

# Quantum Mechanics 1

PHYS 3143

ALEX FENG

2024

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# Chapter 1

## Stern-Gerlach Experiments

### 1.1 The Original Stern-Gerlach Experiment

Particles have an intrinsic spin  $\mathbf{S}$ , a form of angular momentum; although the spin angular momentum is real angular momentum, it is different from the classical orbital angular momentum. To understand the relationship between the angular momentum and magnetic moment of a charged particle, consider a classical of charge  $q$  moving in a circular orbit of radius  $\mathbf{r}$  and velocity  $\mathbf{v}$ . The magnetic moment (in Gaussian units)  $\boldsymbol{\mu}$  is given by

$$\boldsymbol{\mu} = \frac{I\mathbf{A}}{c} = \frac{q\mathbf{r} \times \mathbf{b}}{2c} = \frac{q}{2mc}\mathbf{L}$$

When it comes to intrinsic spin, we write

$$\boldsymbol{\mu} = \frac{gq}{2mc}\mathbf{S}$$

for a constant  $g$  experimentally determined for different particles. Changing the mass distribution of the classical model similarly results in such a factor, but it can not be applied to the intrinsic spin model.

In the Stern-Gerlach experiment, a beam of silver atoms is directed through an inhomogeneous magnetic field. Recall that the force the particles experience is only dependent on field gradient and magnetic moment:

$$\mathbf{F} = \nabla(\boldsymbol{\mu} \cdot \mathbf{B})$$

Surprisingly, the silver atoms only built up in two spots. This would mean that their magnetic moments could only take on two values (we now know that these correspond to the spins  $\pm\hbar/2$ ).

### 1.2 Four Experiments

#### Definition 1.2.1: Ket vector

The symbol  $|+\mathbf{n}\rangle$  is a vector denoting positive spin in the positive  $\mathbf{n}$  direction.

Suppose a particle exited an SG $\mathbf{z}$  device in state  $|+\mathbf{z}\rangle$ , i.e.  $S_z = +\hbar/2$ . When a beam of these particles are sent through another SG $\mathbf{z}$  device, all the particle will exit with the same state,  $|+\mathbf{z}\rangle$ .

Now, instead of sending the beam of particles in state  $|+\mathbf{z}\rangle$  through the SG $\mathbf{z}$  device, send it through an SG $\mathbf{x}$  device. We find that half the particles exit with state  $|+\mathbf{x}\rangle$  and half with state  $|-\mathbf{x}\rangle$ . Note that starting with particles in state  $|+\mathbf{z}\rangle$  yields the same results.

For the third experiment, send the particles in state  $|+\mathbf{z}\rangle$  through an SG $\mathbf{x}$  device, and send the resulting particles with state  $|+\mathbf{x}\rangle$  through another SG $\mathbf{z}$  device. Surprisingly, half the remaining particles have state  $|+\mathbf{z}\rangle$  and the other half are in state  $|-\mathbf{z}\rangle$ . This indicates that the Quantum world is different from our everyday classical experiences.

Before moving on to the fourth experiment, consider the modified SG $\mathbf{n}$  device, which sends particles through one SG $\mathbf{n}$  device, two SG $\mathbf{n}$  devices with their polarities reversed, and another SG $\mathbf{n}$  device at the end. Now, send particles in state  $|+\mathbf{z}\rangle$  through the modified SG $\mathbf{x}$  device, then directly through an SG $\mathbf{z}$  device. Based on the previous experiments, we might expect half the particles to be in state  $|+\mathbf{x}\rangle$ ; going through the SG $\mathbf{z}$  device

results in half of these  $|+\mathbf{x}\rangle$  particles being in state  $|+\mathbf{z}\rangle$ . However, we find that all the exiting particles remained in state  $|+\mathbf{z}\rangle$ . We will later see that these effects can be explained using probability amplitudes.

### 1.3 The Quantum State Vector

#### Definition 1.3.1: Bra vector

For all  $|\psi\rangle$ , there exists a bra vector  $\langle\psi|$ , which is an element of the dual space. The inner product of  $\langle\psi|$  and  $|\phi\rangle$  is  $\langle\psi|\phi\rangle \in \mathbb{C}$ , which is the probability amplitude of finding a particle in state  $|\phi\rangle$  to be in state  $|\psi\rangle$ .

From the first experiment, we see that  $\langle-\mathbf{z}|+\mathbf{z}\rangle = 0$ , so we can think of  $|+\mathbf{z}\rangle$  and  $|-\mathbf{z}\rangle$  as orthogonal. Additionally, it will be convenient to require these state vectors to be unit vectors. An arbitrary spin state  $|\psi\rangle$  can be created by sending spin- $\frac{1}{2}$  particles through an SG device oriented in an arbitrary direction and selecting particles with positive spin.  $|+\mathbf{z}\rangle$  and  $|-\mathbf{z}\rangle$  form a basis, thus we will describe the state  $|\psi\rangle$  as

$$|\psi\rangle = c_+ |+\mathbf{z}\rangle + c_- |-\mathbf{z}\rangle$$

Multiplying  $\langle\pm\mathbf{z}|$  shows that

$$\langle\psi| = \langle+\mathbf{z}|\psi\rangle \langle+\mathbf{z}| + \langle-\mathbf{z}|\psi\rangle \langle-\mathbf{z}|$$

Using the same technique,

$$\langle\psi| = \langle\psi|+\mathbf{z}\rangle \langle+\mathbf{z}| + \langle\psi|-\mathbf{z}\rangle \langle-\mathbf{z}|$$

We will later find that  $\langle\psi|\phi\rangle = \langle\phi|\psi\rangle^*$ . Using this,

$$\langle\psi|\psi\rangle = 1 = |\langle+\mathbf{z}|\psi\rangle|^2 + |\langle-\mathbf{z}|\psi\rangle|^2$$

We interpret  $|\langle+\mathbf{z}|\psi\rangle|^2$  to be the probability that the particle in state  $|\psi\rangle$  will be found in state  $|+\mathbf{z}\rangle$ . When  $\langle+\mathbf{z}|\psi\rangle$  and  $\langle-\mathbf{z}|\psi\rangle$  are both non-zero, then the particle in state  $|\psi\rangle$  is actually in a superposition, instead of being in the definite state that classical mechanics expects.

### 1.4 Analysis of Experiment 3

We know that  $|\langle+\mathbf{z}|+\mathbf{x}\rangle|^2 = |\langle-\mathbf{z}|+\mathbf{x}\rangle|^2 = \frac{1}{2}$ , thus,

$$\langle+\mathbf{z}|+\mathbf{x}\rangle = \frac{e^{i\delta_+}}{\sqrt{2}} \text{ and } \langle-\mathbf{z}|+\mathbf{x}\rangle = \frac{e^{i\delta_-}}{\sqrt{2}}$$

We can use these values to calculate expected value  $\langle S_z \rangle$  and uncertainty  $\Delta S_z$ :

$$\begin{aligned} (\Delta S_z)^2 &= \langle (S_z - \langle S_z \rangle)^2 \rangle \\ &= \langle S_z^2 \rangle - \langle S_z \rangle^2 \end{aligned}$$

#### Example 1.4.1 (Expected Value and Uncertainty)

Consider the spin- $\frac{1}{2}$  particle in state

$$|\psi\rangle = \frac{1}{2} |+\mathbf{z}\rangle + \frac{i\sqrt{3}}{2} |-\mathbf{z}\rangle$$

To find the expected value,

$$\begin{aligned} \langle S_z \rangle &= |\langle+\mathbf{z}|\psi\rangle|^2 \frac{\hbar}{2} - |\langle-\mathbf{z}|\psi\rangle|^2 \frac{\hbar}{2} \\ &= \frac{1}{4} \frac{\hbar}{2} - \frac{3}{4} \frac{\hbar}{2} \\ &= -\frac{\hbar}{4} \end{aligned}$$

To find the uncertainty, we first find  $\langle S_z^2 \rangle$ ,

$$\begin{aligned}\langle S_z \rangle &= |\langle +\mathbf{z}|\psi \rangle|^2 \left(\frac{\hbar}{2}\right)^2 + |\langle -\mathbf{z}|\psi \rangle|^2 \left(-\frac{\hbar}{2}\right)^2 \\ &= \frac{1}{4} \frac{\hbar^2}{4} - \frac{3}{4} \frac{\hbar^2}{4} \\ &= \frac{\hbar^2}{4}\end{aligned}$$

It follows that

$$\Delta S_z = \frac{\sqrt{3}}{4} \hbar$$

## 1.5 Experiment 5

In this experiment, send particles with state  $|+\mathbf{z}\rangle$  through an SG $\mathbf{x}$  device, then make measurements of  $S_y$  on the particles exiting with state  $|+\mathbf{x}\rangle$ . From the third experiment, we already know that 50 percent of the particles have  $S_y = \hbar/2$  and 50 percent have  $S_y = -\hbar/2$ . Another observer could be using different x/y/z axes and the results would be the same; this type of argument tells us that switching the SG $\mathbf{x}$  and SG $\mathbf{y}$  devices will not change the results of the third experiment. This argument has important implications. First, we already know that

$$|+\mathbf{y}\rangle = \frac{e^{i\gamma_+}}{\sqrt{2}} |+\mathbf{z}\rangle + \frac{e^{i\gamma_-}}{\sqrt{2}} |-\mathbf{z}\rangle = \frac{e^{i\gamma_+}}{\sqrt{2}} [|+\mathbf{z}\rangle + e^{i\gamma} |-\mathbf{z}\rangle]$$

for  $\gamma = \gamma_- - \gamma_+$ . Similarly,

$$|+\mathbf{x}\rangle = \frac{e^{i\delta_+}}{\sqrt{2}} [|+\mathbf{z}\rangle + e^{i\delta} |-\mathbf{z}\rangle]$$

it follows that

$$\langle +\mathbf{y} | +\mathbf{x} \rangle = \frac{e^{i(\delta_+ - \gamma_+)}}{2} [1 + e^{i(\delta - \gamma)}]$$

and finally,

$$\begin{aligned}|\langle +\mathbf{y} | +\mathbf{x} \rangle|^2 &= \frac{1}{2} [1 + \cos(\delta - \gamma)] \\ |\langle +\mathbf{y} | +\mathbf{x} \rangle|^2 &= \frac{1}{2} \implies \delta - \gamma = \pm \frac{\pi}{2}\end{aligned}$$

By convention,  $\delta = 0$ , and if we ignore the phases  $\delta_+$  and  $\gamma_+$ , we see that

$$|+\mathbf{x}\rangle = \frac{1}{\sqrt{2}} |+\mathbf{z}\rangle + \frac{1}{\sqrt{2}} |-\mathbf{z}\rangle$$

and

$$|+\mathbf{y}\rangle = \frac{1}{\sqrt{2}} |+\mathbf{z}\rangle + \frac{i}{\sqrt{2}} |-\mathbf{z}\rangle$$

Note that we have chosen  $\gamma = \pi/2$ , which corresponds to a right-handed coordinate system. Results such as

$$|-\mathbf{y}\rangle = \frac{1}{\sqrt{2}} |+\mathbf{z}\rangle - \frac{i}{\sqrt{2}} |-\mathbf{z}\rangle$$

arise from using  $\gamma = -\pi/2$  (left-handed coordinate system).

## Chapter 2

# Rotation of Basis States and Matrix Mechanics

### 2.1 The Beginnings of Matrix Mechanics

We can represent kets as column vectors in any basis we choose. For example, in the  $S_z$  basis,

$$|\psi\rangle \xrightarrow{S_z} \begin{pmatrix} \langle +z|\psi\rangle \\ \langle -z|\psi\rangle \end{pmatrix}$$

Additionally,

$$|+z\rangle \xrightarrow{S_z} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \text{ and } |-z\rangle \xrightarrow{S_z} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Similarly, we express bra vectors as row vectors:

$$\langle\psi| \xrightarrow{S_z} (\langle\psi| + z, \langle\psi| - z)$$

Thus, we can evaluate inner products using matrix mechanics, for example,

$$\langle\psi|\psi\rangle = (\langle\psi| + z, \langle\psi| - z) \begin{pmatrix} \langle +z|\psi\rangle \\ \langle -z|\psi\rangle \end{pmatrix} = 1$$

### 2.2 Rotation Operators

#### Definition 2.2.1: Rotation Operator

The rotation operator  $\hat{R}(\theta\mathbf{n})$  acts on kets by rotating them an angle  $\theta$  counterclockwise around axis  $\mathbf{n}$ .

Note that all operators will have a hat. Consider  $\hat{R}(\frac{\pi}{2}\mathbf{j})$ . This operator rotates kets 90 degrees clockwise around the y axis, so

$$|+x\rangle = \hat{R}\left(\frac{\pi}{2}\mathbf{j}\right)|+z\rangle$$

We write the corresponding bra equation as

$$\langle+x| = \langle+z| \hat{R}^\dagger\left(\frac{\pi}{2}\mathbf{j}\right)$$

where  $\hat{R}^\dagger$  is the adjoint operator of  $\hat{R}$ . Since

$$1 = \langle+x|+x\rangle = \langle+z| \hat{R}^\dagger\left(\frac{\pi}{2}\mathbf{j}\right) \hat{R}\left(\frac{\pi}{2}\mathbf{j}\right)|+z\rangle = \langle+z|+z\rangle$$

we know that  $\hat{R}^\dagger$  and  $\hat{R}$  are inverses, and, in general, an operator  $\hat{U}$  satisfying  $U^\dagger U = 1$  is called a unitary operator.

### Definition 2.2.2: Hermitian Operator

Any operator that is equal to its adjoint (self-adjoint) is called Hermitian.

Now, consider an infinitesimal rotation operator, which we will express as

$$\hat{R}(d\phi\mathbf{k}) = 1 - \frac{i}{\hbar} \hat{J}_z d\phi$$

First, notice that this form satisfies the conditions for rotation operators above. Also, note that  $\hat{J}_z$  must have the same dimensions as  $\hbar$ , which are units of angular momentum. Taking the adjoint of  $\hat{R}(d\phi\mathbf{k})$ , we get

$$\hat{R}^\dagger(d\phi\mathbf{k}) = 1 + \frac{i}{\hbar} \hat{J}_z^\dagger d\phi$$

since we know that complex numbers are replaced by their conjugate when moving from kets to bras. We also know that the composition of the rotation operator and its adjoint is 1. Thus

$$\begin{aligned} \hat{R}^\dagger(d\phi\mathbf{k})\hat{R}(d\phi\mathbf{k}) &= \left(1 + \frac{i}{\hbar} \hat{J}_z^\dagger d\phi\right) \left(1 - \frac{i}{\hbar} \hat{J}_z d\phi\right) \\ &= 1 + \frac{i}{\hbar} (\hat{J}_z^\dagger - \hat{J}_z) d\phi + O(d\phi^2) = 1 \end{aligned}$$

Thus,  $\hat{J}_z$  is Hermitian. To find the rotation operator for a finite angle  $\phi$ ,

$$\begin{aligned} d\phi &= \lim_{N \rightarrow \infty} \frac{\phi}{N} \\ \hat{R}(\phi\mathbf{k}) &= \lim_{N \rightarrow \infty} \left[ 1 - \frac{i}{\hbar} \hat{J}_z \left( \frac{\phi}{N} \right) \right]^N = e^{-i\hat{J}_z\phi/\hbar} \end{aligned}$$

Intuitively,  $\hat{R}(\phi\mathbf{k})|+\mathbf{z}\rangle$  does not change the state of  $|+\mathbf{z}\rangle$ , thus,  $\hat{R}(\phi\mathbf{k})$  must only act as a overall phase factor. In general, if an operator acting on a state only changes the state by a constant factor, the state is called an eigenstate and the constant is the eigenvalue. Then, the Taylor series expansion of the rotation operator shows that  $|+\mathbf{z}\rangle$  must be an eigenstate (or eigenket) of  $\hat{J}_z$ . We claim that the eigenvalue of  $|\pm\mathbf{z}\rangle$  is  $\pm\hbar/2$ , which we will demonstrate is consistent later. Substituting  $\hat{J}_z$  with  $\hbar/2$  for  $|+\mathbf{z}\rangle$  yields that

$$\hat{R}(\phi\mathbf{k})|+\mathbf{z}\rangle = e^{-i\phi/2}|+\mathbf{z}\rangle$$

To show why the eigenvalues of  $|+\mathbf{z}\rangle$  and  $|-\mathbf{z}\rangle$  are different for  $\hat{J}_z$ , consider

$$|+\mathbf{x}\rangle = \frac{1}{\sqrt{2}}|+\mathbf{z}\rangle + \frac{1}{\sqrt{2}}|-\mathbf{z}\rangle$$

$\hat{R}(\phi\mathbf{k})$  must not multiply  $|+\mathbf{z}\rangle$  and  $|-\mathbf{z}\rangle$  by the same overall phase factor, otherwise  $|+\mathbf{x}\rangle$  does not get rotated. Thus,  $|+\mathbf{z}\rangle$  and  $|-\mathbf{z}\rangle$  must have different eigenvalues. Using

$$\hat{J}_z|-\mathbf{z}\rangle = -\frac{\hbar}{2}|-\mathbf{z}\rangle$$

we find that

$$\hat{R}(\phi\mathbf{k})|-\mathbf{z}\rangle = e^{i\phi/2}|-\mathbf{z}\rangle$$

Now consider

$$\hat{R}\left(\frac{\pi}{2}\mathbf{k}\right)|+\mathbf{x}\rangle = e^{-i\pi/4} \left( \frac{1}{\sqrt{2}}|+\mathbf{z}\rangle + \frac{e^{i\pi/2}}{\sqrt{2}}|-\mathbf{z}\rangle \right) = e^{-i\pi/4}|+\mathbf{y}\rangle$$

This result is correct, and only holds when  $\hat{J}_z|\pm\mathbf{z}\rangle = \pm\hbar/2|\pm\mathbf{z}\rangle$ . Thus, the eigenvalues of the operator generating rotations about the z axis acting on  $|\pm\mathbf{z}\rangle$  are the values of the intrinsic spin angular momentum that characterizes these states! Finally, note that

$$\hat{R}(2\pi\mathbf{k})|+\mathbf{z}\rangle = e^{-i\pi}|+\mathbf{z}\rangle = -|+\mathbf{z}\rangle$$

and

$$\hat{R}(2\pi\mathbf{k})|-\mathbf{z}\rangle = e^{i\pi}|-\mathbf{z}\rangle = -|-\mathbf{z}\rangle$$

Thus, rotating a spin- $\frac{1}{2}$  state by 360 degrees and ending up where we started causes the state to pick up a minus sign.

## 2.3 The Identity and Projection Operators

### Definition 2.3.1: Identity and Projection Operators

The identity operator can be expressed as

$$1 = |+\mathbf{z}\rangle \langle +\mathbf{z}| + |-\mathbf{z}\rangle \langle -\mathbf{z}|$$

which are composed of the projection operators:

$$\hat{P}_+ = |+\mathbf{z}\rangle \langle +\mathbf{z}|$$

$$\hat{P}_- = |-\mathbf{z}\rangle \langle -\mathbf{z}|$$

We see that multiplying any spin- $\frac{1}{2}$  state  $|\psi\rangle$  by the identity operator yields the original state  $|\psi\rangle$ . Multiplying  $|\psi\rangle$  by the projection operators  $\hat{P}_+$  and  $\hat{P}_-$  yields the  $|+\mathbf{z}\rangle$  and  $|-\mathbf{z}\rangle$  components of  $|\psi\rangle$  respectively. Note that the relation

$$\hat{P}_+ + \hat{P}_- = 1$$

is referred to as a completeness relation. We can think of the projection operators as a modified SG device that blocks certain pathways that a particle can take.

It is convenient to introduce the following notation for basis states  $|1\rangle$  and  $|2\rangle$ :

$$\sum_i |i\rangle \langle i| = 1$$

for  $i = 1, 2$

## 2.4 Matrix Representations of Operators

If we let

$$\hat{A}|\psi\rangle = |\phi\rangle$$

and we write

$$|\psi\rangle = |+\mathbf{z}\rangle \langle +\mathbf{z}|\psi\rangle + |-\mathbf{z}\rangle \langle -\mathbf{z}|\psi\rangle$$

$$|\phi\rangle = |+\mathbf{z}\rangle \langle +\mathbf{z}|\phi\rangle + |-\mathbf{z}\rangle \langle -\mathbf{z}|\phi\rangle$$

then  $\hat{A}|\psi\rangle = |\phi\rangle$  becomes

$$\hat{A}(|+\mathbf{z}\rangle \langle +\mathbf{z}|\psi\rangle + |-\mathbf{z}\rangle \langle -\mathbf{z}|\psi\rangle) = |+\mathbf{z}\rangle \langle +\mathbf{z}|\phi\rangle + |-\mathbf{z}\rangle \langle -\mathbf{z}|\phi\rangle$$

Multiplying by  $\langle \pm\mathbf{z}|$ , we get

$$\langle +\mathbf{z}|\hat{A}|+\mathbf{z}\rangle \langle +\mathbf{z}|\psi\rangle + \langle +\mathbf{z}|\hat{A}|-\mathbf{z}\rangle \langle -\mathbf{z}|\psi\rangle = \langle +\mathbf{z}|\phi\rangle$$

$$\langle -\mathbf{z}|\hat{A}|+\mathbf{z}\rangle \langle +\mathbf{z}|\psi\rangle + \langle -\mathbf{z}|\hat{A}|-\mathbf{z}\rangle \langle -\mathbf{z}|\psi\rangle = \langle -\mathbf{z}|\phi\rangle$$

We can express this in matrix form as

$$\begin{pmatrix} \langle +\mathbf{z}|\hat{A}|+\mathbf{z}\rangle & \langle +\mathbf{z}|\hat{A}|-\mathbf{z}\rangle \\ \langle -\mathbf{z}|\hat{A}|+\mathbf{z}\rangle & \langle -\mathbf{z}|\hat{A}|-\mathbf{z}\rangle \end{pmatrix} \begin{pmatrix} \langle +\mathbf{z}|\psi\rangle \\ \langle -\mathbf{z}|\psi\rangle \end{pmatrix} = \begin{pmatrix} \langle +\mathbf{z}|\phi\rangle \\ \langle -\mathbf{z}|\phi\rangle \end{pmatrix}$$

which is represented in the  $S_z$  basis. We indicate a representation through an arrow:

$$\hat{A} \xrightarrow{S_z} \begin{pmatrix} \langle +\mathbf{z}|\hat{A}|+\mathbf{z}\rangle & \langle +\mathbf{z}|\hat{A}|-\mathbf{z}\rangle \\ \langle -\mathbf{z}|\hat{A}|+\mathbf{z}\rangle & \langle -\mathbf{z}|\hat{A}|-\mathbf{z}\rangle \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}$$

In general, for basis states  $|1\rangle$  and  $|2\rangle$  we can express matrix elements  $A_{ij}$  as

$$A_{ij} = \langle i|\hat{A}|j\rangle$$



We can express  $\hat{P}_+$  as

$$\hat{P}_+ \xrightarrow{s_z} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

and similarly,

$$\hat{P}_- \xrightarrow{s_z} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

Thus, the completeness relation in matrix form becomes

$$\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = \mathbb{I}$$

We can also express  $\hat{J}_z$  in matrix form by using its eigenvalues:

$$\hat{J}_z \xrightarrow{s_z} \begin{pmatrix} \langle +\mathbf{z} | \hat{J}_z | +\mathbf{z} \rangle & \langle +\mathbf{z} | \hat{J}_z | -\mathbf{z} \rangle \\ \langle -\mathbf{z} | \hat{J}_z | +\mathbf{z} \rangle & \langle -\mathbf{z} | \hat{J}_z | -\mathbf{z} \rangle \end{pmatrix} = \begin{pmatrix} \hbar/2 & 0 \\ 0 & -\hbar/2 \end{pmatrix}$$

To find the form of the matrix representing an adjoint, consider the operator  $\hat{A}$ , and states  $\chi$ ,  $\psi$ , and  $\phi$ .

$$\langle \chi | \hat{A} | \psi \rangle = \langle \chi | \phi \rangle$$

$$\langle \psi | \hat{A}^\dagger | \chi \rangle = \langle \phi | \chi \rangle$$

Thus, we find that

$$\langle \psi | \hat{A}^\dagger | \chi \rangle = \langle \chi | \hat{A} | \psi \rangle^*$$

It follows that

$$\langle i | \hat{A}^\dagger | j \rangle = \langle j | \hat{A} | i \rangle^*$$

#### Definition 2.4.1: Adjoint Matrix

We define the adjoint matrix  $\mathbb{A}^\dagger$  as the transpose conjugate of the matrix  $\mathbb{A}$ , i.e.,  $A_{ij}^\dagger = A_{ji}^*$ .

Since the matrix representation of a Hermitian operator equals its conjugate transpose by definition, operators such as  $\hat{P}_+$  or  $\hat{J}_z$  must be Hermitian.

To find the product of two operators  $\hat{A}$  and  $\hat{B}$ , we first form the matrix element

$$\langle i | \hat{A} \hat{B} | j \rangle$$

Inserting the identity element, we find that

$$\langle i | \hat{A} \hat{B} | j \rangle = \langle i | \hat{A} \left( \sum_k |k\rangle \langle k| \right) \hat{B} | j \rangle = \sum_k \langle i | \hat{A} | k \rangle \langle k | \hat{B} | j \rangle$$

which is the same as usual matrix multiplication. Intuitively,

$$(\hat{A} \hat{B})^\dagger = \hat{B}^\dagger \hat{A}^\dagger$$

## 2.5 Changing Representations

Consider the following equation:

$$|\psi'\rangle \xrightarrow{s_z} \begin{pmatrix} \langle +\mathbf{z} | \psi' \rangle \\ \langle -\mathbf{z} | \psi' \rangle \end{pmatrix} = \begin{pmatrix} \langle +\mathbf{z} | \hat{R}^\dagger(\frac{\pi}{2}\mathbf{j}) | \psi \rangle \\ \langle -\mathbf{z} | \hat{R}^\dagger(\frac{\pi}{2}\mathbf{j}) | \psi \rangle \end{pmatrix} = \begin{pmatrix} \langle +\mathbf{x} | \psi \rangle \\ \langle -\mathbf{x} | \psi \rangle \end{pmatrix} \xleftarrow{s_x} |\psi\rangle$$

The subtlety is that left side involves the state  $|\psi\rangle$  being rotated (active transformation); the right side simply has a rotated basis (passive transformation).

In general, we can change the basis of any state by using the rotation operator  $\hat{R}^\dagger$ , for example,

$$\begin{aligned} \begin{pmatrix} \langle +\mathbf{x}|\psi \rangle \\ \langle -\mathbf{x}|\psi \rangle \end{pmatrix} &= \begin{pmatrix} \langle +\mathbf{x}|\mathbf{z} \rangle & \langle +\mathbf{x}|\mathbf{-z} \rangle \\ \langle -\mathbf{x}|\mathbf{z} \rangle & \langle -\mathbf{x}|\mathbf{-z} \rangle \end{pmatrix} \begin{pmatrix} \langle +\mathbf{z}|\psi \rangle \\ \langle -\mathbf{z}|\psi \rangle \end{pmatrix} \\ &= \begin{pmatrix} \langle +\mathbf{z}|\hat{R}^\dagger(\frac{\pi}{2}\mathbf{j})|\mathbf{z} \rangle & \langle +\mathbf{z}|\hat{R}^\dagger(\frac{\pi}{2}\mathbf{j})|\mathbf{-z} \rangle \\ \langle -\mathbf{z}|\hat{R}^\dagger(\frac{\pi}{2}\mathbf{j})|\mathbf{z} \rangle & \langle -\mathbf{z}|\hat{R}^\dagger(\frac{\pi}{2}\mathbf{j})|\mathbf{-z} \rangle \end{pmatrix} \begin{pmatrix} \langle +\mathbf{z}|\psi \rangle \\ \langle -\mathbf{z}|\psi \rangle \end{pmatrix} \end{aligned}$$

We call the matrix in the example above  $\mathbb{S}^\dagger$  (or more specifically  $\mathbb{S}^\dagger(\frac{\pi}{2}\mathbf{j})$ ). Let  $\hat{A}$  be an operator represented as a matrix in the  $S_z$  basis. We can transform it to the  $S_x$  basis by using the  $\mathbb{S}^\dagger$  from above and writing

$$\hat{A} \xrightarrow{S_x} \mathbb{S}^\dagger \hat{A} \mathbb{S}$$

## 2.6 Expectation Values

Observe that

$$\begin{aligned} \langle S_z \rangle &= \frac{\hbar}{2} |\langle +\mathbf{z}|\psi \rangle|^2 - \frac{\hbar}{2} |\langle -\mathbf{z}|\psi \rangle|^2 \\ &= (\langle \psi | +\mathbf{z} \rangle, \langle \psi | -\mathbf{z} \rangle) \begin{pmatrix} \frac{\hbar}{2} & 0 \\ 0 & -\frac{\hbar}{2} \end{pmatrix} \begin{pmatrix} \langle +\mathbf{z}|\psi \rangle \\ \langle -\mathbf{z}|\psi \rangle \end{pmatrix} \end{aligned}$$

Thus, we can simply express expected value in the form

$$\langle S_z \rangle = \langle \psi | \hat{J}_z | \psi \rangle$$

## Chapter 3

# Angular Momentum

### 3.1 Rotations Do Not Commute and Neither Do the Generators

Consider the matrix equation

$$\begin{pmatrix} A'_x \\ A'_y \\ A'_z \end{pmatrix} = \begin{pmatrix} \cos \phi & -\sin \phi & 0 \\ \sin \phi & \cos \phi & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} A_x \\ A_y \\ A_z \end{pmatrix}$$

which rotates the vector by an angle  $\phi$  counterclockwise about the  $z$  axis; we express this matrix as

$$\mathbb{S}(\phi \mathbf{k}) = \begin{pmatrix} \cos \phi & -\sin \phi & 0 \\ \sin \phi & \cos \phi & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

For a small angle  $\Delta\phi$ , we approximate this as

$$\mathbb{S}(\Delta\phi \mathbf{k}) = \begin{pmatrix} 1 - \Delta\phi^2/2 & -\Delta\phi & 0 \\ \Delta\phi & 1 - \Delta\phi^2/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

rotations about other axes can be obtained from the cyclic substitution  $x \rightarrow y, y \rightarrow z, z \rightarrow x$ . Thus,

$$\mathbb{S}(\Delta\phi \mathbf{i}) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \Delta\phi & -\sin \Delta\phi \\ 0 & \sin \Delta\phi & \cos \Delta\phi \end{pmatrix} \approx \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 - \Delta\phi^2/2 & -\Delta\phi \\ 0 & \Delta\phi & 1 - \Delta\phi^2/2 \end{pmatrix}$$

Similarly,

$$\mathbb{S}(\Delta\phi \mathbf{j}) = \begin{pmatrix} 1 - \Delta\phi^2/2 & 0 & \Delta\phi \\ 0 & 1 & 0 \\ -\Delta\phi & 0 & 1 - \Delta\phi^2/2 \end{pmatrix}$$

We know that the  $\mathbb{S}$  matrices are representation of the rotation operators. Thus

$$\mathbb{S}(\Delta\phi \mathbf{i})\mathbb{S}(\Delta\phi \mathbf{j}) - \mathbb{S}(\Delta\phi \mathbf{j})\mathbb{S}(\Delta\phi \mathbf{i}) = \begin{pmatrix} 0 & -\Delta\phi^2 & 0 \\ \Delta\phi^2 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \mathbb{S}(\Delta\phi^2 \mathbf{k}) - \mathbb{I}$$

It follows that

$$\begin{aligned}
& \hat{R}(\Delta\phi\mathbf{i})\hat{R}(\Delta\phi\mathbf{j}) - \hat{R}(\Delta\phi\mathbf{j})\hat{R}(\Delta\phi\mathbf{i}) \\
&= e^{i\hat{J}_x\Delta\phi/\hbar}e^{-i\hat{J}_y\Delta\phi/\hbar} - e^{i\hat{J}_y\Delta\phi/\hbar}e^{-i\hat{J}_x\Delta\phi/\hbar} \\
&\approx \left\{1 - \frac{i\hat{J}_x\Delta\phi}{\hbar} - \frac{1}{2}\left(\frac{\hat{J}_x\Delta\phi}{\hbar}\right)^2\right\} \left\{1 - \frac{i\hat{J}_y\Delta\phi}{\hbar} - \frac{1}{2}\left(\frac{\hat{J}_y\Delta\phi}{\hbar}\right)^2\right\} \\
&\quad - \left\{1 - \frac{i\hat{J}_y\Delta\phi}{\hbar} - \frac{1}{2}\left(\frac{\hat{J}_y\Delta\phi}{\hbar}\right)^2\right\} \left\{1 - \frac{i\hat{J}_x\Delta\phi}{\hbar} - \frac{1}{2}\left(\frac{\hat{J}_x\Delta\phi}{\hbar}\right)^2\right\} \\
&\approx \frac{(\hat{J}_y\hat{J}_x - \hat{J}_x\hat{J}_y)\Delta\phi^2}{\hbar^2} \\
&= \left(1 - \frac{i\hat{J}_z\Delta\phi^2}{\hbar}\right) - 1
\end{aligned}$$

### Definition 3.1.1: Commutator

We define the commutator of two operators  $\hat{A}$  and  $\hat{B}$  to be

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$$

Thus, we find that

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

By cyclic substitution,

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

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

These important commutation relations are general and also apply for orbital angular momentum operators.

## 3.2 Commuting Operators

We know that the generators of rotation are Hermitian. Before continuing, consider two linear Hermitian operators  $\hat{A}$  and  $\hat{B}$  satisfying

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} = 0$$

Suppose  $\hat{A}$  only has a single eigenstate,  $|a\rangle$  with eigenvalue  $a$ :

$$\hat{A}|a\rangle = a|a\rangle$$

Then apply operator  $\hat{B}$  so that

$$\hat{B}\hat{A}|a\rangle = \hat{B}a|a\rangle$$

$$\hat{A}(\hat{B}|a\rangle) = a(\hat{B}|a\rangle)$$

Thus we can conclude that

$$\hat{B}|a\rangle = b|a\rangle$$

for a constant  $b$ , i.e.,  $|a\rangle$  is also an eigenstate of  $\hat{B}$  with eigenvalue  $b$ . Thus we can relabel the state  $|a\rangle$  as  $|a, b\rangle$ . If there is more than one eigenstate of the operator  $\hat{A}$  with eigenvalue  $a$ , we say that there is degeneracy. Obviously, if there is degeneracy the linear combinations of the eigenstates of  $\hat{A}$  can form the eigenstates of  $\hat{B}$ . By the fundamental spectral theorem of linear algebra two Hermitian operators that commute have a complete set of eigenstates in common.

### 3.3 The Eigenvalues and Eigenstates of Angular Momentum

Let  $\hat{\mathbf{J}}$  be a vector operator such that

$$\hat{\mathbf{J}} = \hat{J}_x \mathbf{i} + \hat{J}_y \mathbf{j} + \hat{J}_z \mathbf{k}$$

and

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

We use the identity

$$[\hat{A}, \hat{B}\hat{C}] = \hat{B}[\hat{A}, \hat{C}] + [\hat{A}, \hat{B}]\hat{C}$$

to obtain

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

Thus,  $\hat{\mathbf{J}}^2$  and  $\hat{J}_z$  must have simultaneous eigenstates in common. We label the kets  $|\lambda, m\rangle$ , where

$$\hat{\mathbf{J}}^2 |\lambda, m\rangle = \lambda\hbar^2 |\lambda, m\rangle$$

$$\hat{J}_z |\lambda, m\rangle = m\hbar |\lambda, m\rangle$$

We expect that  $\lambda \geq 0$  since it is the square of the magnitude of angular momentum. Consider

$$\langle \lambda, m | \hat{\mathbf{J}}^2 | \lambda, m \rangle = \lambda\hbar^2 \langle \lambda, m | \lambda, m \rangle = \lambda\hbar^2$$

which would include a term

$$\langle \lambda, m | \hat{J}_x^2 | \lambda, m \rangle = \langle \psi | \psi \rangle$$

for  $|\psi\rangle = \hat{J}_x |\lambda, m\rangle$  and  $\langle \psi | = \langle \lambda, m | \hat{J}_x$  we can normalize  $|\psi\rangle$  by using  $|\psi\rangle = c|\phi\rangle$  for a complex constant  $c$  and  $\langle \phi | \phi \rangle = 1$ . We see that  $\langle \psi | \psi \rangle = c^* c \langle \phi | \phi \rangle \geq 0$ ; this holds for also holds for  $\hat{J}_y$  and  $\hat{J}_z$ , thus,  $\lambda \geq 0$ .

It is convinient to introduce two operators  $\hat{J}_{\pm} = \hat{J}_x \pm i\hat{J}_y$  (which are not Hermitian). Observe that

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

By the commutation relation,

$$\begin{aligned} \hat{J}_z \hat{J}_+ |\lambda, m\rangle &= (\hat{J}_+ \hat{J}_z + \hbar\hat{J}_+) |\lambda, m\rangle \\ &= (\hat{J}_+ m\hbar + \hbar\hat{J}_+) |\lambda, m\rangle \\ &= (m+1)\hbar\hat{J}_+ |\lambda, m\rangle \end{aligned}$$

Thus,  $\hat{J}_+ |\lambda, m\rangle$  is an eigenstate of  $\hat{J}_z$ . It's eigenvalue is  $(m+1)\hbar$  so we refer to  $\hat{J}_+$  as a raising operator. Similarly,  $\hat{J}_- |\lambda, m\rangle$  is an eigenstate of  $\hat{J}_z$  with eigenvalue  $(m-1)\hbar$ , hence we refer to  $\hat{J}_-$  as a lowering operator. Observe that  $[\hat{J}_{\pm}, \hat{\mathbf{J}}^2] = 0$  implies  $\hat{J}_{\pm} |\lambda, m\rangle$  is an eigenvalue of  $\hat{\mathbf{J}}^2$  with eigenvalue  $\lambda\hbar^2$ .

Physically, we expect that  $m^2 \leq \lambda$  since the square of the projection of the angular momentum should not exceed the the magnitude of  $\hat{\mathbf{J}}^2$ . Formally,

$$\begin{aligned} \langle \lambda, m | (\hat{J}_x^2 + \hat{J}_y^2) | \lambda, m \rangle &\geq 0 \\ \langle \lambda, m | (\hat{\mathbf{J}}^2 - \hat{J}_z^2) | \lambda, m \rangle &\geq 0 \\ (\lambda - m^2)\hbar^2 \langle \lambda, m | \lambda, m \rangle &\geq 0 \end{aligned}$$

Let's call the maximum  $m$  value  $j$ . We must have

$$\hat{J}_+ |\lambda, j\rangle = 0$$

otherwise,  $\hat{J}_+$  would create a contradictory state  $|\lambda, j+1\rangle$ . We see that

$$\begin{aligned} \hat{J}_- \hat{J}_+ |\lambda, j\rangle &= (\hat{J}_x - i\hat{J}_y)(\hat{J}_x + i\hat{J}_y) |\lambda, j\rangle \\ &= (\hat{J}_x^2 + \hat{J}_y^2 + i[\hat{J}_x, \hat{J}_y]) |\lambda, j\rangle \\ &= (\hat{\mathbf{J}}^2 - \hat{J}_z^2 - \hbar\hat{J}_z) |\lambda, j\rangle \\ &= (\lambda - j^2 - j)\hbar^2 |\lambda, j\rangle = 0 \end{aligned}$$

Thus,  $\lambda = j(j+1)$ . Similarly for a minimum  $m$  value  $j'$ , we have that  $\lambda = j'^2 - j'$ . The solution to  $j^2 + j = j'^2 - j'$  is  $j' = -j$  and  $j' = j+1$ . The second result is contradictory, thus the minimum value must be  $-j$ .