

Chapter 3: Angular Momentum

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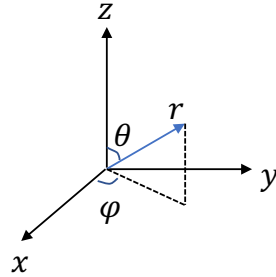
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We have discussed position and momentum operator before, now let's consider the rotation of a system, which leads to angular position and angular momentum. Before we dive in, there's some prerequisites we should know.

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,

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

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

$$|x, y, z\rangle \xrightarrow{\text{rotation}} |x', y', z'\rangle \quad (2)$$

and the corresponding

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

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

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

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

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

and

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

define the spin operator,

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

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

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

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

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

we have

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

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

$$e^{i\phi\hat{\sigma}_x} = I + i\phi\sigma_x - \frac{\phi^2\sigma_x^2}{2!} + \frac{i\phi^3\sigma_x^3}{3!} - \dots \quad (11)$$

we use

$$\begin{cases} e^{\hat{A}} = I + \hat{A} + \frac{\hat{A}^2}{2!} + \dots + \frac{\hat{A}^n}{n!} + \dots \\ \sigma_x^2 = I \end{cases} \quad (12)$$

to get

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

$$= \cos \phi I + i \sin \phi \sigma_x \quad (14)$$

2 Orbital angular momentum

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

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

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

$$\psi(r, \theta, \varphi) \rightarrow \psi(r, \theta, \varphi - d\varphi) \quad (16)$$

and we know

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

we can express this small rotation as

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

here we can see the relationship:

$$\hat{L}_z \stackrel{\varphi \text{ coordinate}}{\longleftrightarrow} -i\hbar \frac{\partial}{\partial \varphi} \longleftrightarrow p_x \stackrel{x \text{ coordinate}}{\longleftrightarrow} -i\hbar \frac{\partial}{\partial x} \quad (19)$$

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

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

rotate axis along z by $d\varphi$

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

so

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

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

we have

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

so

$$\psi(x', y', z') = \psi(x, y, z) + y d\varphi \left(\frac{\hat{p}_x}{-i\hbar} \right) \psi(x, y, z) - x d\varphi \left(\frac{\hat{p}_y}{-i\hbar} \right) \psi(x, y, z) \quad (25)$$

$$= \left(I + \frac{1}{-i\hbar} d\varphi (yp_x - xp_y) \right) \psi(x, y, z) \quad (26)$$

$$= \left(I + \frac{1}{i\hbar} \hat{L}_z \right) \psi(x, y, z) \quad (27)$$

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

$$\hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x \quad (28)$$

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

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

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 .

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

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

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

so

$$[yp_z - zp_y, zp_x - xp_z] = [yp_z, zp_x] + [yp_z, -xp_z] + [-zp_y, zp_x] + [-zp_y, -xp_z] \quad (32)$$

$$= [yp_z, zp_x] + [-zp_y, -xp_z] \quad (33)$$

$$= yp_x[p_z, z] + p_yx[z, p_z] \quad (34)$$

$$= i\hbar (xp_y - yp_x) = i\hbar L_z \quad (35)$$

□

Furthermore, we can easily proof that

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

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

Proof. We know that

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

so

$$[L^2, L_x] = [L_x^2 + L_y^2 + L_z^2, L_x] = [L_x^2, L_x] + [L_y^2, L_x] \quad (37)$$

$$= L_y[L_y, L_x] + [L_y, L_x]L_y + L_z[L_z, L_x] + [L_z, L_x]L_z \quad (38)$$

$$= -i\hbar L_y L_z - i\hbar L_z L_y + i\hbar L_z L_y + i\hbar L_y L_z \quad (39)$$

$$= 0 \quad (40)$$

□

so in total,

Box 2.1: Properties of orbital angular momentum

- 1.

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

- 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

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

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

$$\beta\hbar^2 = \langle y|L^2|y\rangle = \langle y|L_x^2 + L_y^2 + L_z^2|y\rangle \geq \langle y|L_z^2|y\rangle = m^2\hbar^2 \quad (42)$$

so

$$\beta \geq m^2 \quad (43)$$

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 $\lambda = m\hbar$.

$$\langle \theta, \varphi | y \rangle = y(\theta, \varphi) \quad (44)$$

$$\langle \theta, \varphi | L_z | y \rangle = m\hbar \langle \theta, \varphi | y \rangle \quad (45)$$

$$= -i\hbar \frac{\partial}{\partial \varphi} \langle \theta, \varphi | y \rangle \quad (46)$$

then we can solve the equation

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

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

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

so m should be an integer, $m = 0, \pm 1, \pm 2, \dots$, and now we know why we need to set $\lambda = m\hbar$ before. Further, we have the eigen function for L^2

$$\langle \theta, \varphi | L^2 | y \rangle = \beta \hbar^2 \langle \theta, \varphi | y \rangle \quad (49)$$

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

$$\Rightarrow L^2 = -\hbar^2 \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} \right] \quad (50)$$

$$\Rightarrow - \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} \right] y(\theta, \varphi) = \beta y(\theta, \varphi) \quad (51)$$

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

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

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