# Quantum Mechanics

## Algebraic Methods

## Harmonic Oscillator

### ▪ 1D Harmonic Oscillator

### ▪ Hamiltonian

Hamiltonian for the 1D harmonic oscillator

$$H = \frac{1}{2\,m}\,p^2 + \frac{1}{2}\,m\,\omega^2\,x^2. \tag{1}$$

- **Coordinate** operator $x$,
- **Momentum** operator $p$,

Defined by their commutation relation

$$[x,\,p] = i\,\hbar. \tag{2}$$

Let us **rescale the operators** $p$ and $x$

$$p \to p\,\sqrt{\hbar\,m\,\omega}\,,\;\; x \to x\,\sqrt{\frac{\hbar}{m\,\omega}}\,, \tag{3}$$

then the Hamiltonian looks simpler

$$\boxed{H = \frac{1}{2}\,\hbar\,\omega\,\left(p^2 + x^2\right).} \tag{4}$$

- **Energy scale** set by $\hbar\,\omega$.
- New operators $x$ and $p$ are *dimensionless*.

- Commutation relation for the rescaled operators

$$\boxed{[x,\,p] = i.} \tag{5}$$

### ▪ The Idea of Boson

It turns out the eigen energies of the harmonic oscillator Eq. (4) is given by $E_n = \hbar\,\omega(n + 1/2)$

(accept it for now, and we will prove it later).

- Levels are equally spaced: **oscillator** can only absorb/emit energy in *integer* multiples of $\hbar\,\omega$.
- Each unit (quantum) of energy is a **boson**:
  - For *mechanical oscillation* (sound), the boson is also called a **phonon**.
  - For *electromagnetic oscillation* (light), the boson is also called a **photon**.
- Each boson carries energy $\hbar\,\omega \Rightarrow$ can be considered as a *particle*.

Interpretation of boson: **elementary excitation**

| oscillator | | boson |
|---|---|---|
| state $\lvert n\rangle$ | $E_n / \hbar\,\omega$ | |
| $\lvert 0\rangle$ (ground) | 1 / 2 | vacuum |
| $\lvert 1\rangle$ | 3 / 2 | 1 boson |
| $\lvert 2\rangle$ | 5 / 2 | 2 bosons |
| ⋮ | ⋮ | ⋮ |

(6)

The boson can be

- *created* by the operator $a^\dagger$: $\lvert 0\rangle \to \lvert 1\rangle \to \lvert 2\rangle \to \ldots$,
- *annihilated* by the operator $a$: $\ldots \to \lvert 2\rangle \to \lvert 1\rangle \to \lvert 0\rangle$.

## ■ Annihilation and Creation Operators

Introduce the boson **annihilation** and **creation** operators

$$a = \frac{1}{\sqrt{2}}\,(x + i\,p),\;\; a^\dagger = \frac{1}{\sqrt{2}}\,(x - i\,p). \tag{7}$$

- $a$ and $a^\dagger$ are *Hermitian conjugate* to each other.
- Analogy: complex numbers $z = x + i\,y$, $z^* = x - i\,y \Rightarrow$ coordinate ~ real part, momentum ~ imaginary part.

Commutation relation

$$\left[a,\, a^\dagger\right] = 1, \tag{8}$$

meaning $a\,a^\dagger = a^\dagger\,a + 1$.

## ■ Boson Number Basis

Let $\lvert n\rangle$ be the state of $n$ boson excitations ($n = 0, 1, 2, \ldots$). They form a set of basis known as the **Fock state** basis or the boson number basis. Representation of $a$ and $a^\dagger$ on this basis:

$$\boxed{\begin{aligned} a\,|n\rangle &= \sqrt{n}\;\,|n-1\rangle, \\ a^\dagger\,|n\rangle &= \sqrt{n+1}\;\,|n+1\rangle. \end{aligned}} \tag{9}$$

One can verify that

$$a^\dagger\, a\,|n\rangle = n\,|n\rangle,\;\; a\, a^\dagger\,|n\rangle = (n+1)\,|n\rangle, \tag{10}$$

- therefore $a\, a^\dagger = a^\dagger\, a + 1$ indeed holds for all states, as an operator identity.
- $a^\dagger\, a$ is the **boson number operator**, which counts the number of bosons in the *Fock state*.
- The Hilbert space spanned by *Fock states* is called the **Fock space** (or the **occupation number space**).

Can we construct the Fock space from scratch?

Define the operator $\hat{n} = a^\dagger\, a$,

- $\hat{n}$ is Hermitian ($\hat{n}^\dagger = \hat{n}$),
- $\hat{n}$ is positive (semi)definite: $\forall\,|\psi\rangle : \langle\psi|\,\hat{n}\,|\psi\rangle = \langle\psi|\,a^\dagger\, a\,|\psi\rangle \geq 0$,

$\Rightarrow$ $\hat{n}$ has a set of orthogonal eigenstates (denoted as $|n\rangle$, labeled by $n = 0, 1, 2, \ldots$)

$$\hat{n}\,|n\rangle = \lambda_n\,|n\rangle. \tag{11}$$

with $\lambda_n \geq 0$. Because the spectrum is bounded from below, we can always arrange the eigenvalues in ascending order $0 \leq \lambda_0 \leq \lambda_1 \leq \lambda_2 \leq \ldots$, $|0\rangle$ is the "ground state" of $\hat{n}$.

From the following operator identity (use Eq. (8))

$$\hat{n}\, a = a\,(\hat{n} - 1),\;\; \hat{n}\, a^\dagger = a^\dagger\,(\hat{n} + 1), \tag{12}$$

one can show that

$$\hat{n}(a\,|n\rangle) = (\lambda_n - 1)\,(a\,|n\rangle),\;\; \hat{n}\big(a^\dagger\,|n\rangle\big) = (\lambda_n + 1)\,\big(a^\dagger\,|n\rangle\big). \tag{13}$$

If $|n\rangle$ is an eigenstate of $\hat{n}$ with eigenvalue $\lambda_n$, then $a\,|n\rangle$ and $a^\dagger\,|n\rangle$ are also eigenstates of $\hat{n}$ with eigen values $\lambda_n \mp 1$. But there is a caveat: we must make sure that the state is normalizable (the sate has a finite norm). For example $a\,|0\rangle$ must have zero norm, otherwise $a\,|0\rangle$ would be an eigenstate of $\hat{n}$ with eigenvalue $\lambda_0 - 1 < \lambda_0$, which contradict the with the fact that $\lambda_0$ is the smallest eigenvalue, therefore $a\,|0\rangle = 0 \Rightarrow \hat{n}\,|0\rangle = 0 \Rightarrow \lambda_0 = 0$.

Then we consider $a\,|1\rangle$, it is an eigenstate with eigenvalue $\lambda_1 - 1$, but $\lambda_0$ is the only eigenvalue smaller than $\lambda_1$, so $\lambda_1 - 1 = \lambda_0 \Rightarrow \lambda_1 = 1$. Iteratively apply similar argument, one can build up the entire Fock state representation.

## ▪ Matrix Representations

**Fock states** can be represented as *vectors*

$$|0\rangle \doteq \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix},\ |1\rangle \doteq \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix},\ |2\rangle \doteq \begin{pmatrix} 0 \\ 0 \\ 1 \\ \vdots \end{pmatrix}, \ldots \tag{14}$$

Correspondingly, the **creation** and **annihilation operators** are represented as *matrices*

$$\begin{aligned} a_{mn} &= \langle m|\, a\, |n\rangle = \sqrt{n}\ \langle m \mid n-1\rangle = \sqrt{n}\ \delta_{m,n-1}, \\ \left(a^\dagger\right)_{mn} &= \langle m|\, a^\dagger\, |n\rangle = \sqrt{n+1}\ \langle m \mid n+1\rangle = \sqrt{n+1}\ \delta_{m,n+1}, \end{aligned} \tag{15}$$

or more explicitly as

$$a \doteq \begin{pmatrix} 0 & \sqrt{1} & & \\ & 0 & \sqrt{2} & \\ & & 0 & \ddots \\ & & & \ddots \end{pmatrix},\ a^\dagger \doteq \begin{pmatrix} 0 & & & \\ \sqrt{1} & 0 & & \\ & \sqrt{2} & 0 & \\ & & \ddots & \ddots \end{pmatrix}. \tag{16}$$

By matrix multiplication, one can verify that $a^\dagger\, a$ indeed acts as the **number operator** as expected.

$$\hat{n} = a^\dagger\, a \doteq \begin{pmatrix} 0 & & & \\ & 1 & & \\ & & 2 & \\ & & & \ddots \end{pmatrix}. \tag{17}$$

The **coordinate** and **momentum** operators are represented as

$$\begin{aligned} x &= \frac{a + a^\dagger}{\sqrt{2}} \doteq \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & \sqrt{1} & & \\ \sqrt{1} & 0 & \sqrt{2} & \\ & \sqrt{2} & 0 & \ddots \\ & & \ddots & \ddots \end{pmatrix}, \\ p &= \frac{a - a^\dagger}{\sqrt{2}\ i} \doteq \frac{1}{\sqrt{2}\ i} \begin{pmatrix} 0 & \sqrt{1} & & \\ -\sqrt{1} & 0 & \sqrt{2} & \\ & -\sqrt{2} & 0 & \ddots \\ & & \ddots & \ddots \end{pmatrix}. \end{aligned} \tag{18}$$

To have some fun, let us check

$$x\, p \doteq \frac{i}{2} \begin{pmatrix} 1 & 0 & -\sqrt{2} & & \\ 0 & 1 & 0 & -\sqrt{6} & \\ \sqrt{2} & 0 & 1 & 0 & \ddots \\ & \sqrt{6} & 0 & 1 & \ddots \\ & & \ddots & \ddots & \ddots \end{pmatrix}, \tag{19}$$

$$p\,x \doteq \frac{i}{2}\begin{pmatrix} -1 & 0 & -\sqrt{2} & & \\ 0 & -1 & 0 & -\sqrt{6} & \\ \sqrt{2} & 0 & -1 & 0 & \ddots \\ & \sqrt{6} & 0 & -1 & \ddots \\ & & \ddots & \ddots & \ddots \end{pmatrix},$$

so we indeed verify the commutation relation $[x, p] = i$,

$$[x, p] \doteq \begin{pmatrix} i & & & \\ & i & & \\ & & i & \\ & & & \ddots \end{pmatrix} = i\,\mathbb{1}. \tag{20}$$

The **operator algebra** is *basis independent*. Even if the matrices in Eq. (18) do not look like coordinate and momentum in any intuitive way, but their commutation algebra works out just right. So it is the algebra $[x, p] = i$ that should be considered as the defining property of $x$ and $p$ operators.

## ■ Energy Spectrum

In terms of $a$ and $a^\dagger$, the oscillator Hamiltonian becomes

$$H = \hbar\,\omega\left(a^\dagger\,a + \frac{1}{2}\right), \tag{21}$$

So the eigen energies are given by

$$E_n = \hbar\,\omega\left(n + \frac{1}{2}\right). \tag{22}$$

The constant $\hbar\,\omega/2$ is known as the **zero-point energy** or the **vacuum energy**. The corresponding eigenstate $|n\rangle$ can be raised from the ground state by

$$|n\rangle = \frac{1}{\sqrt{n!}}\left(a^\dagger\right)^n|0\rangle. \tag{23}$$

To verify that $|n\rangle$ is indeed an eigenstate of $\hat{n}$ with eigenvalue $n$, we try

$$\begin{aligned} \hat{n}\,|n\rangle &= a^\dagger\,a\,|n\rangle \\ &= \frac{1}{\sqrt{n!}}\,a^\dagger\,a\left(a^\dagger\right)^n|0\rangle \\ &= \ldots \end{aligned}$$

$$= \frac{1}{\sqrt{n!}}\, a^\dagger\left(\left(a^\dagger\right)^n a + n\left(a^\dagger\right)^{n-1}\right)|0\rangle$$

$$= \frac{1}{\sqrt{n!}}\, a^\dagger\left(\left(a^\dagger\right)^n a\,|0\rangle + n\left(a^\dagger\right)^{n-1}|0\rangle\right)$$

$$= \frac{1}{\sqrt{n!}}\, a^\dagger\left(0 + n\left(a^\dagger\right)^{n-1}|0\rangle\right)$$

$$= \frac{1}{\sqrt{n!}}\, n\left(a^\dagger\right)^n|0\rangle$$

$$= n\,|n\rangle.$$

**HW 1**

Complete the missing steps in Eq. (24) by proving that
$a\left(a^\dagger\right)^n = \left(a^\dagger\right)^n a + n\left(a^\dagger\right)^{n-1}$ (for $n = 0, 1, 2, \ldots$).
Hint: consider mathematical induction.

## ■ Wave Functions

The ground state is defined by $a\,|0\rangle = 0 \Rightarrow (x + i\,p)\,|0\rangle = 0$, where $p = -i\,\partial_x$, so the ground state wave function $\psi_0(x)$ must satisfy the differential equation

$$(x + \partial_x)\,\psi_0(x) = 0, \tag{25}$$

the solution is

$$\psi_0(x) = \frac{1}{\pi^{1/4}}\, e^{-\frac{1}{2}x^2}. \tag{26}$$

The excited state can be raised from the ground state by applying $a^\dagger$. For example $|1\rangle = a^\dagger\,|0\rangle$ implies

$$\psi_1(x) = \frac{1}{\sqrt{2}}\,(x - \partial_x)\,\psi_0(x) = \frac{1}{\pi^{1/4}}\,\sqrt{2}\; x\, e^{-\frac{1}{2}x^2}. \tag{27}$$

Iteratively, we can obtain the wave functions for all eigenstates

$$\psi_n(x) = \frac{1}{\pi^{1/4}\,\sqrt{2^n\,n!}}\, H_n(x)\, e^{-\frac{1}{2}x^2}, \tag{28}$$

where $H_n(x)$ is known as the **Hermite polynomial**.

| n | $\psi_n(x)$ | $H_n(x)$ | plot of $\psi_n(x)$ |
|---|---|---|---|
| 0 | $\frac{e^{-\frac{x^2}{2}}}{\pi^{1/4}}$ | $1$ |  |
| 1 | $\frac{\sqrt{2}\, e^{-\frac{x^2}{2}} x}{\pi^{1/4}}$ | $2x$ |  |
| 2 | $\frac{e^{-\frac{x^2}{2}} (-1+2x^2)}{\sqrt{2}\,\pi^{1/4}}$ | $2(-1+2x^2)$ |  |
| 3 | $\frac{e^{-\frac{x^2}{2}} x (-3+2x^2)}{\sqrt{3}\,\pi^{1/4}}$ | $4x(-3+2x^2)$ |  |
| 4 | $\frac{e^{-\frac{x^2}{2}} (3-12x^2+4x^4)}{2\sqrt{6}\,\pi^{1/4}}$ | $4(3-12x^2+4x^4)$ |  |
| 5 | $\frac{e^{-\frac{x^2}{2}} x (15-20x^2+4x^4)}{2\sqrt{15}\,\pi^{1/4}}$ | $8x(15-20x^2+4x^4)$ |  |

Momentum space wave function

$$\tilde{\psi}_n(p) = \frac{1}{\pi^{1/4}\sqrt{2^n\, n!}}\, H_n(p)\, e^{-\frac{1}{2}p^2}. \tag{29}$$

- Comparing Eq. (28) and Eq. (29), there is an SO(2) *rotational* symmetry in the 2D **phase space** of $(x, p)$, which is evident in Eq. (4).
  - This also corresponds to the **U(1) symmetry**:

    $$a \to e^{i\theta}\, a,\ \ a^\dagger \to e^{-i\theta}\, a^\dagger. \tag{30}$$

  - U(1) symmetry ⇒ *conservation* of the boson **number**.

## ■ Uncertainty Relation

The **uncertainty relation** states that

$$(\text{std}\, x)\,(\text{std}\, p) \geq \frac{1}{2}\,|[x, p]| = \frac{1}{2}, \tag{31}$$

for the *rescaled* operators $x$ and $p$ (s.t. $[x, p] = i$).

Let us check it on the Fock state $|n\rangle$. We will use

$$x = \frac{a + a^\dagger}{\sqrt{2}},\ \ p = \frac{a - a^\dagger}{\sqrt{2}\, i}. \tag{32}$$

The one can evaluate

$$\begin{aligned} \langle n|\, x\, |n\rangle &= \frac{1}{\sqrt{2}}\, \langle n|\, a + a^\dagger\, |n\rangle \\ &= \frac{1}{\sqrt{2}} \left( \sqrt{n}\ \langle n \mid n-1\rangle + \sqrt{n+1}\ \langle n \mid n+1\rangle \right) \end{aligned} \tag{33}$$

$$
\begin{aligned}
&= 0, \\
\langle n|\, x^2\, |n\rangle &= \frac{1}{2}\, \langle n|\, \left(a + a^\dagger\right)^2\, |n\rangle \\
&= \frac{1}{2}\, \left(\langle n|\, a\, a\, |n\rangle + \langle n|\, a\, a^\dagger\, |n\rangle + \langle n|\, a^\dagger\, a\, |n\rangle + \langle n|\, a^\dagger\, a^\dagger\, |n\rangle\right) \\
&= \frac{1}{2}\, (0 + (n+1) + n + 0) \\
&= n + 1/2.
\end{aligned}
\tag{34}
$$

So the position uncertainty is given by

$$(\text{std}\, x)^2 = \langle n|\, x^2\, |n\rangle - \langle n|\, x\, |n\rangle^2 = n + 1/2. \tag{35}$$

Similarly, for the momentum uncertainty

$$(\text{std}\, p)^2 = \langle n|\, p^2\, |n\rangle - \langle n|\, p\, |n\rangle^2 = n + 1/2. \tag{36}$$

Therefore, the uncertainty relation holds for all Fock states $|n\rangle$,

$$(\text{std}\, x)\, (\text{std}\, p) = n + 1/2 \geq 1/2. \tag{37}$$

But specifically, the **ground state** $|0\rangle$ *saturates* the uncertainty relation. We say $|0\rangle$ is a **minimal uncertainty state**. The fact that the ground state possesses a finite amount of **zero-point energy** has to do with the *uncertainty relation*. Given that

$$\left\langle x^2\right\rangle \left\langle p^2\right\rangle \geq \frac{1}{4}\, |[x, p]|^2 = \frac{1}{4}, \tag{38}$$

the expectation value of the Hamiltonian is therefore bounded

$$E = \langle H\rangle = \frac{\hbar\, \omega}{2}\, \left(\left\langle p^2\right\rangle + \left\langle x^2\right\rangle\right) \geq \frac{\hbar\, \omega}{2}\, \left(\left\langle p^2\right\rangle + \frac{1}{4\left\langle p^2\right\rangle}\right) \geq \frac{\hbar\, \omega}{2}. \tag{39}$$

To saturates the *minimal energy bound*, the state must *first* saturates the *uncertainty bound*, which is the case for the ground state $|0\rangle$.

**HW 2** Exercise: Calculate the expectation value $\langle 0|\, x^4\, |0\rangle$ of the $x^4$ operator on the ground state $|0\rangle$.

## ■ Coherent States

### ■ Definition

Are there any other minimal uncertainty states besides $|0\rangle$?

Yes, they are known as the **coherent state** (or called **Glauber state**). Each coherent state $|\alpha\rangle$ is labeled by a *complex number* $\alpha \in \mathbb{C}$ and defined as the the *eigenstate* of the *annihilation operator* $a$ with the *eigenvalue* $\alpha$.

$$\boxed{a\,|\alpha\rangle = \alpha\,|\alpha\rangle.} \tag{40}$$

The parameter $\alpha = |\alpha|\, e^{i\varphi}$corresponds to the *complex* **wave amplitude** of the **boson** (under the **wave-particle duality**). This should be distinguished from the wave function $\psi_\alpha(x) = \langle x \mid \alpha\rangle$ of the *oscillator*.

- Note that $a$ is *non-Hermitian*,
  - its eigenvalues $\alpha$ can be *complex*,
  - its eigenstates with different eigenvalues may *not* be *orthogonal*, i.e. $\langle\alpha_1 \mid \alpha_2\rangle \neq \delta(\alpha_1 - \alpha_2)$.
  - Nevertheless, we do assume that $|\alpha\rangle$ is *normalized*, i.e. $\langle\alpha \mid \alpha\rangle = 1$.
- Eq. (40) also implies

$$\boxed{\langle\alpha|\, a^\dagger = \langle\alpha|\, \alpha^*.} \tag{41}$$

Using Eq. (40) and Eq. (41), one can show that

$$\begin{aligned}
\langle\alpha|\, x\,|\alpha\rangle &= \frac{1}{\sqrt{2}}\,\langle\alpha|\, a + a^\dagger\,|\alpha\rangle \\
&= \frac{1}{\sqrt{2}}\,(\alpha + \alpha^*)\,\langle\alpha \mid \alpha\rangle \\
&= \sqrt{2}\ \mathrm{Re}\,\alpha,
\end{aligned} \tag{42}$$

$$\begin{aligned}
\langle\alpha|\, x^2\,|\alpha\rangle &= \frac{1}{2}\,\langle\alpha|\,\left(a + a^\dagger\right)^2\,|\alpha\rangle \\
&= \frac{1}{2}\left(\langle\alpha|\, a\, a\,|\alpha\rangle + \langle\alpha|\, a\, a^\dagger\,|\alpha\rangle + \langle\alpha|\, a^\dagger\, a\,|\alpha\rangle + \langle\alpha|\, a^\dagger\, a^\dagger\,|\alpha\rangle\right) \\
&= \frac{1}{2}\left(\langle\alpha|\, a\, a\,|\alpha\rangle + \langle\alpha|\,\left(a^\dagger\, a + 1\right)|\alpha\rangle + \langle\alpha|\, a^\dagger\, a\,|\alpha\rangle + \langle\alpha|\, a^\dagger\, a^\dagger\,|\alpha\rangle\right) \\
&= \frac{1}{2}\left(\alpha^2 + 2\,\alpha^*\,\alpha + \alpha^{*2} + 1\right) \\
&= 2\,(\mathrm{Re}\,\alpha)^2 + 1/2,
\end{aligned} \tag{43}$$

So the position uncertainty is given by

$$\begin{aligned}
(\mathrm{std}\ x)^2 &= \langle\alpha|\, x^2\,|\alpha\rangle - \langle\alpha|\, x\,|\alpha\rangle^2 \\
&= 2\,(\mathrm{Re}\,\alpha)^2 + 1/2 - 2\,(\mathrm{Re}\,\alpha)^2 \\
&= 1/2.
\end{aligned} \tag{44}$$

Similarly, for the momentum uncertainty,

$$\begin{aligned}
&\langle\alpha|\, p\,|\alpha\rangle = \sqrt{2}\ \mathrm{Im}\,\alpha,\\
&\langle\alpha|\, p^2\,|\alpha\rangle = 2\,(\mathrm{Im}\,\alpha)^2 + 1/2,\\
&(\mathrm{std}\ p)^2 = \langle\alpha|\, p^2\,|\alpha\rangle - \langle\alpha|\, p\,|\alpha\rangle^2 = 1/2.
\end{aligned} \tag{45}$$

Therefore the uncertainty relation is indeed *saturated* for *coherent states*, regardless the choice of $\alpha$ ⇒ All **coherent states** are **minimal uncertainty states**. ⇒ The *quantum* fluctuations are *minimal* in coherent states. A quantum harmonic oscillator in the *coherent state* behaves as close as possible to its *classical* counterpart (without violating the rules of quantum mechanics).

## ■ Fock State Representation

In terms of the Fock state basis $|n\rangle$, a coherent state $|\alpha\rangle$ can be represented as

$$\boxed{|\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}}\,|n\rangle.} \tag{46}$$

This claim can be verified as follows.

$$\begin{aligned}
a\,|\alpha\rangle &= e^{-\frac{1}{2}|\alpha|^2}\left(\sum_{n=1}^{\infty} \frac{\alpha^n}{\sqrt{n!}}\, a\,|n\rangle + a\,|0\rangle\right)\\
&= e^{-\frac{1}{2}|\alpha|^2}\left(\sum_{n=1}^{\infty} \frac{\alpha^n}{\sqrt{n!}}\,\sqrt{n}\ |n-1\rangle + 0\right)\\
&= e^{-\frac{1}{2}|\alpha|^2} \sum_{n=1}^{\infty} \frac{\alpha^n}{\sqrt{(n-1)!}}\,|n-1\rangle,
\end{aligned} \tag{47}$$

by $m = n-1$,

$$\begin{aligned}
a\,|\alpha\rangle &= e^{-\frac{1}{2}|\alpha|^2} \sum_{m=0}^{\infty} \frac{\alpha^{m+1}}{\sqrt{m!}}\,|m\rangle\\
&= \alpha\,|\alpha\rangle.
\end{aligned} \tag{48}$$

So $|\alpha\rangle$ is indeed the eigenstate of $a$ with eigen value $\alpha$.

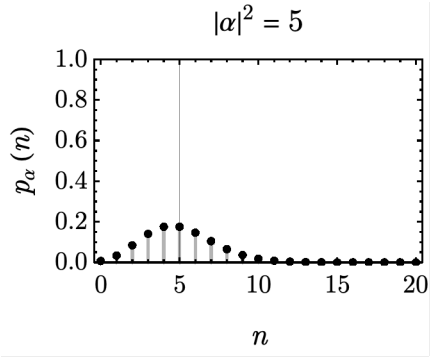
- In particular, the **ground state** (vacuum state) $|0\rangle$ is a coherent state with $\alpha = 0$.
  - Note: $|\alpha = 0\rangle = |n = 0\rangle$ is the *only* case when the coherent state index $\alpha \in \mathbb{C}$ and the Fock state index $n \in \mathbb{Z}$ coincide. In general, $\alpha = n$ does *not* imply $|\alpha\rangle$ and $|n\rangle$ to be the same state. For example,

$$\begin{aligned}
|\alpha = 1\rangle &= e^{-1/2} \sum_{n=0}^{\infty} \frac{1}{\sqrt{n!}}\,|n\rangle\\
&= e^{-1/2}\left(|n=0\rangle + |n=1\rangle + \frac{1}{\sqrt{2}}\,|n=2\rangle + \frac{1}{\sqrt{6}}\,|n=3\rangle + \ldots\right)
\end{aligned} \tag{49}$$

$\neq |n = 1\rangle$.

- Based on Eq. (46), the probability to observe $n$ **bosons** in the coherent state $|\alpha\rangle$ is given by

$$p_\alpha(n) = |\langle n \mid \alpha\rangle|^2 = \frac{|\alpha|^{2\,n}}{n!}\, e^{-|\alpha|^2}. \tag{50}$$




- The **mean boson number** is determined by the *expectation value* of the *boson number operator* $\hat{n} = a^\dagger\, a$,

$$\langle n\rangle_\alpha = \langle\alpha|\, \hat{n}\, |\alpha\rangle = |\alpha|^2. \tag{51}$$

because by Eq. (40) and Eq. (41)

$$\begin{aligned} &\langle\alpha|\, \hat{n}\, |\alpha\rangle = \langle\alpha|\, a^\dagger\, a\, |\alpha\rangle \\ &= \langle\alpha|\, \alpha^*\, \alpha\, |\alpha\rangle \\ &= |\alpha|^2\, \langle\alpha \mid \alpha\rangle \\ &= |\alpha|^2. \end{aligned} \tag{52}$$

We can rewrite Eq. (50) as

$$p_\alpha(n) = \frac{\langle n\rangle_\alpha^n}{n!}\, e^{-\langle n\rangle_\alpha}, \tag{53}$$

which follows the **Poisson distribution**.

## ■ Time Evolution

The **coherent states** (except $|0\rangle$) are *not* energy eigenstates. ⇒ They evolve with time. The **time-evolution operator** $U(t)$ of the harmonic oscillator:

$$U(t) = e^{-i\,H\,t/\hbar} = e^{-\frac{i\,\omega\,t}{2}}\; e^{-i\,\omega\,t\,\hat{n}}. \tag{54}$$

Applying $U(t)$ to $|\alpha\rangle$:

$$U(t)\,|\alpha\rangle = \left(e^{-\frac{i\,\omega\,t}{2}}\; e^{-i\,\omega\,t\,\hat{n}}\right)\left(e^{-\frac{1}{2}|\alpha|^2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}}\, |n\rangle\right)$$

$$= e^{-\frac{i\omega t}{2}}\ e^{-\frac{1}{2}|\alpha|^2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}}\ e^{-i\omega t \hat{n}}\,|n\rangle$$

$$= e^{-\frac{i\omega t}{2}}\ e^{-\frac{1}{2}|\alpha|^2} \sum_{n=0}^{\infty} \frac{\left(\alpha\ e^{-i\omega t}\right)^n}{\sqrt{n!}}\,|n\rangle$$

$$= e^{-\frac{i\omega t}{2}}\ e^{-\frac{1}{2}\left|\alpha\ e^{-i\omega t}\right|^2} \sum_{n=0}^{\infty} \frac{\left(\alpha\ e^{-i\omega t}\right)^n}{\sqrt{n!}}\,|n\rangle.$$

We can rewrite it as

$$U(t)\,|\alpha\rangle = e^{-\frac{i\omega t}{2}}\ \left|\alpha\ e^{-i\omega t}\right\rangle = e^{-\frac{i\omega t}{2}}\ |\alpha(t)\rangle. \tag{56}$$

So up to an overall phase factor $e^{-i\omega t/2}$ (originated from the zero-point energy), the **amplitude** $\alpha$ evolves as

$$\alpha(t) = \alpha(0)\ e^{-i\omega t}. \tag{57}$$

From Eq. (42), Eq. (45) and Eq. (51), we learnt that

$$\begin{aligned}
\langle x\rangle_{\alpha(t)} &= \langle\alpha(t)|\ x\,|\alpha(t)\rangle = \sqrt{2}\ \mathrm{Re}\,\alpha(t),\\
\langle p\rangle_{\alpha(t)} &= \langle\alpha(t)|\ p\,|\alpha(t)\rangle = \sqrt{2}\ \mathrm{Im}\,\alpha(t),\\
\langle n\rangle_{\alpha(t)} &= \langle\alpha(t)|\ \hat{n}\,|\alpha(t)\rangle = |\alpha(t)|^2.
\end{aligned} \tag{58}$$

Suppose we start with a coherent state at $\alpha(0) = A\,/\,\sqrt{2}$ (for a real positive $A$), then

$$\begin{aligned}
\langle x\rangle_{\alpha(t)} &= A\cos\omega t,\\
\langle p\rangle_{\alpha(t)} &= -A\sin\omega t,\\
\langle n\rangle_{\alpha(t)} &= \frac{1}{2}A^2.
\end{aligned} \tag{59}$$

- The *expectation values* of **coordinate** and **momentum** do *oscillate* following the *classical* behavior of a harmonic oscillator.
- The *expectation value* of the **boson number** remains constant. As a consequence, the **energy** of the oscillator is conserved.

$$\langle H\rangle_{\alpha(t)} = \hbar\,\omega\left(\langle n\rangle_{\alpha(t)} + \frac{1}{2}\right) = \frac{\hbar\,\omega}{2}\left(A^2+1\right). \tag{60}$$

## ▪ U(1) Symmetry

Conservation laws in two different languages:

| | **oscillator** | **boson** |
|---|---|---|
| conserved quantity | energy $H$ | particle number $\hat{n}$ |
| $U(1)$ symmetry | $\begin{cases} x \to x\cos\theta - p\sin\theta, \\ p \to p\cos\theta + x\sin\theta, \end{cases}$ | $a \to e^{i\,\theta}\, a$ |

Which Hermitian operator generates the U(1) symmetry transformation?

**Noether's theorem**: what is *conserved* is what *generates* the symmetry. The **U(1) symmetry** is *generated* by the **boson number operator** $\hat{n}$.

$$U(\theta) = e^{i\,\theta\,\hat{n}}. \tag{61}$$

The creation/annihilation operators transform as

$$\begin{aligned} &U(\theta)^{\dagger}\; a\; U(\theta) = e^{i\,\theta}\; a, \\ &U(\theta)^{\dagger}\; a^{\dagger}\; U(\theta) = e^{-i\,\theta}\; a. \end{aligned} \tag{62}$$

The U(1) transformation also rotates the amplitude $\alpha$ of the coherent state $|\alpha\rangle$

$$U(\theta)\,|\alpha\rangle = \left|e^{i\,\theta}\,\alpha\right\rangle. \tag{63}$$

The **time evolution** of the harmonic oscillator is actually a uniform U(1)=SO(2) **phase space rotation**, with $\theta = -\omega\, t$.

## ■ Real Space Representation

Real space (coordinate space) **wave function** of the coherent state $|\alpha\rangle$

$$\psi_{\alpha}(x) = \langle x \mid \alpha\rangle = \frac{1}{\pi^{1/4}} \exp\left(i\,\langle p\rangle_{\alpha}\, x - \frac{1}{2}\,(x - \langle x\rangle_{\alpha})^2\right), \tag{64}$$

where $\langle x\rangle_{\alpha} = \langle\alpha|\, x\,|\alpha\rangle$ and $\langle p\rangle_{\alpha} = \langle\alpha|\, p\,|\alpha\rangle$ are the expectation values of coordinate and momentum for the coherent state $|\alpha\rangle$, s.t.

$$\alpha = \frac{\langle x\rangle_{\alpha} + i\,\langle p\rangle_{\alpha}}{\sqrt{2}}. \tag{65}$$

- Be aware, we are switching among three sets of basis! Don't get confused.

$$\begin{aligned} &\text{coordinate basis}: \ \hat{x}\,|x\rangle = x\,|x\rangle, \\ &\text{Fock state basis}: \hat{n}\,|n\rangle = n\,|n\rangle, \\ &\text{coherent state "basis"}: a\,|\alpha\rangle = \alpha\,|\alpha\rangle. \end{aligned} \tag{66}$$

To show Eq. (64), we need to check that the wave function $\psi_{\alpha}(x)$ indeed represents an eigenstate of the annihilation operator $a$ with eigenvalue $\alpha$. Given that $p = -i\,\partial_x$ (when it acts on a wave function),

$$a = \frac{x + i\,p}{\sqrt{2}} = \frac{x + \partial_x}{\sqrt{2}}, \tag{67}$$

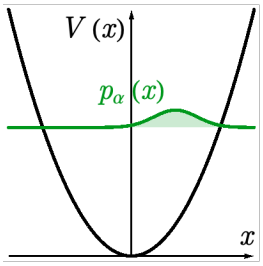
we can verify that

$$\begin{aligned} a\,\psi_\alpha(x) &= \frac{x + \partial_x}{\sqrt{2}}\,\frac{1}{\pi^{1/4}}\exp\left(i\,\langle p\rangle_\alpha\,x - \frac{1}{2}\,(x - \langle x\rangle_\alpha)^2\right) \\ &= \frac{x + i\,\langle p\rangle_\alpha - (x - \langle x\rangle_\alpha)}{\sqrt{2}}\,\frac{1}{\pi^{1/4}}\exp\left(i\,\langle p\rangle_\alpha\,x - \frac{1}{2}\,(x - \langle x\rangle_\alpha)^2\right) \\ &= \frac{\langle x\rangle_\alpha + i\,\langle p\rangle_\alpha}{\sqrt{2}}\,\psi_\alpha(x) \\ &= \alpha\,\psi_\alpha(x). \end{aligned} \tag{68}$$

The probability to find the **oscillator** at position $x$ in the coherent sate $\alpha$ is given by

$$p_\alpha(x) = |\psi_\alpha(x)|^2 = \frac{1}{\pi^{1/2}}\,e^{-(x - \langle x\rangle_\alpha)^2}. \tag{69}$$

As $\langle x\rangle_{\alpha(t)} = A\cos\omega\,t$ oscillates in time, the probability distribution of the coherent state will be a oscillating Gaussian wave packet with constant width, i.e. the wave packet of the coherent state is not spreading and remains the minimal uncertainty.




These properties make the *coherent state* a quantum state in closest analogy to the *classical* oscillator.

## ■ Baker-Campbell-Hausdorff Formula*

**Operator expansion formula**: let $A$, $B$ be two operators

$$\begin{aligned} &e^A\,B\,e^{-A} = e^{[A,\bullet]}\,B \\ &= B + [A,\,B] + \frac{1}{2!}[A,\,[A,\,B]] + \frac{1}{3!}[A,\,[A,\,[A,\,B]]] + \ldots. \end{aligned} \tag{70}$$

To prove this, we first define

$$B(\lambda) = e^{\lambda\,A}\,B\,e^{-\lambda\,A}. \tag{71}$$

It can be shown that $B(\lambda)$ must satisfy the differential equation

$$\begin{aligned}
\partial_\lambda B(\lambda) &= \partial_\lambda\left(e^{\lambda A}\, B\, e^{-\lambda A}\right)\\
&= \left(\partial_\lambda e^{\lambda A}\right) B\, e^{-\lambda A} + e^{\lambda A}\, B\left(\partial_\lambda e^{-\lambda A}\right)\\
&= A\, e^{\lambda A}\, B\, e^{-\lambda A} + e^{\lambda A}\, B\, e^{-\lambda A}(-A)\\
&= A\, B(\lambda) - B(\lambda)\, A\\
&= [A,\, B(\lambda)],
\end{aligned}$$

starting with the initial condition that $B(\lambda = 0) = B$. Then we propose the solution of this differential equation is given as follows

$$B(\lambda) = B + \lambda[A,\, B] + \frac{\lambda^2}{2!}[A,\, [A,\, B]] + \frac{\lambda^3}{3!}[A,\, [A,\, [A,\, B]]] + \ldots. \tag{73}$$

To verify this claim, we check that

$$\begin{aligned}
&\partial_\lambda B(\lambda) = [A,\, B] + \lambda\,[A,\, [A,\, B]] + \frac{\lambda^2}{2!}[A,\, [A,\, [A,\, B]]] + \ldots = [A,\, B(\lambda)],\\
&B(\lambda = 0) = B + 0 + 0 + 0 + \ldots = B,
\end{aligned} \tag{74}$$

therefore Eq. (73) is indeed the solution of Eq. (72). Then combining Eq. (71) and Eq. (73) at $\lambda = 1$, we obtain the operator expansion in Eq. (70).

If $[A,\, B] = \text{const}$ is a **constant operator** (i.e. a constant number times the identity operator $\mathbb{1}$), the operator expansion in Eq. (70) can be reduced to

$$e^{A}\, B\, e^{-A} = e^{[A,\bullet]}\, B = B + [A,\, B], \tag{75}$$

because $[A,\, [A,\, B]] = 0$ and hence all the higher order commutators vanish.

With this, we can prove a *weak version* of the **Baker-Campbell-Hausdorff (BCH) Formula**.

$$\boxed{\text{If } [A,\, B] = \text{const}: e^{A+B} = e^{A}\, e^{B}\, e^{[B,A]/2} = e^{B}\, e^{A}\, e^{[A,B]/2}.} \tag{76}$$

To show this, let $g(\lambda) = e^{\lambda A}\, e^{\lambda B}$,

$$\begin{aligned}
\partial_\lambda g(\lambda) &= \partial_\lambda\left(e^{\lambda A}\, e^{\lambda B}\right)\\
&= \left(\partial_\lambda e^{\lambda A}\right) e^{\lambda B} + e^{\lambda A}\left(\partial_\lambda e^{\lambda B}\right)\\
&= A\, e^{\lambda A}\, e^{\lambda B} + e^{\lambda A}\, B\, e^{\lambda B}\\
&= A\, e^{\lambda A}\, e^{\lambda B} + e^{\lambda A}\, B\, e^{-\lambda A}\, e^{\lambda A}\, e^{\lambda B}\\
&= \left(A + e^{\lambda A}\, B\, e^{-\lambda A}\right) g(\lambda),
\end{aligned} \tag{77}$$

using Eq. (75),

$$\partial_\lambda g(\lambda) = (A + B + \lambda[A,\, B])\, g(\lambda), \tag{78}$$

whose solution is (try to verify this)

$$g(\lambda) = e^{\lambda(A+B) + \frac{\lambda^2}{2}[A,B]}. \tag{79}$$

At $\lambda = 1$, we have

$$e^A\, e^B = e^{A+B+\frac{1}{2}[A,B]} = e^{A+B}\, e^{[A,B]/2}, \tag{80}$$

where the last equality holds because $[A, B]$ is a constant. $e^{[A,B]/2}$ is like a number, which can be further moved to the other side of the equation, therefore the BCH formula in Eq. (76) is proved.

## ■ Displacement Operator*

The **displacement operator** $D(\alpha)$ is defined by

$$\boxed{D(\alpha) = e^{\alpha\, a^\dagger - \alpha^*\, a}.} \tag{81}$$

- $D(\alpha)$ is *unitary*,

$$\boxed{D(\alpha)^\dagger = D(\alpha)^{-1} = D(-\alpha),} \tag{82}$$

which can be verified directly

$$D(\alpha)^\dagger = \left(e^{\alpha\, a^\dagger - \alpha^*\, a}\right)^\dagger = e^{\alpha^*\, a - \alpha\, a^\dagger} = \left(e^{\alpha\, a^\dagger - \alpha^*\, a}\right)^{-1} = D(\alpha)^{-1}. \tag{83}$$

- $D(\alpha)$ implements **phase space displacement**,

$$\boxed{\begin{aligned} &D(\alpha)^\dagger\, a\, D(\alpha) = a + \alpha, \\ &D(\alpha)^\dagger\, a^\dagger\, D(\alpha) = a^\dagger + \alpha^*. \end{aligned}} \tag{84}$$

To see this, let $A = \alpha^*\, a - \alpha\, a^\dagger$. We can see

$$[A,\, a] = \left[\alpha^*\, a - \alpha\, a^\dagger,\, a\right] = -\alpha\left[a^\dagger,\, a\right] = \alpha, \tag{85}$$

which is a constant (operator). Then by the operator expansion in Eq. (75)

$$D(\alpha)^\dagger\, a\, D(\alpha) = e^A\, a\, e^{-A} = a + [A,\, a] = a + \alpha. \tag{86}$$

The case for $a^\dagger$ follows by Hermitian conjugating both sides.

- **Composition** of displacements

$$\boxed{D(\alpha)\, D(\beta) = e^{i\, \mathrm{Im}\, \alpha\, \beta^*}\, D(\alpha + \beta).} \tag{87}$$

Let $A = \alpha\, a^\dagger - \alpha^*\, a$, $B = \beta\, a^\dagger - \beta^*\, a$, we can see

$$\begin{aligned} [A,\, B] &= \left[\alpha\, a^\dagger - \alpha^*\, a,\, \beta\, a^\dagger - \beta^*\, a\right] \\ &= -\alpha\, \beta^*\left[a^\dagger,\, a\right] - \alpha^*\, \beta\left[a,\, a^\dagger\right] \\ &= \alpha\, \beta^* - \alpha^*\, \beta \\ &= 2\, i\, \mathrm{Im}\, \alpha\, \beta^*, \end{aligned} \tag{88}$$

which is a constant (operator). Then by the BCH formula in Eq. (76)

$$\begin{aligned} D(\alpha+\beta) &= e^{A+B} \\ &= e^{A}\, e^{B}\, e^{-[A,B]/2} \\ &= D(\alpha)\, D(\beta)\, e^{-i\,\mathrm{Im}\,\alpha\,\beta^*}. \end{aligned} \tag{89}$$

All these heavy math is to get us prepared for a beautiful statement: the **coherent state** $|\alpha\rangle$ is *displaced* from the **vacuum state** $|0\rangle$ by the **displacement operator** $D(\alpha)$

$$\boxed{|\alpha\rangle = D(\alpha)\,|0\rangle.} \tag{90}$$

- To prove this, we want to show that $|\alpha\rangle$ obtain in this way is indeed an eigenstate of $a$ with eigenvalue $\alpha$.

$$\begin{aligned} a\,|\alpha\rangle &= a\, D(\alpha)\,|0\rangle \\ &= D(\alpha)\, D(\alpha)^{\dagger}\, a\, D(\alpha)\,|0\rangle \\ &= D(\alpha)\,(a+\alpha)\,|0\rangle \\ &= D(\alpha)\,(a\,|0\rangle + \alpha\,|0\rangle) \\ &= D(\alpha)\,\alpha\,|0\rangle \\ &= \alpha\, D(\alpha)\,|0\rangle \\ &= \alpha\,|\alpha\rangle. \end{aligned} \tag{91}$$

Moreover, $|\alpha\rangle$ obtained in this way is automatically normalized (given that $|0\rangle$ is normalized).

$$\langle\alpha\mid\alpha\rangle = \langle 0|\, D(\alpha)^{\dagger}\, D(\alpha)\,|0\rangle = \langle 0\mid 0\rangle = 1. \tag{92}$$

- Another more explicit way to show Eq. (90) is to recall Eq. (23) and Eq. (46),

$$\begin{aligned} |n\rangle &= \frac{1}{\sqrt{n!}}\left(a^{\dagger}\right)^{n}|0\rangle, \\ |\alpha\rangle &= e^{-\frac{1}{2}|\alpha|^2}\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}\,|n\rangle, \end{aligned} \tag{93}$$

then we have

$$|\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2}\sum_{n=0}^{\infty}\frac{\left(\alpha\, a^{\dagger}\right)^n}{n!}\,|0\rangle = e^{-\frac{1}{2}|\alpha|^2}\, e^{\alpha\, a^{\dagger}}\,|0\rangle. \tag{94}$$

Since $a\,|0\rangle = 0$, $e^{-\alpha^*\, a}\,|0\rangle = |0\rangle$, so Eq. (94) can be written as

$$|\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2}\, e^{\alpha\, a^{\dagger}}\, e^{-\alpha^*\, a}\,|0\rangle. \tag{95}$$

Let $A = \alpha\, a^{\dagger}$ and $B = -\alpha^*\, a$, then $[A,\, B] = |\alpha|^2$, by the BCH formula in Eq. (76),

$$D(\alpha) = e^{\alpha\, a^{\dagger} - \alpha^*\, a} = e^{A+B} = e^{A}\, e^{B}\, e^{-[A,B]/2} = e^{\alpha\, a^{\dagger}}\, e^{-\alpha^*\, a}\, e^{-\frac{1}{2}|\alpha|^2}. \tag{96}$$

Plugging Eq. (96) into Eq. (95), we obtain Eq. (90).

## ■ Overcomplete Basis*

**Scalar product** of two coherent states

$$\boxed{\langle\beta \mid \alpha\rangle = e^{-\frac{1}{2}\left(|\alpha|^2+|\beta|^2\right)+\alpha\,\beta^*}.} \tag{97}$$

We use Eq. (96) to show that

$$\begin{aligned}\langle\beta \mid \alpha\rangle &= \langle 0|\, D(\beta)^\dagger\, D(\alpha)\,|0\rangle \\ &= \langle 0|\, e^{-\beta\, a^\dagger}\, e^{\beta^*\, a}\, e^{\alpha\, a^\dagger}\, e^{-\alpha^*\, a}\,|0\rangle\, e^{-\frac{1}{2}\left(|\alpha|^2+|\beta|^2\right)} \\ &= \langle 0|\, e^{\beta^*\, a}\, e^{\alpha\, a^\dagger}\,|0\rangle\, e^{-\frac{1}{2}\left(|\alpha|^2+|\beta|^2\right)}.\end{aligned} \tag{98}$$

According to the BCH formula in Eq. (76),

$$e^{\beta^*\, a}\, e^{\alpha\, a^\dagger} = e^{\alpha\, a^\dagger}\, e^{\beta^*\, a}\, e^{[\beta^*\, a,\alpha\, a^\dagger]} = e^{\alpha\, a^\dagger}\, e^{\beta^*\, a}\, e^{\alpha\,\beta^*}, \tag{99}$$

therefore

$$\begin{aligned}\langle\beta \mid \alpha\rangle &= \langle 0|\, e^{\alpha\, a^\dagger}\, e^{\beta^*\, a}\,|0\rangle\, e^{-\frac{1}{2}\left(|\alpha|^2+|\beta|^2\right)+\alpha\,\beta^*} \\ &= \langle 0 \mid 0\rangle\, e^{-\frac{1}{2}\left(|\alpha|^2+|\beta|^2\right)+\alpha\,\beta^*} \\ &= e^{-\frac{1}{2}\left(|\alpha|^2+|\beta|^2\right)+\alpha\,\beta^*}.\end{aligned} \tag{100}$$

The **transition probability** from state $|\alpha\rangle$ to $|\beta\rangle$ is *decays* with their **phase space distance** $|\alpha-\beta|$ as

$$\boxed{|\langle\beta \mid \alpha\rangle|^2 = e^{-|\alpha-\beta|^2}.} \tag{101}$$

- The non-vanishing scalar product (or transition probability) indicates that the coherent states are *not orthogonal*.
- The transition probability only vanish in the limit of $|\alpha-\beta| \gg 1$.

**Completeness relation** for coherent states:

$$\boxed{\frac{1}{\pi}\int_{\mathbb{C}} d\!\!{}^2\alpha\,|\alpha\rangle\,\langle\alpha| = \mathbb{1}.} \tag{102}$$

In fact, the coherent states are "overcomplete", which means that, as a consequence of their non-orthogonality, any coherent state can be expanded in terms of all the other coherent states, i.e. they are not linearly independent, e.g.

$$|\alpha\rangle = \frac{1}{\pi}\int_{\mathbb{C}} d\!\!{}^2\beta\,|\beta\rangle\,\langle\beta \mid \alpha\rangle = \frac{1}{\pi}\int_{\mathbb{C}} d\!\!{}^2\beta\,|\beta\rangle\, e^{-\frac{1}{2}\left(|\alpha|^2+|\beta|^2\right)+\alpha\,\beta^*}. \tag{103}$$

We can prove Eq. (102) by recalling Eq. (46)

$$|\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle, \tag{104}$$

so that

$$\frac{1}{\pi} \int_{\mathbb{C}} d\!\!\!^{-}\alpha \, |\alpha\rangle \langle\alpha| = \frac{1}{\pi} \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \frac{1}{\sqrt{m!\, n!}} \int_{\mathbb{C}} d\!\!\!^{-}\alpha \; e^{-|\alpha|^2} \alpha^m \alpha^{*n} |m\rangle \langle n|. \tag{105}$$

The complex plane integral can be solved using polar coordinates $\alpha = r\, e^{i\varphi}$,

$$\begin{aligned}
&\int_{\mathbb{C}} d\!\!\!^{-}\alpha \; e^{-|\alpha|^2} \alpha^m \alpha^{*n} = \int_0^{\infty} r \, d\!\!\!^{-} r \; e^{-r^2} \, r^{m+n} \int_0^{2\pi} d\!\!\!^{-}\varphi \; e^{i(m-n)\varphi} \\
&= 2\pi \, \delta_{mn} \int_0^{\infty} r \, d\!\!\!^{-} r \; e^{-r^2} \, r^{m+n} \\
&= \pi \, \delta_{mn} \int_0^{\infty} d\!\!\!^{-} r^2 \; e^{-r^2} \, r^{2n} \\
&= \pi \, \delta_{mn} \int_0^{\infty} d\!\!\!^{-} t \; e^{-t} \, t^n \\
&= \pi \, \delta_{mn} \, \Gamma(n+1) \\
&= \pi \, \delta_{mn} \, n!.
\end{aligned} \tag{106}$$

We used some knowledge about the Gamma function.

```
Integrate[Exp[-t] t^n, {t, 0, ∞}, Assumptions → n > 0]
```

```
Gamma[1 + n]
```

Therefore we can finally write down

$$\frac{1}{\pi} \int_{\mathbb{C}} d\!\!\!^{-}\alpha \, |\alpha\rangle \langle\alpha| = \sum_{n=0}^{\infty} |n\rangle \langle n| = \mathbb{1}. \tag{107}$$

# 3D Harmonic Oscillator

## Hamiltonian

Hamiltonian of a 3D harmonic oscillator

$$H = \frac{\hbar\, \omega}{2} \left(\boldsymbol{p}^2 + \boldsymbol{x}^2\right). \tag{108}$$

- Coordinate $\boldsymbol{x} = (x_1, x_2, x_3)$,
- Momentum $\boldsymbol{p} = (p_1, p_2, p_3)$.

They satisfies

$$\begin{aligned}
&[x_a, p_b] = i\, \delta_{ab}, \\
&[x_a, x_b] = [p_a, p_b] = 0.
\end{aligned} \tag{109}$$

The boson now has three **polarizations** (three oscillation directions)

- boson **annihilation** $\boldsymbol{a} = (a_1, a_2, a_3)$ and **creation** $\boldsymbol{a}^\dagger = \left(a_1^\dagger, a_2^\dagger, a_3^\dagger\right)$ operators

$$\boldsymbol{a} = \frac{1}{\sqrt{2}}(\boldsymbol{x} + i\,\boldsymbol{p}),\ \ \boldsymbol{a}^\dagger = \frac{1}{\sqrt{2}}(\boldsymbol{x} - i\,\boldsymbol{p}). \tag{110}$$

They satisfy the commutation relation

$$\begin{aligned} &\left[a_a,\, a_b^\dagger\right] = \delta_{ab}, \\ &[a_a,\, a_b] = \left[a_a^\dagger,\, a_b^\dagger\right] = 0. \end{aligned} \tag{111}$$

In terms of the boson operators,

$$\begin{aligned} H &= \hbar\,\omega\left(\boldsymbol{a}^\dagger \cdot \boldsymbol{a} + \frac{3}{2}\right) \\ &= \hbar\,\omega\left(a_1^\dagger\, a_1 + a_2^\dagger\, a_2 + a_3^\dagger\, a_3 + \frac{3}{2}\right). \end{aligned} \tag{112}$$

## ■ Energy Level and Degeneracy

Each boson (regardless of polarization) carries the same energy $\hbar\,\omega$, so the total energy is proportional to the **total number** $N$ of bosons.

$$\begin{aligned} &E = \hbar\,\omega\left(N + \frac{3}{2}\right), \\ &N = n_1 + n_2 + n_3. \end{aligned} \tag{113}$$

- Eigen state: $|n_1\ n_2\ n_3\rangle$
- Degeneracy

$$\sum_{n_1, n_2, n_3} \delta_{N = n_1 + n_2 + n_3} = \frac{1}{2}(N+1)(N+2). \tag{114}$$

```
Assuming[N ∈ Integers && N ≥ 0,
 Factor@Sum[KroneckerDelta[n1 + n2 + n3, N], {n1, 0, ∞}, {n2, 0, ∞}, {n3, 0, ∞}]]
```

```
1/2 (1 + N) (2 + N)
```

| | 0 | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|---|
| $E$ | $\frac{3}{2}$ | $\frac{5}{2}$ | $\frac{7}{2}$ | $\frac{9}{2}$ | $\frac{11}{2}$ | $\frac{13}{2}$ |
| deg. | 1 | 3 | 6 | 10 | 15 | 21 |

Question: How are the *degenerate states* differed from each other?

Classical picture: they have the same energy ⇒ oscillation amplitude is the same, but oscillation

direction can be different ⇒ *rotational degrees of freedom* may help to explain the degeneracy (but only partially).

## ■ Angular Momentum

The **angular momentum** $\boldsymbol{L} = (L_1, L_2, L_3)$ operators

$$\boldsymbol{L} = \boldsymbol{x} \times \boldsymbol{p}. \tag{115}$$

In component form, $L_a = \epsilon_{abc}\, x_b\, p_c$. ($\epsilon_{abc}$: Levi-Civita tensor, totally antisymmetric tensor) (*Einstein summation* is assumed hereinafter).

In terms of the boson operators,

$$\boxed{L_a = -i\, \epsilon_{abc}\, a_b^\dagger\, a_c.} \tag{116}$$

- The angular momentum operator generates the SO(3) *rotation* among different *polarization* modes.
- The (quadratic) **Casimir operator** (the square of angular momentum) $\boldsymbol{L}^2$.

$$\boldsymbol{L}^2 = L_1^2 + L_2^2 + L_3^2 = \sum_{a \neq b} \left(\hat{n}_a(\hat{n}_b + 1) - a_a^\dagger\, a_a^\dagger\, a_b\, a_b\right). \tag{117}$$

To verify Eq. (117), (the following summations are implicit)

$$\begin{aligned} \boldsymbol{L}^2 &= L_a\, L_a = -\epsilon_{abc}\, \epsilon_{ade}\, a_b^\dagger\, a_c\, a_d^\dagger\, a_e \\ &= -(\delta_{bd}\, \delta_{ce} - \delta_{be}\, \delta_{cd})\, a_b^\dagger\, a_c\, a_d^\dagger\, a_e \\ &= -a_b^\dagger\, a_c\, a_b^\dagger\, a_c + a_b^\dagger\, a_c\, a_c^\dagger\, a_b. \end{aligned} \tag{118}$$

In the summation of $b$, $c$, the terms with $b = c$ vanish, so we can restrict the summation to $b \neq c$, (the following summation is explicit)

$$\begin{aligned} \boldsymbol{L}^2 &= \sum_{b \neq c} \left(a_b^\dagger\, a_c\, a_c^\dagger\, a_b - a_b^\dagger\, a_c\, a_b^\dagger\, a_c\right) \\ &= \sum_{b \neq c} \left(a_b^\dagger\, a_b \left(a_c^\dagger\, a_c + 1\right) - a_b^\dagger\, a_b^\dagger\, a_c\, a_c\right). \end{aligned} \tag{119}$$

## ■ Fock State Basis

Represent the angular momentum operator in each subspace of fixed total boson number $N = n_1 + n_2 + n_3$.

$$\begin{aligned} L_1 &= -i\, \sqrt{(n_2 + 1)\, n_3}\ |n_1,\, n_2 + 1,\, n_3 - 1\rangle\, \langle n_1\, n_2\, n_3| + h.c., \\ L_2 &= -i\, \sqrt{(n_3 + 1)\, n_1}\ |n_1 - 1,\, n_2,\, n_3 + 1\rangle\, \langle n_1\, n_2\, n_3| + h.c., \\ L_3 &= -i\, \sqrt{(n_1 + 1)\, n_2}\ |n_1 + 1,\, n_2 - 1,\, n_3\rangle\, \langle n_1\, n_2\, n_3| + h.c.\,. \end{aligned} \tag{120}$$

For example in the $N = 1$ sector, we have 3 basis states

$$\{|100\rangle, |010\rangle, |001\rangle\}. \tag{121}$$

The angular momentum operators $L_{1,2,3}$ are represented as $3\times 3$ matrices.

$$L_1 \doteq \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix},\ L_2 \doteq \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix},\ L_3 \doteq \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{122}$$

The $\boldsymbol{L}^2 = L_1^2 + L_2^2 + L_3^2$operator can be obtained by matrix square and summation,

$$\boldsymbol{L}^2 \doteq \begin{pmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}. \tag{123}$$

Use the explicit matrix representation to verify the **commutation relation**

$$\boxed{[L_a, L_b] = i\,\epsilon_{abc}\,L_c.} \tag{124}$$

This is the defining relation of the angular momentum operators (which applies to all angular momentum sectors).

**HW 3** Prove $[L_a, L_b] = i\,\epsilon_{abc}\,L_c$ using $L_a = -i\,\epsilon_{abc}\,a_b^\dagger\,a_c$ and the commutation relations of $a_a$ and $a_a^\dagger$.

## ■ Angular Momentum Basis

Easy to see that $\boldsymbol{L}^2$ and $L_3$ commute ⇒ their simultaneous eigenstates span the degenerate subspace. Introduce $l$ and $m$ to label the common eigenstates.

$$\boxed{\begin{aligned} &\boldsymbol{L}^2\,|l, m\rangle = l(l+1)\,|l, m\rangle, \\ &L_3\,|l, m\rangle = m\,|l, m\rangle. \end{aligned}} \tag{125}$$

Diagonalize the matrices in Eq. (122),

$$\begin{aligned} &|l = 1, m = \pm 1\rangle = \frac{1}{\sqrt{2}}\left(\left|100\right\rangle \pm i\left|010\right\rangle\right), \\ &|l = 1, m = 0\rangle = \left|001\right\rangle. \end{aligned} \tag{126}$$

- Classical picture:
  - $|l = 1, m = \pm 1\rangle$ - uniform circular rotation in the $xy$-plane, ± sign corresponds to counterclockwise or clockwise.
  - $|l = 1, m = 0\rangle$ - linear oscillation along the $z$-direction.
- Quantum wave function:
  - Fock state basis

$$\psi_{n_1\, n_2\, n_3}(x_1,\, x_2,\, x_3) = \psi_{n_1}(x_1)\, \psi_{n_2}(x_2)\, \psi_{n_3}(x_3), \tag{127}$$

where $\psi_n(x)$ is the wave function of a 1D harmonic oscillator, given by Eq. (28).

$|100\rangle$ $|010\rangle$ $|001\rangle$

- Angular momentum basis

| $l$ | $m$ | $N=1$ sector state | |
|---|---|---|---|
| 1 | 1 | $\frac{i\,\lvert 010\rangle + \lvert 100\rangle}{\sqrt{2}}$ |  |
| 1 | 0 | $\lvert 001\rangle$ |  |
| 1 | −1 | $\frac{-i\,\lvert 010\rangle + \lvert 100\rangle}{\sqrt{2}}$ |  |

### ▫ More Examples

## ■ U(3) Symmetry*

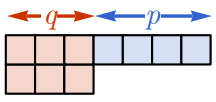
The SO(3) symmetry explains the 3-fold degeneracy of the *first* excited state. But the degeneracy of higher angular momentum states goes as $2\,l+1$ (like 1, 3, 5, 7, ...), which is *smaller* than the observed degeneracies (1, 3, 6, 10, ...) in Eq. (114). This suggest the 3D harmonic oscillator has *larger symmetry*!

In fact, the following $U \in$U(3) transformation leaves the Hamiltonian invariant,

$$\boldsymbol{a} \to U\, \boldsymbol{a}. \tag{128}$$

So the 3D harmonic oscillator actually has **U(3) symmetry**.

- The Abelian U(1) subgroup does not lead to degeneracy.
- The non-Abelian **SU(3) subgroup** ⇒ irreducible representations $D_{pq}$ are labeled by two quantum numbers $p$, $q = 0, 1, 2, \ldots$




and their dimensions are

$$\dim D_{pq} = \frac{1}{2}(p+1)(q+1)(p+q+2). \tag{129}$$

For bosonic systems, only $q = 0$ representations can appear, the corresponding dimensions $\dim D_{p0} = \frac{1}{2}(p+1)(p+2)$ (for $p = 0, 1, 2, \ldots$) fully explain the degeneracies of the entire spectrum, as in Eq. (114).

# Angular Momentum

## ■ Operator Algebra

### ■ Definition

Motivation: classical mechanics: *orbital* angular momentum $\boldsymbol{L} = (L_1, L_2, L_3)$

$$\boxed{\boldsymbol{L} = \boldsymbol{x} \times \boldsymbol{p}.} \tag{130}$$

In component form, $L_a = \epsilon_{abc}\, x_b\, p_c$. ($\epsilon_{abc}$: Levi-Civita tensor, totally antisymmetric tensor) (Einstein summation is assumed here). From

$$[x_a, p_b] = i\,\delta_{ab}, \tag{131}$$

(set $\hbar = 1$ for simplicity) ⇒ the angular momentum operators satisfy

$$[L_a, L_b] = i\,\epsilon_{abc}\, L_c. \tag{132}$$

We may treat this *commutation relation* as the definition for angular momentum.

Definition: the **angular momentum** operator $\boldsymbol{J} = (J_1, J_2, J_3)$ consist of three Hermitian operators, satisfying

$$\boxed{[J_a, J_b] = i\,\epsilon_{abc}\, J_c.} \tag{133}$$

- Equivalently, in vector form, $\boldsymbol{J} \times \boldsymbol{J} = i\,\boldsymbol{J}$.
- This general definition applies to **orbital** and **spin** angular momenta. The spin angular momentum goes beyond the classical definition of $\boldsymbol{x} \times \boldsymbol{p}$.
- The Hermitian operators $\boldsymbol{J}$ generate a unitary group - the SU(2) group.

### ■ Casimir Operator

A **Casimir operator** is a operator that commutes with all components of $\boldsymbol{J}$. It turns out that for SU(2) group, there is only one such operator: the **squared angular momentum** $\boldsymbol{J}^2 = \boldsymbol{J} \cdot \boldsymbol{J}$,

$$\boxed{\boldsymbol{J}^2 = J_1^2 + J_2^2 + J_3^2.} \tag{134}$$

- $\boldsymbol{J}^2$ is Hermitian.
- By Eq. (133), one can verify that (for $a = 1, 2, 3$)

$$\left[\boldsymbol{J}^2, J_a\right] = 0. \tag{135}$$

## ■ Common Eigenstates

$\boldsymbol{J}^2$ and $J_3$ commute ⇒ they share the same set of eigenstates, which can be labeled by two independent quantum number: $|j, m\rangle$ ⇒ as a common eigenstate, $|j, m\rangle$ must satisfy the eigen equation for both operators

$$\begin{aligned} \boldsymbol{J}^2 |j, m\rangle &= \lambda_j |j, m\rangle, \\ J_3 |j, m\rangle &= m |j, m\rangle, \end{aligned} \tag{136}$$

where $\lambda_j$ is a function of $j$ (to be determined later).

- $\lambda_j$ is the the eigenvalue of $\boldsymbol{J}^2$ on $|j, m\rangle$,
- $m$ is the the eigenvalue of $J_3$ on $|j, m\rangle$.

## ■ Raising and Lowering Operators

Define the **raising** $J_+$ and **lowering** $J_-$ operators

$$\boxed{J_\pm = J_1 \pm i\, J_2.} \tag{137}$$

- In analogy to $e^{\pm i\,\theta} = \cos\theta \pm i \sin\theta$.
- $J_\pm$ are *not* Hermitian. Under Hermitian conjugate: $J_\pm^\dagger = J_\mp$.

By definition,

$$\boxed{J_3\, J_\pm = J_\pm (J_3 \pm 1).} \tag{138}$$

To show this,

$$\begin{aligned} J_3\, J_\pm &= J_3 (J_1 \pm i\, J_2) \\ &= (J_1\, J_3 + i\, J_2) \pm i\, (J_2\, J_3 - i\, J_1) \\ &= (J_1 \pm i\, J_2)\, (J_3 \pm 1) \\ &= J_\pm (J_3 \pm 1). \end{aligned} \tag{139}$$

From Eq. (138), $J_3\, J_\pm |j, m\rangle = J_\pm (J_3 \pm 1) |j, m\rangle = (m \pm 1)\, J_\pm |j, m\rangle$ ⇒ the state $J_\pm |j, m\rangle$ (as long as it is not zero) is also an eigenstate of $J_3$ but with the eigenvalue $(m \pm 1)$ ⇒ $J_\pm |j, m\rangle$ is just the $|j, m \pm 1\rangle$ state (up to overall coefficient)

$$J_\pm |j, m\rangle = c_m^\pm |j, m \pm 1\rangle. \tag{140}$$

- Therefore $J_\pm$ is called the *raising/lowering* operator.
- Also note that, under the action of $J_\pm$, the quantum number $m$ can only change by 1 (not change continuously) ⇒ *angular momentum quantization.*

## ■ Bounds on Quantum Numbers

By definition in Eq. (137),

$$\boxed{\begin{aligned} J_+ J_- &= J^2 - J_3^2 + J_3, \\ J_- J_+ &= J^2 - J_3^2 - J_3. \end{aligned}} \tag{141}$$

To show this,

$$\begin{aligned} J_+ J_- &= (J_1 + i J_2)(J_1 - i J_2) \\ &= J_1^2 + i J_2 J_1 - i J_1 J_2 + J_2^2 \\ &= \left(J_1^2 + J_2^2\right) - i(J_1 J_2 - J_2 J_1) \\ &= \left(J^2 - J_3^2\right) + J_3. \end{aligned} \tag{142}$$

$|j, m\rangle$ is also the eigenstate of $J_+ J_-$ and $J_- J_+$.

$$\begin{aligned} \langle j, m| J_+ J_- |j, m\rangle &= \lambda_j - m^2 + m, \\ \langle j, m| J_- J_+ |j, m\rangle &= \lambda_j - m^2 - m. \end{aligned} \tag{143}$$

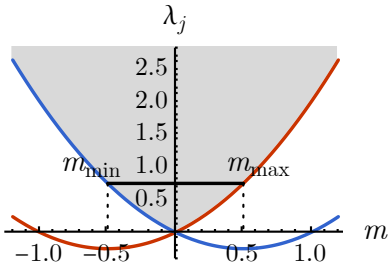
On the other hand, using Eq. (140),

$$\begin{aligned} \langle j, m| J_+ J_- |j, m\rangle &= \langle j, m| J_-^\dagger J_- |j, m\rangle = |c_m^-|^2 \geq 0, \\ \langle j, m| J_- J_+ |j, m\rangle &= \langle j, m| J_+^\dagger J_+ |j, m\rangle = |c_m^+|^2 \geq 0. \end{aligned} \tag{144}$$

Combining Eq. (143) and Eq. (144),

$$\begin{aligned} &\lambda_j - m(m \pm 1) \geq 0 \;\Rightarrow \\ &-\frac{1}{2}\left(\sqrt{1 + 4\lambda_j} - 1\right) \leq m \leq \frac{1}{2}\left(\sqrt{1 + 4\lambda_j} - 1\right). \end{aligned} \tag{145}$$

So $m$ is bounded from both above and below ⇒ denote the upper (lower) bound as $m_{\max}$ ($m_{\min}$).




# ■ Representation Theory

## ■ Highest and Lowest Weight State

Denote:

- **Highest weight state**: $|j, m_{\max}\rangle$, corresponds to $m = m_{\max}$. It can not be further raised by $J_+ \Rightarrow J_+ |j, m_{\max}\rangle = 0$.
- **Lowest weight state**: $|j, m_{\min}\rangle$, corresponds to $m = m_{\min}$. It can not be further lowered by $J_- \Rightarrow J_- |j, m_{\min}\rangle = 0$.

Therefore

$$\begin{aligned} 0 &= \langle j, m_{\min}| J_+ J_- |j, m_{\min}\rangle = \lambda_j - m_{\min}^2 + m_{\min}, \\ 0 &= \langle j, m_{\max}| J_- J_+ |j, m_{\max}\rangle = \lambda_j - m_{\max}^2 - m_{\max}. \end{aligned} \tag{146}$$

Eliminate $\lambda_j$,

$$(m_{\max} + m_{\min})(m_{\max} - m_{\min} + 1) = 0, \tag{147}$$

As $m_{\max} \geq m_{\min} \Rightarrow m_{\max} - m_{\min} + 1 \geq 1 > 0 \Rightarrow$ to satisfy Eq. (147), we must have $m_{\max} + m_{\min} = 0$, i.e. $m_{\max} = -m_{\min}$.

We have not specify the meaning of the quantum number $j$ yet. According to the convention, we give $j$ such a physical meaning that $j$ is the maximal value that $|m|$ can take, i.e.

$$m_{\max} = j, \; m_{\min} = -j \Rightarrow -j \leq m \leq j. \tag{148}$$

Then by Eq. (146)

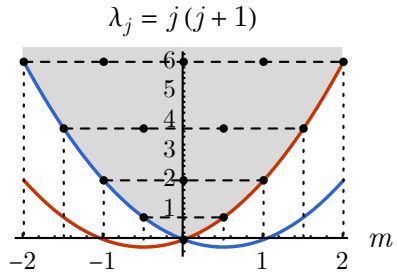
$$\lambda_j = j(j+1). \tag{149}$$

This also makes Eq. (148) consistent with Eq. (145).

## ■ Angular Momentum Quantization

Because $m$ can only change by $\pm 1 \Rightarrow$ the difference between $m_{\max}$ and $m_{\min}$ must be an integer $\Rightarrow m_{\max} - m_{\min} = 2\,j = 0, 1, 2, \ldots$, therefore

- $j$ can only be integer or half-integer: $j = 0, 1/2, 1, 3/2, 2, \ldots$
- $m$ takes values in $m = -j, -j+1, \ldots, j-1, j$.
- For **orbital** angular momentum $j$ takes *integer* values. For **spin** angular momentum $j$ can also be *half-integer*.




## ■ Representation

Now we want to determine the coefficients $c_m^{\pm}$ in Eq. (140). From Eq. (143) and Eq. (144), $|c_m^{\pm}|^2 = j(j+1) - m(m \pm 1)$. It is a gauge choice to fix $c_m^{\pm}$to be real and positive, so we take

$$c_m^{\pm} = \sqrt{j(j+1) - m(m\pm 1)}\ . \tag{150}$$

In conclusion, we have obtained the following representations for angular momentum operators (from Eq. (136) and Eq. (140))

$$\boxed{\begin{aligned} &\boldsymbol{J}^2\,|j,\,m\rangle = j(j+1)\,|j,\,m\rangle,\\ &J_3\,|j,\,m\rangle = m\,|j,\,m\rangle,\\ &J_\pm\,|j,\,m\rangle = \sqrt{j(j+1) - m(m\pm 1)}\ \,|j,\,m\pm 1\rangle. \end{aligned}} \tag{151}$$

Induction implies that all basis states can be

- either *raised* from the *lowest weight* state,

$$|j,\,m\rangle = \left(\frac{(j-m)!}{(2\,j)!\,(j+m)!}\right)^{1/2} J_+^{j+m}\,|j,\,-j\rangle, \tag{152}$$

- or *lowered* from the *highest weight* state,

$$|j,\,m\rangle = \left(\frac{(j+m)!}{(2\,j)!\,(j-m)!}\right)^{1/2} J_-^{j-m}\,|j,\,j\rangle. \tag{153}$$

This is just like the Harmonic oscillator.

To make the analogy more precise, take the large-$j$ limit,

$$\begin{aligned} &\frac{J_+}{\sqrt{2\,j}}\,|j,\,-j+n\rangle = \sqrt{n+1}\ \,|j,\,-j+n+1\rangle + O\big(j^{-1/2}\big),\\ &\frac{J_-}{\sqrt{2\,j}}\,|j,\,-j+n\rangle = \sqrt{n}\ \,|j,\,-j+n-1\rangle + O\big(j^{-1/2}\big). \end{aligned} \tag{154}$$

Under the following correspondence

$$\begin{aligned} &|j,\,-j+n\rangle \to |n\rangle,\\ &(2\,j)^{-1/2}\,J_- \to a,\ (2\,j)^{-1/2}\,J_+ \to a^\dagger, \end{aligned} \tag{155}$$

the boson creation/annihilation algebra Eq. (9) can be reproduced approximately (to the leading order). In this sense, *spin excitations* can also be treated as bosons, called **magnons**.

## ■ Spin-1/2

In the $j = 1/2$ subspace, the (spin) angular momentum operators $\boldsymbol{S} = (S_1,\,S_2,\,S_3)$ can be represented as **Pauli matrices**,

$$\boxed{\boldsymbol{S} = \frac{1}{2}\,\boldsymbol{\sigma}.} \tag{156}$$

- Basis: $\{|\uparrow\rangle = |1/2, +1/2\rangle, |\downarrow\rangle = |1/2, -1/2\rangle\}$.
- Matrix representations:

$$S_1 \doteq \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\ S_2 \doteq \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},\ S_3 \doteq \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{157}$$

- Eigenstates and eigenvalues

$$\begin{aligned} S_1 &: \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \to +\frac{1}{2},\ \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} \to -\frac{1}{2}, \\ S_2 &: \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix} \to +\frac{1}{2},\ \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix} \to -\frac{1}{2}, \\ S_1 &: \begin{pmatrix} 1 \\ 0 \end{pmatrix} \to +\frac{1}{2},\ \begin{pmatrix} 0 \\ 1 \end{pmatrix} \to -\frac{1}{2}. \end{aligned} \tag{158}$$

## ■ Spin-1

The $j = 1$ subspace: dimension $= 3 \Rightarrow 3$ basis states, and angular momentum operator represented as 3×3 matrices.

- Basis: $\{|1, +1\rangle, |1, 0\rangle, |1, -1\rangle\}$.
- Matrix representations (the same matrices also represent spin-1)

$$L_1 \doteq \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix},\ L_2 \doteq \frac{1}{\sqrt{2}\,i}\begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix},\ L_3 \doteq \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \tag{159}$$

Switch to another set of basis ($p$-wave orbitals)

- Basis transformation

$$\begin{pmatrix} |1, +1\rangle \\ |1, 0\rangle \\ |1, -1\rangle \end{pmatrix} = \begin{pmatrix} \frac{i}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & -i \\ \frac{-i}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \end{pmatrix}\begin{pmatrix} |x\rangle \\ |y\rangle \\ |z\rangle \end{pmatrix}. \tag{160}$$

- Denote the transformation matrix by $U$, the operators transform as $L_a \to U^\dagger\, L_a\, U$,

$$L_1 \doteq \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix},\ L_2 \doteq \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix},\ L_3 \doteq \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{161}$$

## ■ Rotation Operators

**Rotation operators** are generated **angular momentum operators** by

$$\boxed{R(\boldsymbol{\theta}) = e^{i\,\boldsymbol{\theta}\cdot\boldsymbol{J}}.} \tag{162}$$

The physical meaning of $\boldsymbol{\theta} = (\theta_1, \theta_2, \theta_3)$

- **direction** of $\boldsymbol{\theta}$: the direction of the rotational *axis* (following the *right-handed* rule),
- **magnitude** of $\boldsymbol{\theta}$: the amount of *angle* to rotate.
  Examples: rotate along (0, 0, 1) axis by $\theta \Rightarrow \boldsymbol{\theta} = (0, 0, \theta)$.
- Spin-1/2 representation, in the $\{|\uparrow\rangle, |\downarrow\rangle\}$ basis,

$$R_{1/2}(\boldsymbol{\theta}) \doteq \begin{pmatrix} e^{i\,\theta/2} & 0 \\ 0 & e^{-i\,\theta/2} \end{pmatrix}. \tag{163}$$

- Spin-1 representation, in the $\{|x\rangle, |y\rangle, |z\rangle\}$ basis,

$$R_1(\boldsymbol{\theta}) \doteq \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{164}$$

When $\theta = 2\,\pi$, a rotation by $2\,\pi$ should do nothing,

- This is indeed the case for spin-1 representation

$$R_1(0, 0, 2\,\pi) \doteq \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \doteq \mathbb{1}. \tag{165}$$

- But not for spin-1/2,

$$R_{1/2}(0, 0, 2\,\pi) \doteq \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} \doteq -\mathbb{1}, \tag{166}$$

The extra minus sign means that spin-1/2 is a **projective representation** of SO(3). Nevertheless, it is a **linear representation** of SU(2).

# ■ Addition of Angular Momentum

## ■ Example: Fusion of Spins

Combine two spin-1/2 systems together,

- **State** tensor products:

$$\{|\uparrow\rangle, |\downarrow\rangle\}_A \times \{|\uparrow\rangle, |\downarrow\rangle\}_B = \{|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle\}. \tag{167}$$

- **Angular momentum** adds:

$$\boxed{\boldsymbol{S} = \boldsymbol{S}_A + \boldsymbol{S}_B,} \tag{168}$$

where $\boldsymbol{S}_A$ and $\boldsymbol{S}_B$ are represented as

$$\begin{aligned}\boldsymbol{S}_A &= \frac{1}{2}\,\boldsymbol{\sigma}_A \otimes \mathbb{1}_B \doteq \frac{1}{2}\left(\sigma^{10}, \sigma^{20}, \sigma^{30}\right),\\ \boldsymbol{S}_B &= \frac{1}{2}\,\mathbb{1}_A \otimes \boldsymbol{\sigma}_B \doteq \frac{1}{2}\left(\sigma^{01}, \sigma^{02}\,\sigma^{03}\right).\end{aligned} \tag{169}$$

The operator $\boldsymbol{S}$ qualifies as an *angular momentum* operator, because it satisfies the defining relation $\boldsymbol{S}\times\boldsymbol{S} = i\,\boldsymbol{S}$ ⇒ In fact, $\boldsymbol{S}$ corresponds to the **total angular momentum** of the combined system. ⇒ They are **generators** of the *global* SU(2) symmetry.

$$\begin{aligned}\boldsymbol{S}^2 &= (\boldsymbol{S}_A + \boldsymbol{S}_B)^2 = \boldsymbol{S}_A^2 + \boldsymbol{S}_B^2 + 2\,\boldsymbol{S}_A\cdot\boldsymbol{S}_B\\ &= \frac{3}{2}\mathbb{1} + 2\,\boldsymbol{S}_A\cdot\boldsymbol{S}_B.\end{aligned} \tag{170}$$

The operator $\boldsymbol{S}_A\cdot\boldsymbol{S}_B$ describes the *spin coupling*.

$$\boldsymbol{S}_A\cdot\boldsymbol{S}_B \doteq \frac{1}{4}\left(\sigma^{11}+\sigma^{22}+\sigma^{33}\right) = \frac{1}{4}\begin{pmatrix}1 & 0 & 0 & 0\\ 0 & -1 & 2 & 0\\ 0 & 2 & -1 & 0\\ 0 & 0 & 0 & 1\end{pmatrix}. \tag{171}$$

Diagonalize $\boldsymbol{S}_A\cdot\boldsymbol{S}_B$:

- Spin **singlet** state, $\boldsymbol{S}_A\cdot\boldsymbol{S}_B = -3/4 \Rightarrow \boldsymbol{S}^2 = 0$ $(s=0)$:

$$\boxed{|0,0\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right).} \tag{172}$$

- Spin **triplet** states, $\boldsymbol{S}_A\cdot\boldsymbol{S}_B = 1/4 \Rightarrow \boldsymbol{S}^2 = 2$ $(s=1)$:

$$\boxed{\begin{aligned}&|1,+1\rangle = |\uparrow\uparrow\rangle,\\ &|1,0\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right),\\ &|1,-1\rangle = |\downarrow\downarrow\rangle.\end{aligned}} \tag{173}$$

Under the basis transformation $\boldsymbol{S}$ is block diagonalized,

| space: | $\frac{1}{2}\otimes\frac{1}{2}$ | $0\oplus 1$ |
|---|---|---|
| basis: | $\lvert\uparrow\uparrow\rangle, \lvert\uparrow\downarrow\rangle, \lvert\downarrow\uparrow\rangle, \lvert\downarrow\downarrow\rangle$ | $\lvert 0,0\rangle; \lvert 1,+1\rangle, \lvert 1,0\rangle, \lvert 1,-1\rangle$ |

$$S_1 \doteq \begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{2} & 0 & 0 & \frac{1}{2} \\ \frac{1}{2} & 0 & 0 & \frac{1}{2} \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix} \qquad \left(\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \hline 0 & 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & 0 & \frac{1}{\sqrt{2}} & 0 \end{array}\right)$$

$$S_2 \doteq \begin{pmatrix} 0 & -\frac{i}{2} & -\frac{i}{2} & 0 \\ \frac{i}{2} & 0 & 0 & -\frac{i}{2} \\ \frac{i}{2} & 0 & 0 & -\frac{i}{2} \\ 0 & \frac{i}{2} & \frac{i}{2} & 0 \end{pmatrix} \qquad \left(\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \hline 0 & 0 & -\frac{i}{\sqrt{2}} & 0 \\ 0 & \frac{i}{\sqrt{2}} & 0 & -\frac{i}{\sqrt{2}} \\ 0 & 0 & \frac{i}{\sqrt{2}} & 0 \end{array}\right)$$

$$S_3 \doteq \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \qquad \left(\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \hline 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{array}\right)$$

$$\boldsymbol{S}^2 \doteq \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix} \qquad \left(\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \hline 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix}\right)$$

- The original basis $\{\lvert\uparrow\uparrow\rangle, \lvert\uparrow\downarrow\rangle, \lvert\downarrow\uparrow\rangle, \lvert\downarrow\downarrow\rangle\}$ form a **reducible representation** of SU(2).
- The new basis $\{\lvert 0,0\rangle\}$ and $\{\lvert 1,+1\rangle, \lvert 1,0\rangle, \lvert 1,-1\rangle\}$ respectively form **irreducible representations** of SU(2).

The two bases are related by basis transformations:

- $1/2 \otimes 1/2 \to 0$ channel:

$$(\lvert 0,0\rangle) = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \end{pmatrix} \begin{pmatrix} \lvert\uparrow\uparrow\rangle \\ \lvert\uparrow\downarrow\rangle \\ \lvert\downarrow\uparrow\rangle \\ \lvert\downarrow\downarrow\rangle \end{pmatrix}. \tag{174}$$

- $1/2 \otimes 1/2 \to 1$ channel:

$$\begin{pmatrix} \lvert 1,+1\rangle \\ \lvert 1,0\rangle \\ \lvert 1,-1\rangle \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \lvert\uparrow\uparrow\rangle \\ \lvert\uparrow\downarrow\rangle \\ \lvert\downarrow\uparrow\rangle \\ \lvert\downarrow\downarrow\rangle \end{pmatrix}. \tag{175}$$

The matrix elements are called **Clebsch-Gordan coefficients**. They tell us how the composition

of two spin-1/2 systems splits into a spin-0 and a spin-1 system.

## ■ Fusion Rules

Spins are irreducible representations of the SU(2) group. They are building blocks for more general (reducible) representations. All **representations** of SU(2) form a **category**:

- **Irreducible representations** are *simple objects* in the category, labeled by their spin quantum numbers $j = 0, 1/2, 1, \ldots$
- Other **reducible representations** are not simple. They can be considered as *spin systems*.
  - **Semisimple property**: each reducible representation (spin system) can split in to direct sum of irreducible representations (spins).

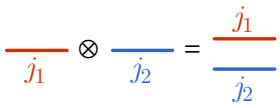
Each representation can be associated with a **representation space** (which is a Hilbert space). For example, spin-1/2 has a 2-dim representation space, spanned by $\{|\uparrow\rangle, |\downarrow\rangle\}$. For an irreducible representation of spin-$j$, the **representation dimension** is $2j+1$.

- Matrix representation of group element $g \in \mathrm{SU}(2)$ in representation $j$ can be depicted as


Example: rotation $\boldsymbol{\theta} = (0, 0, \theta)$, c.f. Eq. (163) and Eq. (164)

$$\begin{aligned} R(\boldsymbol{\theta}) &= \begin{pmatrix} e^{i\theta/2} & 0 \\ 0 & e^{-i\theta/2} \end{pmatrix}, \\ R(\boldsymbol{\theta}) &= \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}. \end{aligned} \tag{176}$$

The representation category of SU(2) is actually a **tensor category**, i.e. a category equipped with **tensor product** structures, meaning that the tensor product two representations is still a representation (which can then be further decomposed into irreducible representations).



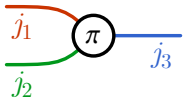

- The tensor structure specifies the **fusion rule**:

$$j_1 \otimes j_2 \to |j_1 - j_2| \oplus (|j_1 - j_2| + 1) \oplus \ldots \oplus (j_1 + j_2 - 1) \oplus (j_1 + j_2). \tag{177}$$

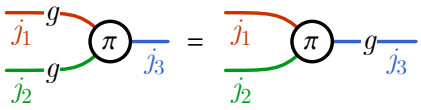
  - Composition of a spin-$j_1$ and a spin-$j_2$ systems is a spin system that contains irreducible representations ranging from $|j_1 - j_2|$ to $j_1 + j_2$ (each of them appear once).
  - Example: $1/2 \otimes 1/2 \to 0 \oplus 1$.
  - Notice that the *representation dimensions* add up correctly

$$\dim \mathcal{H}_{j_1 \otimes j_2} = \sum_{j_3=|j_1-j_2|}^{j_1+j_2} (2\,j_3+1) = (2\,j_1+1)\,(2\,j_2+1). \tag{178}$$

- The decomposition is implemented by the **fusion vertex** (a *projective morphism*), which can be viewed as three-leg tensors preserving the SU(2) symmetry.




such that $\forall\ g \in \mathrm{SU}(2)$:




- Example: fusion of two spin-1/2s, c.f. Eq. (174) and Eq. (175)

$$\begin{aligned}
&\pi_0 : 1/2 \otimes 1/2 \to 0,\\
&\pi_0 \doteq \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \end{pmatrix},\\
&\pi_1 : 1/2 \otimes 1/2 \to 1,\\
&\pi_1 \doteq \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.
\end{aligned} \tag{179}$$

Tensor elements of the *fusion vertex* are **Clebsch-Gordan coefficients** (CG coefficients).

$$\left(\begin{array}{cc|c} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{array}\right) = \langle j_3,\, m_3 \mid j_1,\, m_1;\, j_2,\, m_2 \rangle. \tag{180}$$

They can be used to implement basis transformations

$$\pi(j_1 \otimes j_2 \to j_3) = \sum_{m_1,m_2,m_3} |j_3,\, m_3\rangle \left(\begin{array}{cc|c} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{array}\right) \langle j_1,\, m_1;\, j_2,\, m_2|. \tag{181}$$

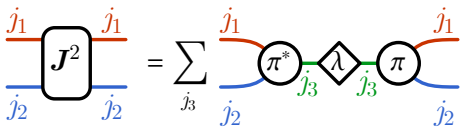
To obtain the CG coefficient,

- either look up in *Mathematica*:

```
ClebschGordan[{1/2, -1/2}, {1/2, 1/2}, {1, 0}]
```

$$\frac{1}{\sqrt{2}}$$

- or calculate as eigenbasis of the *Casimir operator* $\boldsymbol{J}^2$:




- Represent $\boldsymbol{J}^2$ in the $j_1 \otimes j_2$ space.
- Diagonalize $\boldsymbol{J}^2$, group eigenvectors by eigenvalues.
- Within each degenerated subspace: the eigenvalue $\lambda_{j_3} = j_3(j_3+1)$ or the degeneracy $2\,j_3+1$ infers the spin quantum number $j_3$, the eigenvectors form the fusion vertex $\pi(j_1 \otimes j_2 \to j_3)$.

### Code Example

Representation of $\boldsymbol{J}$ on spin-$j$ space.

$$\left\{\begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & 0 \end{pmatrix}, \begin{pmatrix} 0 & -\frac{i}{\sqrt{2}} & 0 \\ \frac{i}{\sqrt{2}} & 0 & -\frac{i}{\sqrt{2}} \\ 0 & \frac{i}{\sqrt{2}} & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}\right\}$$

Given $j_1 = 1/2$ and $j_2 = 1$, construct the representation of $\boldsymbol{J}^2$ in the $1/2 \otimes 1$ space.

$$\begin{pmatrix} \frac{15}{4} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{11}{4} & 0 & \sqrt{2} & 0 & 0 \\ 0 & 0 & \frac{7}{4} & 0 & \sqrt{2} & 0 \\ 0 & \sqrt{2} & 0 & \frac{7}{4} & 0 & 0 \\ 0 & 0 & \sqrt{2} & 0 & \frac{11}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{15}{4} \end{pmatrix}$$

Find the eigenvalues of $\boldsymbol{J}^2$

$$\left\{\frac{15}{4}, \frac{15}{4}, \frac{15}{4}, \frac{15}{4}, \frac{3}{4}, \frac{3}{4}\right\}$$

| $\lambda_j = j(j+1)$ | deg. $= 2j+1$ | $j$ |
|---|---|---|
| $3/4$ | 2 | $1/2$ |
| $15/4$ | 4 | $3/2$ |

(182)

This indicates that $1/2 \otimes 1 \to 1/2 \oplus 3/2$. Group the eigenvectors by their eigenvalues. Each degenerated subspace corresponds to a irreducible representation. The corresponding eigenbasis form the fusion vertex.

$$\left\langle \left| \frac{15}{4} \to \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & \frac{1}{\sqrt{3}} & 0 & \sqrt{\frac{2}{3}} & 0 \\ 0 & \sqrt{\frac{2}{3}} & 0 & \frac{1}{\sqrt{3}} & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \frac{3}{4} \to \begin{pmatrix} 0 & 0 & -\sqrt{\frac{2}{3}} & 0 & \frac{1}{\sqrt{3}} & 0 \\ 0 & -\frac{1}{\sqrt{3}} & 0 & \sqrt{\frac{2}{3}} & 0 & 0 \end{pmatrix} \right| \right\rangle$$

One can check the representation of $J_3$ in the spin-1/2 subspace

$$\begin{pmatrix} -\frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}$$

It is not guaranteed that the basis vectors will be the canonical ones. We may further diagonalize this matrix and rearrange its basis vectors.

In conclusion, the fusion vertex of $1/2 \otimes 1 \to 1/2$ is given by

$$\pi(1/2 \otimes 1 \to 1/2) = \begin{pmatrix} 0 & -\frac{1}{\sqrt{3}} & 0 & \sqrt{\frac{2}{3}} & 0 & 0 \\ 0 & 0 & -\sqrt{\frac{2}{3}} & 0 & \frac{1}{\sqrt{3}} & 0 \end{pmatrix}. \tag{183}$$

One can also obtain the fusion vertex of $1 \otimes 1/2 \to 1/2$ simply by rearranging the columns of the matrix in Eq. (183)

$$\pi(1 \otimes 1/2 \to 1/2) = \begin{pmatrix} 0 & \sqrt{\frac{2}{3}} & -\frac{1}{\sqrt{3}} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{\sqrt{3}} & -\sqrt{\frac{2}{3}} & 0 \end{pmatrix}, \tag{184}$$

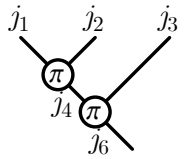
since their basis states are related by:

| $1/2 \otimes 1$ basis | $1 \otimes 1/2$ basis |
|---|---|
| $\lvert 1/2, +1/2; 1, +1\rangle$ | $\lvert 1, +1; 1/2, +1/2\rangle$ |
| $\lvert 1/2, +1/2; 1, 0\rangle$ | $\lvert 1, +1; 1/2, -1/2\rangle$ |
| $\lvert 1/2, +1/2; 1, -1\rangle$ | $\lvert 1, 0; 1/2, +1/2\rangle$ |
| $\lvert 1/2, -1/2; 1, +1\rangle$ | $\lvert 1, 0; 1/2, -1/2\rangle$ |
| $\lvert 1/2, -1/2; 1, 0\rangle$ | $\lvert 1, -1; 1/2, +1/2\rangle$ |
| $\lvert 1/2, -1/2; 1, +1\rangle$ | $\lvert 1, -1; 1/2, -1/2\rangle$ |

(185)

## ■ F-Symbols

Fusion vertices can be **composed** to fuse *multiple* spins.




- The composition follows from the *tensor network contraction*.

Given incoming representations $j_1, j_2, j_3$ and the outgoing representation $j_6$, there could still be multiple fusion channels, depending on the choice of $j_4$.

Example: $(1/2 \otimes 1/2) \otimes 1/2 \to 1/2$

- For $j_4 = 0$,

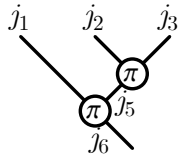
$$\begin{aligned}
\alpha_0 &= \pi(1/2 \otimes 1/2 \to 0) \circ \pi(0 \otimes 1/2 \to 1/2) \\
&\doteq \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \left[ \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \right] \\
&= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 0 & \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} & 0 & 0 \end{pmatrix} \\
&= \begin{pmatrix} 0 & 0 & \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} & 0 & 0 \end{pmatrix},
\end{aligned} \tag{186}$$

- For $j_4 = 1$,

$$\begin{aligned}
\alpha_1 &= \pi(1/2 \otimes 1/2 \to 1) \circ \pi(1 \otimes 1/2 \to 1/2) \\
&\doteq \begin{pmatrix} 0 & \sqrt{\frac{2}{3}} & -\frac{1}{\sqrt{3}} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{\sqrt{3}} & -\sqrt{\frac{2}{3}} & 0 \end{pmatrix} \left[ \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \right] \\
&= \begin{pmatrix} 0 & \sqrt{\frac{2}{3}} & -\frac{1}{\sqrt{3}} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{\sqrt{3}} & -\sqrt{\frac{2}{3}} & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}
\end{aligned} \tag{187}$$

$$= \begin{pmatrix} 0 & \sqrt{\frac{2}{3}} & -\frac{1}{\sqrt{6}} & 0 & -\frac{1}{\sqrt{6}} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{\sqrt{6}} & 0 & \frac{1}{\sqrt{6}} & -\sqrt{\frac{2}{3}} & 0 \end{pmatrix}.$$

However, we can also fuse the spin in a different order.




Now depending on $j_5$, there could be multiple fusion channels.

Example: $1/2 \otimes (1/2 \otimes 1/2) \to 1/2$

- For $j_5 = 0$,

$$\beta_0 = \pi(1/2 \otimes 1/2 \to 0) \circ \pi(1/2 \otimes 0 \to 1/2)$$

$$\doteq \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \left[ \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \end{pmatrix} \right]$$

$$= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \end{pmatrix} \tag{188}$$

$$= \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \end{pmatrix},$$

- For $j_5 = 1$,

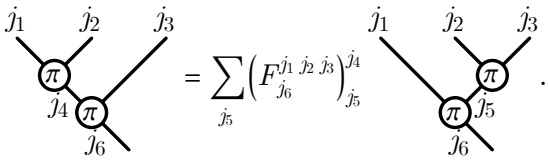
$$\beta_1 = \pi(1/2 \otimes 1/2 \to 1) \circ \pi(1/2 \otimes 1 \to 1/2)$$

$$\doteq \begin{pmatrix} 0 & -\frac{1}{\sqrt{3}} & 0 & \sqrt{\frac{2}{3}} & 0 & 0 \\ 0 & 0 & -\sqrt{\frac{2}{3}} & 0 & \frac{1}{\sqrt{3}} & 0 \end{pmatrix} \left[ \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \right]$$

$$= \begin{pmatrix} 0 & -\frac{1}{\sqrt{3}} & 0 & \sqrt{\frac{2}{3}} & 0 & 0 \\ 0 & 0 & -\sqrt{\frac{2}{3}} & 0 & \frac{1}{\sqrt{3}} & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

$$= \begin{pmatrix} 0 & -\frac{1}{\sqrt{6}} & -\frac{1}{\sqrt{6}} & 0 & \sqrt{\frac{2}{3}} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\sqrt{\frac{2}{3}} & 0 & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} & 0 \end{pmatrix}.$$

The incoming and outgoing representation remains the same, just by changing the fusion order, the resulting fusion tensors are different. For consistency, the two different **fusion trees** must be related. The relation is a *natural transformation* in category theory, which is a *linear transformation* among fusion trees,




(190)

In the example of $1/2 \otimes 1/2 \otimes 1/2 \to 1/2$

$$\begin{pmatrix} \alpha_0 \\ \alpha_1 \end{pmatrix} = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix}. \tag{191}$$

- The matrix $F^{j_1\, j_2\, j_3}_{j_6}$ is called ***F*-matrix**, whose elements are called ***F*-symbols**. The $F$-matrix is *unitary*.
- $F$-symbol is related to **Wigner 6 *j*-symbol** by a normalization factor

$$\left(F^{j_1\, j_2\, j_3}_{j_6}\right)^{j_4}_{j_5} = (-)^{j_1+j_2+j_3+j_6} \sqrt{(2\,j_4+1)\,(2\,j_5+1)} \begin{Bmatrix} j_1 & j_2 & j_4 \\ j_3 & j_6 & j_5 \end{Bmatrix}. \tag{192}$$

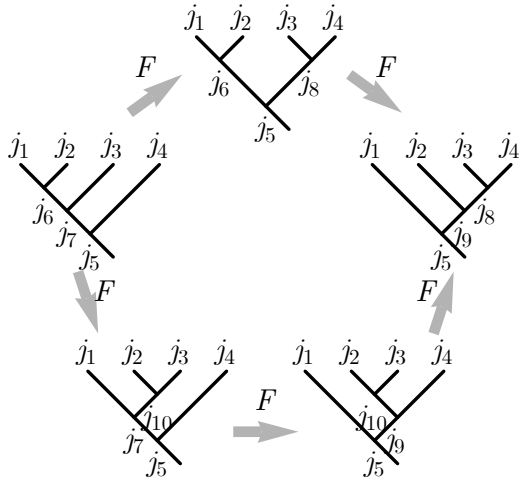
*Mathematica* knows how to calculate the 6 $j$-symbol.

```
SixJSymbol[{1 / 2, 1 / 2, 0}, {1 / 2, 1 / 2, 0}]
```

$$-\frac{1}{2}$$

**Pentagon Relation**: the consistency equation of $F$-symbols. The left-most and right-most fusion trees of four spins can be related to each other by $F$-moves in two different sequences. The

diagram must commute.




$$\left(F^{j_6\, j_3\, j_4}_{j_5}\right)^{j_7}_{j_8}\left(F^{j_1\, j_2\, j_8}_{j_5}\right)^{j_6}_{j_9} = \sum_{j_{10}}\left(F^{j_1\, j_2\, j_3}_{j_7}\right)^{j_6}_{j_{10}}\left(F^{j_1\, j_{10}\, j_4}_{j_5}\right)^{j_7}_{j_9}\left(F^{j_2\, j_3\, j_4}_{j_9}\right)^{j_{10}}_{j_8}. \tag{193}$$

Fortunately, a mathematical theorem guarantees that the *pentagon relations* are all that need to be satisfied, i.e. all other consistencies are consequences of the pentagon relations.

# Hydrogen Atom

## ▪ Classical Mechanical Background

## ▪ Classical Equation of Motion

- A **hydrogen atom** is a bound state of a single **electron** and a single **proton**.
  - The proton is much *heavier* than the electron (mass ratio $m_p \,/\, m_e \approx 1836$), it is essentially pinned at the center of mass.
  - Consider electron moving in the *electric static potential* created by the proton.

    $$V(r) = -\frac{k}{r}, \tag{194}$$

    where $k = e^2 \,/\, (4\,\pi\,\epsilon_0)$ describes the strength of the Coulomb force.
- The **Energy** (Hamiltonian) of the *electron* is given by

$$\boxed{E = \frac{\boldsymbol{p}^2}{2\,m} - \frac{k}{r},} \tag{195}$$

  - $\boldsymbol{r}$ is the **displacement** from the proton and $r = |\boldsymbol{r}|$ is the electron-proton distance.

- $\boldsymbol{p} = m\,\dot{\boldsymbol{r}}$ is the **momentum**.
- $m$ is the **mass** of electron (or more precisely the *reduced mass* of the electron in this two-body problem).

- The **angular momentum**

$$\boxed{\boldsymbol{L} = \boldsymbol{r} \times \boldsymbol{p}.} \tag{196}$$

- The **classical equation of motion**:

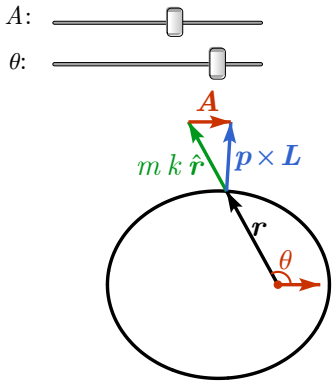
$$\dot{\boldsymbol{r}} = \frac{\boldsymbol{p}}{m},\ \dot{\boldsymbol{p}} = -\frac{k\,\boldsymbol{r}}{r^3}. \tag{197}$$

- $\dot{\boldsymbol{L}} = \dot{\boldsymbol{r}} \times \boldsymbol{p} + \boldsymbol{r} \times \dot{\boldsymbol{p}} = 0$ from Eq. (197) $\Rightarrow$ the angular momentum is *conserved*. ($\because$ the Hamiltonian has the SO(3) *rotation symmetry*)

## ■ Laplace-Runge-Lenz (LRL) Vector

- The **Laplace-Runge-Lenz** (LRL) vector is defined to be

$$\boxed{\boldsymbol{A} = \boldsymbol{p} \times \boldsymbol{L} - m\,k\,\frac{\boldsymbol{r}}{r}.} \tag{198}$$




- The LRL vector is *conserved* (there must be an *symmetry* associate to it, what is it?)

$$\boxed{\dot{\boldsymbol{A}} = 0.} \tag{199}$$

Using Eq. (197),

$$\dot{\boldsymbol{A}} = \dot{\boldsymbol{p}} \times \boldsymbol{L} - m\,k\,\frac{\dot{\boldsymbol{r}}}{r} + m\,k\,\frac{\boldsymbol{r}}{r^2}\,\dot{r}$$

$$= -\frac{k}{r^3}\,\boldsymbol{r} \times (\boldsymbol{r} \times \boldsymbol{p}) - \frac{k}{r}\,\boldsymbol{p} + m\,k\,\frac{\boldsymbol{r}}{r^2}\,\dot{r}$$

$$= -\frac{k}{r^3}\left(\boldsymbol{r}\,(\boldsymbol{r}\cdot\boldsymbol{p}) - r^2\,\boldsymbol{p}\right) - \frac{k}{r}\,\boldsymbol{p} + m\,k\,\frac{\boldsymbol{r}}{r^2}\,\dot{r}$$
$$= -m\,k\,\frac{\boldsymbol{r}}{r^3}\,(\boldsymbol{r}\cdot\dot{\boldsymbol{r}}) + m\,k\,\frac{\boldsymbol{r}}{r^2}\,\dot{r} = 0$$

This conservation law can be used to derive the **Kepler orbit**. Consider

$$\boldsymbol{A}\cdot\boldsymbol{r} = A\,r\cos\theta = \boldsymbol{r}\cdot(\boldsymbol{p}\times\boldsymbol{L}) - m\,k\,r, \tag{200}$$

where $\theta$ is the angle between $\boldsymbol{r}$ and $\boldsymbol{A}$. Permuting the scalar triple product $\boldsymbol{r}\cdot(\boldsymbol{p}\times\boldsymbol{L}) = \boldsymbol{L}\cdot(\boldsymbol{r}\times\boldsymbol{p}) = L^2$, Eq. (200) ⇒ the orbit equation

$$\frac{1}{r} = \frac{m\,k}{L^2}\left(1 + \frac{A}{m\,k}\cos\theta\right). \tag{201}$$

- Conservation of the *magnitude* $A = |\boldsymbol{A}|$ ⇒ conservation of the *eccentricity* of the orbit (in fact $e \equiv c\,/\,a = A\,/\,m\,k$).
- Conservation of the *direction* of $\boldsymbol{A}$ ⇒ conservation of the *periapsis* (the point of closest approach) with respect to the force center.

So the LRL vector is conserved.

- $\boldsymbol{L}$ and $\boldsymbol{A}$ are always perpendicular ($\boldsymbol{L}\cdot\boldsymbol{A} = 0$), they fully specifies a *unique* Kepler orbit (shape and orientation are both determined).
- As the orbit is specified, its energy must be determined too ⇒ so the energy $E$ is *not* an independent conserved quantity, in fact

$$\boxed{A^2 = 2\,m\,E\,L^2 + m^2\,k^2.} \tag{202}$$

- Given the *magnitude* of $L$ and $A$,
  - All orbits of different orientations are *degenerated* in energy ⇒ they are related by **symmetry**.
  - Each orbit orientation ⇔ a pair of *perpendicular unit* vectors ($\boldsymbol{L}\,/\,L$, $\boldsymbol{A}\,/\,A$) ⇔ a particular rotation in 3D space, i.e., a group element of SO(3) ⇔ a point on (half of) a **4D sphere**! (more precisely a point on $\mathrm{RP}^3$)
    - An explicit construction: every 4-dim unit vector ($n_1$, $n_2$ $n_3$, $n_4$) ⇔ two orthogonal 3-dim unit vectors

$$\begin{aligned}\boldsymbol{L}\,/\,L &= \left(n_1^2 + n_2^2 - n_3^2 - n_4^2,\ 2\,(n_2\,n_3 - n_1\,n_4),\ 2\,(n_1\,n_3 + n_2\,n_4)\right),\\ \boldsymbol{A}\,/\,A &= \left(2\,(n_2\,n_3 + n_1\,n_4),\ n_1^2 - n_2^2 + n_3^2 - n_4^2,\ 2\,(n_3\,n_4 - n_1\,n_2)\right).\end{aligned} \tag{203}$$

  - The symmetry that keeps the 4D sphere *invariant* is **SO(4)** (more precisely, to keep $\mathrm{RP}^3$ invariant, the symmetry is actually $\mathrm{SO}(4)\,/\,\mathbb{Z}_2$).
  - SO(4) group has *six* generators, all of them must be *conserved* ⇒ corresponding to the conservation of both $\boldsymbol{L}$ and $\boldsymbol{A}$.

> Let us represent the SO(4) group as 4×4 orthogonal matrices. (a) Show that orthogonal matrices $O = e^{i\,\theta\,A}$ are generated by imaginary antisymmetric matrices $A$ (i.e., if

$O^{\mathrm{T}}\, O = \mathbb{1}$ and $O \in \mathbb{R}$, then $A^{\mathrm{T}} = -A$ and $A \in \mathbb{I}$). (b) Verify that the following six matrices form a complete basis of generators (i.e. any imaginary antisymmetric matrix can be represented as a linear combination of them with real coefficient)

$$T_1 = \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix}, \qquad T_2 = \frac{1}{2}\begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & -i \\ i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{pmatrix},$$

$$T_3 = \frac{1}{2}\begin{pmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & i \\ 0 & 0 & -i & 0 \end{pmatrix};$$

$$S_1 = \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & -i & 0 \\ 0 & i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix}, \; S_2 = \frac{1}{2}\begin{pmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{pmatrix}, \; S_3 = \frac{1}{2}\begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & i \\ i & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \end{pmatrix}.$$

(c) Verify the following commutation relations
$[T_i,\, T_j] = i\, \epsilon_{ijk}\, T_k$, $[S_i,\, S_j] = i\, \epsilon_{ijk}\, S_k$, $[T_i,\, S_j] = 0$.
Compare with Eq. (133), we learn that $\mathrm{so}(4) \cong \mathrm{su}(2) \times \mathrm{su}(2)$.

# ■ Quantum Mechanical Treatment

## ■ Operator Algebra

We promote *classical observables* to **Hermitian operators**:

- **Coordinate** $\boldsymbol{r}$ and **momentum** $\boldsymbol{p}$ operators, satisfying $[r_a,\, p_b] = i\, \delta_{ab}$. See Eq. (131).
- **Angular momentum** operator $\boldsymbol{L} = \boldsymbol{r} \times \boldsymbol{p}$. See Eq. (130).
- **Quantum LRL** operator

$$\boldsymbol{A} = \frac{1}{2}\,(\boldsymbol{p} \times \boldsymbol{L} - \boldsymbol{L} \times \boldsymbol{p}) - m\, k\, \frac{\boldsymbol{r}}{r}. \tag{204}$$

Compared with the classical case Eq. (198), the additional "anti-symmetrization" is to ensure $\boldsymbol{A}$ to be Hermitian.

- **Hamiltonian** operator

$$H = \frac{\boldsymbol{p}^2}{2\, m} - \frac{k}{r}. \tag{205}$$

One can verify the following commutation relations

$$\begin{aligned} &[H,\, L_a] = 0, \\ &[H,\, A_a] = 0, \\ &[L_a,\, L_b] = i\, \epsilon_{abc}\, L_c, \\ &[L_a,\, A_b] = i\, \epsilon_{abc}\, A_c, \end{aligned} \tag{206}$$

$$[A_a,\, A_b] = -i\, 2\, m\, \epsilon_{abc}\, L_c\, H,$$

and the following operator equations

$$\begin{aligned} &\boldsymbol{A}\cdot\boldsymbol{L} = \boldsymbol{L}\cdot\boldsymbol{A} = 0, \\ &\boldsymbol{A}^2 = 2\, m\, H\big(\boldsymbol{L}^2 + 1\big) + m^2\, k^2. \end{aligned} \tag{207}$$

## ■ SO(4) Generators

Suppose there exist *bound states* with energy $E < 0$. In the subspace of a *fixed eigen energy* $E$ (i.e. replacing $H \to E$), it makes sense to rescale the quantum LRL operator $\boldsymbol{A}$ by a scalar

$$\tilde{\boldsymbol{A}} = \frac{1}{\sqrt{-2\, m\, E}}\, \boldsymbol{A}, \tag{208}$$

then Eq. (206) is simplified to

$$\begin{aligned} &[H,\, L_a] = 0, \\ &[H,\, A_a] = 0, \\ &[L_a,\, L_b] = i\, \epsilon_{abc}\, L_c, \\ &\big[L_a,\, \tilde{A}_b\big] = i\, \epsilon_{abc}\, \tilde{A}_c, \\ &\big[\tilde{A}_a,\, \tilde{A}_b\big] = i\, \epsilon_{abc}\, L_c. \end{aligned} \tag{209}$$

Define the SO(4) generators

$$\boldsymbol{T} = \frac{1}{2}\big(\boldsymbol{L} + \tilde{\boldsymbol{A}}\big),\ \ \boldsymbol{S} = \frac{1}{2}\big(\boldsymbol{L} - \tilde{\boldsymbol{A}}\big). \tag{210}$$

- How do we know they form SO(4) generators? We check their commutation relations

$$\begin{aligned} &[H,\, T_a] = 0, \\ &[H,\, S_a] = 0, \\ &[T_a,\, T_b] = i\, \epsilon_{abc}\, T_c, \\ &[S_a,\, S_b] = i\, \epsilon_{abc}\, S_c, \\ &[T_a,\, S_b] = 0. \end{aligned} \tag{211}$$

- $\boldsymbol{A}\cdot\boldsymbol{L} = \boldsymbol{L}\cdot\boldsymbol{A} = 0$ further implies $\boldsymbol{T}^2 = \boldsymbol{S}^2$.
- $\boldsymbol{T}$ and $\boldsymbol{S}$ are two sets of independent "angular-momentum-like" operators.
- Common eigen states of $\boldsymbol{T}$ and $\boldsymbol{S}$ are labeled by three quantum numbers $t$, $m_t$, $m_s$:

$$\begin{aligned} &\boldsymbol{T}^2\, |t,\, m_t,\, m_s\rangle = \boldsymbol{S}^2\, |t,\, m_t,\, m_s\rangle = t(t+1)\, |t,\, m_t,\, m_s\rangle, \\ &T_3\, |t,\, m_t,\, m_s\rangle = m_t\, |t,\, m_t,\, m_s\rangle, \\ &S_3\, |t,\, m_t,\, m_s\rangle = m_s\, |t,\, m_t,\, m_s\rangle, \end{aligned} \tag{212}$$

- $t = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots$. For each fixed $t \Rightarrow (2\,t+1)^2$ degeneracy.
- $m_t, m_s = -t, -t+1, \ldots, t-1, t$.

## ■ Energy Levels

From Eq. (207), Eq. (208), Eq. (210),

$$\begin{aligned} 4\,\boldsymbol{T}^2 &= \boldsymbol{L}^2 + \tilde{\boldsymbol{A}}^2 \\ &= \boldsymbol{L}^2 + \frac{1}{-2\,m\,E}\,\boldsymbol{A}^2 \\ &= \boldsymbol{L}^2 - \frac{1}{2\,m\,E}\left(2\,m\,E\left(\boldsymbol{L}^2+1\right) + m^2\,k^2\right) \\ &= -1 - \frac{m\,k^2}{2\,E}. \end{aligned} \tag{213}$$

- Acting on the state $|t, m_t, m_s\rangle$, $\boldsymbol{T}^2\,|t, m_t, m_s\rangle = t(t+1)\,|t, m_t, m_s\rangle$,

$$E = -\frac{m\,k^2}{2\left(4\,\boldsymbol{T}^2+1\right)} = -\frac{m\,k^2}{2\,(4\,t(t+1)+1)} = -\frac{m\,k^2}{2\,(2\,t+1)^2}. \tag{214}$$

- Given $t = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots$, define the **principal quantum number**

$$n = 2\,t+1 = 1, 2, 3, 4, 5, \ldots \tag{215}$$

The **energy levels** are given by $n \in \mathbb{Z}_+$

$$\boxed{E_n = -\frac{m\,k^2}{2\,n^2}.} \tag{216}$$

- The corresponding eigenstates $|t, m_t, m_s\rangle$ (with $t = (n-1)/2$) are labeled by $m_t, m_s = -t, -t+1, \ldots, t-1, t \Rightarrow$ level degeneracy: $(2\,t+1)^2 = n^2$.

## ■ Ground State

Which state is the ground state?

- The energy $E_n = -m\,k^2/\left(2\,n^2\right)$ is minimized when $n = 1$ (or $t = 0$).
- When $t = 0$, $m_t$ and $m_s$ has only one choice, i.e. $m_t = m_s = 0$.
- So the ground state corresponds to the $|0, 0, 0\rangle$ state.

How to find its wave function $\psi_{1\,s}(\boldsymbol{r})$? This amount to solve the differential equation $\boldsymbol{T}^2\,\psi_{1\,s} = 0$, which is equivalent to

$$H\,\psi_{1\,s} = E_1\,\psi_{1\,s}, \tag{217}$$

or more explicitly as

$$\left(\frac{\boldsymbol{p}^2}{2\,m} - \frac{k}{r}\right)\psi_{1\,s} = -\frac{m\,k^2}{2}\,\psi_{1\,s}. \tag{218}$$

We guess a trial wave function

$$\psi_{1\,s}(\boldsymbol{r}) \propto e^{-r/a}, \tag{219}$$

Eq. (218) implies $a\,k\,m - 1 = 0$, i.e. $a = 1/(k\,m)$.

In conclusion, the (normalized) **ground state wave function** of the electron in the hydrogen atom reads

$$\boxed{\psi_{1\,s}(\boldsymbol{r}) = \frac{2}{a^{3/2}}\,e^{-r/a},} \tag{220}$$

- $a = 1/(k\,m)$ is called the **Bohr radius**.
- The ground state energy is given by

$$\boxed{E_1 = -\frac{k}{2\,a},} \tag{221}$$

*as if* the electron in orbiting the proton in a circular orbital of radius $a$ (the classical picture).

- The electron is observed randomly in a probability cloud, called the **electron cloud**.

$$p(\boldsymbol{r}) = |\psi(\boldsymbol{r})|^2 \propto e^{-2\,r/a}. \tag{222}$$

## ■ Excited States

Excited states are labeled by higher *principal quantum numbers* $n = 2, 3, \ldots$ (or $t = \frac{1}{2}, 1, \ldots$).

- States with the same principal quantum numbers are degenerated in energy.
- Within each degenerated sectors, the states $|t, m_t, m_s\rangle$ form a complete set of basis (with $m_t, m_s = -t, \ldots, t$), which can be viewed as a combined system of two "spins" of the same angular momentum $t$.

The *orbital* angular momentum $\boldsymbol{L}$ of electron is the total angular momentum of the fictitious spins,

$$\boxed{\boldsymbol{L} = \boldsymbol{T} + \boldsymbol{S}.} \tag{223}$$

According to the fusion rules of spins, we anticipate their total angular momentum to take $l = 0, 1, \ldots, 2\,t$ (each representation will appear once). So the excited states may as well be labeled by

$$|n, l, m\rangle \tag{224}$$

- $n$ - **principal** quantum number ($n = 1, 2, \ldots$),
- $l$ - **angular** quantum number ($l = 0, 1, \ldots, n-1$)

- $m$ - **magnetic** quantum number $(m = -l, -l+1, \ldots, l-1, l)$

$|n, l, m\rangle$ and $|t, m_t, m_s\rangle$ are just differed by a basis transformation, but the former basis is more commonly used as **atomic orbitals**, because the electron-electron interaction will break the SO(4) symmetry down to SO(3).

# Code