Angular Momentum

Angular momentum: is as important in classical mechanics as in quantum mechanics. It is particularly useful for studying the dynamics of systems that move under the influence of *spherically symmetric*, or *central*, potentials, $V(\vec{r}) = V(r)$, for the orbital angular momenta of these systems are *conserved*.

One of the cornerstones of Bohr's model of the hydrogen atom (where the electron moves in the proton's Coulomb potential, a central potential) is based on the quantization of angular momentum.

The total angular momentum,$(\vec{J})$, combines both the spin and orbital angular momentum of a particle (or a system), namely $\vec{J} = \vec{L} + \vec{S}$.

where $\vec{L}$ is orbital angular momentum, $\vec{S}$ is spin angular momentum or just spin.

Additionally, angular momentum plays a critical role in the description of molecular rotations, the motion of electrons in atoms, and the motion of nucleons in nuclei.

I. Orbital angular momentum (L)

A. General Formalism of angular momentum

In classical physics the angular momentum of a particle with momentum $\vec{p}$ and position $\vec{r}$ is defined by

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

$$\vec{L} = (yp_z - zp_y)\hat{\imath} + (zp_x - xp_z)\hat{\jmath} + (xp_y - yp_x)\hat{k}$$

The orbital angular momentum operator $\hat{\vec{L}}$ can be obtained at once by replacing $\vec{r}$ and $\vec{p}$ by the corresponding operators in the position representation, $\hat{\vec{R}}$ and $\hat{\vec{P}} = -i\hbar\vec{\nabla} = \frac{\hbar}{i}\vec{\nabla}$:

$$\hat{\vec{L}} = \hat{\vec{R}} \times \hat{\vec{P}} = -i\hbar(\hat{\vec{R}} \times \vec{\nabla})$$

The Cartesian components of $\hat{\vec{L}}$ are

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

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

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

Clearly, angular momentum does not exist in a one-dimensional space. We should mention that the components $\hat{L}_x$, $\hat{L}_y$, $\hat{L}_z$, and the square of $\hat{\vec{L}}$,

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

$$\hat{\vec{L}}^2 = r^2p^2 - (r \cdot p)^2 + i\hbar r \cdot p$$

are all Hermitian.

In quantum mechanics the classical vectors $\hat{\vec{R}}$, $\hat{\vec{P}}$ and $\hat{\vec{L}}$ become operators. More precisely, they give us triplets of operators:

$$\hat{\vec{R}} \to (\hat{X}, \hat{Y}, \hat{Z}), \quad \hat{\vec{P}} \to (\hat{P}_x, \hat{P}_y, \hat{P}_z), \quad \hat{\vec{L}} \to (\hat{L}_x, \hat{L}_y, \hat{L}_z)$$

Commutators

$$[A, B] = AB - BA$$

B. Properties of Angular Momentum

Since $\hat{X}$, $\hat{Y}$, and $\hat{Z}$ mutually commute and so do $\hat{P}_x$, $\hat{P}_y$, and $\hat{P}_z$, and since

$[\hat{X}, \hat{P}_x] = i\hbar, [\hat{Y}, \hat{P}_y] = i\hbar, [\hat{Z}, \hat{P}_z] = i\hbar$, we have

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

Similar calculation yields the other two commutation relations; but it is much simpler to infer them from equation above by means of a *cyclic permutation* of the xyz components, $x \to y \to z \to x$:

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

The three equations are equivalent to the vectorial commutation relation:

$$\hat{L} \times \hat{L} = i\hbar\hat{L} ,$$

Note that this can only be true for operators; since, for regular vectors, $\hat{L} \times \hat{L} = \mathbf{0}$.

It is easy to show that $\hat{\vec{L}}^2$ does commute with each of the three components: $\hat{L}_x, \hat{L}_y$ *or* $\hat{L}_z$

For example (using $[\hat{L}_x^2, \hat{L}_x] = 0$):

$$[\hat{\vec{L}}^2, \hat{L}_x] = [\hat{L}_y^2 + \hat{L}_z^2, \hat{L}_x] = [\hat{L}_y^2, \hat{L}_x] + [\hat{L}_z^2, \hat{L}_x]$$
$$= \hat{L}_y[\hat{L}_y, \hat{L}_x] + [\hat{L}_y, \hat{L}_x]\hat{L}_y + \hat{L}_z[\hat{L}_z, \hat{L}_x] + [\hat{L}_z, \hat{L}_x]\hat{L}_z$$
$$= -i\hbar(\hat{L}_y\hat{L}_z + \hat{L}_z\hat{L}_y) + i\hbar(\hat{L}_z\hat{L}_y + \hat{L}_y\hat{L}_z) = 0$$

Similarly,

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

which can be summarized as

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

Physically, this means that one can find simultaneous eigenfunctions of $\vec{L}^2$ and one of the components of $\vec{L}$, implying that both the magnitude of the angular momentum and one of its components can be precisely determined. Once these are known, they fully specify the angular momentum.

Example:

(a) Calculate the commutators: $[\hat{X}, \hat{L}_x], [\hat{X}, \hat{L}_y]$, and $[\hat{X}, \hat{L}_z]$.
(b) Calculate the commutators: $[\hat{P}_x, \hat{L}_x], [\hat{P}_x, \hat{L}_y]$ and $[\hat{P}_x, \hat{L}_z]$.
(c) Use the results of (a) and (b) to $[\hat{X}, \hat{\vec{L}}^2]$ and $[\hat{P}_x, \hat{\vec{L}}^2]$.

Solution:

(a) The only nonzero commutator which involves $\hat{X}$, and the various components of , $\hat{L}_x$, $\hat{L}_y$, $\hat{L}_z$ is $[\hat{X}, \hat{P}_x] = i\hbar$. Having stated this result, we can easily evaluate the needed commutators.

First, since $\hat{L}_x = \hat{Y}\hat{P}_z - \hat{Z}\hat{P}_y$ involves no $\hat{P}$, the operator $\hat{X}$ commutes separately with $\hat{Y}$, $\hat{P}_z$, $\hat{Z}$, and $\hat{P}_y$; hence

$$[\hat{X}, \hat{L}_x] = [\hat{X}, \hat{Y}\hat{P}_z - \hat{Z}\hat{P}_y] = 0$$

The evaluation of the other two commutators is straightforward:

$$[\hat{X}, \hat{L}_y] = [\hat{X}, \hat{Z}\hat{P}_x - \hat{X}\hat{P}_z] = [\hat{X}, \hat{Z}\hat{P}_x] = \hat{Z}[\hat{X}, \hat{P}_x] = i\hbar\hat{Z},$$
$$[\hat{X}, \hat{L}_z] = [\hat{X}, \hat{X}\hat{P}_y - \hat{Y}\hat{P}_x] = -[\hat{X}, \hat{Y}\hat{P}_x] = -\hat{Y}[\hat{X}, \hat{P}_x] = -i\hbar\hat{Y},$$

(b) The only commutator between $\hat{P}_x$ and the components of $\hat{L}_x$, $\hat{L}_y$, $\hat{L}_z$ that survives is again $[\hat{P}_x, \hat{X}] = -i\hbar$. We may thus infer

$$[\hat{P}_x, \hat{L}_x] = [\hat{P}_x, \hat{Y}\hat{P}_z - \hat{Z}\hat{P}_y] = 0,$$

$$[\hat{P}_x, \hat{L}_y] = [\hat{P}_x, \hat{Z}\hat{P}_x - \hat{X}\hat{P}_z] = -[\hat{P}_x, \hat{X}\hat{P}_z] = -[\hat{P}_x, \hat{X}]\hat{P}_z = i\hbar\hat{P}_z,$$

$$[\hat{P}_x, \hat{L}_z] = [\hat{P}_x, \hat{X}\hat{P}_y - \hat{Y}\hat{P}_x] = [\hat{P}_x, \hat{X}\hat{P}_y] = [\hat{P}_x, \hat{X}]\hat{P}_y = -i\hbar\hat{P}_y,$$

(c) Using the commutators derived in (a) and (b), we infer

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

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

In order to obtain the eigenvalues of $\vec{L}^2$ and one of the components of $\vec{L}$ (typically, $\hat{L}_z$), it is convenient to express the angular momentum operators in spherical polar coordinates: r, θ, ϕ, rather than the Cartesian coordinates x, y, z. The spherical coordinates are related to the Cartesian ones via

$$x = r sin\theta cos\phi;$$
$$y = r sin\theta sin\phi;$$
$$z = r cos\theta;$$

After some algebra, one gets:

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

We thus find that the operators $\hat{L}_x, \hat{L}_y, \hat{L}_z$ and $\vec{L}^2$ depend on θ and ϕ only, that is they are independent on the radial coordinate r. All these operators therefore commute with any function of r,

$$[\hat{L}_x, f(r)] = [\hat{L}_y, f(r)] = [\hat{L}_z, f(r)] = [\vec{L}^2, f(r)] = 0$$

Also, obviously, if a wavefunction depends only on r (but not on θ, ϕ) it can be simultaneously an eigenfunction of $\hat{L}_x, \hat{L}_y, \hat{L}_z$ and $\vec{L}^2$. In all cases, the corresponding eigenvalue will be 0. (This is the only exception to the rule that that eigenvalues of one component (e.g., $\hat{L}_x$) cannot be simultaneously eigenfunctions of the two other components of $\hat{L}$).

Example: Derive equation of $\hat{L}_z$ in Spherical coordinates.
From relation of $\hat{L}_z$ in Cartesian coordinates

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

We can develop the desired partial differentials from the relation between azimuthal angle and position coordinates, or

$$\phi = tan^{-1}(y/x) \quad \Rightarrow y = xtan\phi$$

$$\Rightarrow \frac{\partial y}{\partial \phi} = x\partial(tan\phi) = xsec^2\phi = \frac{x}{cos^2\phi}$$

$$\Rightarrow \partial y = \frac{x\partial\phi}{cos^2\phi}$$

The same relation gives us

$$x = \frac{y}{tan\phi} = y\frac{cos\phi}{sin\phi} = ycos\phi sin^{-1}\phi$$

$$\Rightarrow \frac{\partial x}{\partial \phi} = y(-sins\phi sin^{-1}\phi + cos\phi(-1)sin^{-2}\phi cos\phi)$$

$$= y\left(1 + \frac{cos^2\phi}{sin^2\phi}\right) = -y\left(\frac{sin^2\phi + cos^2\phi}{sin^2\phi}\right) = \frac{-y}{sin^2\phi}$$

$$\Rightarrow \partial x = \frac{-y\partial\phi}{sin^2\phi}$$

Using the partial differentials in the Cartesian formulation for the z component of angular momentum,

$$\hat{L}_z = i\hbar\left(-xcos^2\phi\frac{\partial}{x\partial\phi} + y\left(-sin^2\phi\frac{\partial x}{y\partial\phi}\right)\right)$$

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

$$= -i\hbar\frac{\partial}{\partial\phi}$$

C. Eigenvalues and eigenfunctions of L^2 and L_z

Let us find now the common eigenfunctions to L^2 and L_z, for a single particle. The choice of L_z (rather than, e.g., L_x) is motivated by the simpler expression**.**

I. Eigenvalues of L_z

Since, in spherical coordinates L_z depends only on $\emptyset$, we can denote its eigenvalue by $m\hbar$ and the corresponding eigenfunctions by $\Phi_m(\phi)$. We thus have:

$$\boldsymbol{L_z}\Phi_m(\phi) = m\hbar\Phi_m(\phi)$$

Namely

$$-i\frac{\partial}{\partial\emptyset}\Phi_m(\phi) = m\Phi_m(\phi)$$

The solutions to this equation are

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

This is satisfied for any value of m; however, physically we require the wave function to be single valued (alternatively: continuous), namely $\Phi_m(2\pi) = \Phi_m(0)$, from which we find

$$\boldsymbol{e^{i2\pi m\emptyset} = 0}$$

This equation is satisfied for $m = 0, \pm1, \pm2, \pm3, \ldots$. The eigenvalues of the operator $\boldsymbol{L_z}$ are thus $m\hbar$, with m being integer (positive or negative) or zero. The number m is called the magnetic quantum number, due to the role it plays in the motion of charged particles in magnetic fields.

This means, that when measuring the z-component of an orbital angular momentum, one can only obtain $0, \pm\hbar, \pm2\hbar, \ldots$. Since the choice of the z direction was arbitrary, we see that the component of the orbital angular momentum about any axis is quantized.

II. Simultaneous eigenvalues of $\boldsymbol{L^2}$ and $\boldsymbol{L_z}$

The compatibility theorem tells us that L^2 and L_z thus have simultaneous eigenfunctions. These turn out to be the spherical harmonics, $Y_l^m(\theta,\phi)$. In particular, the eigenvalue equation for L^2 is

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

Where $l = 0,1,2,3,\ldots$ and as we know that

$$Y_l^m(\theta,\phi) = (-1)^m\left[\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}\right]^{1/2} P_L^m(\cos\theta)e^{im\phi}$$

The eigenvalue $l(l+1)\hbar^2$ is degenerate; there exist $(2l+1)$ eigenfunctions corresponding to a given l and they are distinguished by the label m which can take any of the $(2l+1)$ values

$$m = l, l-1, \ldots, l$$

In fact it is easy to show that m labels the eigenvalues of L_z. Since

$$Y_l^m(\theta,\phi) \propto e^{im\phi}$$

We obtain directly that

$$L_z Y_l^m(\theta,\phi) = -i\hbar\frac{\partial}{\partial\emptyset}Y_l^m(\theta,\phi) = m\hbar Y_l^m(\theta,\phi)$$

Confirming that the spherical harmonics are also eigenfunctions of L_z with eigenvalues $m\hbar$.

D. Representation of Angular Momentum Operators

We would like to have matrix operators for the angular momentum operators l_x, l_y, and l_z. The idea is to find three 3 X 3 matrix operators that satisfy relations (Angular Momentum Commutation Relations), which are

$$[l_x, l_y] = i\hbar l_z,\quad [l_y, l_z] = i\hbar l_x,\quad [l_z, l_x] = i\hbar l_y,$$

One such group of objects is

$$l_x = \frac{1}{\sqrt{2}}\begin{pmatrix}0&1&0\\1&0&1\\0&1&0\end{pmatrix}\hbar,\quad l_y = \frac{1}{\sqrt{2}}\begin{pmatrix}0&-i&0\\i&0&-i\\0&i&0\end{pmatrix}\hbar,\quad l_z = \begin{pmatrix}1&0&0\\0&0&0\\0&0&-1\end{pmatrix}\hbar,$$

There are other ways to express these matrices in subspace C^3 of an infinite dimensional Hilbert space. Relations above are dominantly the most popular. Since the three operators do not commute, we arbitrarily have selected a basis for one of them, and then expressed the other two in that basis. Notice l_z is diagonal. That means the basis selected is natural for l_z. The terminology usually used is the operators in equations above are in the l_z basis.

Example: - Show $[l_x, l_y] = i\hbar l_z,$ using matrix operator relations

$$[l_x, l_y] = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}\hbar \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} - \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}\hbar \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}\hbar$$

$$= \frac{\hbar^2}{2}\begin{pmatrix} i & 0 & -i \\ 0 & -i+i & 0 \\ i & 0 & -i \end{pmatrix} - \frac{\hbar^2}{2}\begin{pmatrix} -i & 0 & -i \\ 0 & i-i & 0 \\ i & 0 & i \end{pmatrix} = \frac{\hbar^2}{2}\begin{pmatrix} i+i & 0 & -i+i \\ 0 & 0 & 0 \\ i-i & 0 & -i-i \end{pmatrix}$$

$$= \frac{\hbar^2}{2}\begin{pmatrix} 2i & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -2i \end{pmatrix} = i\hbar\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}\hbar$$

$$= i\hbar l_z.$$

Again, the other two relations can be calculated using similar procedures.

Remember l is comparable to a vector sum of the three component operators, so in vector/matrix notation would look like

$$l = \begin{pmatrix} l_x \\ l_y \\ l_z \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}\hbar \\ \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}\hbar \\ \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}\hbar \end{pmatrix}$$

Again, this operator will normally be denoted just l. The l operator is a different sort of object than the component operators. It is a different object in a different space. Yet, we would like a way to address angular momentum with a 3 X 3 matrix which is in the same subspace asthe components. We can do this if we use l^2. This operator is

$$l^2 = 2\hbar^2 I = 2\hbar^2\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Where I is the identity matrix.

Example: - Show that $l^2 = 2\hbar^2 I$

$$l^2 = \langle l|l\rangle = \left\langle \frac{1}{\sqrt{2}}\begin{pmatrix}0&1&0\\1&0&1\\0&1&0\end{pmatrix}, \frac{1}{\sqrt{2}}\begin{pmatrix}0&-i&0\\i&0&-i\\0&i&0\end{pmatrix}\hbar, \begin{pmatrix}1&0&0\\0&0&0\\0&0&-1\end{pmatrix}\hbar, \middle| \begin{matrix}\frac{1}{\sqrt{2}}\begin{pmatrix}0&1&0\\1&0&1\\0&1&0\end{pmatrix}\hbar\\ \frac{1}{\sqrt{2}}\begin{pmatrix}0&-i&0\\i&0&-i\\0&i&0\end{pmatrix}\hbar\\ \begin{pmatrix}1&0&0\\0&0&0\\0&0&-1\end{pmatrix}\hbar\end{matrix}\right\rangle$$

$$= \tfrac{1}{\sqrt{2}}\begin{pmatrix}0&1&0\\1&0&1\\0&1&0\end{pmatrix}\tfrac{1}{\sqrt{2}}\begin{pmatrix}0&1&0\\1&0&1\\0&1&0\end{pmatrix} + \tfrac{1}{\sqrt{2}}\begin{pmatrix}0&-i&0\\i&0&i\\0&i&0\end{pmatrix}\tfrac{1}{\sqrt{2}}\begin{pmatrix}0&-i&0\\i&0&i\\0&i&0\end{pmatrix} + \begin{pmatrix}1&0&0\\0&0&0\\0&0&-1\end{pmatrix}\hbar\begin{pmatrix}1&0&0\\0&0&0\\0&0&-1\end{pmatrix}\hbar$$

$$= \tfrac{1}{2}\begin{pmatrix}1&0&1\\0&1+1&0\\1&0&1\end{pmatrix}\hbar^2 + \tfrac{1}{2}\begin{pmatrix}1&0&-1\\0&1+1&0\\-1&0&1\end{pmatrix}\hbar^2 + \begin{pmatrix}1&0&0\\0&0&0\\0&0&1\end{pmatrix}\hbar^2$$

$$= \begin{pmatrix}1/2&0&1/2\\0&1&0\\1/2&0&1/2\end{pmatrix}\hbar^2 + \frac{1}{2}\begin{pmatrix}1/2&0&-1/2\\0&1&0\\-1/2&0&1/2\end{pmatrix}\hbar^2 + \begin{pmatrix}1&0&0\\0&0&0\\0&0&1\end{pmatrix}\hbar^2$$

$$= \begin{pmatrix}1&0&0\\0&2&0\\0&0&1\end{pmatrix}\hbar^2 + \begin{pmatrix}1&0&0\\0&0&0\\0&0&1\end{pmatrix}\hbar^2 = \begin{pmatrix}2&0&0\\0&2&0\\0&0&2\end{pmatrix}\hbar^2 = 2\hbar^2 I$$

E. Precurser to the Hydrogen Atom

The Hamiltonian for a spherically symmetric potential commutes with l^2 and the three component angular momentum operators. So H; l^2, and one of the three component angular momentum operators, congenitally Lz , is a complete set of commuting observables for a spherically symmetric potential.

We will use a Hamiltonian with a Coulomb potential for the hydrogen atom. The Coulomb potential is rotationally invariant, or spherically symmetric. We have indicated H; l^2, and l_z form a complete set of commuting observables for such a system. You may be familiar with the principal quantum number n, the angular momentum quantum number l, and the magnetic quantum number m. We will find there is a correspondence between these two sets of three quantities, which is n comes from application of H, l comes from application of l^2, and m comes from application of l_z.

F. Ladder Operators for Angular Momentum

As already mentioned, and since $\hat{L}^2$ and $\hat{L}_z$ commute, they share common eigenfunctions. We can point out the eigenvalues of $\hat{L}^2$ and $\hat{L}_z$ by α and β, respectively so that:

$$\hat{L}^2 Y_\alpha^\beta(\theta,\phi) = \alpha Y_\alpha^\beta(\theta,\phi), \quad \hat{L}^2 Y_\alpha^\beta(\theta,\phi) = \beta Y_\alpha^\beta(\theta,\phi),$$

It is convenient to define the raising and lowering operators (note the similarity to the Harmonic oscillator!):

$$L_{\pm} = \hat{L}_x \pm i\hat{L}_y$$

Which satisfy the commutation relations;

$$[L_+, L_-] = 2\hbar l_z, \quad [L_Z, L_{\pm}] = \pm\hbar L_{\pm}, \quad [L_{\pm}, l^2] = 0,$$

These relations are relatively easy to prove using the commutation relations we've already mentioned:

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

For example:

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

The raising and lowering operators have a peculiar effect on the eigenvalue of l_z :

$$\hat{L}_z(L_{\pm}Y_{\alpha}^{\beta}) = ([\hat{L}_z, L_{\pm}] + L_{\pm}\hat{L}_z)Y_{\alpha}^{\beta} = (\pm\hbar L_{\pm} + L_{\pm}\beta)Y_{\alpha}^{\beta} = (\beta \pm\hbar)(L_{\pm}Y_{\alpha}^{\beta})$$

Thus, L_+ (L_-) raises (lowers) the eigenvalue of $\hat{L}_z$ by $\hbar$, hence the names. Since the raising and lowering operators commute with $\hat{L}^2$ they do not change the value of α and so we can write

$$L_{\pm}Y_{\alpha}^{\beta} \propto Y_{\alpha}^{\beta\pm\hbar}$$

and so the eigenvalues of $\hat{L}_z$ are evenly spaced!

What are the limits on this ladder of eigenvalues? Recall that for the harmonic oscillator, we found that there was a minimum eigenvalue and the eigenstates could be created by successive applications of the raising operator to the lowest state. There is also a minimum eigenvalue in this case. To see this, note that

$$\langle\hat{L}_x^2 + \hat{L}_y^2\rangle = \langle\hat{L}_x^2\rangle + \langle\hat{L}_y^2\rangle \geq 0$$

This result simply reflects the fact that if you take any observable operator and square it, you must get back a positive number. To get a negative value for the average value of $\hat{L}_x^2$ or $\hat{L}_y^2$ would imply an imaginary eigenvalue of $\hat{L}_x$ or $\hat{L}_y$, which is impossible since these operators are Hermitian. Besides, what would an imaginary angular momentum mean? We now apply the above equation for the specific wavefunction Y_{α}^{β} :

$$\int Y_{\alpha}^{\beta*}(\hat{L}_x^2 + \hat{L}_y^2)Y_{\alpha}^{\beta} = \int Y_{\alpha}^{\beta*}(\hat{L}^2 - \hat{L}_z^2)Y_{\alpha}^{\beta} = \int Y_{\alpha}^{\beta*}(\alpha - \beta^2)Y_{\alpha}^{\beta} = \alpha - \beta^2$$

Hence $\beta^2 \leq \alpha$ and therefore $-\alpha \leq \beta \leq \alpha$. Which means that there are both maximum and minimum values that β can take on for a given α. If we denote these values by β_{max} and β_{min}, respectively, then it is clear that

$$L_+Y_{\alpha}^{\beta_{max}} = 0, \qquad L_-Y_{\alpha}^{\beta_{min}} = 0,$$

We can then use this knowledge and some algebra tricks trick to determine the relationship between α and β_{max} (or β_{min}). First note that:

$$\Rightarrow L_+ L_- Y_{\alpha}^{\beta_{max}} = 0 \quad L_- L_+ Y_{\alpha}^{\beta_{min}} = 0$$

We can expand this explicitly in terms of $\hat{L}_x$ and $\hat{L}_y$:

$$\Rightarrow \left(\hat{L}_x^2 + \hat{L}_y^2 - i(\hat{L}_y\hat{L}_x - \hat{L}_x\hat{L}_y)\right)Y_{\alpha}^{\beta_{max}} = 0 \quad \left(\hat{L}_x^2 + \hat{L}_y^2 + i(\hat{L}_y\hat{L}_x - \hat{L}_x\hat{L}_y)\right)Y_{\alpha}^{\beta_{min}} = 0$$

However, this is not the most convenient form for the operators, because we don't know what $\hat{L}_x$ or $\hat{L}_y$ gives when acting on Y_α^β . However, we can rewrite the same expression in terms of $l^2$and $\hat{L}_z$:

$$\underbrace{\hat{L}_x^2+\hat{L}_y^2}_{\hat{L}^2-\hat{L}_z^2} \pm i\left(\underbrace{\hat{L}_y\hat{L}_x-\hat{L}_x\hat{L}_y}_{-i\hbar\hat{L}_z}\right)$$

So then we have;

$$\Rightarrow \left(\hat{L}^2-\hat{L}_z^2-\hbar\hat{L}_z\right)Y_\alpha^{\beta_{max}}=0 \qquad \left(\hat{L}^2-\hat{L}_z^2+\hbar\hat{L}_z\right)Y_\alpha^{\beta_{min}}=0$$

$$\Rightarrow (\alpha-\beta_{max}^2-\hbar\beta_{max})Y_\alpha^{\beta_{max}}=0 \qquad (\alpha-\beta_{min}^2+\hbar\beta_{min})Y_\alpha^{\beta_{min}}=0$$

$$\Rightarrow \alpha=\beta_{max}(\beta_{max}+\hbar)=\beta_{min}(\beta_{min}-\hbar)$$

$$\beta_{max}=-\beta_{min}=\hbar l$$

where in the last line we have simply defined a new variable, l, that is dimensionless (notice that $\hbar$ has the units of angular momentum). So combining these minimum and maximum values we have that $-\hbar l \le \beta \le \hbar l$. Further, since we can get from the lowest to the highest eigenvalue in increments of $\hbar$ by successive applications of the raising operator, it is clear that the difference between the highest and lowest values [$\hbar j-(-\hbar j)=2\hbar l$] must be an integer multiple of $\hbar$. Thus, l itself must either be an integer or a half-integer.
Putting all these facts together, we conclude (Define $m \equiv \beta / \hbar$):

$$\boxed{\begin{array}{c} \hat{L}^2Y_l^m=\hbar^2 l(l+1)Y_l^m \quad l=0,\frac{1}{2},1,\frac{3}{2},2,\dots. \\ \text{And} \\ \hat{L}_zY_l^m=m\hbar Y_l^m \quad m=-l,-l+1,\dots,l-1,l \end{array}}$$

where we have replaced α with l and β with m so that Y_α^β becomes Y_l^m . Also, in the first equation, we have noted that $0 \le \langle\hat{L}^2\rangle=\hbar^2 l\,(l+1)$ implies $l \ge 0$. These are the fundamental eigenvalue equations for all forms of angular momentum.
At first, you might think this means we made a mistake in our derivation above and that l should only be an integer and not a half integer. However, there is no error. The difference arises because our derivation above is valid for any kind of angular momentum. Thus, while certain values of l may not appear for certain types of angular momentum, we will see later on that they can appear for other types of angular momentum. Most notably, electrons have an intrinsic spin angular momentum with $l=\frac{1}{2}$. Thus, while individual systems may have additional restrictions on the allowed values of l, angular momentum states always obey the above eigenvalue relations.

Important remark:
The four angular momentum operators are related as

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

The sum of the two components $\hat{L}_x^2+\hat{L}_y^2$would appear to factor

$$\left(\hat{L}_x+i\hat{L}_y\right)\left(\hat{L}_x-i\hat{L}_y\right)$$

and they would if the factors were scalars, but they are operators which do not commute, so this is not factoring. Just like the SHO, it is a good mnemonic, nevertheless.

Example: Show $\hat{L}_x^2 + \hat{L}_y^2 = (\hat{L}_x + i\hat{L}_y)(\hat{L}_x - i\hat{L}_y)$

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

where the expression in the next to last line is a significant intermediate result, and we will have reason to refer to it.

Like the SHO, the idea is to take advantage of the angular momentum commutation relations. We will use the notation

$$L_+ = \hat{L}_x + i\hat{L}_y$$
$$L_- = \hat{L}_x - i\hat{L}_y$$

which together are often denoted $L_\mp$.We need commutators for $L_\mp$, which are

$$\left[\hat{\vec{L}}^2, L_\mp\right] = 0$$
$$\left[\hat{L}_z, L_\mp\right] = \mp\hbar L_\mp$$

Example: Show $\left[\hat{\vec{L}}^2, L_+\right] = 0$

$$\left[\hat{\vec{L}}^2, L_+\right] = \left[\hat{\vec{L}}^2, \hat{L}_x + i\hat{L}_y\right] = \left[\hat{\vec{L}}^2, \hat{L}_x\right] + i\left[\hat{\vec{L}}^2, \hat{L}_y\right] = 0 + i(0) = 0$$

Example: Show $\left[\hat{L}_z, L_+\right] = \hbar L_+$

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

We will proceed essentially as we did the raising and lowering operators of the SHO. Since $\hat{\vec{L}}^2$ and $\hat{L}_z$ commute, they share a common eigenbasis.

Example: Show $\hat{\vec{L}}^2$ and $\hat{L}_z$ commute

$$\begin{aligned}\left[\hat{\vec{L}}^2, L_z\right] &= [\hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2, L_z] = [\hat{L}_x^2, L_z] + [\hat{L}_y^2, L_z] + [\hat{L}_z^2, / L_z] \\ &= [\hat{L}_x\hat{L}_x, L_z] + [\hat{L}_y\hat{L}_y, L_z] \\ &= \hat{L}_x[\hat{L}_x, L_z] + [\hat{L}_x, L_z]\hat{L}_x + \hat{L}_y[\hat{L}_y, L_z] + [\hat{L}_y, L_z]\hat{L}_y \\ &= \hat{L}_x(-i\hbar L_y) + (-i\hbar L_y)\hat{L}_x + \hat{L}_y(i\hbar L_x) + (i\hbar L_x)\hat{L}_y \\ &= (-i\hbar L_x\hat{L}_y + i\hbar L_x\hat{L}_y) + (-i\hbar L_y\hat{L}_x + i\hbar L_y\hat{L}_x) \\ &= 0\end{aligned}$$

Example: Given the spherical coordinate representations of L_x and L_y, show that, we can write the ladder operator of orbital angular momentum as;

$L_\pm = \pm\hbar e^{\pm i\phi}\left(\frac{\partial}{\partial\theta} \pm i cot\theta \frac{\partial}{\partial\phi}\right)$ Sherical coordinate,

$L_\pm = \hat{L}_x + i\hat{L}_y$ Cartesian coordinate,

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

$$= \hbar\left[isin\phi\frac{\partial}{\partial\theta} + icos\phi cot\theta\frac{\partial}{\partial\phi} + cos\phi\frac{\partial}{\partial\theta} - sin\phi cot\theta\frac{\partial}{\partial\phi}\right]$$

$$= \hbar\left[(cos\phi + isin\phi)\frac{\partial}{\partial\theta} + i(cos\phi - sin\phi)cot\theta\frac{\partial}{\partial\phi}\right]$$

$$= \hbar\left[(cos\phi + isin\phi)\frac{\partial}{\partial\theta} + i(cos\phi + isin\phi)cot\theta\frac{\partial}{\partial\phi}\right]$$

$$= \hbar\left[\left(e^{i\phi}\right)\frac{\partial}{\partial\theta} + i\left(e^{i\phi}\right)cot\theta\frac{\partial}{\partial\phi}\right]$$

$$= \hbar e^{i\phi}\left[\frac{\partial}{\partial\theta} + icot\theta\frac{\partial}{\partial\phi}\right]$$

G. **Geometrical Representation of Angular Momentum**

The relationship between the angular momentum and its *z*-component can be represented geometrically as follows. For a fixed value of l, the total angular momentum $\hat{\vec{L}}$ may be represented by a vector whose length, as displayed in Figure below, is given by $\sqrt{\langle\hat{\vec{L}}^2\rangle} = \hbar\sqrt{l(l+1)}$ and whose *z*-component is $\langle\hat{L}_Z\rangle = m\hbar$. Since $\hat{L}_x$ and $\hat{L}_y$ are separately undefined, only their sum $\hat{L}_x^2 + \hat{L}_y^2 = \hat{\vec{L}}^2 - \hat{L}_z^2$, which lies within the *xy* plane, is well defined.

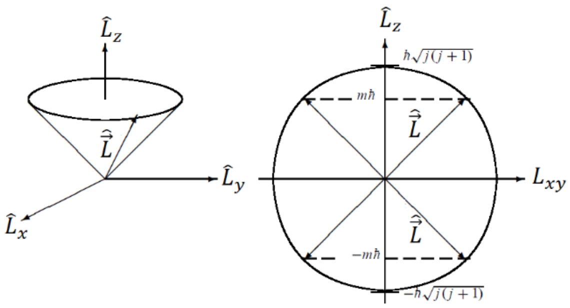

Figure: Geometrical representation of the angular momentum $\hat{\vec{L}}$: the vector $\hat{\vec{L}}$ rotates along the surface of a cone about its axis; the cone's height is equal to $m\hbar$, the projection of $\hat{\vec{L}}$on the cone's axis. The tip of $\hat{\vec{L}}$ lies, within the $\hat{L}_z$ L_{xy} plane, on a circle of radius $\hbar\sqrt{l(l+1)}$.

In classical terms, we can think of $\hat{\vec{L}}$ as representable graphically by a vector, whose endpoint lies on a circle of radius $\hbar\sqrt{l(l+1)}$, rotating along the surface of a cone of half-angle

$$\theta = cos^{-1}\left(\frac{m}{\sqrt{l(l+1)}}\right)$$

such that its projection along the *z*-axis is always $m\hbar$. Notice that, as the values of the quantum number m are limited to $m = -l, -l+1, \ldots, l-1, l$, the angle θ is quantized; the only possible values of θ consist of a discrete set of $2l + 1$ values:

$$\theta = cos^{-1}\left(\frac{-l}{\sqrt{l(l+1)}}\right), cos^{-1}\left(\frac{-l+1}{\sqrt{l(l+1)}}\right), \ldots, cos^{-1}\left(\frac{l-1}{\sqrt{l(l+1)}}\right), cos^{-1}\left(\frac{l}{\sqrt{l(l+1)}}\right).$$

Since all orientations of $\hat{\vec{L}}$ on the surface of the cone are equally likely, the projection of $\hat{\vec{L}}$ on both the x and y axes average out to zero:

$$\langle \hat{L}_x \rangle = \langle \hat{L}_y \rangle = 0$$

where $\langle \hat{L}_x \rangle$ stands for $\langle l, m|\hat{L}_x|l, m\rangle$.

As an example, Figure below shows the graphical representation for the $l = 2$ case. As specified in the equation θ, θ takes only a discrete set of values. In this case where $l = 2$ the angle θ takes only five values corresponding respectively to $m = -2, -1,0,1,2$; they are given by;

$$\theta = -35.26^{\circ}, -65.91^{\circ}, 90^{\circ}, 35.26^{\circ}, 65.91^{\circ}$$

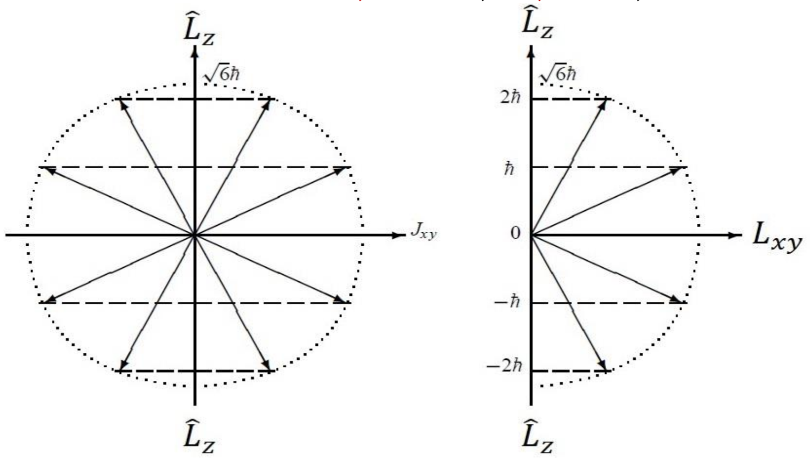

Figure: Graphical representation of the angular momentum $l = 2$ for the state $|s, m\rangle$ with $m = -2, -1,0,1,2$. The radius of the circle is $\hbar\sqrt{2(2+1)} = \sqrt{6}\hbar$.

II. Spin angular momentum (S)

The spin operator, S, represents another type of angular momentum, associated with "intrinsic rotation" of a particle around an axis; Spin is an intrinsic property of a particle (nearly all elementary particles have spin), that is unrelated to its spatial motion. The existence of spin angular momentum is inferred from experiments, such as the **Stern-Gerlach experiment**, in which particles are observed to possess angular momentum that cannot be accounted for by orbital angular momentum alone.

The spin angular momentum of a particle does not depend on its spatial degrees of freedom. The spin, an intrinsic degree of freedom, is a purely quantum mechanical concept with no classical analog. Unlike the orbital angular momentum, *the spin cannot be described by a differential operator*.

Unlike the spatial coordinates, **spin** can only take a discrete set of values. Proportional to the spin angular momentum is a magnetic momentum, $\vec{M}_S \propto \vec{S}$.The proton also has **spin** of equal magnitude, but the magnetic momentum due to the proton spin is much smaller and can be neglected in the **Stern-Gerlach** experiment. The magnetic momentum due to the spin of the paired core electrons cancels.

By analogy with the orbital angular momentum of a particle, which is characterized by two quantum numbers—the orbital number l and the azimuthal number m or same time write m_l

$(m = -l, -l+1, \dots, l-1, l)$—the spin angular momentum is also characterized by two quantum numbers, the spin s and its projection m_s on the z-axis (the direction of the magnetic field), where $(m_s = -s, -s+1, \dots, s-1, s)$. Since only two components were observed in the Stern–Gerlach experiment,we must have $2s+1=2$. The quantum numbers for the electron must then be given by $s=\frac{1}{2}$ and $m_s = \pm\frac{1}{2}$.

In nature it turns out that every fundamental particle has a specific spin. Some particles have integer spins $s = 0,1,2,3,..$ (the pi mesons have spin $s=0$, the photons have spin $s=1$, and so on) and others have half-odd-integer spins $s = \frac{1}{2},\frac{3}{2},\frac{5}{2},$ (the electrons, protons, andneutrons have spin $s=\frac{1}{2}$, the deltas have spin $s=\frac{3}{2}$ and so on.

A. General Theory of Spin

The theory of spin is identical to the general theory of angular momentum**.** By analogy with the vector angular momentum $\vec{\hat{L}}$, the spin is also represented by a vector operator $\vec{S}$ whose components $\hat{S}_x$, $\hat{S}_y$, $\hat{S}_z$ obey the same commutation relations as $\hat{L}_x$, $\hat{L}_x$, $\hat{L}_x$:

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

and therefore, all the general relations for angular momentum are satisfied, in particular, $\hat{S}^2$ and $\hat{S}_z$commute; hence they have common eigenvalues

$$\hat{S}^2 Y_l^m = \hbar^2 s(s+1) Y_l^m$$
$$\hat{S}_z Y_l^m = m_s \hbar Y_l^m$$

For a given value of s, we have $2s+1$ m_s-values

$$m_s = -s, -s+1, \dots, s-1, s$$

Where $\quad s = \frac{integer}{2} \geq 0$

There are no boundary conditions restricting the value of s, so we can have both integer and half-integer values.

By another way, we can write;

$$\hat{S}^2 |s, m_s\rangle = \hbar^2 s(s+1) |s, m_s\rangle$$
$$\hat{S}_z |s, m_s\rangle = m_s \hbar |s, m_s\rangle$$

Similarly, we have

$$\hat{S}_\pm |s, m_s\rangle = \hbar\sqrt{s(s+1) - m_s(m_s \pm 1)}\, |s, m_s \pm 1\rangle$$

Where $\hat{S}_\pm = \hat{S}_x \pm i\hat{S}_y$, and

$$\langle \hat{S}_x^2 \rangle = \langle \hat{S}_y^2 \rangle = \frac{1}{2}\left(\langle \hat{S}^2 \rangle - \langle \hat{S}_z^2 \rangle\right) = \frac{\hbar^2}{2}[s(s+1) - m_s]$$

The spin states form an orthonormal and complete basis

$$\sum_{m_s=-s}^{s} |s, m_s\rangle = I$$

where I is the unit matrix.

Each elementary particle has a fixed magnitude of the spin vector, given by the quantum number s. However, the projection of the spin onto one axis, typically chosen to be the z-axis, is needed in addition to the coordinates (or momenta) to fully specify the state of the particle. A complete description of spin requires relativistic Quantum Mechanics.

B. **Spin $1/2$ and the Pauli Matrices**

For a particle with spin $\frac{1}{2}$ the quantum number m_s takes only two values: $m_s = -\frac{1}{2}$ and $\frac{1}{2}$. The particle can thus be found in either of the following two states: $|s, m_s\rangle = \left|\frac{1}{2}, \frac{1}{2}\right\rangle$and $\left|\frac{1}{2}, -\frac{1}{2}\right\rangle$.

The eigenvalues of $\hat{S}^2$ and $\hat{S}_z$ are given by

$$\hat{S}^2\left|\frac{1}{2}, \pm\frac{1}{2}\right\rangle = \frac{3}{4}\hbar^2\left|\frac{1}{2}, \pm\frac{1}{2}\right\rangle, \qquad \hat{S}_z\left|\frac{1}{2}, \pm\frac{1}{2}\right\rangle = \pm\frac{\hbar}{2}\left|\frac{1}{2}, \pm\frac{1}{2}\right\rangle$$

Hence the spin may be represented graphically, as shown in Figure below, by a vector of length $|\hat{S}| = \sqrt{3}\hbar/2$, whose endpoint lies on a circle of radius $|\hat{S}| = \sqrt{3}\hbar/2$, rotating along the surface of a cone with half-angle

$$\theta = cos^{-1}\left(\frac{|m_s|}{\sqrt{s(s+1)}}\right) = cos^{-1}\left(\frac{\hbar/2}{\sqrt{3}\hbar/2}\right) = cos^{-1}\left(\frac{1}{\sqrt{3}}\right) = 54.73^{\circ}$$

The projection of $\hat{S}$ on the z-axis is restricted to two values only: $\pm\frac{\hbar}{2}$ corresponding to spin up and spin-down.

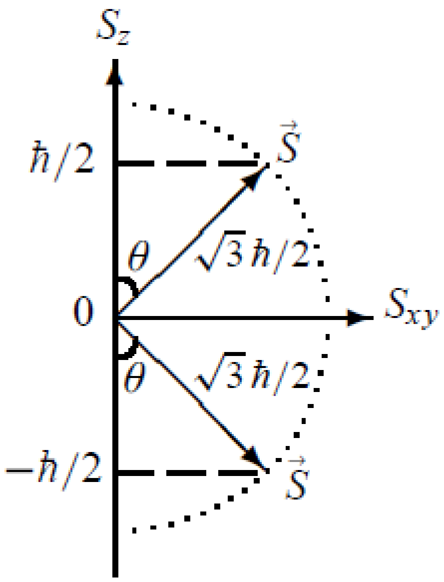

Figure: Graphical representation of spin $\frac{1}{2}$ the tip of $\hat{S}$ lies on a circle of radius $|\hat{S}| = \sqrt{3}\hbar/2$ so that its projection on the z-axis takes only two values, $\pm\frac{\hbar}{2}$, with $\theta = 54.73^{\circ}$.

Let us now study the matrix representation of the spin $s = \frac{1}{2}$. Using above we can represent the operators $\hat{S}^2$ and $\hat{S}_z$ within the $\{|s, m_s\rangle\}$basis by the following matrices:

$$\hat{S}^2 = \begin{pmatrix} \left\langle \frac{1}{2},\frac{1}{2}\middle|\hat{S}^2\middle|\frac{1}{2},\frac{1}{2}\right\rangle & \left\langle \frac{1}{2},\frac{1}{2}\middle|\hat{S}^2\middle|\frac{1}{2},-\frac{1}{2}\right\rangle \\ \left\langle \frac{1}{2},-\frac{1}{2}\middle|\hat{S}^2\middle|\frac{1}{2},\frac{1}{2}\right\rangle & \left\langle \frac{1}{2},-\frac{1}{2}\middle|\hat{S}^2\middle|\frac{1}{2},-\frac{1}{2}\right\rangle \end{pmatrix} = \frac{3\hbar^2}{4}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad \text{(A)}$$

$$\hat{S}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad \text{(B)}$$

The matrices $\hat{S}_+$ and $\hat{S}_-$ of can be inferred from (A)

$$\hat{S}_+ = \hbar\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad \hat{S}_- = \hbar\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \qquad \text{(C)}$$

and since $\hat{S}_x = \frac{\hbar}{2}(\hat{S}_+ + \hat{S}_-)$ and $\hat{S}_y = \frac{\hbar}{2}(\hat{S}_+ - \hat{S}_-)$, we have

$$\hat{S}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \hat{S}_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \text{(D)}$$

The joint eigenvectors of $\hat{S}^2$ and $\hat{S}_z$ are expressed in terms of two-element column matrices, known as *spinors*:

$$\left|\frac{1}{2},\frac{1}{2}\right\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \left|\frac{1}{2},-\frac{1}{2}\right\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \qquad \text{(E)}$$

It is easy to verify that these eigenvectors form a basis that is complete,

$$\sum_{m_s=\frac{1}{2}}^{\frac{1}{2}} \left|\frac{1}{2},m_s\right\rangle\left\langle\frac{1}{2},m_s\right| = \begin{pmatrix} 1 \\ 0 \end{pmatrix}(0 \quad 1) + \begin{pmatrix} 1 \\ 0 \end{pmatrix}(1 \quad 0) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad \text{(G)}$$

And orthonormal

$$\left\langle\frac{1}{2},\frac{1}{2}\middle|\frac{1}{2},\frac{1}{2}\right\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}(0 \quad 1) = 1 \qquad \text{(H)}$$

$$\left\langle\frac{1}{2},-\frac{1}{2}\middle|\frac{1}{2},-\frac{1}{2}\right\rangle = (0 \quad 1)\begin{pmatrix} 0 \\ 1 \end{pmatrix} = 1 \qquad \text{(I)}$$

$$\left\langle\frac{1}{2},\frac{1}{2}\middle|\frac{1}{2},-\frac{1}{2}\right\rangle = \left\langle\frac{1}{2},-\frac{1}{2}\middle|\frac{1}{2},\frac{1}{2}\right\rangle = 0 \qquad \text{(J)}$$

Let us now find the eigenvectors of $\hat{S}_x$ and $\hat{S}_y$. First, note that the basis vectors $|s,m_s\rangle$ are eigenvectors of neither $\hat{S}_x$ nor $\hat{S}_y$; their eigenvectors can, however, be expressed in terms of $|s,m_s\rangle$ as follows:

$$|\psi_x\rangle_\pm = \frac{1}{\sqrt{2}}\left[\left|\frac{1}{2},\frac{1}{2}\right\rangle \pm \left|\frac{1}{2},-\frac{1}{2}\right\rangle\right] = 0 \qquad \text{(K)}$$

$$|\psi_y\rangle_\pm = \frac{1}{\sqrt{2}}\left[\left|\frac{1}{2},\frac{1}{2}\right\rangle \pm i\left|\frac{1}{2},-\frac{1}{2}\right\rangle\right] = 0 \qquad \text{(L)}$$

The eigenvalue equations for $\hat{S}_x$ and $\hat{S}_y$ are thus given by

$$\hat{S}_x\,|\psi_y\rangle_\pm = \frac{\hbar}{2}|\psi_x\rangle_\pm, \quad \hat{S}_y\,|\psi_y\rangle_\pm = \frac{\hbar}{2}|\psi_y\rangle_\pm, \qquad \text{(M)}$$

C. State vectors for electron spin

A general state of electron spin can be represented by a linear combination of two basis states, one corresponding to the "spin-up" state, written as $|\uparrow\rangle, \left|\frac{1}{2},\frac{1}{2}\right\rangle$ or $\begin{bmatrix}1\\0\end{bmatrix}$and the other corresponding to a "spin-down" state, written as as $|\downarrow\rangle, \left|\frac{1}{2},-\frac{1}{2}\right\rangle$ or $\begin{bmatrix}0\\1\end{bmatrix}$.The "up" and "down" refer to the *z* direction, conventionally, though any axis in space can be chosen. A general electron spin state can therefore be written as

$$|s\rangle = a_{1/2}\left|\frac{1}{2},\frac{1}{2}\right\rangle + a_{-1/2}\left|\frac{1}{2},-\frac{1}{2}\right\rangle = a_{1/2}|\uparrow\rangle + a_{-1/2}|\downarrow\rangle = \begin{bmatrix}a_{1/2}\\a_{-1/2}\end{bmatrix}$$

D. Spin operators

By analogy with orbital angular momentum operators, spin operators $\hat{S}_x$, $\hat{S}_y$, and $\hat{S}_z$ can be defined with analogous commutation relations. More commonly, the operators

$$\hat{\sigma}_x=2\hat{S}_x/\hbar,\ \hat{\sigma}_y=2\hat{S}_y/\hbar,\ \hat{\sigma}_z=2\hat{S}_z/\hbar,$$

are used, with commutation relations

$$[\hat{\sigma}_x,\hat{\sigma}_y] = 2i\hat{\sigma}_z$$
$$[\hat{\sigma}_y,\hat{\sigma}_z] = 2i\hat{\sigma}_x$$
$$[\hat{\sigma}_z,\hat{\sigma}_x] = 2i\hat{\sigma}_y$$

These operators can be written as the Pauli spin matrices

$$\hat{\sigma}_x = \begin{bmatrix}0 & 1\\1 & 0\end{bmatrix},\ \hat{\sigma}_y = \begin{bmatrix}0 & -i\\i & 0\end{bmatrix},\ \hat{\sigma}_z = \begin{bmatrix}1 & 0\\0 & -1\end{bmatrix},$$

The vector spin operator

$$\hat{\sigma} = i\hat{\sigma}_x + j\hat{\sigma}_y + k\hat{\sigma}_z = i\begin{bmatrix}0 & 1\\1 & 0\end{bmatrix} + j\begin{bmatrix}0 & -i\\i & 0\end{bmatrix} + k\begin{bmatrix}1 & 0\\0 & -1\end{bmatrix}$$

Spinor

A spinor is a vector in the direct product space of the spatial (or space and time) and spin basis functions, and corresponds to a vector with a possibly different spatial (or space and time) function for each spin direction, i.e.,

$$|\Psi\rangle = \begin{bmatrix}\psi_\uparrow(r,t)\\\psi_\downarrow(r,t)\end{bmatrix} = \psi_\uparrow(r,t)\begin{bmatrix}1\\0\end{bmatrix} + \psi_\downarrow(r,t)\begin{bmatrix}0\\1\end{bmatrix}$$

A spinor can represent any possible state of a single electron, including spin.

Example: Show that $[\hat{S}_x,\hat{S}_y] = i\hbar\hat{S}_z$

$$[\hat{S}_x,\hat{S}_y] = \left\{\frac{\hbar}{2}\begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}\frac{\hbar}{2}\begin{pmatrix}0 & -i\\i & 0\end{pmatrix} - \frac{\hbar}{2}\begin{pmatrix}0 & -i\\i & 0\end{pmatrix}\frac{\hbar}{2}\begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}\right\}$$
$$= \frac{\hbar^2}{4}\left\{\begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}\begin{pmatrix}0 & -i\\i & 0\end{pmatrix} - \begin{pmatrix}0 & -i\\i & 0\end{pmatrix}\begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}\right\}$$
$$= \frac{\hbar^2}{4}\left\{\begin{pmatrix}i & 0\\0 & -i\end{pmatrix} - \begin{pmatrix}-i & 0\\0 & i\end{pmatrix}\right\} = \frac{\hbar^2}{2}\left\{\begin{pmatrix}i & 0\\0 & -i\end{pmatrix}\right\}$$
$$= i\hbar\frac{\hbar}{2}\left\{\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}\right\} = i\hbar\hat{S}_z$$

In the same manner

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

Example: Show that

(i) $\hat{\sigma}_x^2 = I$ and (ii) the commutator $[\hat{\sigma}_x, \hat{\sigma}_y] = 2i\hat{\sigma}_z$

(i) $\hat{\sigma}_x^2 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = I,$

(ii) $[\hat{\sigma}_x, \hat{\sigma}_y] = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} - \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$

$$= \begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix} - \begin{bmatrix} -i & 0 \\ 0 & i \end{bmatrix} = \begin{bmatrix} 2i & 0 \\ 0 & -2i \end{bmatrix} = 2i\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = 2i\,\hat{\sigma}_z$$