H-atom will be a product of spherical harmonic Y and a radial function R(r).