Chapter 3: Angular Momentum

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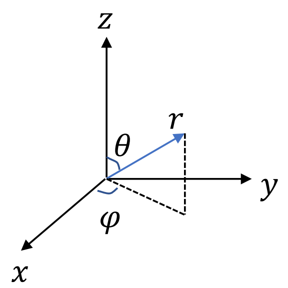
We have discussed position and momentum operator before, now let's consider the rotation of a system, which leads to angular position and angular momentum. Before we dive in, there's some prerequisites we should know.

1 Some prerequisites

In a 3D system, we use $\vec{r} = (x, y, z)$ to represent the coordinate, and the momentum is $\vec{p} = (p_x, p_y, p_z)$. In position representation, we have $p_x \leftrightarrow -i\hbar\frac{\partial}{\partial x}$, $p_y \leftrightarrow -i\hbar\frac{\partial}{\partial y}$, and $p_z \leftrightarrow -i\hbar\frac{\partial}{\partial z}$, together we get $\vec{p} = (-i\hbar\frac{\partial}{\partial x}, -i\hbar\frac{\partial}{\partial y}, -i\hbar\frac{\partial}{\partial z}) = -i\hbar\vec{\nabla}$.

Now let's switch to spherical coordinate (r, θ, φ).



For a point in space, we use a ket $|\psi\rangle$ to represent it,

$$\begin{cases} x = r\sin\theta\cos\varphi \\ y = r\sin\theta\sin\varphi \\ z = r\cos\theta \end{cases} \Rightarrow r = \sqrt{x^2 + y^2 + z^2} \tag{1}$$

now let's consider a rotation along $\hat{z}$ direction. Here φ becomes $\varphi + d\varphi$, and r, θ remain the same. We have

$$|x, y, z\rangle \xrightarrow{\text{rotation}} |x', y', z'\rangle \tag{2}$$

and the corresponding

$$(r, \theta, \varphi) \xrightarrow{\text{rotation}} (r, \theta, \varphi + d\varphi) \tag{3}$$

then we try to find out the expression of x', y', z' in terms of $r, \theta, \varphi, d\varphi$

$$\begin{cases} x' = r\sin\theta\cos(\varphi + d\varphi) \simeq r\sin\theta\cos\varphi - r\sin\theta\sin\varphi d\varphi \\ y' = r\sin\theta\sin(\varphi + d\varphi) \simeq r\sin\theta\sin\varphi + r\sin\theta\cos\varphi d\varphi \\ z' = r\cos\theta = z \end{cases} \Rightarrow \begin{cases} x' = x - yd\varphi \\ y' = y + xd\varphi \\ z' = z \end{cases} \tag{4}$$

On a spin-$\frac{1}{2}$ system, we have Pauli operators $\sigma_x, \sigma_y, \sigma_z$. In the σ_z basis, we have

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{5}$$

and

$$[\sigma_k, \sigma_l] = 2i\varepsilon_{klm}\sigma_m, \quad \varepsilon_{klm} = \begin{cases} 1 & \text{if } k, l, m \text{ in order} \\ -1 & \text{if out of order} \end{cases} \tag{6}$$

define the spin operator,

$$\begin{cases} \vec{S} = \frac{\hbar}{2}\vec{\sigma}, \ S_z = \frac{\hbar}{2}\sigma_z \\ \vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z) \end{cases} \tag{7}$$

here we should mention that $\boxed{[S_k, S_l] = i\hbar\varepsilon_{klm}S_m}$ is generally true for angular momentum operators, including spin-$\frac{1}{2}$ operators.

$$\vec{S}^2 = S_x^2 + S_y^2 + S_z^2 = \frac{\hbar^2}{4}\left(\sigma_x^2 + \sigma_y^2 + \sigma_z^2\right) = \frac{3}{4}\hbar^2 I \tag{8}$$

notice that for each k in x, y, z, we have $\boxed{\sigma_k^2 = I}$ so $\vec{S}^2 \propto I$, and we also have $\boxed{[\vec{S}^2, S_k] = 0}$. If we define unite length vector

$$\vec{n} = (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta) \tag{9}$$

we have

$$\vec{\sigma}\cdot\vec{n} = \sigma_x\sin\theta\cos\varphi + \sigma_y\sin\theta\sin\varphi + \sigma_z\cos\theta \tag{10}$$

Noticed that if you try to use Mathematica to implement $\vec{\sigma}\cdot\vec{n}$, use the expression $\vec{n}\cdot\vec{\sigma}$ instead. When we are dealing with matrix exponential, we use Taylor expansion

$$e^{i\phi\hat{\sigma}_x} = I + i\phi\sigma_x - \frac{\phi^2\sigma_x^2}{2!} + \frac{i\phi^3\sigma_x^3}{3!} - ... \tag{11}$$

we use

$$\begin{cases} e^{\hat{A}} = I + \hat{A} + \frac{\hat{A}^2}{2!} + ... + \frac{\hat{A}^n}{n!} + ... \\ \sigma_x^2 = I \end{cases} \tag{12}$$

to get

$$e^{i\phi\hat{\sigma}_x} = \left(I - \frac{\phi^2}{2!}I + \frac{\phi^4}{4!}I - ...\right) + i\sigma_x\left(\phi - \frac{\phi^3}{3!} + \frac{\phi^5}{5!} - ...\right) \tag{13}$$

$$= \cos\phi I + i\sin\phi\sigma_x \tag{14}$$

2 Orbital angular momentum

Let's consider a small rotation: $\varphi \to \varphi + d\varphi$,

$$\begin{cases} x' \simeq x - yd\varphi \\ y' \simeq y + xd\varphi \\ z' = z \end{cases} \tag{15}$$

if we have a state $|\psi\rangle$ expressed in position coordinate $\langle x, y, z|\psi\rangle = \psi(x, y, z)$ (we can also write it in spherical basis $\psi(r, \theta, \varphi)$, as we discussed above), then we apply a rotation to the state, we get from

$$\psi(r, \theta, \varphi) \to \psi(r, \theta, \varphi - d\varphi) \tag{16}$$

and we know

$$\psi(r, \theta, \varphi - d\varphi) \simeq \psi(r, \theta, \varphi) - d\varphi \cdot \frac{\partial}{\partial \varphi}\psi(r, \theta, \varphi) \tag{17}$$

we can express this small rotation as

$$I - \frac{\partial}{\partial \varphi} = I + \frac{1}{i\hbar}\hat{L}_z \tag{18}$$

here we can see the relationship:

$$\hat{L}_z \xlongequal{\varphi \text{ coordinate}} -i\hbar\frac{\partial}{\partial \varphi} \longleftrightarrow p_x \xlongequal{x \text{ coordinate}} -i\hbar\frac{\partial}{\partial x} \tag{19}$$

then we express $\hat{L}_z$ in x, y, z coordinates,

$$\psi(x, y, z) \xrightarrow{I - \frac{\partial}{\partial \varphi}} \psi(x', y', z') \tag{20}$$

rotate axis along z by $d\varphi$

$$\begin{cases} x' = x - yd\varphi \\ y' = y + xd\varphi \\ z' = z \end{cases} \xrightarrow{\text{want } -d\varphi} \begin{cases} x' = x + yd\varphi \\ y' = y - xd\varphi \\ z' = z \end{cases} \tag{21}$$

so

$$\psi(x', y', z') \simeq \psi(x + yd\varphi, y - xd\varphi, z) \tag{22}$$

$$= \psi(x, y, z) + yd\varphi\frac{\partial}{\partial x}\psi(x, y, z) - xd\varphi\frac{\partial}{\partial y}\psi(x, y, z) \tag{23}$$

we have

$$p_x \leftrightarrow -i\hbar\frac{\partial}{\partial x},\ \ p_y \leftrightarrow -i\hbar\frac{\partial}{\partial y} \tag{24}$$

so

$$
\begin{aligned}
\psi(x', y', z') &= \psi(x, y, z) + y d\varphi \left(\frac{\hat{p}_x}{-i\hbar} \right) \psi(x, y, z) - x d\varphi \left(\frac{\hat{p}_y}{-i\hbar} \right) \psi(x, y, z) && (25) \\
&= \left(I + \frac{1}{-i\hbar} d\varphi (y p_x - x p_y) \right) \psi(x, y, z) && (26) \\
&= \left(I + \frac{1}{i\hbar} \hat{L}_z \right) \psi(x, y, z) && (27)
\end{aligned}
$$

So $\hat{L}_z$ expressed with x, y, z coordinate with respected operators should be

$$
\hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x \tag{28}
$$

similarly, we can write out the $\hat{L}_x$ and $\hat{L}_y$. In total,

$$
\boxed{\begin{cases} \hat{L}_x = \hat{y}\hat{p}_z - \hat{z}\hat{p}_y \\ \hat{L}_y = \hat{z}\hat{p}_x - \hat{x}\hat{p}_z \\ \hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x \end{cases}} \tag{29}
$$

which is the same as classical mechanics $\vec{L} = \vec{r} \times \vec{p}$, so we get an orbital angular momentum operator in analog to classical. For now, we've already find out the $\hat{L}_x, \hat{L}_y, \hat{L}_z$ represented in x, y, z coordinate. Let's try to write them in r, θ, φ coordinate. We can replace the $\hat{p}_i$ as $-i\hbar\frac{\partial}{\partial i}$, and use (1) to replace x, y, z to r, θ, φ.

$$
\begin{cases} L_x = i\hbar \left(\sin\varphi \frac{\partial}{\partial \varphi} + \cot\theta \cos\varphi \frac{\partial}{\partial \varphi} \right) \\ L_y = i\hbar \left(-\cos\varphi \frac{\partial}{\partial \theta} + \cot\theta \sin\varphi \frac{\partial}{\partial \varphi} \right) \\ L_z = -i\hbar \frac{\partial}{\partial \varphi} \end{cases} \tag{30}
$$

After defined L_i in both x, y, z and r, θ, φ coordinates, we can now explore some properties of orbital angular momentum.

1. $[L_x, L_y] = i\hbar L_z$

   Proof. We already know

$$
\begin{cases} [x, p_x] = i\hbar \\ [x, y] = [x, p_y] = [p_x, p_y] = 0 \end{cases} \tag{31}
$$

   so

$$
\begin{aligned}
[y p_z - z p_y, z p_x - x p_z] &= [y p_z, z p_x] + [y p_z, -x p_z] + [-z p_y, z p_x] + [-z p_y, -x p_z] && (32) \\
&= [y p_z, z p_x] + [-z p_y, -x p_z] && (33) \\
&= y p_x [p_z, z] + p_y x [z, p_z] && (34) \\
&= i\hbar \left(x p_y - y p_x \right) = i\hbar L_z && (35)
\end{aligned}
$$

   □

Furthermore, we can easily proof that

$$\boxed{[L_k, L_l] = i\hbar\varepsilon_{k,l,m}L_m,\ \ \varepsilon_{klm} = \begin{cases} 1 & \text{if } k,l,m \text{ in order} \\ -1 & \text{if out of order} \end{cases}} \tag{36}$$

2. $\boxed{[L^2, L_i] = 0}$, which is similar to $[S^2, S_i] = 0$.

   Proof. We know that

$$L^2 = L_x^2 + L_y^2 + L_z^2,\ \ [A^2, B] = A[A, B] + [A, B]A$$

   so

$$\begin{aligned} [L^2, L_x] &= [L_x^2 + L_y^2 + L_z^2, L_x] = [L_y^2, L_x] + [L_z^2, L_x] && (37) \\ &= L_y[L_y, L_x] + [L_y, L_x]L_y + L_z[L_z, L_x] + [L_z, L_x]L_z && (38) \\ &= -i\hbar L_yL_z - i\hbar L_zL_y + i\hbar L_zL_y + i\hbar L_yL_z && (39) \\ &= 0 && (40) \end{aligned}$$

   □

so in total,

Box 2.1: Properties of orbital angular momentum

1.
$$[L_k, L_l] = i\hbar\varepsilon_{k,l,m}L_m,\ \ \varepsilon_{klm} = \begin{cases} 1 & \text{if } k,l,m \text{ in order} \\ -1 & \text{if out of order} \end{cases}$$

2.
$$[L^2, L_i] = 0$$

Now let's consider the eigen equation with L^2 and L_z. Recall that if $\hat{A}, \hat{B}$ are Hermitian, and $[\hat{A}, \hat{B}] = 0$, then there exists $\{|\psi\rangle\}$ giving

$$\begin{cases} \hat{A}|\psi\rangle = a|\psi\rangle \\ \hat{B}|\psi\rangle = b|\psi\rangle \end{cases}$$

or we can say $\{|\psi\rangle\}$ is the mutual eigen state. Here we already have $[L^2, L_z] = 0$, let $|y\rangle$ to be one of these states, so

$$\begin{cases} L_z|y\rangle = m\hbar|y\rangle \\ L^2|y\rangle = \beta\hbar^2|y\rangle \end{cases} \tag{41}$$

where m, β are numbers. $|y\rangle$ needs to be normalized, $\langle y|y\rangle = 1$

$$\beta\hbar^2 = \langle y|L^2|y\rangle = \langle y|L_x^2 + L_y^2 + L_z^2|y\rangle \geq \langle y|L_z^2|y\rangle = m^2\hbar^2 \tag{42}$$

so

$$\beta \geq m^2 \tag{43}$$

in spherical coordinate, as above we can express L^2, L_z all in just θ, φ without r. L^2, L_z only relates to angular coordinates $\{\theta, \varphi\}$ as the angular representation. The eigen function for L_z in coordinates $\{\theta, \varphi\}$ is $\langle\theta, \varphi|L_z|y\rangle = \lambda\langle\theta, \varphi|y\rangle$. To make the expression more convenient (we will know the reason soon), let's set $\lambda = m\hbar$.

$$\begin{aligned} \langle\theta, \varphi|y\rangle &= y(\theta, \varphi) &(44)\\ \langle\theta, \varphi|L_z|y\rangle &= m\hbar\langle\theta, \varphi|y\rangle &(45)\\ &= -i\hbar\frac{\partial}{\partial\varphi}\langle\theta, \varphi|y\rangle &(46) \end{aligned}$$

then we can solve the equation

$$-i\hbar\frac{\partial}{\partial\varphi}y(\theta, \varphi) = m\hbar y(\theta, \varphi) \Rightarrow y(\theta, \varphi) \propto e^{im\varphi} \tag{47}$$

and $\varphi \to \varphi + 2\pi$ should give the same wave function, so we have

$$e^{im\varphi} = e^{im(\varphi+2\pi)} \Rightarrow e^{i2\pi m} = 1 \tag{48}$$

so m should be an integer, $m = 0, \pm1, \pm2, ...$, and now we know why we need to set $\lambda = m\hbar$ before. Further, we have the eigen function for L^2

$$\langle\theta, \varphi|L^2|y\rangle = \beta\hbar^2\langle\theta, \varphi|y\rangle \tag{49}$$

notice that the original eigen function is $\langle\theta, \varphi|L^2|y\rangle = \lambda'\langle\theta, \varphi|y\rangle$, and the reason to let $\lambda' = \beta\hbar^2$ is similar to the former one, we will see it soon. By using (30) to calculate $L^2 = L_x^2 + L_y^2 + L_z^2$, we get

$$\begin{aligned} &\Rightarrow L^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right] &(50)\\ &\Rightarrow -\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]y(\theta, \varphi) = \beta y(\theta, \varphi) &(51) \end{aligned}$$

use (47) we can get $\frac{\partial^2}{\partial\varphi^2}y(\theta, \varphi) = -m^2 y(\theta, \varphi)$,

$$\Rightarrow \left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{m^2}{\sin^2\theta} - \beta\right]y(\theta, \varphi) = 0 \tag{52}$$

There's a solution proportional to a spherical function $P_l^m(\cos\theta)$ called associated Legendre polynomial. We need

$$\begin{cases} \beta = l(l+1),\ l = 0, 1, 2, ... \\ m = -l, -l+1, ..., l-1, l \end{cases} \tag{53}$$

the full solution is called Spherical Harmonics function

$$Y_{lm} = y(\theta, \varphi) = \sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}} P_l^m(\cos\theta)e^{im\varphi} \tag{54}$$

as a normalized solution, with $\begin{cases} l = 0, 1, 2, ... \\ m = -l, -l+1, ..., l-1, l \end{cases}$ as quantum number (the solution Y_{lm} needs two numbers to specify, just like an ID). As we discussed above, Y_{lm} is normalized, which means

$$\int_0^{2\pi} d\varphi \int_0^{\pi} \sin\theta Y^*_{l'm'} Y_{lm} d\theta = \delta_{ll'}\delta_{mm'} = \begin{cases} 1 & \text{if } l = l', m = m' \\ 0 & \text{otherwise} \end{cases} \tag{55}$$

From Y_{lm}, we know $|y\rangle = |l, m\rangle$. $\{|l, m\rangle\}$ form a basis, which has $2l + 1$ dimension.

3 General properties of angular momentum

This section corresponds to section 3.5 of *Sakurai*. Similar to $\vec{S}, \vec{L}$, we use $\vec{J}$ for general case, and the corresponding eigen state is $|j, m\rangle$, with

1. $[J_k, J_l] = i\hbar\varepsilon_{klm}J_m$
2. $[J^2, J_i] = 0$
3. $J_z|j, m\rangle = m\hbar|j, m\rangle$
4. $J^2|j, m\rangle = \beta\hbar^2|j, m\rangle$

and we will proof $\beta = j(j + 1)$ soon.