

Angular momentum operator

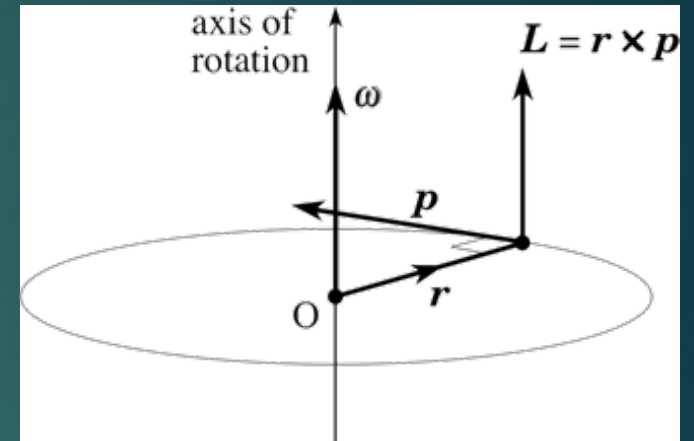
Angular momentum

We may work in a similar way for constructing the operators of other observables:

Angular momentum in 3D

classical operator

$$L = r \times p \quad \rightarrow \quad \hat{L} = \hat{r} \times \hat{p}$$



- Since this expression involves the product of the potentially non-commuting operators, one has to be careful with the order of the multiplication
- One also needs to make sure that the resulting operator is Hermitian

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$$\mathbf{L} = \mathbf{r} \times \mathbf{p} \quad \rightarrow \quad \hat{\mathbf{L}} = \hat{\mathbf{r}} \times \hat{\mathbf{p}}$$

In cartesian components:

$$L_x = y p_z - z p_y$$

$$L_y = z p_x - x p_z$$

$$L_z = x p_y - y p_x$$

$$\hat{L}_x = \hat{y} \hat{p}_z - \hat{z} \hat{p}_y$$

$$\hat{L}_y = \hat{z} \hat{p}_x - \hat{x} \hat{p}_z$$

$$\hat{L}_z = \hat{x} \hat{p}_y - \hat{y} \hat{p}_x$$

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We can write down a quantum mechanical angular momentum operator

$$\hat{\mathbf{L}} = \hat{\mathbf{r}} \times \hat{\mathbf{p}} \equiv -i\hbar(\mathbf{r} \times \nabla)$$

Angular momentum

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classical operator

$$\mathbf{L} = \mathbf{r} \times \mathbf{p} \rightarrow \hat{\mathbf{L}} = \hat{\mathbf{r}} \times \hat{\mathbf{p}}$$

In cartesian components:

$$L_x = y p_z - z p_y$$

$$L_y = z p_x - x p_z$$

$$L_z = x p_y - y p_x$$

$$\hat{L}_x = \hat{y} \hat{p}_z - \hat{z} \hat{p}_y$$

$$\hat{L}_y = \hat{z} \hat{p}_x - \hat{x} \hat{p}_z$$

$$\hat{L}_z = \hat{x} \hat{p}_y - \hat{y} \hat{p}_x$$

$$\begin{aligned} \mathbf{L} &= \mathbf{r} \times \mathbf{p} = \\ &= c r p \sin\theta = \\ &= \begin{vmatrix} e_x & e_y & e_z \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix} \end{aligned}$$

Angular momentum

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operator

$$\mathbf{L} = \mathbf{r} \times \mathbf{p} \quad \rightarrow \quad \hat{\mathbf{L}} = \hat{\mathbf{r}} \times \hat{\mathbf{p}}$$

$$\begin{aligned}\hat{L}_x &= \hat{y}\hat{p}_z - \hat{z}\hat{p}_y \\ \hat{L}_y &= \hat{z}\hat{p}_x - \hat{x}\hat{p}_z \\ \hat{L}_z &= \hat{x}\hat{p}_y - \hat{y}\hat{p}_x\end{aligned}$$

- One has to be careful with the order of the multiplication
- ✓ the order in which are placed the operators is not important because all components being multiplied correspond to commuting components of the position and momentum vectors

Angular momentum

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Angular momentum in 3D

classical operator

$$\mathbf{L} = \mathbf{r} \times \mathbf{p} \quad \rightarrow \quad \hat{\mathbf{L}} = \hat{\mathbf{r}} \times \hat{\mathbf{p}}$$

$$\begin{aligned}\hat{L}_x &= \hat{y}\hat{p}_z - \hat{z}\hat{p}_y \\ \hat{L}_y &= \hat{z}\hat{p}_x - \hat{x}\hat{p}_z \\ \hat{L}_z &= \hat{x}\hat{p}_y - \hat{y}\hat{p}_x\end{aligned}$$

$$L_x = -i\hbar y \frac{\partial}{\partial z} + i\hbar z \frac{\partial}{\partial y}$$

$$L_y = -i\hbar z \frac{\partial}{\partial x} + i\hbar x \frac{\partial}{\partial z}$$

$$L_z = -i\hbar x \frac{\partial}{\partial y} + i\hbar y \frac{\partial}{\partial x}$$

By exploiting the position representation:

Angular momentum

We may work in a similar way for constructing the operators of other observables:

Angular momentum in 3D

classical operator

$$\mathbf{L} = \mathbf{r} \times \mathbf{p} \quad \rightarrow \quad \hat{\mathbf{L}} = \hat{\mathbf{r}} \times \hat{\mathbf{p}}$$

$$\begin{aligned}\hat{L}_x &= \hat{y}\hat{p}_z - \hat{z}\hat{p}_y \\ \hat{L}_y &= \hat{z}\hat{p}_x - \hat{x}\hat{p}_z \\ \hat{L}_z &= \hat{x}\hat{p}_y - \hat{y}\hat{p}_x\end{aligned}$$

- One needs to verify that each component of the Angular momentum operator is Hermitian

$$\hat{L}_x^\dagger = (\hat{y}\hat{p}_z - \hat{z}\hat{p}_y)^\dagger = (\hat{y}\hat{p}_z)^\dagger - (\hat{z}\hat{p}_y)^\dagger = \hat{p}_z\hat{y} - \hat{p}_y\hat{z} = \hat{L}_x$$

OK

One can show that also the other components are Hermitian operator

Angular momentum

The most interesting observation is property of the angular momentum is that the different component do not commute

$$[L_x, L_y] = [(y p_z - z p_y), (z p_x - x p_z)]$$

*let me avoid ^

Note:

$$\begin{aligned} [A-B, C-D] &= (A-B)(C-D) - (C-D)(A-B) = \\ &= (A-B)C - (A-B)D - C(A-B) + D(A-B) = \\ &= AC - BC - AD + BD - CA + CB + DA - DB = \\ &= [A, C] - [B, C] - [A, D] + [B, D] \end{aligned}$$

Angular momentum

The most interesting observation is property of the angular momentum is that the different component do not commute

$$[L_x, L_y] = [(yp_z - zp_y), (zp_x - xp_z)]$$

A B C D

*let me avoid ^

Note:

$$[A-B, C-D] = [A, C] - [B, C] - [A, D] + [B, D]$$

$$[L_x, L_y] = [yp_z, zp_x] - [zp_y, zp_x] - [yp_z, xp_z] + [zp_y, xp_z]$$

Angular momentum

The most interesting observation is property of the angular momentum is that the different component do not commute

$$[L_x, L_y] = [(y p_z - z p_y), (z p_x - x p_z)]$$

A B C D

*let me omit ^

Note:

$$[A-B, C-D] = [A, C] - [B, C] - [A, D] + [B, D]$$

$$[L_x, L_y] = [y p_z, z p_x] - [z p_y, z p_x] - [y p_z, x p_z] + [z p_y, x p_z]$$

$$[z p_y, z p_x] = z p_y z p_x - z p_x z p_y = z z p_y p_x - z z p_x p_y = 0$$

Angular momentum

The most interesting observation is property of the angular momentum is that the different component do not commute

$$[L_x, L_y] = [(yp_z - zp_y), (zp_x - xp_z)]$$

A B C D

*let me avoid ^

Note:

$$[A-B, C-D] = [A, C] - [B, C] - [A, D] + [B, D]$$

$$[L_x, L_y] = [yp_z, zp_x] - \cancel{[zp_y, zp_x]} - \cancel{[yp_z, xp_z]} + [zp_y, xp_z]$$

$$[L_x, L_y] = [yp_z, zp_x] + [zp_y, xp_z]$$

Angular momentum

$$\begin{aligned} [L_x, L_y] &= [y p_z, z p_x] + [z p_y, x p_z] = \\ &= y p_z z p_x - z p_x y p_z + z p_y x p_z - x p_z z p_y = \\ &= y p_x p_z z - y p_x z p_z + p_y x z p_z - x p_y p_z z = \\ &= y p_x [p_z, z] + x p_y [z, p_z] \end{aligned}$$

..but.. $[\hat{r}_i, \hat{p}_j] = i\hbar \delta_{ij}$

$$[L_x, L_y] = i\hbar [-y p_x + x p_y] = i\hbar L_z$$

Angular momentum

If you repeat the calculations for the other commutators:

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

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

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

The three components of the angular momentum operator are incompatible observables and do not represent mutually consistent observables

If a quantum system is in a state in which one of the Cartesian components of the angular momentum is known with certainty, measurements of two other components will produce uncertain results

Angular momentum

But what about L^2 , the square of the magnitude of the angular momentum

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

$$[\hat{L}^2, L_x] = [L_x^2, L_x] + [L_y^2, L_x] + [L_z^2, L_x]$$

↓

I can use $[L_x, L_y] = i\hbar L_z = L_x L_y - L_y L_x$

$$[L_y L_y, L_x] = L_y L_y L_x - L_x L_y L_y = L_y L_y L_x - i\hbar L_z L_y - L_y L_x L_y$$

$$[L_y L_y, L_x] = L_y [L_y, L_x] - i\hbar L_z L_y = -i\hbar (L_y L_z + L_z L_y)$$

Angular momentum

But what about L^2 , the square of the magnitude of the angular momentum

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

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

$$[\hat{L}_y \hat{L}_y, \hat{L}_x] = -i\hbar(\hat{L}_y \hat{L}_z + \hat{L}_z \hat{L}_y)$$

similarly one obtains

$$[\hat{L}_z \hat{L}_z, \hat{L}_x] = i\hbar(\hat{L}_y \hat{L}_z + \hat{L}_z \hat{L}_y)$$

Angular momentum

Thus:

$$\begin{aligned} [L^2, L_x] &= [\cancel{L_x^2}, L_x] + [L_y^2, L_x] + [L_z^2, L_x] = \\ &= -i\hbar(L_y L_z + L_z L_y) + i\hbar(L_y L_z + L_z L_y) = 0 \end{aligned}$$

Similarly one obtains

$$[L^2, L_y] = 0$$

$$[L^2, L_z] = 0$$

Angular momentum

Thus:

$$[\hat{L}^2, \hat{L}_x] = 0$$

$$[\hat{L}^2, \hat{L}_y] = 0$$

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

The operator of the square of the angular momentum and any component of the angular momentum are compatible observables

Obviously they have common eigenvectors...

Angular momentum

The angular momentum operator is fundamental in quantum theory

The main reason is the fact that many fundamental interactions in nature are described by central potentials (e.g. Coulomb potential between electrically charged particles)

In classical mechanics, systems with a central potential do conserve the angular momentum.

In a quantum mechanical system characterized by a central potential, its Hamiltonian commutes with all components of the angular momentum and L^2

Angular momentum

In a quantum mechanical system characterized by a central potential, its Hamiltonian commutes with all components of the angular momentum and L^2

To prove that one should show that the L^2 and $L_{x,y,z}$ commute both with the kinetic energy and with the potential energy.

The former part can be easily shown by $[L^2, p] = [L_{x,y,z}, p] = 0$. For the latter part we would need to know the central potential expression...

However, vanishing of the commutators of angular momentum operators and the Hamiltonian means that they have common eigenvectors. This can significantly simplify finding eigenvalues and eigenvectors of the Hamiltonian

Angular momentum

In a quantum mechanical system characterized by a central potential, its Hamiltonian commutes with all components of the angular momentum and L^2

Vanishing of the commutators of angular momentum operators and the Hamiltonian means that they have common eigenvectors

The eigenvalues of L^2 and $L_{x,y,z}$ can be found using only the commutations relations seen previously.

Repres. of Orbital Angular Momentum

Let's use spherical coordinates :

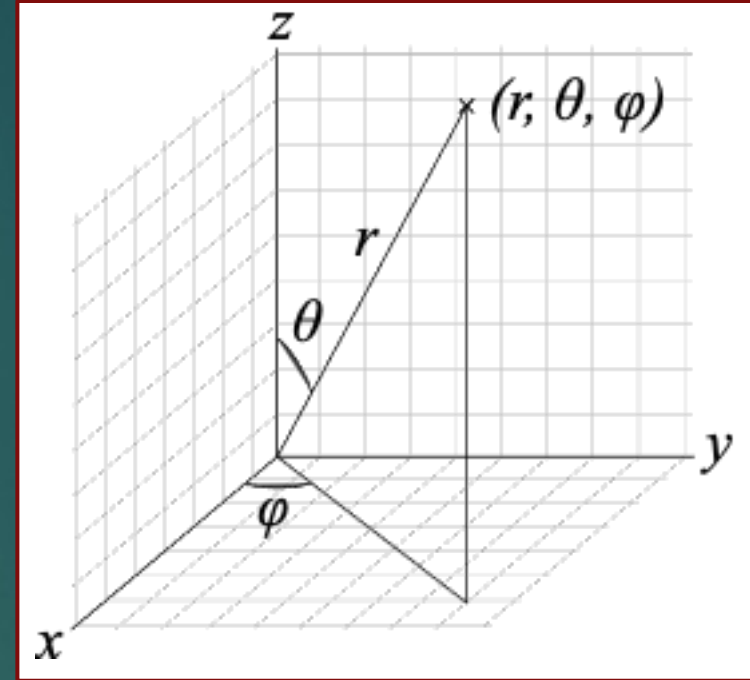
$$x = r \sin \theta \cos \varphi$$

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

$$z = r \cos \theta$$

$$r = \sqrt{x^2 + y^2 + z^2}$$

$$\frac{\partial r}{\partial x} = \frac{x}{\sqrt{x^2 + y^2 + z^2}} = \frac{x}{r} = \frac{\cancel{r} \sin \theta \cos \varphi}{\cancel{r}}$$



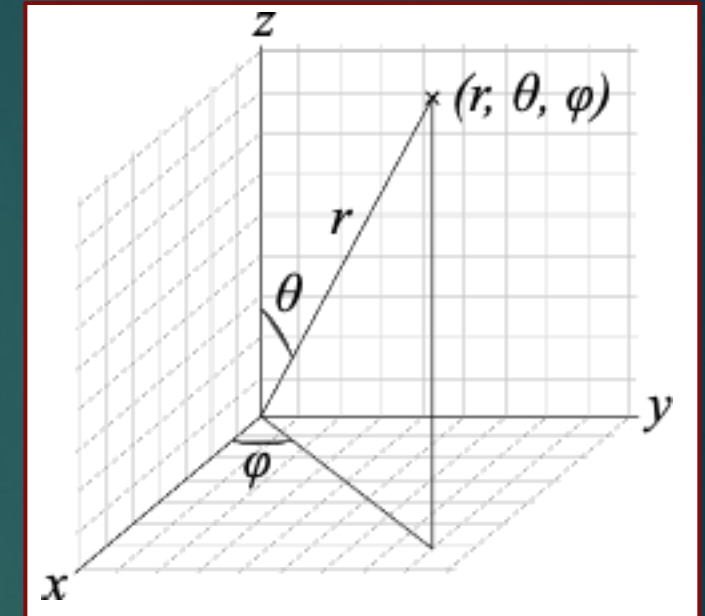
Repres. of Orbital Angular Momentum

Let's use spherical coordinates :

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

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

$$z = r \cos \theta$$



$$\cos \theta = \frac{z}{\sqrt{x^2 + y^2 + z^2}}$$

and $\tan \theta = y/x$

$$\frac{\partial \theta}{\partial x} = \frac{\cos \theta \cos \varphi}{r}$$

and similarly

$$\frac{\partial \varphi}{\partial x} = \frac{\sin \varphi}{r \sin \theta}$$

Repres. of Orbital Angular Momentum

Let's use spherical coordinates :

$$\frac{\partial r}{\partial x} = \sin \theta \cos \varphi \qquad \frac{\partial \theta}{\partial x} = \frac{\cos \theta \cos \varphi}{r} \qquad \frac{\partial \varphi}{\partial x} = \frac{\sin \varphi}{r \sin \theta}$$

We can write (chain rule):

$$\begin{aligned} \frac{\partial}{\partial x} &= \frac{\partial r}{\partial x} \frac{\partial}{\partial r} + \frac{\partial \theta}{\partial x} \frac{\partial}{\partial \theta} + \frac{\partial \varphi}{\partial x} \frac{\partial}{\partial \varphi} \\ &= \sin \theta \cos \varphi \frac{\partial}{\partial r} + \frac{\cos \theta \cos \varphi}{r} \frac{\partial}{\partial \theta} + \frac{\sin \varphi}{r \sin \theta} \frac{\partial}{\partial \varphi} \end{aligned}$$

Repres. of Orbital Angular Momentum

Working similarly with dy and dz we obtain:

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

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

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

which can be now inserted in the expression of momentum coord.:

$$L_x = -i\hbar y \frac{\partial}{\partial z} + i\hbar z \frac{\partial}{\partial y}$$

$$L_y = -i\hbar z \frac{\partial}{\partial x} + i\hbar x \frac{\partial}{\partial z}$$

$$L_z = -i\hbar x \frac{\partial}{\partial y} + i\hbar y \frac{\partial}{\partial x}$$

Repres. of Orbital Angular Momentum

Using these equations together:

$$\begin{aligned}\frac{\partial}{\partial x} &= \sin \theta \cos \varphi \frac{\partial}{\partial r} + \frac{\cos \theta \cos \varphi}{r} \frac{\partial}{\partial \theta} - \frac{\sin \varphi}{r \sin \theta} \frac{\partial}{\partial \varphi} \\ \frac{\partial}{\partial y} &= \sin \theta \sin \varphi \frac{\partial}{\partial r} + \frac{\cos \theta \sin \varphi}{r} \frac{\partial}{\partial \theta} + \frac{\cos \varphi}{r \sin \theta} \frac{\partial}{\partial \varphi} \\ \frac{\partial}{\partial z} &= \cos \theta \frac{\partial}{\partial r} - \frac{\sin \theta}{r} \frac{\partial}{\partial \theta}\end{aligned}$$

$$L_x = -i\hbar y \frac{\partial}{\partial z} + i\hbar z \frac{\partial}{\partial y}$$

$$L_y = -i\hbar z \frac{\partial}{\partial x} + i\hbar x \frac{\partial}{\partial z}$$

$$L_z = -i\hbar x \frac{\partial}{\partial y} + i\hbar y \frac{\partial}{\partial x}$$

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

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

$$z = r \cos \theta$$

e.g for L_z :

$$\begin{aligned}L_z &= -i\hbar x \frac{\partial}{\partial y} + i\hbar y \frac{\partial}{\partial x} = -i\hbar r \sin \theta \cos \varphi \left(\sin \theta \sin \varphi \frac{\partial}{\partial r} + \frac{\cos \theta \sin \varphi}{r} \frac{\partial}{\partial \theta} + \frac{\cos \varphi}{r \sin \theta} \frac{\partial}{\partial \varphi} \right) \\ &\quad + i\hbar r \sin \theta \sin \varphi \left(\sin \theta \cos \varphi \frac{\partial}{\partial r} + \frac{\cos \theta \cos \varphi}{r} \frac{\partial}{\partial \theta} - \frac{\sin \varphi}{r \sin \theta} \frac{\partial}{\partial \varphi} \right)\end{aligned}$$

Repres. of Orbital Angular Momentum

Using these equations together...

e.g for L_z :

$$L_z = -i\hbar x \frac{\partial}{\partial y} + i\hbar y \frac{\partial}{\partial x} = -i\hbar r \sin \theta \cos \varphi \left(\sin \theta \sin \varphi \frac{\partial}{\partial r} + \frac{\cos \theta \sin \varphi}{r} \frac{\partial}{\partial \theta} + \frac{\cos \varphi}{r \sin \theta} \frac{\partial}{\partial \varphi} \right) \\ + i\hbar r \sin \theta \sin \varphi \left(\sin \theta \cos \varphi \frac{\partial}{\partial r} + \frac{\cos \theta \cos \varphi}{r} \frac{\partial}{\partial \theta} - \frac{\sin \varphi}{r \sin \theta} \frac{\partial}{\partial \varphi} \right) =$$

$$= -i\hbar r \sin \theta \cos \varphi \left(\frac{\cos \varphi}{r \sin \theta} \frac{\partial}{\partial \varphi} \right) + i\hbar r \sin \theta \sin \varphi \left(-\frac{\sin \varphi}{r \sin \theta} \frac{\partial}{\partial \varphi} \right)$$

$$= -i\hbar (\sin^2 \varphi + \cos^2 \varphi) \frac{\partial}{\partial \varphi} = -i\hbar \frac{\partial}{\partial \varphi}$$

||
1

Repres. of Orbital Angular Momentum

Similarly for L_x and L_y , I can obtain:

$$L_x = -i \hbar \left(-\sin \varphi \frac{\partial}{\partial \theta} - \cos \varphi \cot \theta \frac{\partial}{\partial \varphi} \right)$$

$$L_y = -i \hbar \left(\cos \varphi \frac{\partial}{\partial \theta} - \sin \varphi \cot \theta \frac{\partial}{\partial \varphi} \right)$$

$$L_z = -i \hbar \frac{\partial}{\partial \varphi}$$

And also L^2 :

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

All angular momentum operators can be naturally represented as differential operators involving spherical coordinates...

Repres. of Orbital Angular Momentum

Moreover, if you write the Laplacian operator in spherical coordinates you will get:

$$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2} \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} \right]$$

Hey, the second part is identical to the square of the ang. Momentum

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

Thus, we can rewrite the kinetic energy operator in spherical coordinates as:

$$K = \frac{-\hbar^2 \nabla^2}{2m} = \frac{-\hbar^2}{2m r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{L^2}{2m r^2}$$

Eigenvectors of Angular Momentum

Let's start with L_z because it contains derivatives with respect just to φ :

$$L_z = -i\hbar \frac{\partial}{\partial \varphi}$$

I can write the eigen equation as:

$$L_z \Phi(\varphi) = m\hbar \Phi(\varphi)$$

We have chosen to write the eigenvalue in the form $m\hbar$.

By using the expression of L_z I can write:

$$-i\hbar \frac{d\Phi_m}{d\varphi} = m\hbar \Phi_m$$

with an obvious solution:

$$\Phi_m(\varphi) = \frac{1}{\sqrt{2\pi}} e^{im\varphi}$$

Eigenvectors of Angular Momentum

Let's start with L_z :

$$L_z = -i\hbar \frac{\partial}{\partial \varphi}$$

I can write the eigen equation as:

$$L_z \Phi(\varphi) = m\hbar \Phi(\varphi)$$

With:
$$\Phi_m(\varphi) = \frac{1}{\sqrt{2\pi}} e^{im\varphi}$$

To ensure that L_z is Hermitian, this function and its derivative must be continuous:

$$\Phi_m(\varphi + 2\pi) = \Phi_m(\varphi)$$

thus, m must be integer

Eigenvectors of Angular Momentum

With: $\Phi_m(\varphi) = \frac{1}{\sqrt{2\pi}} e^{im\varphi}$

To ensure that L_z is Hermitian, this function must be continuous*:

$\Phi_m(\varphi + 2\pi) = \Phi_m(\varphi)$ thus, m must be integer

* Two motivations for the continuity of the function:

1. $|\Phi_m|^2 = \text{probability density} \Rightarrow$ must be continuous
2. to ensure L_z is Hermitian

$$\langle \Phi | L_z | \Phi \rangle^* = \langle \Phi | L_z | \Phi \rangle \Rightarrow \left(\int \Phi^* L_z \Phi d\varphi \right)^* = \int \Phi^* L_z \Phi d\varphi$$

Eigenvectors of Angular Momentum

With:
$$\Phi_m(\varphi) = \frac{1}{\sqrt{2\pi}} e^{im\varphi}$$

To ensure that L_z is Hermitian, this function must be continuous*:

$$\Phi_m(\varphi + 2\pi) = \Phi_m(\varphi) \quad \text{thus, } m \text{ must be integer}$$

Hence, we find that the angular momentum around the z axis is quantized, with units of angular momentum of \hbar .

Eigenvectors of Angular Momentum

With:
$$\Phi_m(\varphi) = \frac{1}{\sqrt{2\pi}} e^{im\varphi}$$

To ensure that L_z is Hermitian, this function must be continuous*:

$$\Phi_m(\varphi + 2\pi) = \Phi_m(\varphi) \quad \text{thus, } m \text{ must be integer}$$

Our choice of the z axis was quite arbitrary, and we could equally well have chosen the x or y axes as the polar axes for our coordinate system, in which case we would see quite clearly that the eigenfunctions of the L_x or L_y operators are of similar form to those of L_z , but they are not the same!

Eigenfunctions of L^2

Remembering that for L_x , L_y and L_z :

$$L_x = -i \hbar \left(-\sin \varphi \frac{\partial}{\partial \theta} - \cos \varphi \cot \theta \frac{\partial}{\partial \varphi} \right)$$

$$L_y = -i \hbar \left(\cos \varphi \frac{\partial}{\partial \theta} - \sin \varphi \cot \theta \frac{\partial}{\partial \varphi} \right)$$

$$L_z = -i \hbar \frac{\partial}{\partial \varphi}$$

And also L^2 :

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

All angular momentum operators can be naturally represented as differential operators involving spherical coordinates...

Eigenfunctions of L^2

Moreover, if you write the Laplacian operator in spherical coordinates you will get:

$$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2} \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} \right]$$

If we take the θ and φ part of the Laplacian operator in spherical polar coordinates, with the notation:

$$\nabla_{\theta, \varphi}^2 = \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \varphi^2}$$

Then:

$$L^2 = -\hbar^2 \nabla_{\theta, \varphi}^2$$

Eigenfunctions of L^2

We have already found the eigenvalue of L_z , let's now try to get the eigenvectors that we know are in common, for L^2 and L_z .

We should find functions that are simultaneously satisfying:

$$\nabla_{\theta,\varphi}^2 Y_{l,m}(\theta, \varphi) = -l(l+1) Y_{l,m}(\theta, \varphi)$$

And also the previous eq.:

$$-i\hbar \frac{d\Phi_m}{d\varphi} = m\hbar \Phi_m$$

We anticipate the solution by writing the eigenvalue in the form $-l(l+1)$ which are just arbitrary numbers to be determined, still a guess now

$Y_{l,m}(\theta, \phi)$ are these functions in question, also anticipating the answer.

Of course, $Y_{l,m}(\theta, \phi)$ must be orthonormal

Separation of variables

The simultaneous eigenstates of L^2 and L_z , $Y_{l,m}(\theta, \varphi)$, are known as the spherical harmonics.

I can write the eigenstate in the separable form (this is a still a guess, but we will see that this hypothesis is true):

$$Y_{l,m}(\theta, \varphi) = \Theta_{l,m}(\theta) \Phi_m(\varphi)$$

Substituting this into

$$L^2 Y_{l,m}(\theta, \varphi) = l(l+1) \hbar^2 Y_{l,m}(\theta, \varphi)$$

or

$$\nabla_{\theta,\varphi}^2 Y_{l,m}(\theta, \varphi) = -l(l+1) Y_{l,m}(\theta, \varphi)$$

Separation of variables

$$Y_{l,m}(\theta, \varphi) = \Theta_{l,m}(\theta) \Phi_m(\varphi)$$

Substituting this into

$$\nabla_{\theta,\varphi}^2 Y_{l,m}(\theta, \varphi) = -l(l+1) Y_{l,m}(\theta, \varphi)$$

Gives:

$$\frac{\Phi_m(\varphi)}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) \Theta_{l,m}(\theta) + \frac{\Theta_{l,m}(\theta)}{\sin^2 \theta} \frac{\partial^2 \Phi_m(\varphi)}{\partial \varphi^2} = -l(l+1) \Theta_{l,m}(\theta) \Phi_m(\varphi)$$

Separation of variables

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$$\frac{\Phi_m(\varphi)}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) \Theta_{l,m}(\theta) + \frac{\Theta_{l,m}(\theta)}{\sin^2 \theta} \frac{\partial^2 \Phi_m(\varphi)}{\partial \varphi^2} = -l(l+1) \Theta_{l,m}(\theta) \Phi_m(\varphi)$$

And multiplying by $\sin^2 \theta / \Theta_{l,m}(\theta) \Phi_m(\varphi)$ and rearranging it:

$$\frac{1}{\Phi_m(\varphi)} \frac{\partial^2 \Phi_m(\varphi)}{\partial \varphi^2} = -l(l+1) \sin^2 \theta - \frac{\sin \theta}{\Theta_{l,m}(\theta)} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) \Theta_{l,m}(\theta)$$

The left hand part depends only on φ

While the right hand side depends only on θ

And they must be equal to a constant which we choose to be $-m^2$

Separation of variables

Gives:

$$\frac{\Phi_m(\varphi)}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) \Theta_{l,m}(\theta) + \frac{\Theta_{l,m}(\theta)}{\sin^2 \theta} \frac{\partial^2 \Phi_m(\varphi)}{\partial \varphi^2} = -l(l+1) \cancel{\Theta_{l,m}(\theta)} \cancel{\Phi_m(\varphi)} = \text{constant}$$

And multiplying by $\sin^2 \theta / \Theta_{l,m}(\theta) \Phi_m(\varphi)$ and rearranging it:

$$\frac{1}{\Phi_m(\varphi)} \frac{\partial^2 \Phi_m(\varphi)}{\partial \varphi^2} = -l(l+1) \sin^2 \theta - \frac{\sin \theta}{\Theta_{l,m}(\theta)} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) \Theta_{l,m}(\theta)$$

The left-hand part depends only on φ

While the right-hand side depends only on θ

And they must be equal to a constant which we choose to be $-m^2$

Eigenfunctions of L^2

Taking the left-hand side of

$$\frac{1}{\Phi_m(\varphi)} \frac{\partial^2 \Phi_m(\varphi)}{\partial \varphi^2} = -l(l+1) \sin^2 \theta - \frac{\sin \theta}{\Theta_{l,m}(\theta)} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) \Theta_{l,m}(\theta) = -m^2$$

We have:

$$\frac{d^2 \Phi_m(\varphi)}{d\varphi^2} = -m^2 \Phi_m(\varphi)$$

The solutions to an equation like this are of the form $\sin(m\varphi)$, $\cos(m\varphi)$ or $\exp(im\varphi)$.

We choose the exponential form, so it is also a solution of the L_z eigen equation

$$L_z \Phi(\varphi) = m\hbar \Phi(\varphi)$$

Eigenfunctions of L^2

Taking the left hand side of

$$\frac{1}{\Phi_m(\varphi)} \frac{\partial^2 \Phi_m(\varphi)}{\partial \varphi^2} = -l(l+1) \sin^2 \theta - \frac{\sin \theta}{\Theta_{l,m}(\theta)} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) \Theta_{l,m}(\theta) = -m^2$$

We have:

$$\frac{d^2 \Phi_m(\varphi)}{d\varphi^2} = -m^2 \Phi_m(\varphi)$$

We choose the exponential form $\exp(im\varphi)$

We expect that it and its derivative are continuous.

As a result, this wavefunction must be cyclic every 2π of angle φ .

Hence, m must be an integer.

Legendre functions

Taking the right-hand side of

$$\frac{1}{\Phi_m(\varphi)} \frac{\partial^2 \Phi_m(\varphi)}{\partial \varphi^2} = -l(l+1) \sin^2 \theta - \frac{\sin \theta}{\Theta_{l,m}(\theta)} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) \Theta_{l,m}(\theta) = -m^2$$

And multiplying by $\Theta_{l,m}(\theta) / \sin^2 \theta$ we have:

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

This is the **Legendre equation**,

and the solutions to it are the associated Legendre functions,

$$\Theta(\theta) = P_l^m(\cos \theta)$$

Legendre functions

The solutions $\Theta(\theta) = P_l^m(\cos\theta)$ to this equation

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

Require that

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

$$-l \leq m \leq l \quad (\text{with } m \text{ integer})$$

The associated Legendre functions can be defined by the formula:

$$P_l^m(x) = (-1)^l \frac{(1-x^2)^{m/2}}{2^l l!} \left(\frac{d}{dx} \right)^{l+m} (1-x^2)^l,$$

Legendre functions

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

$$-l \leq m \leq l \quad (\text{with } m \text{ integer})$$

The associated Legendre functions can be defined by the formula:

$$P_l^m(x) = (-1)^m \frac{(1-x^2)^{m/2}}{2^l l!} \left(\frac{d}{dx} \right)^{l+m} (1-x^2)^l,$$

For example, for $l=0$ and $m=0$

$$P_0^0(x) = 1$$

for $l=1$ and $m=0$

$$P_1^0(x) = x$$

Legendre functions

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

$$-l \leq m \leq l \quad (\text{with } m \text{ integer})$$

The associated Legendre functions can be defined by the formula:

$$P_l^m(x) = (-1)^m \frac{(1-x^2)^{m/2}}{2^l l!} \left(\frac{d}{dx}\right)^{l+m} (1-x^2)^l,$$

$l=0$

$$m=0 \quad P_0^0(x) = 1$$

$l=1$

$$P_1^0(x) = x$$

$$m=1 \quad P_1^1(x) = (1-x^2)^{1/2}$$

$$m=-1 \quad P_1^{-1}(x) = -\frac{1}{2}(1-x^2)^{1/2}$$

$l=2$

$$P_2^0(x) = \frac{1}{2}(3x^2 - 1)$$

$$P_2^1(x) = 3x(1-x^2)^{1/2}$$

$$P_2^{-1}(x) = -\frac{1}{2}x(1-x^2)^{1/2}$$

$$m=2 \quad P_2^2(x) = 3(1-x^2)$$

$$m=-2 \quad P_2^{-2}(x) = \frac{1}{8}(1-x^2)$$

Legendre functions

We can see by inspection that these functions $P_m(x)$ have the following:

- the highest power of the argument x is always x^l ;
- the functions for a given l for $+m$ and $-m$ are identical (other than for differences in numerical prefactors).

	$l=0$	$l=1$	$l=2$
$m=0$	$P_0^0(x) = 1$	$P_1^0(x) = x$	$P_2^0(x) = \frac{1}{2}(3x^2 - 1)$
$m=1$		$P_1^1(x) = (1-x^2)^{1/2}$	$P_2^1(x) = 3x(1-x^2)^{1/2}$
$m=-1$		$P_1^{-1}(x) = -\frac{1}{2}(1-x^2)^{1/2}$	$P_2^{-1}(x) = -\frac{1}{2}x(1-x^2)^{1/2}$
		$m=2$	$P_2^2(x) = 3(1-x^2)$
		$m=-2$	$P_2^{-2}(x) = \frac{1}{8}(1-x^2)$

Eigenvectors of Angular Momentum

Putting all together, we have again the eigen equation:

$$L^2 Y_{l,m}(\theta, \varphi) = l(l+1) \hbar^2 Y_{l,m}(\theta, \varphi)$$

Where $Y_{l,m}$ are the **spherical harmonics** as eigenfunction

$$Y_{l,m}(\theta, \varphi) = P_{l,m}(\cos \theta) e^{im\varphi}$$

And they must be normalized

Eigenvectors of Angular Momentum

We finally have:

$$Y_{l,m}(\theta, \varphi) = (-1)^m \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} P_{l,m}(\cos \theta) e^{im\varphi}$$

Where $P_{l,m}$ are the associated Legendre Polynomials

$$P_l^m(x) = (-1)^l \frac{(1-x^2)^{m/2}}{2^l l!} \left(\frac{d}{dx}\right)^{l+m} (1-x^2)^l,$$

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

$-l \leq m \leq l$ (with m integer)

Eigenvectors of Angular Momentum

We finally have:

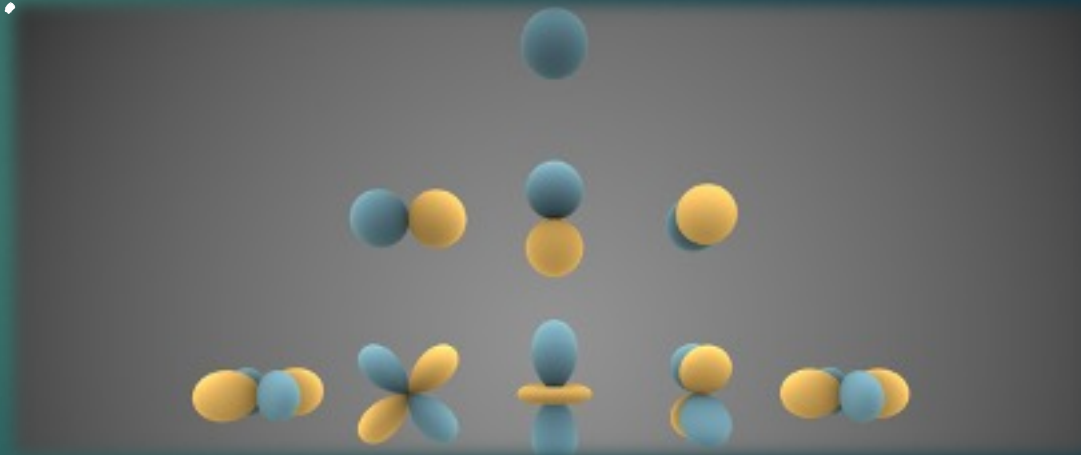
$$Y_{l,m}(\theta, \varphi) = (-1)^m \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} P_{l,m}(\cos \theta) e^{im\varphi}$$

The spherical harmonics for $l=0,1,2$ are:

$$Y_{0,0} = \frac{1}{\sqrt{4\pi}}$$

$$Y_{1,0} = \sqrt{\frac{3}{4\pi}} \cos \theta \quad Y_{1,\pm 1} = \mp \sqrt{\frac{3}{8\pi}} \sin \theta e^{\pm i\varphi}$$

$$Y_{2,0} = \sqrt{\frac{5}{16\pi}} (3 \cos^2 \theta - 1) \quad Y_{2,\pm 1} = \mp \sqrt{\frac{15}{8\pi}} \sin \theta \cos \theta e^{\pm i\varphi} \quad Y_{2,\pm 2} = \sqrt{\frac{15}{32\pi}} \sin^2 \theta e^{\pm 2i\varphi}$$



“s,p,d,f” notation

$$Y_{l,m}(\theta, \varphi) = (-1)^m \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} P_{l,m}(\cos \theta) e^{im\varphi}$$

Spherical

harmonics plots

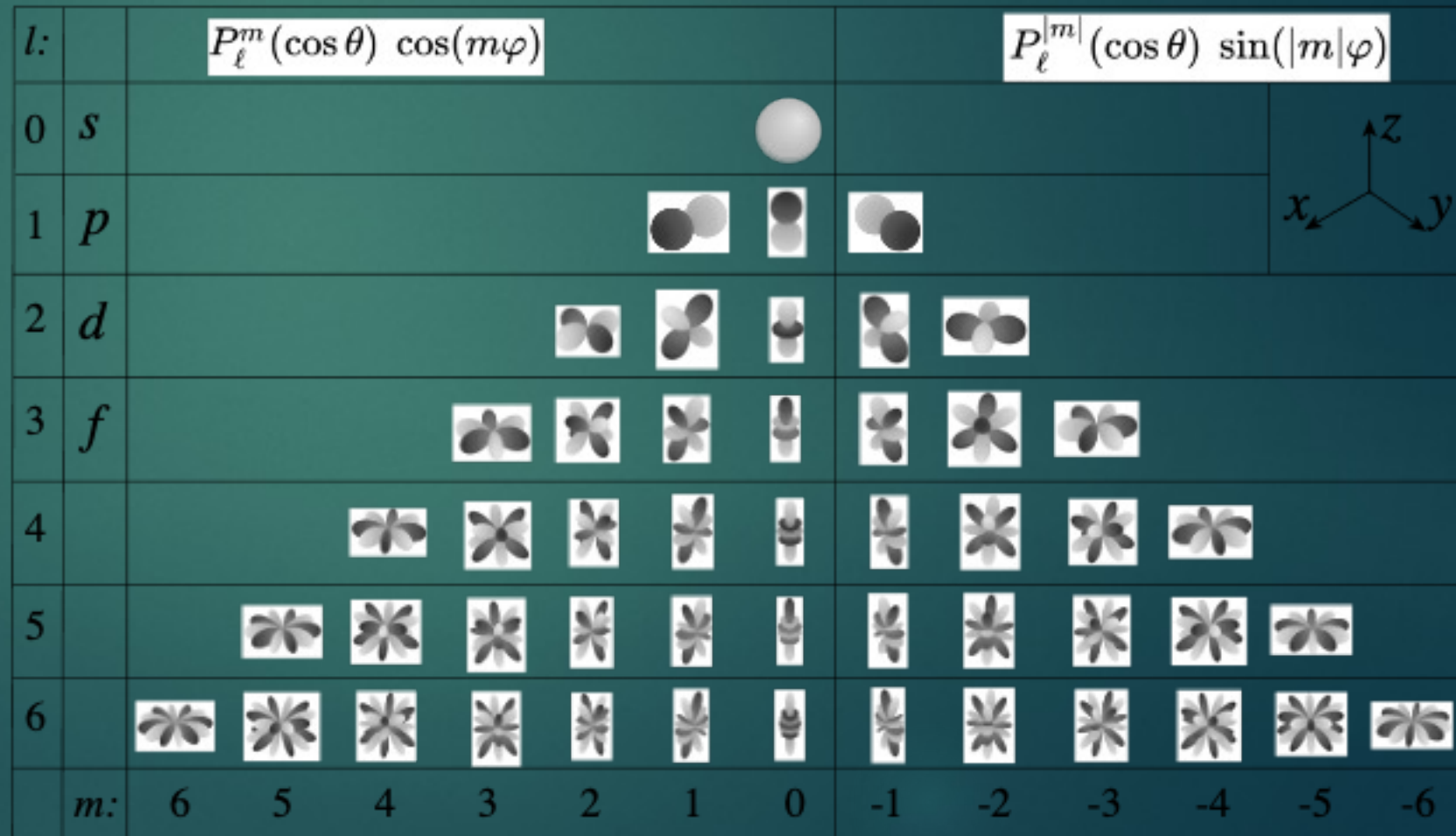
$r = Y_{l,m}(\Phi, \varphi)$:

s: “spectral”

p: “principal”

d: “diffuse”

f: “fundamental”



Eigenvectors of Angular Momentum

One can easily check that the spherical harmonics are also eigenfunctions of the L_z operator

$$L_z Y_{l,m}(\theta, \varphi) = m \hbar Y_{l,m}(\theta, \varphi)$$

With $m \hbar$ eigenvalues of L_z

Angular momentum

1. The eigenvalue of operator L^2 is equal to $\hbar^2 l(l+1)$, where l determines the maximum eigenvalue of the operator L_z , $\hbar l$
2. l can take integer values: 0;1;2;3...
3. The eigenvalue of operator L_z is equal to $\hbar m$. Allowed values of m start at $-l$ and advance increasing by one until it reaches l

For instance, for $l=0$; the only possible value of m is zero; for $l=1$, we can have states with $m=-1,0,1$; in general for integer l $m = -l, -l+1, \dots, 0, \dots, l-1, l$

Dirac notation for angular momentum

The eigenvalue of operator L^2 is equal to $\hbar^2 l(l+1)$, where l determines the maximum eigenvalue of the operator L_z , $\hbar l$ while a general eigenvalue m is $-l \leq m \leq l$

l is often referred to as the "angular momentum," and m is often called a "magnetic" quantum number

Then the eigenvectors of operators L^2 and L_z , are usually indicated by the Dirac notation:

$$|l, m\rangle$$

Dirac notation for angular momentum

Then the eigenvectors of operators L^2 and L_z , are usually indicated by the Dirac notation:

$$|l, m\rangle$$

Then the eigenvalue equations for L^2 and L_z are:

$$\hat{L}^2 |l, m\rangle = l(l + 1)\hbar^2 |l, m\rangle$$

Instead of

$$L^2 Y_{l,m}(\theta, \varphi) = l(l + 1)\hbar^2 Y_{l,m}(\theta, \varphi)$$

And

$$\hat{L}_z |l, m\rangle = m\hbar |l, m\rangle$$

Instead of

$$L_z Y_{l,m}(\theta, \varphi) = m\hbar Y_{l,m}(\theta, \varphi)$$