

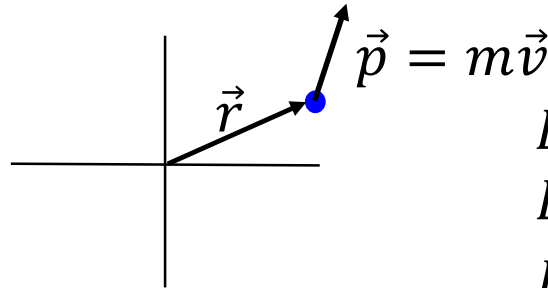
Angular momentum

(A lot of mathematics; I will try to explain as simple as possible)

Classical mechanics

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

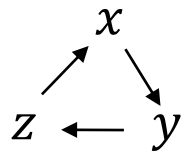
(angular momentum)



$$L_x = y p_z - z p_y$$

$$L_y = z p_x - x p_z$$

$$L_z = x p_y - y p_x$$



Quantum mechanics

The same, but $\hat{p}_x = -i\hbar \frac{\partial}{\partial x}$

$$\hat{p}_y = -i\hbar \frac{\partial}{\partial y}$$

$$\hat{p}_z = -i\hbar \frac{\partial}{\partial z}$$

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

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

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

To find quantized values of angular momentum, we can solve 3D differential equations to find eigenvalues and eigenstates. However, there is a simpler way, similar to the trick for oscillator.

Commutation relations

Simple to show:
(check yourself)

$$\begin{aligned} [\hat{L}_x, \hat{L}_y] &= i\hbar \hat{L}_z \\ [\hat{L}_y, \hat{L}_z] &= i\hbar \hat{L}_x \\ [\hat{L}_z, \hat{L}_x] &= i\hbar \hat{L}_y \end{aligned}$$

Most of the theory of angular momentum (and spin) can be derived from these commutation relations.

Will not write hats below for brevity

First observation: L_x, L_y, L_z are all incompatible (do not commute), so if L_x has a definite value, then L_y and L_z do not have definite values (except when all are zero, $\sigma_{L_x} \sigma_{L_y} \geq \frac{\hbar}{2} |\langle L_z \rangle|$).

However, $L^2 = L_x^2 + L_y^2 + L_z^2$ commutes with each component.

Simple to show:

$$\left. \begin{aligned} [L^2, L_x] &= 0 \\ [L^2, L_y] &= 0 \\ [L^2, L_z] &= 0 \end{aligned} \right\} [L^2, \vec{L}] = 0$$

Therefore, L^2 (square of total angular momentum) and one component can have definite values at the same time (usually z-component is chosen)

Eigenvalues of L^2 and L_z

We want to find eigenvalues of operators L^2 and L_z (they are the quantized values for the angular momentum).

Need to solve:
$$\begin{cases} L^2 f = \lambda f \\ L_z f = \mu f \end{cases}$$
 Will show
(next goal):
(f is not very important)

$$\begin{aligned} \lambda &= \hbar^2 l(l+1) \\ \mu &= \hbar m \\ l &= 0, \frac{1}{2}, 1, \frac{3}{2}, \dots \\ m &= -l, -l+1, \dots, l \end{aligned}$$

Trick of ladder operators

Let us introduce operators $L_{\pm} = L_x \pm iL_y$

These operators are not Hermitian (unphysical), while L_x, L_y, L_z are of course Hermitian

$$[L_z, L_{\pm}] = [L_z, L_x] \pm i[L_z, L_y] = i\hbar L_y \pm i(-i\hbar)L_x = \pm\hbar L_{\pm}$$

Thus

$$\begin{cases} [L_z, L_{\pm}] = \pm\hbar L_{\pm} \\ [L^2, L_{\pm}] = 0 \end{cases}$$

Lemma If f is an eigenvector of both L^2 (with eigenvalue λ) and L_z (with eigenvalue μ), then $L_{\pm}f$ are also eigenvectors, with the same λ , but $\mu \rightarrow \mu \pm \hbar$.

Proof

$$L^2(L_{\pm}f) = L_{\pm}(L^2f) = \lambda L_{\pm}f$$

$$\begin{cases} [L_z, L_{\pm}] = \pm \hbar L_{\pm} \\ [L^2, L_{\pm}] = 0 \end{cases}$$

$$L_z(L_{\pm}f) = [L_z, L_{\pm}]f + L_{\pm}L_zf = \pm \hbar L_{\pm}f + \mu L_{\pm}f = (\mu \pm \hbar)L_{\pm}f$$

Now the same logic as for oscillator: apply L_+ many times, the process should stop at some point (since L_z^2 cannot exceed L^2), therefore $L_+f_{\text{top}} = 0$.

$$\begin{array}{l} \text{---} f_{\text{top}} \\ \vdots \\ \text{---} (L_+)^2 f \\ \text{---} L_+ f \\ \text{---} f \end{array}$$

$$\begin{cases} L_z f_{\text{top}} = \hbar l f_{\text{top}} & \text{(so far } l \text{ is arbitrary)} \\ L^2 f_{\text{top}} = \lambda f_{\text{top}} & \text{Let us show } \boxed{\lambda = \hbar^2 l(l+1)} \text{ (eigenvalues are related!)} \end{cases}$$

Use formula $L^2 = L_-L_+ + L_z^2 + \hbar L_z$ (simple to derive explicitly), then

$$\lambda f_{\text{top}} = (\hbar l)^2 f_{\text{top}} + \hbar^2 l f_{\text{top}} = \hbar^2 l(l+1) f_{\text{top}}$$

Similarly, applying L_- many times, we should eventually get $L_- f_{\text{bottom}} = 0$.

Then similarly $L_z f_{\text{bottom}} = \hbar l' f_{\text{bottom}}$ (with arbitrary l'),
and can show the relation between eigenvalues:

$$\lambda = \hbar^2 l'(l' - 1)$$

Comparing these two equations, we obtain $l' = -l$.

But they are related by integer number (integer number of applying L_{\pm}).

Therefore, l is integer or half-integer.

Thus, result:

Eigenvalues of L^2 (i.e., possible measured values) are
 $\lambda = \hbar^2 l(l + 1)$, where $l = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \dots$,
eigenvalues of L_z (i.e., possible measured values) are
 $\mu = \hbar m$, where $m = -l, -l + 1, \dots, l - 1, l$

If we denote the corresponding eigenvectors by f_l^m , then

$$\begin{cases} L^2 f_l^m = \hbar^2 l(l + 1) f_l^m \\ L_z f_l^m = \hbar m f_l^m \end{cases}$$

Interesting that $L_z^2 \rightarrow \hbar^2 m^2 \leq \hbar^2 l^2$
is always smaller than $L^2 \rightarrow \hbar^2 l(l + 1)$.
So, z-component cannot be parallel to \vec{L} .
(If it would, then $L_x = L_y = 0$, impossible.)

Eigenvectors of L^2 and L_z

We found eigenvalues of L^2 and L_z :

$$\begin{cases} L^2 f_l^m = \hbar^2 l(l+1) f_l^m \\ L_z f_l^m = \hbar m f_l^m \end{cases}$$

What are the eigenvectors f_l^m ?

This is not simple. Discuss only the result (not the derivation).

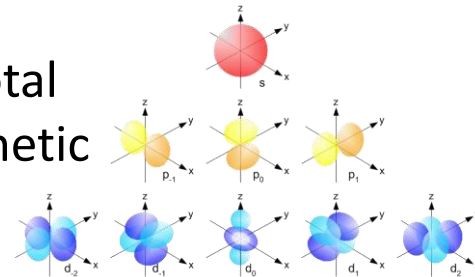
If the eigenvector f_l^m is represented by ψ -function in real space, $\psi(r, \theta, \varphi)$, then

l is integer (not half-integer) and $\psi(r, \theta, \varphi) = \underbrace{R(r)}_{\text{any}} \underbrace{Y_l^m(\theta, \varphi)}_{\text{spherical harmonics}}$

is the eigenfunction, $L^2 \psi = \hbar^2 l(l+1) \psi$

$$L_z \psi = \hbar m \psi$$

Thus, azimuthal quantum number l means that square of the total angular momentum is $L^2 = \hbar^2 l(l+1)$ (s, p, d, f orbitals). Magnetic quantum number m means that $L_z = \hbar m$ (degeneracy $2l+1$).



However, **half-integer l values really exist: spin** (consider next).

Spin

Existence of half-integer values of l is experimental fact (Stern-Gerlach, 1922: neutral silver atoms travel through inhomogeneous magnetic field, split into two beams)

Cannot explain as $\psi(r, \theta, \varphi) \Rightarrow$ something else. It is an angular momentum, which does not correspond to motion in $(x, y, z) \Rightarrow$ intrinsic angular momentum (spin).

The theory of spin is essentially the same as theory of angular momentum, just no $\psi(r, \theta, \varphi)$, only operator formalism.

$$\begin{aligned} [\hat{S}_x, \hat{S}_y] &= i\hbar \hat{S}_z \\ [\hat{S}_y, \hat{S}_z] &= i\hbar \hat{S}_x \\ [\hat{S}_z, \hat{S}_x] &= i\hbar \hat{S}_y \end{aligned}$$

Denote eigenstates of S^2 and S_z as $|s, m\rangle$

total spin \nearrow \nwarrow z-component

This is jargon, actually $\sqrt{S^2} = \hbar\sqrt{s(s+1)}$, $S_z = \hbar m$

More correctly,
$$\begin{cases} S^2 |s, m\rangle = \hbar^2 s(s+1) |s, m\rangle \\ S_z |s, m\rangle = \hbar m |s, m\rangle \end{cases}$$

Useful relation:
$$S_{\pm} |s, m\rangle = \hbar\sqrt{s(s+1) - m(m \pm 1)} |s, m \pm 1\rangle$$

Total spin: $s = 0, \frac{1}{2}, 1, \frac{3}{2}, \dots$

z-component: $m = -s, -s+1, \dots, s$

$s = 0$: pi-mesons, Higgs boson,

$s = 1/2$: electron, proton, neutron, quarks,

$s = 1$: photon, W, Z, $s = 3/2$: deltas, omega,

$s = 2$: graviton, etc.

The case $s = 1/2$ (spin one-half)

(simplest and most important)

$$S^2 = \hbar^2 \frac{1}{2} \frac{3}{2} = \frac{3}{4} \hbar^2 \quad S_z: m\hbar = \pm \frac{\hbar}{2}$$

What is the wavefunction? It cannot depend on x, y, z .

Let us introduce **something** that satisfies formalism (commutation relations).

Spinor $\chi = \begin{pmatrix} a \\ b \end{pmatrix} = a \underbrace{\begin{pmatrix} 1 \\ 0 \end{pmatrix}}_{\text{spin-up}} + b \underbrace{\begin{pmatrix} 0 \\ 1 \end{pmatrix}}_{\text{spin-down}}$ (χ is chosen to resemble ψ)

Normalization: $|a|^2 + |b|^2 = 1$

spin-up χ_{\uparrow} spin-down χ_{\downarrow}

Spin operators

These operators satisfy desired commutation relations:

$$[S_x, S_y] = i\hbar S_z, \quad [S_y, S_z] = i\hbar S_x, \\ [S_z, S_x] = i\hbar S_y$$

Also, as desired


$$S^2 = S_x^2 + S_y^2 + S_z^2 = \frac{\hbar^2}{4} (\sigma_x^2 + \sigma_y^2 + \sigma_z^2) \\ = \frac{3}{4} \hbar^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \frac{3}{4} \hbar^2$$

$\sigma_x, \sigma_y, \sigma_z$ are called Pauli matrices

Eigenvectors and eigenvalues

We know that S_z has eigenvalues $\pm\hbar/2$; what are the eigenvectors?

$$S_z \begin{pmatrix} a \\ b \end{pmatrix} = \lambda \begin{pmatrix} a \\ b \end{pmatrix}$$

$\pm\frac{\hbar}{2}$ 

$$S_z = \frac{\hbar}{2} \Rightarrow \chi = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad (\text{spin-up})$$


$$\text{Check: } S_z \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

Similarly

$$S_z = -\frac{\hbar}{2} \Rightarrow \chi = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad (\text{spin-down})$$

However, z-direction is not different from other directions, therefore the same eigenvalues for S_x and S_y .

$$S_x \begin{pmatrix} a \\ b \end{pmatrix} = \lambda \begin{pmatrix} a \\ b \end{pmatrix}$$


$\pm\frac{\hbar}{2}$ 

$$S_x = \frac{\hbar}{2} \Rightarrow \chi = \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$
$$S_x = -\frac{\hbar}{2} \Rightarrow \chi = \begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

$$\text{Check: } S_x \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix} \quad (\text{similar for } -\hbar/2)$$

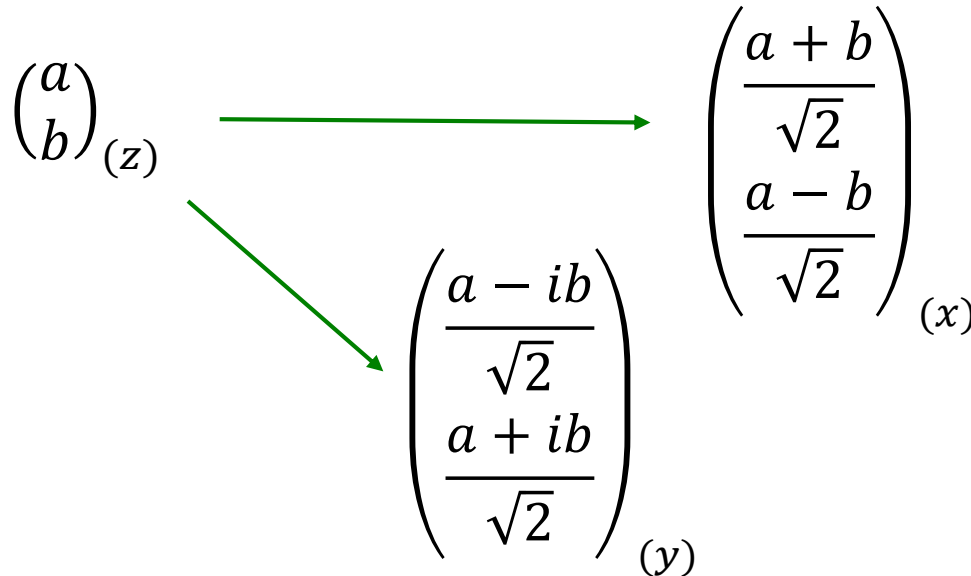
Similarly find eigenvectors for S_y

$$S_y \begin{pmatrix} a \\ b \end{pmatrix} = \lambda \begin{pmatrix} a \\ b \end{pmatrix}$$

$\pm \frac{\hbar}{2}$ 

$$S_y = \frac{\hbar}{2} \Rightarrow \chi = \begin{pmatrix} 1/\sqrt{2} \\ i/\sqrt{2} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix}$$
$$S_y = -\frac{\hbar}{2} \Rightarrow \chi = \begin{pmatrix} 1/\sqrt{2} \\ -i/\sqrt{2} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix}$$

Actually, S_x and S_y correspond to new bases of eigenstates, and everything can also be considered in these new bases



(we will consider only the standard z-basis)

not included into this course

Measurement of spin

$$\chi = \begin{pmatrix} a \\ b \end{pmatrix} \quad (\text{in standard z-representation})$$

Measure S_z : get $S_z = \hbar/2$ with probability $P_{z+} = |a|^2$, after that $\chi = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$
get $S_z = -\hbar/2$ with probability $P_{z-} = |b|^2$, after that $\chi = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

Measure S_x : get $S_x = \hbar/2$ with probability

$$P_{x+} = \left| \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} \right|^2 = \frac{1}{2} |a + b|^2 \quad \text{after that } \chi = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$S_x = -\hbar/2 \text{ with } P_{x-} = \left| \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} \right|^2 = \frac{1}{2} |a - b|^2 \quad \text{then } \chi = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

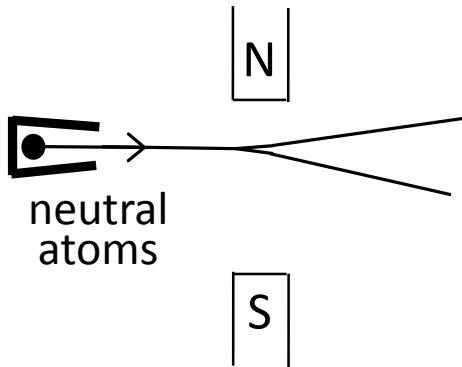
Measure S_y : get $S_y = \hbar/2$ with probability

$$P_{y+} = \left| \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{-i}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} \right|^2 = \frac{1}{2} |a - ib|^2 \quad \text{then } \chi = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix}$$

$$S_y = -\hbar/2 \text{ with } P_{y-} = \left| \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{+i}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} \right|^2 = \frac{1}{2} |a + ib|^2 \quad \text{then } \chi = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix}$$

(not included into this course)

Experimental measurement of spin (Stern-Gerlach experiment, 1922)



inhomogeneous magnetic field produces force onto a magnetic moment

$$H = -\gamma \vec{B} \vec{S}$$

angular momentum (or spin)
magnetic field
gyromagnetic ratio

If B is inhomogeneous (not constant), then $\vec{F} = -\nabla H = \gamma \nabla (\vec{B} \vec{S})$

So, force depends on \vec{S} .

If $\vec{B}(x, y, z) = (B_0 + \alpha z)\vec{k} - \underbrace{\alpha x \vec{i}}_{\text{not important}}$ (for magnetic field $\frac{\partial B_x}{\partial x} + \frac{\partial B_y}{\partial y} + \frac{\partial B_z}{\partial z} = 0$),

then $\vec{F} = \gamma \alpha (S_z \vec{k} - \underbrace{S_x \vec{i}}_{\text{not important}})$

not important (oscillates because of Larmor precession about z-axis, so zero on average)

$$F_z = \gamma \alpha S_z$$

spin-up is deflected down ($\gamma < 0$),
spin-down is deflected up

(particle should be neutral because otherwise charge will circle in magnetic field)