130A Quantum Physics

Part 2. Algebraic Methods

Introduction

■ Functions are Vectors

■ Wave Function

Both **functions** and **vectors** as *mappings*:

- A **function** maps *inputs* to *outputs*: it takes in an input, does some processing, and returns an output. For example, a complex function

$$\begin{aligned} \psi : \mathbb{R} &\to \mathbb{C} \\ x &\mapsto \psi(x) \end{aligned} \tag{1}$$

- A **vector** is also a mapping: it maps *indices* to *values*, like looking up a table. For example, a complex vector

$$\begin{aligned} \psi : \mathbb{Z} &\to \mathbb{C} \\ i &\mapsto \psi_i \end{aligned} \tag{2}$$

By this analogy, every function can be viewed as a vector with *continuous* index and *infinite* dimension, vice versa.

When a **quantum state** $|\psi\rangle$ is described by

- a vector ψ_i, we call it a **state vector**.

$$|\psi\rangle = \sum_i \psi_i \, |i\rangle. \tag{3}$$

  - **Statistical interpretation**: the value of the state vector describes the *probability* to observe the state $|\psi\rangle$ behaving like the state $|i\rangle$,

$$p(i \,|\, \psi) = |\psi_i|^2. \tag{4}$$

- a function $\psi(x)$, we call it a **wave function**.

$$|\psi\rangle = \int dx \, \psi(x) \, |x\rangle. \tag{5}$$

  - **Statistical interpretation**: the value of the wave function describes the *probability density* to observe the state $|\psi\rangle$ behaving like the state $|x\rangle$ (continuously labeled),

$$p(x \,|\, \psi) = |\psi(x)|^2. \tag{6}$$

■ Dirac Delta

Dirac delta function - the continuous limit of the Kronecker delta symbol. It is defined by the following property under integration

$$\forall\, f : \int dx\, \delta(x)\, f(x) = f(0). \tag{7}$$

- By a shift of variable, Eq. (7) implies

$$\boxed{\int dx\, \delta(x - x')\, f(x) = f(x').} \tag{8}$$

Exc 1 Show Eq. (8) based on Eq. (7).

This behavior is similar to

$$\sum_i \delta_{ij}\, v_i = v_j. \tag{9}$$

- Intuitively, $\delta(x)$ describes a **unit impulse** located at $x = 0$. It can be considered as the limit of Gaussian functions at $\sigma \to 0$

$$\delta(x) = \lim_{\sigma \to 0} \frac{1}{\sqrt{2\,\pi}\ \sigma}\ e^{-\frac{x^2}{2\,\sigma^2}}. \tag{10}$$

Loosely speaking, it looks like

$$\delta(x) = \begin{cases} 0 & \text{if } x \neq 0, \\ \infty & \text{if } x = 0 \text{ (ill–defined).} \end{cases} \tag{11}$$

while the area under the curve remains unity as the limit is taken

$$\int dx\, \delta(x) = 1. \tag{12}$$

■ Position and Momentum

■ Discrete v.s. Continuous

Continuous observables are observables (Hermitian operators) whose *eigenvalues* can take *continuous real* values.

- Examples: **position** x of a quantum particle.

$$\hat{x}\,|x\rangle = x\,|x\rangle. \tag{13}$$

where

- $\hat{x}$ denotes the position operator (a Hermitian operator corresponding to the position observable of the particle)
- $x \in \mathbb{R}$ is the position eigenvalue.
- $|x\rangle$ the corresponding position eigenstate (the quantum state that describe the particle at the position x).

- The Hilbert space dimension is *infinite*. It is always helpful to think about the continuous eigen spectrum as the limit of an *infinitely dense* discrete spectrum.

Many notions of states and operators generalize to the continuous limit. The key is to replace every **summation** by **integration**.

	discrete	→	continuous
orthonormal basis	$\langle i\|j\rangle = \delta_{ij}$	→	$\langle x\|x'\rangle = \delta(x-x')$
resolution of identity	$\sum_i \|i\rangle\langle i\| = \mathbb{1}$	→	$\int dx\,\|x\rangle\langle x\| = \mathbb{1}$
state decomposition	$\|v\rangle = \sum_i v_i\,\|i\rangle$	→	$\|\psi\rangle = \int dx\ \psi(x)\,\|x\rangle$
	$v_i = \langle i\|v\rangle$		$\psi(x) = \langle x\|\psi\rangle$
state normalization	$\sum_i \|v_i\|^2 = 1$	→	$\int dx\,\|\psi(x)\|^2 = 1$
scalar product	$\langle u\|v\rangle = \sum_i \langle u\|i\rangle\langle i\|v\rangle$	→	$\langle\phi\|\psi\rangle = \int dx\,\langle\phi\|x\rangle\langle x\|\psi\rangle$
	$= \sum_i u_i^*\ v_i$		$= \int dx\,\phi(x)^*\,\psi(x)$

■ Position Operator

All position eigenstates $|x\rangle$ form a set of *orthonormal basis*, called the **position basis**. The **position operator** can be represented as

$$\hat{x} = \int dx\,|x\rangle\,x\,\langle x|. \tag{14}$$

- The position operator is *diagonal* in its own eigen basis.

Effect of the **position operator** on the **wave function**:

- Suppose the particle is in a state $|\psi\rangle$

$$|\psi\rangle = \int dx\ \psi(x)\,|x\rangle, \tag{15}$$

described by the wave function $\psi(x)$.

- Applying the position operator,

$$\hat{x}\,|\psi\rangle = \int dx\,(x\,\psi(x))\,|x\rangle. \tag{16}$$

So the position operator point-wise multiplies the wave function $\psi(x)$ with the position eigenvalue x, i.e. $\hat{x}:\psi(x)\to x\,\psi(x)$. For this reason, the position operator is often denoted as

$$\hat{x} \doteq x. \tag{17}$$

■ Translation

Translation operator is an operator that translate the particle from one position to another.

$$\hat{T}(a)\,|x\rangle = |x+a\rangle. \tag{18}$$

- Suppose the particle was in the $|x\rangle$ state (at position x).
- After applying the translation operator, the particle is in a new state $|x+a\rangle$ (at position $x+a$).
- Therefore $\hat{T}(a)$ translates the particle by displacement a.

In terms of the position basis, the translation operator can be represented as

$$\hat{T}(a) = \int dx\ |x+a\rangle\,\langle x|. \tag{19}$$

- Translation operator implements a basis transformation (from $|x\rangle$ to $|x+a\rangle$). Every basis transformation is unitary. So the translation operator is **unitary**.

Exc 2

Use the definition Eq. (19) to show that
$\hat{T}(a)^\dagger\ \hat{T}(a) = \hat{T}(a)\ \hat{T}(a)^\dagger = \mathbb{1}$,
thus the translation operator is unitary.

■ Momentum Operator

The **momentum operator** $\hat{p}$ is defined to be the *Hermitian generator* of the unitary operator that translates the position.

$$\hat{T}(a) = \exp\left(-\frac{i\,\hat{p}\,a}{\hbar}\right). \tag{20}$$

Conversely,

$$\begin{aligned}\hat{p} &= i\,\hbar\,\partial_a\,\hat{T}(a)\,|_{a=0} \\ &= i\,\hbar \lim_{a\to 0} \frac{\hat{T}(a)-\hat{T}(0)}{a},\end{aligned} \tag{21}$$

where zero-translation (do-nothing) operator $\hat{T}(0) \equiv \mathbb{1}$ is always equivalent to the identity operator.

Effect of the **momentum operator** on the **wave function**:

- Suppose the particle is in a state $|\psi\rangle$

$$|\psi\rangle = \int dx\ \psi(x)\,|x\rangle, \tag{22}$$

  described by the wave function $\psi(x)$.

- Under translation,

$$\begin{aligned}\hat{T}(a)\,|\psi\rangle &= \int dx\ \psi(x)\,|x+a\rangle \\ &= \int dx\,\psi(x-a)\,|x\rangle.\end{aligned} \tag{23}$$

- Applying the momentum operator,

$$\begin{aligned}\hat{p}\,|\psi\rangle &= i\ \hbar \lim_{a\to 0} \frac{\hat{T}(a)\,|\psi\rangle - \hat{T}(0)\,|\psi\rangle}{a} \\ &= i\ \hbar \int dx \left(\lim_{a\to 0} \frac{\psi\,(x-a) - \psi\,(x)}{a}\right)|x\rangle \\ &= \int dx\,(-i\,\hbar\,\partial_x\psi(x))\,|x\rangle.\end{aligned} \tag{24}$$

The momentum operator maps a wave function $\psi(x)$ to its derivative $\partial_x\psi(x)$ (with additional prefactor $-i\,\hbar$), i.e. $\hat{p}:\psi(x)\to -i\,\hbar\,\partial_x\psi(x)$. Therefore, the momentum operator is often written as

$$\boxed{\hat{p} \doteq -i\,\hbar\,\partial_x,} \tag{25}$$

when acting on a wave function $\psi(x)$. More precisely, its representation in the position basis is given by

$$\boxed{\hat{p} = -i\ \hbar \int dx\,dx'\,|x\rangle\,\partial_x\delta\,(x-x')\,\langle x'|.} \tag{26}$$

Exc 3 Show that Eq. (26) is consistent with Eq. (25) when acting on a state $|\psi\rangle$.

■ Commutation Relation

The **position** and **momentum** operators satisfy the commutation relation

$$[\hat{x}, \hat{p}] = i\,\hbar\,\mathbb{1}. \tag{27}$$

Note: $\mathbb{1}$ denotes the identity operator, which can be omitted.

The simplest way to show this is to check the action of these operators on a wave function $\psi(x)$. Recall that

$$\hat{x} \doteq x,\ \hat{p} \doteq -i\,\hbar\,\partial_x, \tag{28}$$

the commutator acts as

$$\begin{aligned}
&[\hat{x}, \hat{p}]\,|\psi\rangle \doteq [x, -i\,\hbar\,\partial_x]\,\psi(x)\\
&= -i\,\hbar(x\,\partial_x - \partial_x\,x)\,\psi(x)\\
&= i\,\hbar\,\psi(x)\\
&\doteq i\,\hbar\,|\psi\rangle.
\end{aligned} \tag{29}$$

This verifies the commutation relation.

Harmonic Oscillator

■ Operator Algebra

■ Hamiltonian

Hamiltonian $\hat{H}$ for the 1D harmonic oscillator

$$\hat{H} = \frac{1}{2\,m}\,\hat{p}^2 + \frac{1}{2}\,m\,\omega^2\,\hat{x}^2. \tag{30}$$

where the **position** $\hat{x}$ and **momentum** $\hat{p}$ operators are defined by their commutation relation

$$[\hat{x}, \hat{p}] = i\,\hbar\,\mathbb{1}. \tag{31}$$

m - mass of the oscillator, ω - oscillation frequency.

Let us **rescale the operators** $\hat{p}$ and $\hat{x}$

$$\hat{p} \to \hat{p}\,\sqrt{\hbar\,m\,\omega}\,,\ \hat{x} \to \hat{x}\,\sqrt{\frac{\hbar}{m\,\omega}}\,, \tag{32}$$

then the Hamiltonian looks simpler

$$\hat{H} = \frac{1}{2}\,\hbar\,\omega\,(\hat{p}^2 + \hat{x}^2). \tag{33}$$

Exc 4 Show that the Hamiltonian in Eq. (30) gets rescaled to that in Eq. (33).

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

Commutation relation for the rescaled $\hat{x}$ and $\hat{p}$ operators

$$\boxed{[\hat{x},\,\hat{p}] = i\,\mathbb{1}.} \tag{34}$$

We will work with these rescaled $\hat{x}$ and $\hat{p}$ from now on.

■ Concept of Bosons

The goal here is to find the eigen energies and states of the harmonic oscillator, given its Hamiltonian operator $\hat{H}$ in Eq. (33). This amounts to solve the (time-independent) Schrödinger equation

$$\hat{H}\,|n\rangle = E_n\,|n\rangle. \tag{35}$$

It turns out that the eigen energies are given by

$$E_n = \hbar\,\omega\left(n + \frac{1}{2}\right), \tag{36}$$

with quantized levels labeled by $n = 0, 1, 2, \ldots \in \mathbb{N}$ (accept it for now, and we will prove it later).

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

(37)

- Levels are equally spaced: **oscillator** can only absorb/emit energy in *integer* units of $\hbar\,\omega$.
- Each unit of energy (energy quantum) is carried by a **boson** --- an **elementary excitation** of the oscillator.
  - For *mechanical oscillation* (sound), the boson is called **phonon**.
  - For *electromagnetic oscillation* (light), the boson is called **photon**.
- Bosons are *indistinguishable particles*, because each of them carries the same amount of energy (and nothing else to differentiate them).

The boson can be

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

■ Annihilation and Creation Operators

Define the **annihilation** $\hat{a}$ and **creation** $\hat{a}^\dagger$ operators (the names will be evident later) as,

$$\hat{a} = \frac{1}{\sqrt{2}} (\hat{x} + i\,\hat{p}),\ \ \hat{a}^\dagger = \frac{1}{\sqrt{2}} (\hat{x} - i\,\hat{p}). \tag{38}$$

- $\hat{a}$ and $\hat{a}^\dagger$ are *Hermitian conjugate* to each other.
- Analogy: complex numbers $z = x + i\,y$, $z^* = x - i\,y$
  ⇒ position $\hat{x}$ ~ real part of $\hat{a}$, momentum $\hat{p}$ ~ imaginary part of $\hat{a}$.

Commutation relation for $\hat{a}$ and $\hat{a}^\dagger$

$$\left[\hat{a},\, \hat{a}^\dagger\right] = \mathbb{1}, \tag{39}$$

Exc 5 Prove Eq. (39) from Eq. (34).

meaning that

$$\begin{aligned} \hat{a}\,\hat{a}^\dagger &= \hat{a}^\dagger\,\hat{a} + \mathbb{1}, \\ \hat{a}^\dagger\,\hat{a} &= \hat{a}\,\hat{a}^\dagger - \mathbb{1}. \end{aligned} \tag{40}$$

These equations tell us how to commute $\hat{a}$ or $\hat{a}^\dagger$ through each other.

■ Number Operator

Define the **number operator** (the name will be evident later) as

$$\hat{n} = \hat{a}^\dagger\,\hat{a}. \tag{41}$$

In terms of the position and momentum operators

$$\hat{n} = \frac{1}{2}\left(\hat{p}^2 + \hat{x}^2\right) - \frac{\mathbb{1}}{2}. \tag{42}$$

Exc 6 Verify Eq. (42) using Eq. (38).

Compare with Eq. (33), the number operator and the Hamiltonian are related by

$$\hat{H} = \hbar\,\omega\left(\hat{n} + \frac{\mathbb{1}}{2}\right). \tag{43}$$

The goal is to find the eigenvalues and eigenstates of the Hamiltonian $\hat{H}$. However, given the relation Eq. (43), it will be sufficient to find the eigenvalues n and eigenstates $|n\rangle$ of the number operator $\hat{n}$ instead

$$\hat{n}\,|n\rangle = n\,|n\rangle, \tag{44}$$

then $|n\rangle$ are also eigenstates of $\hat{H}$ with shifted and rescaled eigenvalues

$$\hat{H}\,|n\rangle = \hbar\ \omega\ \left(n+\frac{1}{2}\right)|n\rangle, \tag{45}$$

which means the energy eigenvalues are

$$E_n = \hbar\,\omega\left(n+\frac{1}{2}\right). \tag{46}$$

What is left to be understood:

- Why must the eigenvalue n take quantized (discrete integer) values?
- What are the eigenstates $|n\rangle$? (What are the *interrelations* between the states $|n\rangle$ under the action of creation/annihilation operators?)

■ Algebraic Relations

To answer these questions, we should dive deeper into the algebraic relations among $\hat{a}$, $\hat{a}^\dagger$ and $\hat{n} = \hat{a}^\dagger\,\hat{a}$.

- Commute $\hat{a}$ or $\hat{a}^\dagger$through $\hat{n}$:

$$\begin{aligned}&\hat{n}\,\hat{a} = \hat{a}\,(\hat{n}-\mathbb{1}),\\ &\hat{n}\,\hat{a}^\dagger = \hat{a}^\dagger\,(\hat{n}+\mathbb{1}).\end{aligned} \tag{47}$$

Exc 7 Prove Eq. (47) using Eq. (40).

- Physical meaning: suppose $\hat{n}$ counts the number of bosons, counting it before or after the boson annihilation/creation process will result in a ± 1 difference in the boson number results.

- Consider any operator function of $\hat{n}$

$$f(\hat{n}) := c_0\,\mathbb{1} + c_1\,\hat{n} + c_2\,\hat{n}^2 + \ldots = \sum_{k=0}^{\infty} c_k\,\hat{n}^k, \tag{48}$$

conjugating it as $\square \to \hat{a}^\dagger\,\square\,\hat{a}$ shifts the operator $\hat{n}$ by $\mathbb{1}$,

$$\hat{a}^\dagger\,f(\hat{n})\,\hat{a} = \hat{n}\,f(\hat{n}-\mathbb{1}). \tag{49}$$

Exc 8 Show Eq. (49) based on Eq. (47).

- Repeatedly applying Eq. (49), we can show that

$$\begin{aligned}&\hat{a}^\dagger\,\hat{a} = \hat{n},\\ &(\hat{a}^\dagger)^2\,\hat{a}^2 = \hat{n}\,(\hat{n}-\mathbb{1}),\\ &(\hat{a}^\dagger)^3\,\hat{a}^3 = \hat{n}\,(\hat{n}-\mathbb{1})\,(\hat{n}-2\,\mathbb{1}),\\ &\ldots\end{aligned} \tag{51}$$

from which we conclude (for $m \in \mathbb{N}$)

$$(\hat{a}^\dagger)^m\, \hat{a}^m = \prod_{l=0}^{m-1} (\hat{n} - l\,\mathbb{1}). \tag{52}$$

■ Quantum Bootstrap

■ General Principle

Quantum bootstrap [1] is an algebraic technique for finding the common *eigenvalues* and *eigenvectors* for a set of commuting *Hermitian operators*, purely based on algebraic relations, without diagonalizing matrices. It only uses a basic principle in linear algebra:

> The **positivity constraint** --- the *scalar product* between any vector $|\psi\rangle$ and itself must be *non-negative*, i.e. $\langle\psi|\psi\rangle \geq 0$.

Let us see how this simple-enough principle is powerful enough to establish the full energy spectra and eigenstates of a harmonic oscillator.

Consider the Hermitian operator $\hat{n}$ (the number operator) admitting a set of eigenvalues and eigenvectors

$$\hat{n}\,|n\rangle = n\,|n\rangle. \tag{53}$$

Taking any operator $\hat{O}$ acting on $|n\rangle$ will produce a (generally unnormalized) state $|\psi\rangle = \hat{O}\,|n\rangle$, the *positivity constraint* requires

$$\forall\ \hat{O}: \langle n|\ \hat{O}^\dagger\ \hat{O}\,|n\rangle \geq 0. \tag{54}$$

Idea: the eigenvalues n can be determined by solving this set of inequalities.

[1] Xizhi Han, Sean Hartnoll, Jorrit Kruthoff. arXiv:2004.10212.

■ Level Quantization

For the purpose of finding eigenvalues n, it turns out to be sufficient to consider the just following series of operators

$$\hat{O}_m = \hat{a}^m, \tag{55}$$

labeled by $m = 0, 1, 2, \ldots$.

- Substitute Eq. (55) into Eq. (54), the *positivity constraint* requires

$$\forall\ m: \langle n|\ (\hat{a}^\dagger)^m\ \hat{a}^m\,|n\rangle \geq 0. \tag{56}$$

- On the other hand,

$$\langle n|\ (\hat{a}^\dagger)^m\ \hat{a}^m\,|n\rangle \overset{\text{Eq.(52)}}{=} \langle n|\ \prod_{l=0}^{m-1} (\hat{n} - l\,\mathbb{1})\,|n\rangle \tag{57}$$

$$\overset{\text{Eq. (44)}}{=} \prod_{l=0}^{m-1} (n-l) = \frac{n!}{(n-m)!}.$$

Therefore, the possible eigenvalue n must satisfy

$$\forall\, m: \prod_{l=0}^{m-1} (n-l) \geq 0. \tag{58}$$

Eq. (58) gives a series of *inequalities* (for $m = 0, 1, 2, \ldots$) to constrain the value of n:

$$\begin{aligned} &m = 0: 1 \geq 0, \\ &m = 1: n \geq 0, \\ &m = 2: n\,(n-1) \geq 0, \\ &m = 3: n\,(n-1)\,(n-2) \geq 0, \\ &m = 4: n\,(n-1)\,(n-2)\,(n-3) \geq 0, \\ &\ldots \end{aligned} \tag{59}$$

To satisfy all these inequalities, n can only be natural numbers

$$n = 0, 1, 2, \ldots \in \mathbb{N}. \tag{60}$$

- The eigenvalues $n = 0, 1, 2, \ldots$ are *discrete*! For this reason, the operator $\hat{n}$ is called the **number** operator, which counts the number of **bosons** (elementary excitations).
- The $n = 0$ eigenstate, denoted as $|0\rangle$, is also called the **vacuum state**, as it describes a state with no excitations. It is also the **ground state** of the Hamiltonian $\hat{H}$.
- The eigenstates $|n\rangle$ for $n = 1, 2, \ldots$ are **excited states** of the Hamiltonian $\hat{H}$, describing the states of n bosons *occupying* the oscillator **mode** (a mode = a slot that can host particles).

■ Fock Basis Representation

Since the states $|n\rangle$ (for $n \in \mathbb{N}$) are eigenstates of a Hermitian operator $\hat{n}$ (of different eigenvalues), they are automatically orthogonal to each other. Further assuming them to be normalized, they form a set of orthonormal basis

$$\boxed{\langle n|n'\rangle = \delta_{nn'},} \tag{61}$$

The basis is also known as the **Fock state basis** or the boson number basis,

$$\mathcal{B} = \{|n\rangle \mid n \in \mathbb{N}\}, \tag{62}$$

that spans an infinite-dimensional Hilbert space $\mathcal{H} = \operatorname{span} \mathcal{B}$, with the resolution of identity

$$\boxed{\mathbb{1} = \sum_n |n\rangle \langle n|.} \tag{63}$$

Every operator (such as $\hat{a}$ and $\hat{a}^\dagger$) can be represented in the Fock basis as a matrix, but how?

- Applying the operator equality Eq. (47), we have

$$\begin{aligned} \hat{n}\,\hat{a}\,|n\rangle &= \hat{a}\,(\hat{n}-\mathbb{1})\,|n\rangle = (n-1)\,\hat{a}\,|n\rangle, \\ \hat{n}\,\hat{a}^\dagger\,|n\rangle &= \hat{a}^\dagger\,(\hat{n}+\mathbb{1})\,|n\rangle = (n+1)\,\hat{a}^\dagger\,|n\rangle, \end{aligned} \tag{64}$$

  meaning that $\hat{a}\,|n\rangle$ is an (unnormalized) eigenstate of $\hat{n}$ with eigenvalue $(n-1)$, and $\hat{a}^\dagger\,|n\rangle$ is an (unnormalized) eigenstate of $\hat{n}$ with eigenvalue $(n+1)$.

- Since we have already introduced $|n\pm1\rangle$ to denote the normalized eigenstates corresponding to the $n \pm 1$ eigenvalues, we must conclude that

$$\begin{aligned} \hat{a}\,|n\rangle &\propto |n{-}1\rangle, \\ \hat{a}^\dagger\,|n\rangle &\propto |n{+}1\rangle. \end{aligned} \tag{65}$$

- To determine the proportionality constant, we can compute the squared norms

$$\begin{aligned} \langle n|\,\hat{a}^\dagger\,\hat{a}\,|n\rangle &= \langle n|\,\hat{n}\,|n\rangle = n, \\ \langle n|\,\hat{a}\,\hat{a}^\dagger\,|n\rangle &= \langle n|\left(\hat{a}^\dagger\,\hat{a}+\mathbb{1}\right)|n\rangle = \langle n|\,(\hat{n}+\mathbb{1})\,|n\rangle = n+1. \end{aligned} \tag{66}$$

Assuming the number basis states $|n\rangle$ are normalized, we must have

$$\boxed{\begin{aligned} \hat{a}\,|n\rangle &= \sqrt{n}\;|n-1\rangle, \\ \hat{a}^\dagger\,|n\rangle &= \sqrt{n+1}\;|n+1\rangle. \end{aligned}} \tag{67}$$

All exited states $|n\rangle$ can be raised from the ground state by the creation operator

$$\boxed{|n\rangle = \frac{1}{\sqrt{n!}}\left(a^\dagger\right)^n |0\rangle.} \tag{68}$$

Exc 9 Prove Eq. (68) using Eq. (67).

■ Summary

- Annihilation and creation operators

$$\begin{cases} \hat{a} = \frac{1}{\sqrt{2}} (\hat{x} + i\,\hat{p}) \\ \hat{a}^\dagger = \frac{1}{\sqrt{2}} (\hat{x} - i\,\hat{p}) \end{cases}, \quad \begin{cases} \hat{x} = \frac{1}{\sqrt{2}} \left(\hat{a} + \hat{a}^\dagger\right) \\ \hat{p} = \frac{1}{\sqrt{2}\,i} \left(\hat{a} - \hat{a}^\dagger\right) \end{cases}. \tag{69}$$

  They satisfies the commutation relation

$$[\hat{x},\, \hat{p}] = i\,\mathbb{1} \Leftrightarrow \left[\hat{a},\, \hat{a}^\dagger\right] = \mathbb{1}. \tag{70}$$

- Number operator

$$\hat{n} = \hat{a}^\dagger\, \hat{a}. \tag{71}$$

  It defines a discrete spectrum $\hat{n}\,|n\rangle = n\,|n\rangle$ for $n \in \mathbb{N}$. Such that

$$\begin{aligned} \hat{a}\,|n\rangle &= \sqrt{n}\;|n-1\rangle, \\ \hat{a}^\dagger\,|n\rangle &= \sqrt{n+1}\;|n+1\rangle. \end{aligned} \tag{72}$$

- Hamiltonian

$$\hat{H} = \frac{1}{2}\,\hbar\,\omega\left(\hat{p}^2 + \hat{x}^2\right) = \hbar\,\omega\left(\hat{n} + \frac{\mathbb{1}}{2}\right). \tag{73}$$

  - Eigen energies

$$E_n = \hbar\,\omega\left(n + \frac{1}{2}\right). \tag{74}$$

  - Every eigenstate $|n\rangle$ can be raised from the ground state by

$$|n\rangle = \frac{1}{\sqrt{n!}}\,(\hat{a}^\dagger)^n\,|0\rangle. \tag{75}$$

HW 1

Apply quantum bootstrap to determine the eigenvalues and eigenstates of a Hermitian operator $\hat{\beta}$ (i.e. $\hat{\beta}^\dagger = \hat{\beta}$), given that there is another operator $\hat{\alpha}$ acting in the same Hilbert space with the following algebraic relations:
$[\hat{\alpha}, \hat{\beta}] = \hat{\alpha}$,
$\hat{\alpha}^\dagger \hat{\alpha} = \mathbb{1} - \frac{1}{2}\hat{\beta}(\hat{\beta} - \mathbb{1})$,
$\hat{\alpha}\hat{\alpha}^\dagger = \mathbb{1} - \frac{1}{2}\hat{\beta}(\hat{\beta} + \mathbb{1})$.
(i) Use the commutation relation to show: $\hat{\beta}\hat{\alpha} = \hat{\alpha}(\hat{\beta} - \mathbb{1})$ and $\hat{\beta}\hat{\alpha}^\dagger = \hat{\alpha}^\dagger(\hat{\beta} + \mathbb{1})$, similar to Eq. (47).
(ii) Use the result obtained in (i) to express $(\hat{\alpha}^\dagger)^m \hat{\alpha}^m$ and $\hat{\alpha}^m(\hat{\alpha}^\dagger)^m$ as operator functions of $\hat{\beta}$, similar to Eq. (52).
(iii) Applying the positivity constraint associated with $(\hat{\alpha}^\dagger)^m \hat{\alpha}^m$ and $\hat{\alpha}^m(\hat{\alpha}^\dagger)^m$ to determine the eigenvalues of $\hat{\beta}$.
(iv) Study how $\hat{\alpha}$ acts on the eigenstates of $\hat{\beta}$, similar to Eq. (67).
(v) Based on the understanding, represent both operators $\hat{\alpha}$ and $\hat{\beta}$ in matrix forms.

■ Representation Theory

■ Fock State Representations

Fock states can be represented as *vectors*

$$|0\rangle \doteq \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix},\ |1\rangle \doteq \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix},\ |2\rangle \doteq \begin{pmatrix} 0 \\ 0 \\ 1 \\ \vdots \end{pmatrix},\ \ldots \tag{76}$$

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

$$\begin{aligned} a_{mn} &= \langle m|\,\hat{a}\,|n\rangle = \sqrt{n}\,\langle m|n-1\rangle = \sqrt{n}\,\delta_{m,n-1}, \\ \left(a^\dagger\right)_{mn} &= \langle m|\,\hat{a}^\dagger\,|n\rangle = \sqrt{n+1}\,\langle m|n+1\rangle = \sqrt{n+1}\,\delta_{m,n+1}, \end{aligned} \tag{77}$$

or more explicitly as

$$\hat{a} \doteq \begin{pmatrix} 0 & \sqrt{1} & & \\ & 0 & \sqrt{2} & \\ & & 0 & \ddots \\ & & & \ddots \end{pmatrix},\ \hat{a}^\dagger \doteq \begin{pmatrix} 0 & & & \\ \sqrt{1} & 0 & & \\ & \sqrt{2} & 0 & \\ & & \ddots & \ddots \end{pmatrix}. \tag{78}$$

- By matrix multiplication, one can verify that $\hat{a}^\dagger \hat{a}$ indeed acts as the **number operator** $\hat{n}$

$$\hat{n} = \hat{a}^\dagger \hat{a} \doteq \begin{pmatrix} 0 & & & \\ & 1 & & \\ & & 2 & \\ & & & \ddots \end{pmatrix}, \tag{79}$$

which is diagonal in its own eigen basis (i.e. the Fock basis).

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

$$\hat{x} = \frac{\hat{a} + \hat{a}^\dagger}{\sqrt{2}} \doteq \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & \sqrt{1} & & \\ \sqrt{1} & 0 & \sqrt{2} & \\ & \sqrt{2} & 0 & \ddots \\ & & \ddots & \ddots \end{pmatrix},$$
$$\hat{p} = \frac{\hat{a} - \hat{a}^\dagger}{\sqrt{2}\, i} \doteq \frac{1}{\sqrt{2}\, i} \begin{pmatrix} 0 & \sqrt{1} & & \\ -\sqrt{1} & 0 & \sqrt{2} & \\ & -\sqrt{2} & 0 & \ddots \\ & & \ddots & \ddots \end{pmatrix}. \tag{80}$$

- To have some fun, let us check

$$\hat{x}\,\hat{p} \doteq \frac{i}{2} \begin{pmatrix} 1 & 0 & -\sqrt{2} & & \\ 0 & 1 & 0 & -\sqrt{6} & \\ \sqrt{2} & 0 & 1 & 0 & \ddots \\ & \sqrt{6} & 0 & 1 & \ddots \\ & & \ddots & \ddots & \ddots \end{pmatrix},$$
$$\hat{p}\,\hat{x} \doteq \frac{i}{2} \begin{pmatrix} -1 & 0 & -\sqrt{2} & & \\ 0 & -1 & 0 & -\sqrt{6} & \\ \sqrt{2} & 0 & -1 & 0 & \ddots \\ & \sqrt{6} & 0 & -1 & \ddots \\ & & \ddots & \ddots & \ddots \end{pmatrix}, \tag{81}$$

Exc 10 Check the matrix multiplication in Eq. (81).

so we indeed verify the commutation relation $[\hat{x}, \hat{p}] = i\,\mathbb{1}$, as

$$[\hat{x}, \hat{p}] \doteq \begin{pmatrix} i & & & \\ & i & & \\ & & i & \\ & & & \ddots \end{pmatrix} = i\,\mathbb{1}. \tag{82}$$

The **operator algebra** is *basis independent*. Even if the matrices in Eq. (80) do not look like coordinate and momentum in any intuitive way, but their commutation algebra works out just right. So it is the algebra $[\hat{x}, \hat{p}] = i\,\mathbb{1}$ that should be considered as the defining property of $\hat{x}$ and $\hat{p}$ operators.

■ Uncertainty Relation

The **uncertainty relation** states that

$$(\text{std } x)\,(\text{std } p) \geq \frac{1}{2}\,|[\hat{x},\,\hat{p}]| = \frac{1}{2}, \tag{83}$$

given that $[\hat{x},\,\hat{p}] = i\,\mathbb{1}$.

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

$$\hat{x} = \frac{\hat{a} + \hat{a}^\dagger}{\sqrt{2}},\ \hat{p} = \frac{\hat{a} - \hat{a}^\dagger}{\sqrt{2}\ i}. \tag{84}$$

The one can evaluate

$$\begin{aligned}
&\langle n|\,\hat{x}\,|n\rangle = \frac{1}{\sqrt{2}}\,\langle n|\,\hat{a} + \hat{a}^\dagger\,|n\rangle \\
&= \frac{1}{\sqrt{2}}\left(\sqrt{n}\ \langle n \mid n-1\rangle + \sqrt{n+1}\ \langle n \mid n+1\rangle\right) \\
&= 0,
\end{aligned} \tag{85}$$

$$\begin{aligned}
&\langle n|\,\hat{x}^2\,|n\rangle = \frac{1}{2}\,\langle n|\left(\hat{a} + \hat{a}^\dagger\right)^2|n\rangle \\
&= \frac{1}{2}\left(\langle n|\,\hat{a}\ \hat{a}\,|n\rangle + \langle n|\,\hat{a}\ \hat{a}^\dagger\,|n\rangle + \langle n|\,\hat{a}^\dagger\ \hat{a}\,|n\rangle + \langle n|\,\hat{a}^\dagger\ \hat{a}^\dagger\,|n\rangle\right) \\
&= \frac{1}{2}\,(0 + (n+1) + n + 0) \\
&= n + 1/2.
\end{aligned} \tag{86}$$

So the position uncertainty is given by

$$(\text{std } x)^2 = \langle n|\,\hat{x}^2\,|n\rangle - \langle n|\,\hat{x}\,|n\rangle^2 = n + 1/2. \tag{87}$$

Similarly, for the momentum uncertainty

$$(\text{std } p)^2 = \langle n|\,\hat{p}^2\,|n\rangle - \langle n|\,\hat{p}\,|n\rangle^2 = n + 1/2. \tag{88}$$

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

$$(\text{std } x)\,(\text{std } p) = n + 1/2 \geq 1/2. \tag{89}$$

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

$$\left\langle x^2\right\rangle \left\langle p^2\right\rangle \geq \frac{1}{4}\,|[\hat{x},\,\hat{p}]|^2 = \frac{1}{4}, \tag{90}$$

the expectation value of the Hamiltonian is therefore bounded

$$E = \langle H\rangle = \frac{\hbar\,\omega}{2}\left(\left\langle p^2\right\rangle + \left\langle x^2\right\rangle\right) \geq \frac{\hbar\,\omega}{2}\left(\left\langle p^2\right\rangle + \frac{1}{4\left\langle p^2\right\rangle}\right) \geq \frac{\hbar\,\omega}{2}. \tag{91}$$

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

(i) Calculate the expectation value $\langle 0|\,\hat{x}^4\,|0\rangle$ of the $\hat{x}^4$ operator on the harmonic oscillator ground state $|0\rangle$ using creation and annihilation operators.
(ii)* Show that for $m \in \mathbb{N}$: $\langle 0|\,\hat{x}^{2\,m}\,|0\rangle = (2\,m-1)!!\,/\,2^m$, where $(2\,m-1)!! = \prod_{l=1}^{m}(2\,l-1)$ is the double factorial of odd numbers (it is also defined that $(-1)!! = 1$ for the $m = 0$ case).

■ Wave Function Representation

Note that the ground state (vacuum state) $|0\rangle$ can not be further annihilated by $\hat{a} = (\hat{x} + i\,\hat{p})\,/\,\sqrt{2}$,

$$\hat{a}\,|0\rangle = 0 \tag{92}$$

which can be viewed as a *defining* property of $|0\rangle$. This implies

$$(\hat{x} + i\,\hat{p})\,|0\rangle = 0. \tag{93}$$

Introduce:

- $|0\rangle \doteq \psi_0(x)$ the (coordinate space) wave function corresponds to the state $|0\rangle$,
- $\hat{x} \doteq x$ when acting on the wave function in the coordinate space,
- $\hat{p} \doteq -i\,\partial_x$ when acting on the wave function in the coordinate space.

The ground state wave function $\psi_0(x)$ must satisfy the differential equation

$$(x + \partial_x)\,\psi_0(x) = 0, \tag{94}$$

the solution is

$$\psi_0(x) = \frac{1}{\pi^{1/4}}\,e^{-\frac{1}{2}x^2}. \tag{95}$$

Exc 11

Show that Eq. (95) is a normalized solution of the differential equation Eq. (94).

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

$$\psi_1(x) = \frac{1}{\sqrt{2}}\,(x - \partial_x)\,\psi_0(x) = \frac{1}{\pi^{1/4}}\,\sqrt{2}\;x\,e^{-\frac{1}{2}x^2}. \tag{96}$$

Exc 12

Check Eq. (96) by applying the differential operator.

Iteratively, we can obtain the wave functions for all eigenstates

$$\psi_n(x) = \frac{1}{\pi^{1/4}\,\sqrt{2^n\,n!}}\,H_n(x)\,e^{-\frac{1}{2}x^2}, \tag{97}$$

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	$\frac{\sqrt{2}\, e^{-\frac{x^2}{2}}\, x}{\pi^{1/4}}$	$2\,x$	
2	$\frac{e^{-\frac{x^2}{2}}\,(-1+2\,x^2)}{\sqrt{2}\,\pi^{1/4}}$	$2\,(-1+2\,x^2)$	
3	$\frac{e^{-\frac{x^2}{2}}\,x\,(-3+2\,x^2)}{\sqrt{3}\,\pi^{1/4}}$	$4\,x\,(-3+2\,x^2)$	
4	$\frac{e^{-\frac{x^2}{2}}\,(3-12\,x^2+4\,x^4)}{2\,\sqrt{6}\,\pi^{1/4}}$	$4\,(3-12\,x^2+4\,x^4)$	
5	$\frac{e^{-\frac{x^2}{2}}\,x\,(15-20\,x^2+4\,x^4)}{2\,\sqrt{15}\,\pi^{1/4}}$	$8\,x\,(15-20\,x^2+4\,x^4)$	

Angular Momentum

■ Operator Algebra

■ Definition

The **angular momentum** of a quantum system (in 3D space) is described by a set of *three Hermitian operators* $\hat{J}_1$, $\hat{J}_2$, $\hat{J}_3$, jointly written as $\hat{\boldsymbol{J}} = (\hat{J}_1, \hat{J}_2, \hat{J}_3)$, satisfying the following commutation relation

$$\boxed{\left[\hat{J}_a, \hat{J}_b\right] = i\,\epsilon_{abc}\,\hat{J}_c.} \tag{98}$$

- ϵ_{abc} is the Levi-Civita symbol: the *sign* of the abc permutation (e.g. $\epsilon_{123} = +1$, $\epsilon_{321} = -1$).
- Repeated indices are automatically contracted in Eq. (98).
- Equivalently, in vector form, $\hat{\boldsymbol{J}} \times \hat{\boldsymbol{J}} = i\,\hat{\boldsymbol{J}}$.

Examples:

- **Orbital angular momentum** of a particle.

$$\boxed{\hat{\boldsymbol{L}} = \hat{\boldsymbol{x}} \times \hat{\boldsymbol{p}}.} \tag{99}$$

  - $\hat{\boldsymbol{x}} = (\hat{x}_1, \hat{x}_2, \hat{x}_3)$ and $\hat{\boldsymbol{p}} = (\hat{p}_1, \hat{p}_2, \hat{p}_3)$ are position and momentum operators in 3D space.
  - In component form, $\hat{L}_a = \epsilon_{abc}\,\hat{x}_b\,\hat{p}_c$.
  - From $[\hat{x}_a, \hat{p}_b] = i\,\delta_{ab}\,\mathbb{1}$ (set $\hbar = 1$ for simplicity), one can verify that

$$\left[\hat{L}_a, \hat{L}_b\right] = i\,\epsilon_{abc}\,\hat{L}_c. \tag{100}$$

Exc 13 Verify Eq. (100).

- **Spin angular momentum** of a qubit.

$$\hat{\boldsymbol{S}} = \frac{1}{2}\,\hat{\boldsymbol{\sigma}}. \tag{101}$$

  - $\hat{\boldsymbol{\sigma}} = (\hat{\sigma}^x, \hat{\sigma}^y, \hat{\sigma}^z)$ are the Pauli matrices.
  - The commutation relation of Pauli matrices implies

$$\left[\hat{S}_a, \hat{S}_b\right] = i\,\epsilon_{abc}\,\hat{S}_c. \tag{102}$$

We will discuss the *general property* of angular momentum operators without specifying whether it is orbital or spin.

■ Casimir Operator

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

$$\hat{\boldsymbol{J}}^2 = \hat{J}_1^2 + \hat{J}_2^2 + \hat{J}_3^2. \tag{103}$$

- $\hat{\boldsymbol{J}}^2$ is Hermitian.
- By Eq. (98), one can verify that (for $a = 1, 2, 3$)

$$\left[\hat{\boldsymbol{J}}^2, \hat{J}_a\right] = 0. \tag{104}$$

Exc 14 Prove Eq. (104).

■ Raising and Lowering Operators

Define the **raising** $\hat{J}_+$ and **lowering** $\hat{J}_-$ operators

$$\hat{J}_\pm = \hat{J}_1 \pm i\,\hat{J}_2. \tag{105}$$

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

The raising and lower operators $\hat{J}_\pm$ multiply to

$$\hat{J}_\mp\,\hat{J}_\pm = \hat{\boldsymbol{J}}^2 - \hat{J}_3\left(\hat{J}_3 \pm \mathbb{1}\right). \tag{106}$$

Exc 15 Prove Eq. (106).

■ Algebraic Relations

- Commute $\hat{J}_\pm$ through $\hat{\boldsymbol{J}}^2$ and $\hat{J}_3$

$$\begin{aligned} &\hat{\boldsymbol{J}}^2\,\hat{J}_\pm = \hat{J}_\pm\,\hat{\boldsymbol{J}}^2, \\ &\hat{J}_3\,\hat{J}_\pm = \hat{J}_\pm\big(\hat{J}_3 \pm \mathbb{1}\big). \end{aligned} \tag{107}$$

Exc 16 Prove Eq. (107).

  - Physical meaning: $\hat{J}_3$ corresponds to the angular momentum in the z direction, associated to rotations in the xy-plane, while $\hat{J}_\pm$ spins up/down the xy-plane rotation. Observing $\hat{J}_3$ before or after $\hat{J}_\pm$ will result in a ± 1 difference. However, $\hat{\boldsymbol{J}}^2$ commutes with $\hat{J}_\pm$, so it does not care whether $\hat{J}_\pm$ is applied before or after, a consequence of the total angular momentum conservation.

- Consider any operator function f of $\hat{\boldsymbol{J}}^2$ and $\hat{J}_3$, conjugating by $\hat{J}_\pm$ shifts only the $\hat{J}_3$ operator by $\pm\mathbb{1}$,

$$\hat{J}_\mp\, f\Big(\hat{\boldsymbol{J}}^2,\, \hat{J}_3\Big)\,\hat{J}_\pm = \Big(\hat{\boldsymbol{J}}^2 - \hat{J}_3\big(\hat{J}_3 \pm \mathbb{1}\big)\Big)\, f\Big(\hat{\boldsymbol{J}}^2,\, \hat{J}_3 \pm \mathbb{1}\Big), \tag{108}$$

  which can be shown by combining Eq. (106) and Eq. (107).

- Repeatedly applying Eq. (108), we can show that

$$\hat{J}_\mp^{\,l}\,\hat{J}_\pm^{\,l} = \prod_{k=0}^{l-1}\Big(\hat{\boldsymbol{J}}^2 - \big(\hat{J}_3 \pm k\,\mathbb{1}\big)\big(\hat{J}_3 \pm (k+1)\,\mathbb{1}\big)\Big). \tag{109}$$

Exc 17 Prove Eq. (109).

■ Quantum Bootstrap

■ Problem Setup

$\hat{\boldsymbol{J}}^2$ and $\hat{J}_3$ commute ⇒ they share the same set of eigenstates, which can be labeled by two independent quantum numbers, called j and m ⇒ as a common eigenstate $|j, m\rangle$ must satisfy the eigen equation for both operators

$$\begin{aligned} &\hat{\boldsymbol{J}}^2\,|j,m\rangle = \lambda_j\,|j,m\rangle, \\ &\hat{J}_3\,|j,m\rangle = \lambda_m\,|j,m\rangle, \end{aligned} \tag{110}$$

- λ_j is the the eigenvalue of $\hat{\boldsymbol{J}}^2$ of the $|j,m\rangle$ state,
- λ_m is the the eigenvalue of $\hat{J}_3$ of the $|j,m\rangle$ state.

The possible values of λ_j, λ_m can be determined by the **quantum bootstrap** method, by imposing the **positivity constraint**:

$$\forall\ O : \langle j,m|\ \hat{O}^\dagger\ \hat{O}\,|j,m\rangle \geq 0. \tag{111}$$

■ Angular Momentum Quantization

It turns out to be sufficient to consider

$$O_l = \hat{J}_\pm^l, \tag{112}$$

labeled by $l = 0, 1, 2, \ldots$.

- Substitute Eq. (112) into Eq. (111), the *positivity constraint* requires

$$\forall\ l : \langle j,m|\ \hat{J}_\mp^l\ \hat{J}_\pm^l\,|j,m\rangle \geq 0. \tag{113}$$

- On the other hand,

$$\begin{aligned}
&\langle j,m|\ \hat{J}_\mp^l\ \hat{J}_\pm^l\,|j,m\rangle \\
&\overset{\text{Eq. (109)}}{=} \langle j,m|\ \prod_{k=0}^{l-1}\left(\hat{\boldsymbol{J}}^2 - \left(\hat{J}_3 \pm k\,\mathbb{1}\right)\left(\hat{J}_3 \pm (k+1)\,\mathbb{1}\right)\right)|j,m\rangle \\
&\overset{\text{Eq. (110)}}{=} \prod_{k=0}^{l-1}\left(\lambda_j - (\lambda_m \pm k)\,(\lambda_m \pm (k+1))\right).
\end{aligned} \tag{114}$$

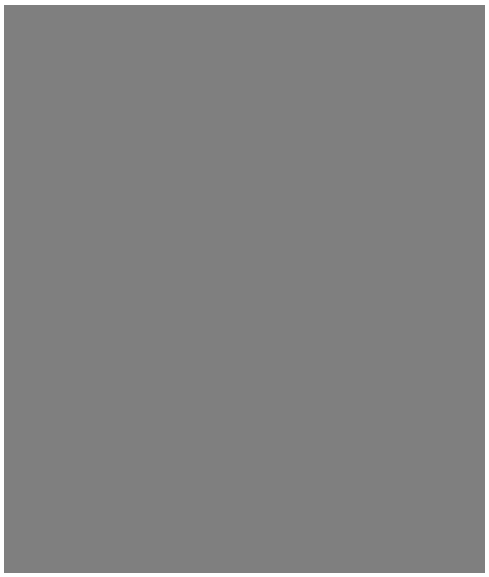
Therefore, the possible eigenvalue pair (λ_j, λ_m) must satisfy

$$\boxed{\forall\ l : \prod_{k=0}^{l-1}\left(\lambda_j - (\lambda_m \pm k)\,(\lambda_m \pm (k+1))\right) \geq 0.} \tag{115}$$

Eq. (115) gives a series of *inequalities* (for $l = 0, 1, 2, \ldots$) to constrain the value of λ_j and λ_m (jointly):

$$\begin{aligned}
&l = 0 : 1 \geq 0, \\
&l = 1 : \lambda_j - \lambda_m(\lambda_m \pm 1) \geq 0, \\
&l = 2 : \left(\lambda_j - \lambda_m(\lambda_m \pm 1)\right)\left(\lambda_j - (\lambda_m \pm 1)\,(\lambda_m \pm 2)\right) \geq 0, \\
&\ldots
\end{aligned} \tag{116}$$

If the inequalities are solved for $l = 1, 2, \ldots, l_{\max}$ (up to a maximal l), the feasible region for λ_m and λ_j looks like:



Solutions are *discrete*! ⇒ **angular momentum quantization**. They are described by

$$\boxed{\begin{aligned} &\lambda_j = j(j+1) \text{ for } j = 0, \tfrac{1}{2}, 1, \tfrac{3}{2}, \ldots \\ &\lambda_m = m \qquad \text{for } m = -j, -j+1, \ldots, j-1, j \end{aligned}} \tag{117}$$

- For **orbital** angular momentum j takes *integer* values.
  For **spin** angular momentum j can also be *half-integers*.
- The eigen equations in Eq. (110) become

$$\begin{aligned} &\hat{\boldsymbol{J}}^2 \,|j,m\rangle = j(j+1)\,|j,m\rangle, \\ &\hat{J}_3 \,|j,m\rangle = m\,|j,m\rangle. \end{aligned} \tag{118}$$

■ Operator Representation

The eigenstates $|j,m\rangle$ ($m = -j, \ldots, j$) for a set of orthonormal basis, on which the raising and lowering operators $\hat{J}_\pm$ can be represented. To find the representation,

- Applying the operator equality Eq. (107), we have

$$\begin{aligned} &\hat{J}_3\, \hat{J}_\pm \,|j,m\rangle = \hat{J}_\pm\big(\hat{J}_3 \pm \mathbb{1}\big)\,|j,m\rangle \\ &= (m \pm 1)\, \hat{J}_\pm \,|j,m\rangle \end{aligned} \tag{119}$$

  ⇒ the state $\hat{J}_\pm\,|j,m\rangle$ (as long as it is not zero) is also an eigenstate of $\hat{J}_3$ but with the eigenvalue $(m \pm 1)$ ⇒ $\hat{J}_\pm\,|j,m\rangle$ is just the $|j,m\pm1\rangle$ state (up to overall coefficient)

$$\hat{J}_\pm \,|j,m\rangle = c^{\pm}_{j,m}\,|j,m\pm1\rangle. \tag{120}$$

- To determine the coefficient $c^{\pm}_{j,m}$, use Eq. (106),

$$\langle j,m|\, \hat{J}_{\mp}\, \hat{J}_{\pm}\, |j,m\rangle = j(j+1) - m(m\pm 1). \tag{121}$$

On the other hand

$$\langle j,m|\, \hat{J}_{\mp}\, \hat{J}_{\pm}\, |j,m\rangle = \left(c^{\pm}_{j,m}\right)^2 \langle j,m\pm 1|j,m\pm 1\rangle = \left(c^{\pm}_{j,m}\right)^2. \tag{122}$$

Combining Eq. (121) and Eq. (122), $c^{\pm}_{j,m}$ can be solved

$$c^{\pm}_{j,m} = \sqrt{j(j+1) - m(m\pm 1)}\,. \tag{123}$$

In conclusion, we have obtained the following representations for angular momentum operators (from Eq. (118) and Eq. (120))

$$\boxed{\begin{aligned} &\hat{\boldsymbol{J}}^2\, |j,\, m\rangle = j(j+1)\, |j,\, m\rangle, \\ &\hat{J}_3\, |j,\, m\rangle = m\, |j,\, m\rangle, \\ &\hat{J}_{\pm}\, |j,\, m\rangle = \sqrt{j(j+1) - m(m\pm 1)}\; |j,\, m\pm 1\rangle. \end{aligned}} \tag{124}$$

Induction implies that all basis states can be

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

$$|j,\, m\rangle = \left(\frac{(j-m)!}{(2\,j)!\,(j+m)!}\right)^{1/2} \hat{J}_+^{j+m}\, |j,\, -j\rangle, \tag{125}$$

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

$$|j,\, m\rangle = \left(\frac{(j+m)!}{(2\,j)!\,(j-m)!}\right)^{1/2} \hat{J}_-^{j-m}\, |j,\, j\rangle. \tag{126}$$

This is just like the Harmonic oscillator.

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

$$\begin{aligned} &\frac{\hat{J}_+}{\sqrt{2\,j}}\; |j,\, -j+n\rangle = \sqrt{n+1}\; |j,\, -j+n+1\rangle + O\left(j^{-1/2}\right), \\ &\frac{\hat{J}_-}{\sqrt{2\,j}}\; |j,\, -j+n\rangle = \sqrt{n}\; |j,\, -j+n-1\rangle + O\left(j^{-1/2}\right). \end{aligned} \tag{127}$$

Under the following correspondence

$$\begin{aligned} &|j,\, -j+n\rangle \to |n\rangle, \\ &(2\,j)^{-1/2}\, \hat{J}_- \to a,\; (2\,j)^{-1/2}\, \hat{J}_+ \to a^{\dagger}, \end{aligned} \tag{128}$$

the boson creation/annihilation algebra Eq. (67) can be reproduced approximately (to the leading order). In this sense, *spin excitations* can also be treated as bosons, called **magnons**.

■ Summary

Angular momentum operator $\hat{\boldsymbol{J}} = \left(\hat{J}_1,\, \hat{J}_2,\, \hat{J}_3\right)$ is defined by the commutation relation

$$\hat{\boldsymbol{J}} \times \hat{\boldsymbol{J}} = i\, \hat{\boldsymbol{J}}. \tag{129}$$

Based on $\hat{\boldsymbol{J}}$, we can define

- The total angular momentum operator

$$\hat{\boldsymbol{J}}^2 = \hat{J}_1^2 + \hat{J}_2^2 + \hat{J}_3^2. \tag{130}$$

- The raising and lowering operators

$$\hat{J}_\pm = \hat{J}_1 \pm i\, \hat{J}_2. \tag{131}$$

They acts on the common eigen basis $|j,m\rangle$ as

$$\begin{aligned} &\hat{\boldsymbol{J}}^2 \,|j,\, m\rangle = j(j+1)\,|j,\, m\rangle, \\ &\hat{J}_3 \,|j,\, m\rangle = m\,|j,\, m\rangle, \\ &\hat{J}_\pm \,|j,\, m\rangle = \sqrt{j(j+1) - m(m\pm 1)}\;|j,\, m\pm 1\rangle, \end{aligned} \tag{132}$$

where

$$\begin{aligned} &j = 0,\, \frac{1}{2},\, 1,\, \frac{3}{2},\, \ldots, \\ &m = -j,\, -j+1,\, \ldots,\, j-1,\, j. \end{aligned} \tag{133}$$

■ Representation Theory

■ Spin-1/2

In the $j = 1/2$ subspace, the (spin) angular momentum operators $\hat{\boldsymbol{S}} = \left(\hat{S}_1,\, \hat{S}_2,\, \hat{S}_3\right)$ can be represented as **Pauli matrices**,

$$\boxed{\hat{\boldsymbol{S}} = \frac{1}{2}\,\hat{\boldsymbol{\sigma}}.} \tag{134}$$

Exc 18

Use Eq. (132) to derive the matrix representation for spin-1/2 angular momentum operators, and show that they are indeed related to Pauli matrices as indicated in Eq. (134).

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

$$\hat{S}_1 \doteq \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\; \hat{S}_2 \doteq \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},\; \hat{S}_3 \doteq \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{135}$$

- Eigenstates and eigenvalues

$$\hat{S}_1 : \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} \to +\frac{1}{2}, \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix} \to -\frac{1}{2},$$
$$\hat{S}_2 : \frac{1}{\sqrt{2}}\begin{pmatrix}1\\i\end{pmatrix} \to +\frac{1}{2}, \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-i\end{pmatrix} \to -\frac{1}{2},$$
$$\hat{S}_3 : \begin{pmatrix}1\\0\end{pmatrix} \to +\frac{1}{2}, \begin{pmatrix}0\\1\end{pmatrix} \to -\frac{1}{2}.$$

■ Spin-1

The $j = 1$ subspace: dimension = 3 ⇒ 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)

$$\hat{L}_1 \doteq \frac{1}{\sqrt{2}}\begin{pmatrix}0 & 1 & 0\\1 & 0 & 1\\0 & 1 & 0\end{pmatrix}, \hat{L}_2 \doteq \frac{1}{\sqrt{2}\,i}\begin{pmatrix}0 & 1 & 0\\-1 & 0 & 1\\0 & -1 & 0\end{pmatrix}, \hat{L}_3 \doteq \begin{pmatrix}1 & 0 & 0\\0 & 0 & 0\\0 & 0 & -1\end{pmatrix}. \tag{137}$$

Exc 19 Use Eq. (132) to derive the matrix representation for spin-1 angular momentum operators in Eq. (137).

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

- Basis transformation

$$\begin{pmatrix}|1, +1\rangle\\|1, 0\rangle\\|1, -1\rangle\end{pmatrix} = \begin{pmatrix}\frac{i}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0\\0 & 0 & -i\\\frac{-i}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0\end{pmatrix}\begin{pmatrix}|x\rangle\\|y\rangle\\|z\rangle\end{pmatrix}. \tag{138}$$

- Denote the transformation matrix by $\hat{U}$, the operators transform as $\hat{L}_a \to \hat{U}^\dagger\, \hat{L}_a\, \hat{U}$,

$$\hat{L}_1 \doteq \begin{pmatrix}0 & 0 & 0\\0 & 0 & -i\\0 & i & 0\end{pmatrix}, \hat{L}_2 \doteq \begin{pmatrix}0 & 0 & i\\0 & 0 & 0\\-i & 0 & 0\end{pmatrix}, \hat{L}_3 \doteq \begin{pmatrix}0 & -i & 0\\i & 0 & 0\\0 & 0 & 0\end{pmatrix}. \tag{139}$$

Exc 20 Implement the basis transformation Eq. (138) to transform Eq. (137) to Eq. (139).

■ Rotation Operators

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

$$\hat{R}(\boldsymbol{\theta}) = e^{i\,\boldsymbol{\theta}\cdot\hat{\boldsymbol{J}}}. \tag{140}$$

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,

$$\hat{R}_{1/2}(\boldsymbol{\theta}) \doteq \begin{pmatrix} e^{i\,\theta/2} & 0 \\ 0 & e^{-i\,\theta/2} \end{pmatrix}. \tag{141}$$

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

$$\hat{R}_1(\boldsymbol{\theta}) \doteq \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{142}$$

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

- This is indeed the case for spin-1 representation

$$\hat{R}_1(0, 0, 2\,\pi) \doteq \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \doteq \mathbb{1}. \tag{143}$$

- But not for spin-1/2,

$$\hat{R}_{1/2}(0, 0, 2\,\pi) \doteq \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} \doteq -\mathbb{1}, \tag{144}$$

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).

■ Fusion Category

■ Example: Fusion of Spins

Combine two spin-1/2 systems together,

- **States** *tensor product* together:

$$\{|\uparrow\rangle, |\downarrow\rangle\}_A \otimes \{|\uparrow\rangle, |\downarrow\rangle\}_B = \{|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle\}. \tag{145}$$

- **Rotation operators** *multiply* together:

$$e^{i\,\boldsymbol{\theta}\cdot\hat{\boldsymbol{S}}_A}\, e^{i\,\boldsymbol{\theta}\cdot\hat{\boldsymbol{S}}_B} = \hat{R}_A(\boldsymbol{\theta})\, \hat{R}_B(\boldsymbol{\theta}) := \hat{R}(\boldsymbol{\theta}) = e^{i\,\boldsymbol{\theta}\cdot\hat{\boldsymbol{S}}}. \tag{146}$$

- **Angular momenta** *add* together:

$$\boxed{\hat{\boldsymbol{S}} = \hat{\boldsymbol{S}}_A + \hat{\boldsymbol{S}}_B,} \tag{147}$$

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

$$\hat{\boldsymbol{S}}_A = \frac{1}{2}\,\hat{\boldsymbol{\sigma}}_A \otimes \mathbb{1}_B,$$
$$\hat{\boldsymbol{S}}_B = \frac{1}{2}\,\mathbb{1}_A \otimes \hat{\boldsymbol{\sigma}}_B. \tag{148}$$

Exc 21 Write down the matrix representation for $\hat{\boldsymbol{S}}_A$ and $\hat{\boldsymbol{S}}_B$. [Hint: altogether six 4×4 matrices]

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

$$\hat{\boldsymbol{S}}^2 = \left(\hat{\boldsymbol{S}}_A + \hat{\boldsymbol{S}}_B\right)^2 = \hat{\boldsymbol{S}}_A^2 + \hat{\boldsymbol{S}}_B^2 + 2\,\hat{\boldsymbol{S}}_A \cdot \hat{\boldsymbol{S}}_B$$
$$= \frac{3}{2}\,\mathbb{1} + 2\,\hat{\boldsymbol{S}}_A \cdot \hat{\boldsymbol{S}}_B. \tag{149}$$

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

$$\hat{\boldsymbol{S}}_A \cdot \hat{\boldsymbol{S}}_B \doteq \frac{1}{4}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{150}$$

Exc 22 Verify the matrix representation in Eq. (150).

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

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

$$|0, 0\rangle = \frac{1}{\sqrt{2}}\,(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle). \tag{151}$$

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

$$|1, +1\rangle = |\uparrow\uparrow\rangle,$$
$$|1, 0\rangle = \frac{1}{\sqrt{2}}\,(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle), \tag{152}$$
$$|1, -1\rangle = |\downarrow\downarrow\rangle.$$

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

space: $\frac{1}{2}\otimes\frac{1}{2}$ $0\oplus 1$

basis: $|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle$ $|0,0\rangle; |1,+1\rangle, |1,0\rangle, |1,-1\rangle$

$$\hat{S}_1 \doteq \begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{2} & 0 & 0 & \frac{1}{2} \\ \frac{1}{2} & 0 & 0 & \frac{1}{2} \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix} \qquad \left(\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \hline 0 & 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & 0 & \frac{1}{\sqrt{2}} & 0 \end{array}\right)$$

$$\hat{S}_2 \doteq \begin{pmatrix} 0 & -\frac{i}{2} & -\frac{i}{2} & 0 \\ \frac{i}{2} & 0 & 0 & -\frac{i}{2} \\ \frac{i}{2} & 0 & 0 & -\frac{i}{2} \\ 0 & \frac{i}{2} & \frac{i}{2} & 0 \end{pmatrix} \qquad \left(\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \hline 0 & 0 & -\frac{i}{\sqrt{2}} & 0 \\ 0 & \frac{i}{\sqrt{2}} & 0 & -\frac{i}{\sqrt{2}} \\ 0 & 0 & \frac{i}{\sqrt{2}} & 0 \end{array}\right)$$

$$\hat{S}_3 \doteq \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \qquad \left(\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \hline 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{array}\right)$$

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

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

The two bases are related by basis transformations:

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

$$(|0,0\rangle) = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \end{pmatrix} \begin{pmatrix} |\uparrow\uparrow\rangle \\ |\uparrow\downarrow\rangle \\ |\downarrow\uparrow\rangle \\ |\downarrow\downarrow\rangle \end{pmatrix}. \tag{153}$$

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

$$\begin{pmatrix} |1,+1\rangle \\ |1,0\rangle \\ |1,-1\rangle \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} |\uparrow\uparrow\rangle \\ |\uparrow\downarrow\rangle \\ |\downarrow\uparrow\rangle \\ |\downarrow\downarrow\rangle \end{pmatrix}. \tag{154}$$

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.

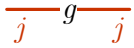
■ Fusion Rules

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 $2j+1$.

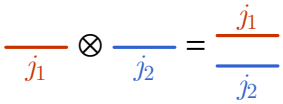
- Matrix representation of group element $g \in \mathrm{SU}(2)$ in representation j can be depicted as



Example: rotation $\boldsymbol{\theta} = (0, 0, \theta)$, c.f. Eq. (141) and Eq. (142)

$$\begin{aligned} &\overline{1/2}\; g\; \overline{1/2} = \begin{pmatrix} e^{i\theta/2} & 0 \\ 0 & e^{-i\theta/2} \end{pmatrix}, \\ &\overline{1}\; g\; \overline{1} = \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}. \end{aligned} \tag{155}$$

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).



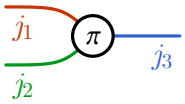
- The tensor structure specifies the **fusion rule**:

$$j_1 \otimes j_2 \to |j_1 - j_2| \oplus (|j_1 - j_2| + 1) \oplus \ldots \oplus (j_1 + j_2 - 1) \oplus (j_1 + j_2). \tag{156}$$

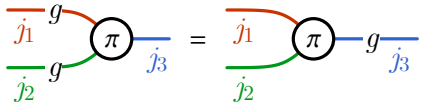
  - Composition of a spin-j_1 and a spin-j_2 systems is a spin system that contains irreducible representations ranging from $|j_1 - j_2|$ to $j_1 + j_2$ (each of them appear once).
  - Example: $1/2 \otimes 1/2 \to 0 \oplus 1$.
  - Notice that the *representation dimensions* add up correctly

$$\dim \mathcal{H}_{j_1 \otimes j_2} = \sum_{j_3 = |j_1 - j_2|}^{j_1 + j_2} (2j_3 + 1) = (2j_1 + 1)(2j_2 + 1). \tag{157}$$

- 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. (153) and Eq. (154)

$$\begin{aligned}
&\pi_0 : 1/2 \otimes 1/2 \to 0,\\
&\pi_0 \doteq \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \end{pmatrix},\\
&\pi_1 : 1/2 \otimes 1/2 \to 1,\\
&\pi_1 \doteq \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.
\end{aligned} \tag{158}$$

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

$$\left(\begin{matrix} j_1 & j_2 \\ m_1 & m_2 \end{matrix} \middle| \begin{matrix} j_3 \\ m_3 \end{matrix} \right) = \langle j_3,\, m_3 \mid j_1,\, m_1;\, j_2,\, m_2 \rangle. \tag{159}$$

They can be used to implement basis transformations

$$\pi(j_1 \otimes j_2 \to j_3) = \sum_{m_1, m_2, m_3} |j_3,\, m_3\rangle \left(\begin{matrix} j_1 & j_2 \\ m_1 & m_2 \end{matrix} \middle| \begin{matrix} j_3 \\ m_3 \end{matrix} \right) \langle j_1,\, m_1;\, j_2,\, m_2|. \tag{160}$$

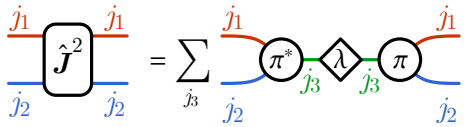
To obtain the CG coefficient,

- 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* $\hat{\boldsymbol{J}}^2$:



- Represent $\hat{\boldsymbol{J}}^2$ in the $j_1 \otimes j_2$ space.

- Diagonalize $\hat{\boldsymbol{J}}^2$, 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 $\pi(j_1 \otimes j_2 \to j_3)$.

Exc 23

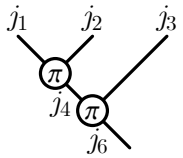
Compute the fusion vertex of $\pi(1/2 \otimes 1 \to 1/2)$ and $\pi(1 \otimes 1/2 \to 1/2)$.

HW 3

Consider a spin-1 particle A interacting with a spin-1/2 particle B via the Hamiltonian $\hat{H} = -\,\hat{\boldsymbol{S}}_A \cdot \hat{\boldsymbol{S}}_B$.
(i) Find the eigenvalues of $\hat{H}$
(ii) Define the projection operator onto the spin-1/2 and spin-3/2 subspaces as
$P_{1/2} = \pi(1/2 \otimes 1 \to 1/2)^\dagger\, \pi(1/2 \otimes 1 \to 1/2)$
$P_{3/2} = \pi(1/2 \otimes 1 \to 3/2)^\dagger\, \pi(1/2 \otimes 1 \to 3/2)$
Show that
$P_{1/2} = -\frac{2}{3}\left(\hat{\boldsymbol{S}}_A \cdot \hat{\boldsymbol{S}}_B - \mathbb{1}/2\right)$
$P_{3/2} = \frac{2}{3}\left(\hat{\boldsymbol{S}}_A \cdot \hat{\boldsymbol{S}}_B + \mathbb{1}\right)$

■ 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 $j_4 = 0$,

$$\alpha_0 = \pi(0 \otimes 1/2 \to 1/2)\,(\pi(1/2 \otimes 1/2 \to 0) \otimes \pi(1/2 \to 1/2))$$
$$\doteq \begin{pmatrix} 0 & 0 & \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} & 0 & 0 \end{pmatrix}. \tag{161}$$

Exc 24

Verify Eq. (161).

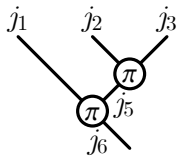
- For $j_4 = 1$,

$$\alpha_1 = \pi(1 \otimes 1/2 \to 1/2)\,(\pi(1/2 \otimes 1/2 \to 1) \otimes \pi(1/2 \to 1/2))$$

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

Exc 25 Verify Eq. (162).

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 $j_5 = 0$,

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

$$\doteq \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \end{pmatrix}. \tag{163}$$

Exc 26 Verify Eq. (163).

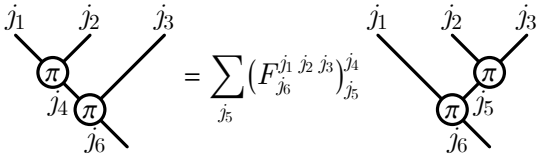
- For $j_5 = 1$,

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

$$\doteq \begin{pmatrix} 0 & -\frac{1}{\sqrt{6}} & -\frac{1}{\sqrt{6}} & 0 & \sqrt{\frac{2}{3}} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\sqrt{\frac{2}{3}} & 0 & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} & 0 \end{pmatrix}. \tag{164}$$

Exc 27 Verify Eq. (164).

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,



(165)

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

$$\begin{pmatrix}\alpha_0\\ \alpha_1\end{pmatrix}=\begin{pmatrix}-\frac{1}{2} & -\frac{\sqrt{3}}{2}\\ \frac{\sqrt{3}}{2} & -\frac{1}{2}\end{pmatrix}\begin{pmatrix}\beta_0\\ \beta_1\end{pmatrix}. \tag{166}$$

- 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

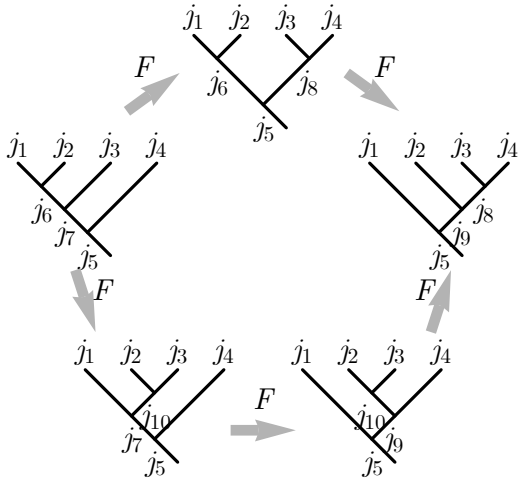
$$\left(F^{j_1\, j_2\, j_3}_{j_6}\right)^{j_4}_{j_5}=(-)^{j_1+j_2+j_3+j_6}\sqrt{(2\,j_4+1)\,(2\,j_5+1)}\begin{Bmatrix} j_1 & j_2 & j_4\\ j_3 & j_6 & j_5\end{Bmatrix}. \tag{167}$$

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.



$$\left(F^{j_6\, j_3\, j_4}_{j_5}\right)^{j_7}_{j_8}\left(F^{j_1\, j_2\, j_8}_{j_5}\right)^{j_6}_{j_9}=\sum_{j_{10}}\left(F^{j_1\, j_2\, j_3}_{j_7}\right)^{j_6}_{j_{10}}\left(F^{j_1\, j_{10}\, j_4}_{j_5}\right)^{j_7}_{j_9}\left(F^{j_2\, j_3\, j_4}_{j_9}\right)^{j_{10}}_{j_8}. \tag{168}$$

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

■ Background: Classical Mechanics

■ Model Hamiltonian

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 $m_p / m_e \approx 1836$). So the proton is essentially pinned at the center of mass (i.e. we can ignore its motion).
- Consider electron moving in the *electric static potential* created by the proton.

$$V(r) = -\frac{\alpha}{r}, \tag{169}$$

where $\alpha = e^2 / (4\pi\epsilon_0)$ is the **fine-structure constant**, describing the strength of the electrostatic Coulomb force.

The **Hamiltonian** (energy) of the *electron* is given by

$$H = \frac{\boldsymbol{p}^2}{2m} - \frac{\alpha}{r}, \tag{170}$$

- $\boldsymbol{r}$ 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).

We can rescale $\boldsymbol{r}$ and $\boldsymbol{p}$ in a manner that preserves the phase space volume, such that their commutation relation (after quantization) will not be modified

$$\boldsymbol{r} \to \frac{\boldsymbol{r}}{m\alpha}, \ \boldsymbol{p} \to m\alpha\,\boldsymbol{p}, \tag{171}$$

accordingly H will also be rescaled

$$H \to m\alpha^2 H. \tag{172}$$

The Hamiltonian Eq. (170) gets simplified to

$$\boxed{H = \frac{\boldsymbol{p}^2}{2} - \frac{1}{r}.} \tag{173}$$

- Every quantity is dimensionless now. The energy $m\alpha^2/2$ is called the **Rydberg unit** of energy.
- The **classical equation of motion** is given by the Hamiltonian equation

$$\frac{d\boldsymbol{r}}{dt} = \frac{\partial H}{\partial \boldsymbol{p}}, \frac{d\boldsymbol{p}}{dt} = -\frac{\partial H}{\partial \boldsymbol{r}}. \tag{174}$$

Substitute in Eq. (173),

$$\frac{d\boldsymbol{r}}{dt} = \boldsymbol{p}, \frac{d\boldsymbol{p}}{dt} = -\frac{\boldsymbol{r}}{r^3}. \tag{175}$$

■ Angular Momentum

The **angular momentum** is defined as

$$\boldsymbol{L} = \boldsymbol{r} \times \boldsymbol{p}. \tag{176}$$

It can be checked that the angular momentum is *conserved*.

$$\frac{d\boldsymbol{L}}{dt} = \boldsymbol{0}. \tag{177}$$

Because the Hamiltonian has an SO(3) *rotation symmetry*.

Exc 28 Check Eq. (177).

■ Laplace-Runge-Lenz (LRL) Vector

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

$$\boldsymbol{A} = \boldsymbol{p} \times \boldsymbol{L} - \frac{\boldsymbol{r}}{r}. \tag{178}$$

The LRL vector is also *conserved* (but why? what is the deeper symmetry reason? - we will come back to this later)

$$\frac{d\boldsymbol{A}}{dt} = \mathbf{0}. \tag{179}$$

Exc 29 Check Eq. (179).

This conservation law is useful in deriving the **Kepler orbit** (of a classical electron, or of a planet).

- Let θ be the angle between $\boldsymbol{r}$ and $\boldsymbol{A}$,

$$\boldsymbol{A}\cdot\boldsymbol{r} = A\, r\cos\theta = \boldsymbol{r}\cdot(\boldsymbol{p}\times\boldsymbol{L}) - r. \tag{181}$$

Permuting the *scalar triple product*

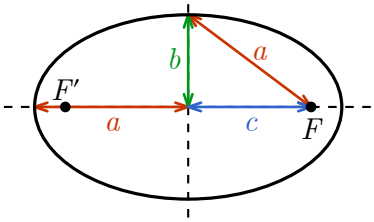
$$\boldsymbol{r}\cdot(\boldsymbol{p}\times\boldsymbol{L}) = \boldsymbol{L}\cdot(\boldsymbol{r}\times\boldsymbol{p}) = \boldsymbol{L}^2, \tag{182}$$

Eq. (181) ⇒ the **orbit equation**

$$\boxed{r = \frac{L^2}{1 + A\cos\theta}.} \tag{183}$$

- This describes an *elliptical* orbit, with

$$a = \frac{L^2}{1 - A^2},\; c = \frac{L^2\, A}{1 - A^2}. \tag{184}$$



The physical meaning of the LRL vector $\boldsymbol{A}$:

- Conservation of the *magnitude* $A = |\boldsymbol{A}|$ ⇒ conservation of the *eccentricity* of the orbit (in fact $e \equiv c/a = A$).
- Conservation of the *direction* of $\boldsymbol{A}$ ⇒ conservation of the *orientation* of the orbit in the orbital plane: the *periapsis* (the point of closest approach) does not move with respect to the force center (focal point) in time.

HW 4

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 $O^{\mathsf{T}} O = \mathbb{1}$ and $O \in \mathbb{R}^{n\times n}$, then $A^{\mathsf{T}} = -A$ and $A \in \mathbb{I}^{n\times n}$).
(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)

$$T_1 = \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix},\ T_2 = \frac{1}{2}\begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & -i \\ i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{pmatrix},\ T_3 = \frac{1}{2}\begin{pmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & i \\ 0 & 0 & -i & 0 \end{pmatrix};$$

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

(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. (98), we learn that the SO(4) group can be covered by two SU(2) groups.

■ SO(4) Symmetry

■ Operator Definition

In quantum mechanics, every *classical observable* is promoted to Hermitian operators:

- **Coordinate** operator: $\hat{\boldsymbol{r}} = (\hat{r}_1,\ \hat{r}_2,\ \hat{r}_3)$. Further define

$$\hat{r} := \sqrt{\hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{r}}} = \sqrt{\hat{r}_1^2 + \hat{r}_2^2 + \hat{r}_3^2}\,. \tag{185}$$

- **Momentum** operator: $\hat{\boldsymbol{p}} = (\hat{p}_1,\ \hat{p}_2,\ \hat{p}_3)$.
- **Hamiltonian** operator:

$$\boxed{\hat{H} = \frac{\hat{\boldsymbol{p}}^2}{2} - \frac{1}{\hat{r}}.} \tag{186}$$

- **Angular momentum** operator: $\hat{\boldsymbol{L}} = \left(\hat{L}_1,\ \hat{L}_2,\ \hat{L}_3\right)$, where

$$\boxed{\hat{\boldsymbol{L}} = \hat{\boldsymbol{r}}\times\hat{\boldsymbol{p}}} \tag{187}$$

or in component form as

$$\hat{L}_a = \epsilon_{abc}\,\hat{r}_b\,\hat{p}_c. \tag{188}$$

- **LRL vector** operator: $\hat{\boldsymbol{A}} = \left(\hat{A}_1,\ \hat{A}_2,\ \hat{A}_3\right)$, where

$$\boxed{\hat{\boldsymbol{A}} = \frac{1}{2}\left(\hat{\boldsymbol{p}} \times \hat{\boldsymbol{L}} - \hat{\boldsymbol{L}} \times \hat{\boldsymbol{p}}\right) - \frac{\hat{\boldsymbol{r}}}{\hat{r}},} \tag{189}$$

or in component form as

$$\hat{A}_a = \frac{1}{2}\,\epsilon_{abc}\left(\hat{p}_b\,\hat{L}_c - \hat{L}_b\,\hat{p}_c\right) - \frac{\hat{r}_a}{\hat{r}}. \tag{190}$$

The expression is modified from the classical definition Eq. (178) to ensure the Hermiticity of the LRL vector as quantum operators.

■ Operator Algebra

The basic commutation relation is that among the coordinate and moment operators

$$[\hat{r}_a,\, \hat{p}_b] = i\,\delta_{ab}\,\mathbb{1}. \tag{191}$$

One can verify the following commutation relations

$$\begin{aligned}
&\left[\hat{H},\, \hat{L}_a\right] = 0,\\
&\left[\hat{H},\, \hat{A}_a\right] = 0,\\
&\left[\hat{L}_a,\, \hat{L}_b\right] = i\,\epsilon_{abc}\,\hat{L}_c,\\
&\left[\hat{L}_a,\, \hat{A}_b\right] = i\,\epsilon_{abc}\,\hat{A}_c,\\
&\left[\hat{A}_a,\, \hat{A}_b\right] = -2\,i\,\epsilon_{abc}\,\hat{L}_c\,\hat{H},
\end{aligned} \tag{192}$$

Exc 30 Verify Eq. (192). [Hint: try writing a computer program to help.]

and the following operator equalities

$$\begin{aligned}
&\hat{\boldsymbol{A}} \cdot \hat{\boldsymbol{L}} = \hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{A}} = 0,\\
&2\,\hat{H}\left(\hat{\boldsymbol{L}}^2 + \mathbb{1}\right) - \hat{\boldsymbol{A}}^2 + \mathbb{1} = 0.
\end{aligned} \tag{193}$$

Exc 31 Verify Eq. (193).

- The conservation laws of angular momentum and LRL vector are manifested by

$$\left[\hat{H},\, \hat{\boldsymbol{L}}\right] = \left[\hat{H},\, \hat{\boldsymbol{A}}\right] = \boldsymbol{0}. \tag{194}$$

- One might expect $\hat{\boldsymbol{L}}$ and $\hat{\boldsymbol{A}}$ to generate a symmetry group, however their algebra is not closed --- in particular, the $\left[\hat{\boldsymbol{A}},\, \hat{\boldsymbol{A}}\right]$ commutator leads to new operators like $\hat{\boldsymbol{L}}\,\hat{H}$, which can not be written as a linear combination of $\hat{\boldsymbol{L}}$ and $\hat{\boldsymbol{A}}$ --- thus the algebra must be further extended.
- Or ... maybe not. If we restrict our focus within each eigen subspace of $\hat{H}$ (the subspace spanned by eigenvectors of $\hat{H}$ with the same eigenvalue), then $\hat{H}$ is effectively reduced to a number (the eigenvalue) in the eigen subspace, and the algebra Eq. (192) is closed.

▪ Emergent SO(4) Symmetry

Assuming there exist *bound states* with energy $E < 0$, in the space of a fixed eigen energy E (i.e. replacing $\hat{H} \to E$), it makes sense to rescale the LRL operator $\hat{\boldsymbol{A}}$ by a scalar, and define

$$\boxed{\hat{\boldsymbol{N}} = \frac{1}{\sqrt{-2\,E}}\,\hat{\boldsymbol{A}},} \tag{195}$$

then Eq. (192) reduces to (the original first two lines are trivialized)

$$\begin{aligned}
&\left[\hat{L}_a,\, \hat{L}_b\right] = i\,\epsilon_{abc}\,\hat{L}_c,\\
&\left[\hat{L}_a,\, \hat{N}_b\right] = i\,\epsilon_{abc}\,\hat{N}_c,\\
&\left[\hat{N}_a,\, \hat{N}_b\right] = i\,\epsilon_{abc}\,\hat{L}_c,
\end{aligned} \tag{196}$$

and Eq. (193) becomes

$$\begin{aligned}
&\hat{\boldsymbol{N}}\cdot\hat{\boldsymbol{L}} = \hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{N}} = 0,\\
&2\,E\left(\hat{\boldsymbol{L}}^2 + \hat{\boldsymbol{N}}^2 + \mathbb{1}\right) + \mathbb{1} = 0.
\end{aligned} \tag{197}$$

Define the SO(4) generators

$$\boxed{\begin{aligned}
\hat{\boldsymbol{T}} &= \frac{1}{2}\left(\hat{\boldsymbol{L}} + \hat{\boldsymbol{N}}\right),\\
\hat{\boldsymbol{S}} &= \frac{1}{2}\left(\hat{\boldsymbol{L}} - \hat{\boldsymbol{N}}\right).
\end{aligned}} \tag{198}$$

- Eq. (196) further reduces to

$$\begin{aligned}
&\left[\hat{T}_a,\, \hat{T}_b\right] = i\,\epsilon_{abc}\,\hat{T}_c,\\
&\left[\hat{S}_a,\, \hat{S}_b\right] = i\,\epsilon_{abc}\,\hat{S}_c,\\
&\left[\hat{T}_a,\, \hat{S}_b\right] = 0.
\end{aligned} \tag{199}$$

Exc 32 Derive Eq. (199) from Eq. (196).

This implies that $\hat{\boldsymbol{T}}$ and $\hat{\boldsymbol{S}}$ generates two independent SU(2) group, which combines into the SO(4) group (roughly speaking), see (HW 4).

- Eq. (197) reduces to the following constraints

$$\begin{aligned}
&\hat{\boldsymbol{T}}^2 = \hat{\boldsymbol{S}}^2,\\
&2\,E\left(4\,\hat{\boldsymbol{T}}^2 + \mathbb{1}\right) + \mathbb{1} = 0.
\end{aligned} \tag{200}$$

Exc 33 Prove Eq. (200).

Therefore, $\hat{\boldsymbol{T}}$ and $\hat{\boldsymbol{S}}$ are two angular-momentum-like operators, subject to a constraint $\hat{\boldsymbol{T}}^2 = \hat{\boldsymbol{S}}^2$. The common eigenstates of $\hat{\boldsymbol{T}}$ and $\hat{\boldsymbol{S}}$ are labeled by three quantum numbers t, m_t, m_s:

$$\begin{aligned} &\hat{\boldsymbol{T}}^2 \,|t,\, m_t,\, m_s\rangle = \hat{\boldsymbol{S}}^2 \,|t,\, m_t,\, m_s\rangle = t(t+1)\,|t,\, m_t,\, m_s\rangle, \\ &\hat{T}_3 \,|t,\, m_t,\, m_s\rangle = m_t \,|t,\, m_t,\, m_s\rangle, \\ &\hat{S}_3 \,|t,\, m_t,\, m_s\rangle = m_s \,|t,\, m_t,\, m_s\rangle, \end{aligned} \tag{201}$$

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

■ Spectrum

■ Energy Levels

Eq. (200) implies that

$$\hat{\boldsymbol{T}}^2 = -\frac{1}{4}\left(\frac{1}{2\,E} + 1\right)\mathbb{1}, \tag{202}$$

when acting in the eigen subspace of E. On the other hand, acting on the state $|t,\, m_t,\, m_s\rangle$, $\hat{\boldsymbol{T}}^2$ takes the eigenvalue $t\,(t+1)$, meaning that

$$-\frac{1}{4}\left(\frac{1}{2\,E} + 1\right) = t\,(t+1), \tag{203}$$

whose solution is

$$E = -\frac{1}{2\,(4\,t\,(t+1)+1)} = -\frac{1}{2\,(2\,t+1)^2}. \tag{204}$$

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

$$n := 2\,t + 1 = 1,\, 2,\, 3,\, 4,\, \ldots \tag{205}$$

- The **energy levels** are labeled by the positive integer $n \in \mathbb{Z}_+$

$$E_n = -\frac{1}{2\,n^2}. \tag{206}$$

Restoring the energy unit by undo the rescaling in Eq. (172), the energy levels are given by

$$E_n = -\frac{m\,\alpha^2}{2\,n^2}. \tag{207}$$

- 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 $E_n = -m\,\alpha^2 \big/ \left(2\,n^2\right)$ 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 has to be the $|0,0,0\rangle$ state (also denoted as the $1\,s$ orbital).

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

$$\hat{H}\,\psi_{1s} = E_1\,\psi_{1s}, \tag{208}$$

or more explicitly as

$$\left(\frac{\hat{\boldsymbol{p}}^2}{2\,m} - \frac{\alpha}{\hat{r}}\right)\psi_{1s} = -\frac{m\,\alpha^2}{2}\,\psi_{1s}. \tag{209}$$

We guess a trial wave function

$$\psi_{1s}(\boldsymbol{r}) \propto e^{-r/a}, \tag{210}$$

Eq. (209) implies $a\,m\,\alpha - 1 = 0$, i.e. $a = 1\,/\,(m\,\alpha)$.

Exc 34 Verify that Eq. (210) is the solution of Eq. (209).

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

$$\boxed{\psi_{1s}(\boldsymbol{r}) = \frac{2}{a^{3/2}}\,e^{-r/a},} \tag{211}$$

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

$$\boxed{E_1 = -\frac{\alpha}{2\,a},} \tag{212}$$

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

- In quantum mechanics, the electron does not move along a deterministic trajectory, instead, it distributes in a probability cloud, called the **electron cloud**.

$$p(\boldsymbol{r}) = |\psi(\boldsymbol{r})|^2 \propto e^{-2\,r/a}. \tag{213}$$

■ 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 $\hat{\boldsymbol{L}}$ of electron is the total angular momentum of the fictitious spins,

$$\boxed{\hat{\boldsymbol{L}} = \hat{\boldsymbol{T}} + \hat{\boldsymbol{S}}.} \tag{214}$$

According to Eq. (156) 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 states may as well be labeled by

$$|n,l,m\rangle \tag{215}$$

- 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).

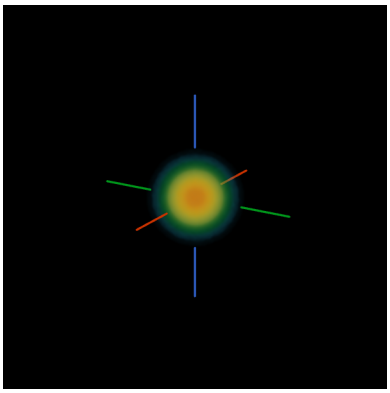
■ Atomic Structure

Each state $|n,l,m\rangle$ is associated with an **electron wave function**

$$\psi_{nlm}(\boldsymbol{r}). \tag{216}$$

It is also called an **atomic orbital**, on which electrons can occupy.

- Atomic orbitals do not depict the exact location of an electron in an atom, but rather provide a *probability distribution* $|\psi_{nlm}(\boldsymbol{r})|^2$ of where the electron is likely to be, which can be visualized as **electron clouds**:



		$n=1$	$n=2$	$n=3$	$n=4$
$l=0$	$m=0$	$1\,s$	$2\,s$	$3\,s$	$4\,s$
$l=1$	$m=0$		$2\,p_z$	$3\,p_z$	$4\,p_z$
	$m=\pm1$		$2\,p_y$	$3\,p_y$	$4\,p_y$
			$2\,p_x$	$3\,p_x$	$4\,p_x$
$l=2$	$m=0$			$3\,d_{z^2}$	$4\,d_{z^2}$
	$m=\pm1$			$3\,d_{y\,z}$	$4\,d_{y\,z}$
				$3\,d_{x\,z}$	$4\,d_{x\,z}$
	$m=\pm2$			$3\,d_{x\,y}$	$4\,d_{x\,y}$
				$3\,d_{x^2-y^2}$	$4\,d_{x^2-y^2}$
$l=3$	$m=0$				$4f_{z^3}$
	$m=\pm1$				$4f_{y\,z^2}$
					$4f_{x\,z^2}$
	$m=\pm2$				$4f_{x\,y\,z}$
					$4f_{(x^2-y^2)\,z}$
	$m=\pm3$				$4f_{3\,x^2\,y-y^3}$
					$4f_{x^3-3\,x\,y^2}$

- n - labels energy shells, controls the radial excitation,
- l - labels energy sub-shells, controls the angular excitation, and are given the following names

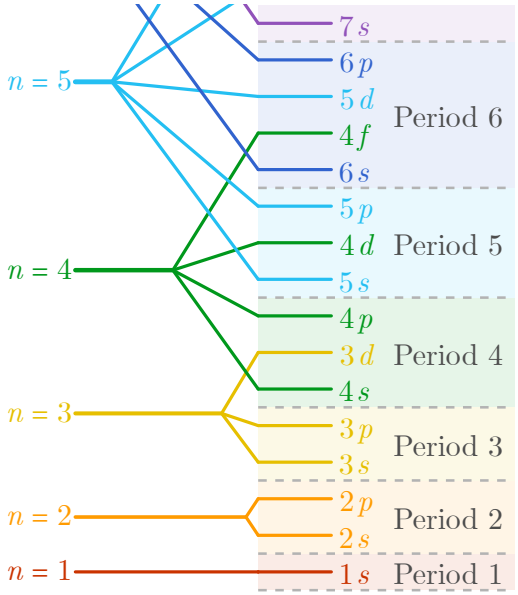
$$\begin{array}{l} l = 0\ 1\ 2\ 3\ 4\ 5\ \ldots \\ \quad\ s\ p\ d\ f\ g\ h\ \ldots \end{array} \tag{217}$$

- m - specifies the orientation of the orbital.

The shape of the orbital are often indicated by the **harmonic polynomials** (e.g. $x\,y$, x^2-y^2), which labels the SO(3) symmetry representation by the behavior of the wave function near the

origin.

In *multi-electron* atoms, due to the modifications from electron *interactions*, the effective potential function *deviates* from the 1/r behavior. As a result, the SO(4) symmetry is *broken* down to SO(3), leading to the further *splitting* of energy shells into sub-shells.



- As the atomic number increases, more electrons will fill the energy sub-shells from the bottom up. The electron configuration determines the chemical properties of the atom.
- **Periodic table in chemistry**: The chemical properties of an element are dependent on its outermost electrons. Therefore, whenever a new s orbital begins to be filled, a new period of elemental properties commences.