Quantum Mechanics

Part III. Quantum Bootstrap*

Harmonic Oscillator

■ 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.

$$\boxed{\hat{x}\,|x\rangle = x\,|x\rangle.} \tag{1}$$

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	$\sum_i \|i\rangle\langle i\| = \mathbb{1}$	→	$\int d\!\!\!{}^{-}x\,\|x\rangle\langle x\| = \mathbb{1}$
state decomposition	$\|v\rangle = \sum_i v_i\,\|i\rangle$	→	$\|\psi\rangle = \int d\!\!\!{}^{-}x\,\psi(x)\,\|x\rangle$
	$v_i = \langle i\|v\rangle$		$\psi(x) = \langle x\|\psi\rangle$
state normalization	$\sum_i \|v_i\|^2 = 1$	→	$\int d\!\!\!{}^{-}x\,\|\psi(x)\|^2 = 1$
scalar product	$\langle u\|v\rangle = \sum_i \langle u\|i\rangle\langle i\|v\rangle$	→	$\langle\phi\|\psi\rangle = \int d\!\!\!{}^{-}x\,\langle\phi\|x\rangle\langle x\|\psi\rangle$
	$= \sum_i u_i^*\,v_i$		$= \int d\!\!\!{}^{-}x\,\phi(x)^*\,\psi(x)$

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

$$\forall f : \int d x\, \delta(x)\, f(x) = f(0). \tag{2}$$

Position Operator

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

$$\boxed{\hat{x} = \int d x\, |x\rangle\, x\, \langle x|.} \tag{3}$$

- 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 $|\psi\rangle$

$$|\psi\rangle = \int d x\, \psi(x)\, |x\rangle, \tag{4}$$

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

- Applying the position operator,

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

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

$$\boxed{\hat{x} \doteq x.} \tag{6}$$

Translation

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

$$\boxed{\hat{T}(a)\, |x\rangle = |x+a\rangle.} \tag{7}$$

- 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

$$\boxed{\hat{T}(a) = \int d x\, |x+a\rangle\, \langle x|.} \tag{8}$$

- 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 1

> Use the definition Eq. (8) 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.

By definition,

$$\hat{T}(a)^\dagger = \int d x\, |x\rangle\, \langle x+a|. \tag{9}$$

We can show that

$$\begin{aligned}
&\hat{T}(a)^\dagger\, \hat{T}(a) = \int d x'\, |x'\rangle\, \langle x'+a| \int d x\, |x+a\rangle\, \langle x| \\
&= \int d x' \int d x\, |x'\rangle\, \langle x'+a|x+a\rangle\, \langle x| \\
&= \int d x' \int d x\, |x'\rangle\, \delta\,(x' + a - x - a)\, \langle x| \\
&= \int d x' \int d x\, |x'\rangle\, \delta\,(x' - x)\, \langle x| \\
&= \int d x\, |x\rangle\, \langle x| \\
&= \mathbb{1}.
\end{aligned} \tag{10}$$

Similarly, $\hat{T}(a)\, \hat{T}(a)^\dagger = \mathbb{1}$. So $\hat{T}(a)$ is unitary.

Momentum Operator

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

$$\boxed{\hat{T}(a) = \exp\left(-\frac{i\, \hat{p}\, a}{\hbar}\right).} \tag{11}$$

Conversely,

$$\begin{aligned}
\hat{p} &= i\, \hbar\, \partial_a\, \hat{T}(a)\, |_{a=0} \\
&= i\, \hbar \lim_{a\to 0} \frac{\hat{T}(a) - \hat{T}(0)}{a},
\end{aligned} \tag{12}$$

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 $|\psi\rangle$

$$|\psi\rangle = \int d\,x\,\psi(x)\,|x\rangle, \tag{13}$$

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

- Under translation,

$$\begin{aligned}\hat{T}(a)\,|\psi\rangle &= \int d\,x\,\psi(x)\,|x+a\rangle \\ &= \int d\,x\,\psi(x-a)\,|x\rangle.\end{aligned} \tag{14}$$

- Applying the momentum operator,

$$\begin{aligned}\hat{p}\,|\psi\rangle &= i\,\hbar \lim_{a\to 0} \frac{\hat{T}(a)\,|\psi\rangle - \hat{T}(0)\,|\psi\rangle}{a} \\ &= i\,\hbar \int d\,x \left(\lim_{a\to 0} \frac{\psi\,(x-a) - \psi\,(x)}{a}\right)|x\rangle \\ &= \int d\,x\,(-i\,\hbar\,\partial_x \psi(x))\,|x\rangle.\end{aligned} \tag{15}$$

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

$$\boxed{\hat{p} \doteq -i\,\hbar\,\partial_x,} \tag{16}$$

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

$$\boxed{\hat{p} = -i\,\hbar \int d\,x\,d\,x'\,|x\rangle\,\partial_x\delta\,(x-x')\,\langle x'|.} \tag{17}$$

Exc 2 Show that Eq. (17) is consistent with Eq. (16) when acting on a state $|\psi\rangle$.

Commutation Relation

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

$$\boxed{[\hat{x},\,\hat{p}] = i\,\hbar.} \tag{19}$$

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

$$\hat{x} \doteq x,\;\; \hat{p} \doteq -i\,\hbar\,\partial_x, \tag{20}$$

the commutator acts as

$$\begin{aligned}[\hat{x}, \hat{p}] |\psi\rangle &\doteq [x, -i \hbar \partial_x] \psi(x) \\ &= -i \hbar (x \partial_x - \partial_x x) \psi(x) \\ &= i \hbar \psi(x) \\ &\doteq i \hbar |\psi\rangle.\end{aligned} \tag{21}$$

This verifies the commutation relation.

Operator Algebra

Hamiltonian

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

$$\hat{H} = \frac{1}{2m} \hat{p}^2 + \frac{1}{2} m \omega^2 \hat{x}^2. \tag{22}$$

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

$$[\hat{x}, \hat{p}] = i \hbar. \tag{23}$$

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

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

$$\hat{p} \to \hat{p} \sqrt{\hbar m \omega}, \ \hat{x} \to \hat{x} \sqrt{\frac{\hbar}{m \omega}}, \tag{24}$$

then the Hamiltonian looks simpler

$$\boxed{\hat{H} = \frac{1}{2} \hbar \omega \left(\hat{p}^2 + \hat{x}^2\right).} \tag{25}$$

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

- Commutation relation for the rescaled operators

$$\boxed{[\hat{x}, \hat{p}] = i \mathbb{1}.} \tag{26}$$

Annihilation and Creation Operators

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

$$\boxed{\hat{a} = \frac{1}{\sqrt{2}} (\hat{x} + i \hat{p}), \ \hat{a}^\dagger = \frac{1}{\sqrt{2}} (\hat{x} - i \hat{p}).} \tag{27}$$

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

Commutation relation

$$\boxed{\left[\hat{a}, \hat{a}^\dagger\right] = \mathbb{1},} \tag{28}$$

meaning that

$$\hat{a}\,\hat{a}^\dagger = \hat{a}^\dagger\,\hat{a} + \mathbb{1}. \tag{29}$$

Keep applying Eq. (29), it can be proven that (for l, $m = 0, 1, 2, \ldots$)

$$\hat{a}^l\,(\hat{a}^\dagger)^m = \sum_{k=0}^{\min(m,l)} \frac{m!\,l!}{(m-k)!\,(l-k)!\,k!}\,(\hat{a}^\dagger)^{m-k}\,\hat{a}^{l-k} \tag{30}$$

Exc 3 Prove Eq. (30).

Number Operator

Define the **number operator** as

$$\boxed{\hat{n} = \hat{a}^\dagger\,\hat{a}.} \tag{37}$$

In terms of the position and momentum operators

$$\hat{n} = \frac{1}{2}\left(\hat{p}^2 + \hat{x}^2\right) - \frac{\mathbb{1}}{2}. \tag{38}$$

Exc 4 Verify Eq. (38) using Eq. (27).

Compare with Eq. (25), the number operator and the Hamiltonian are related by

$$\boxed{\hat{H} = \hbar\,\omega\left(\hat{n} + \frac{\mathbb{1}}{2}\right).} \tag{40}$$

The goal is to find the eigenvalues and eigenstates of the Hamiltonian $\hat{H}$. However, given the relation Eq. (40), we can find the eigenvalues n and eigenstates $|n\rangle$ of the number operator $\hat{n}$ instead

$$\boxed{\hat{n}\,|n\rangle = n\,|n\rangle,} \tag{41}$$

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

$$\hat{H}\,|n\rangle = \hbar\,\omega\left(n + \frac{1}{2}\right)|n\rangle, \tag{42}$$

which means the energy eigenvalues are

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

Quantum Bootstrap

General Principles

Quantum bootstrap is an approach to solve the eigen problem of a given Hermitian operator.

Consider a Hermitian operator $\hat{n}$ (say the number operator)

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

For any operator $\hat{O}$, the following consistency conditions must hold:

- **Eigen condition**

$$\boxed{\forall\ n : \langle n| \left[\hat{n}, \hat{O}\right] |n\rangle = 0.} \tag{45}$$

This can be seen from

$$\langle n|\,\hat{n}\,\hat{O}\,|n\rangle = \langle n|\,\hat{O}\,\hat{n}\,|n\rangle = n\,\langle n|\,\hat{O}\,|n\rangle. \tag{46}$$

- **Positivity constraint**

$$\boxed{\forall\ n : \langle n|\,\hat{O}^{\dagger}\,\hat{O}\,|n\rangle \geq 0,} \tag{47}$$

as the squared norm of the state vector $\hat{O}\,|n\rangle$ must always be non-negative.

Level Quantization

Consider a generic operator (for $m, l = 0, 1, 2, \ldots$)

$$\boxed{\hat{O}_{m,l} := (\hat{a}^{\dagger})^{m}\,\hat{a}^{l}.} \tag{48}$$

- This covers the several operators as special cases,

$$\begin{aligned} \hat{O}_{0,0} &= \mathbb{1}, \\ \hat{O}_{0,1} &= \hat{a}, \\ \hat{O}_{1,0} &= \hat{a}^{\dagger}, \\ \hat{O}_{1,1} &= \hat{a}^{\dagger}\,\hat{a} = \hat{n}. \end{aligned} \tag{49}$$

- The indices m, l interchange under Hermitian conjugate

$$\hat{O}_{m,l}^{\dagger} = \hat{O}_{l,m}. \tag{50}$$

- **Operator product expansion**: product of two operators can be expanded into linear combination of operators.

$$\hat{O}_{k,l}\,\hat{O}_{m,n} = \sum_{p=0}^{\min(m,l)} \frac{m!\,l!}{(m-p)!\,(l-p)!\,p!}\,\hat{O}_{k+m-p,l+n-p}. \tag{51}$$

Exc 5 Prove Eq. (51) using Eq. (30).

In particular, if one of the operator is $\hat{O}_{1,1} = \hat{n}$, Eq. (51) reduces to

$$\begin{aligned}\hat{n}\,\hat{O}_{m,l} &= \hat{O}_{m+1,l+1} + m\,\hat{O}_{m,l},\\ \hat{O}_{m,l}\,\hat{n} &= \hat{O}_{m+1,l+1} + l\,\hat{O}_{m,l}.\end{aligned} \tag{53}$$

Therefore, we have the following commutator

$$\left[\hat{n},\,\hat{O}_{m,l}\right] = \hat{n}\,\hat{O}_{m,l} - \hat{O}_{m,l}\,\hat{n} = (m-l)\,\hat{O}_{m,l}, \tag{54}$$

then the **eigen condition** Eq. (45) becomes

$$\langle n|\left[\hat{n},\,\hat{O}_{m,l}\right]|n\rangle = (m-l)\,\langle n|\,\hat{O}_{m,l}\,|n\rangle = 0. \tag{55}$$

- If $m \neq l$ (i.e. $m - l \neq 0$), for Eq. (55) to hold, we must have

$$\langle n|\,\hat{O}_{m,l}\,|n\rangle = 0 \ \text{(for } m \neq l). \tag{56}$$

- If $m = l$, Eq. (55) is automatically satisfied. In this case, the expectation value $\langle n|\,\hat{O}_{m,m}\,|n\rangle$ can take any real number, which we denote as $W_{m|n}$,

$$W_{m|n} := \langle n|\,\hat{O}_{m,m}\,|n\rangle \in \mathbb{R}. \tag{57}$$

To determine $W_{m|n}$, we notice that

$$\begin{aligned}&\langle n|\,\hat{O}_{m,m}\,\hat{n}\,|n\rangle = n\,\langle n|\,\hat{O}_{m,m}\,|n\rangle = n\,W_{m|n},\\ &\langle n|\,\hat{O}_{m,m}\,\hat{n}\,|n\rangle = \langle n|\,\hat{O}_{m+1,m+1}\,|n\rangle + m\,\langle n|\,\hat{O}_{m,m}\,|n\rangle\\ &= W_{m+1|n} + m\,W_{m|n}.\end{aligned} \tag{58}$$

This leads to a recurrent equation

$$W_{m+1|n} = (n-m)\,W_{m|n}. \tag{59}$$

Given the initial condition at $m = 0$ (the normalization of eigenstates)

$$W_{0|n} = \langle n|n\rangle = 1, \tag{60}$$

the solution of Eq. (59) is

$$W_{m|n} = \prod_{l=0}^{m-1}(n-l). \tag{61}$$

Finally, we examine the **positivity constraint** Eq. (47) with $\hat{O}_{0,m} = \hat{a}^m$,

$$\langle n| \hat{O}_{0,m}^{\dagger} \hat{O}_{0,m} |n\rangle = \langle n| (\hat{a}^{\dagger})^m \hat{a}^m |n\rangle = \langle n| \hat{O}_{m,m} |n\rangle = W_{m|n} \geq 0. \tag{62}$$

To ensure $W_{m|n} \geq 0$, according to Eq. (61), we must have

$$\forall\ n,\ m: \prod_{l=0}^{m-1} (n-l) \geq 0 \tag{63}$$

This corresponds to a series of *inequalities*

$$\begin{aligned} &n \geq 0, \\ &n\,(n-1) \geq 0, \\ &n\,(n-1)\,(n-2) \geq 0, \\ &n\,(n-1)\,(n-2)\,(n-3) \geq 0, \\ &\ldots \end{aligned} \tag{64}$$

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

$$\boxed{n = 0, 1, 2, \ldots \in \mathbb{N}.} \tag{65}$$

- 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 *elementary excitations*, called **phonons** (the quanta of sound). The phonon is an example of emergent **boson** in quantum systems.
- The $n = 0$ state, 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 $|n\rangle$ has the following expectation value

$$\langle n| \hat{O}_{m,l} |n\rangle = \langle n| (\hat{a}^{\dagger})^m \hat{a}^l |n\rangle = \begin{cases} 0 & \text{if } m \neq l, \\ n!\,/\,m! & \text{if } m = l. \end{cases} \tag{66}$$

Number Basis Representation

The commutation relation Eq. (54) implies that on any eigenstate $|n\rangle$,

$$\hat{n}\, \hat{O}_{m,l} |n\rangle = (n + m - l)\, \hat{O}_{m,l} |n\rangle, \tag{67}$$

meaning that the state $\hat{O}_{m,l} |n\rangle$ must be an eigenstate of $\hat{n}$ with eigenvalue $n + m - l$. Therefore, it should be identified with the $|n{+}m{-}l\rangle$ state,

$$\hat{O}_{m,l} |n\rangle \propto |n{+}m{-}l\rangle. \tag{68}$$

In particular,

- for $\hat{O}_{0,1} = \hat{a}$,

$$\hat{a} |n\rangle \propto |n{-}1\rangle; \tag{69}$$

- for $\hat{O}_{1,0} = \hat{a}^{\dagger}$,

$$\hat{a}^\dagger |n\rangle \propto |n{+}1\rangle. \tag{70}$$

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

$$\begin{aligned} \langle n|\, \hat{a}^\dagger\, \hat{a}\, |n\rangle &= \langle n|\, \hat{n}\, |n\rangle = n, \\ \langle n|\, \hat{a}\, \hat{a}^\dagger\, |n\rangle &= \langle n| \left(\hat{a}^\dagger\, \hat{a} + \mathbb{1}\right) |n\rangle = \langle n|\, (\hat{n} + \mathbb{1})\, |n\rangle = n + 1. \end{aligned} \tag{71}$$

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

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

Summary

- Annihilation and creation operators

$$\begin{cases} \hat{a} = \frac{1}{\sqrt{2}}\, (\hat{x} + i\, \hat{p}) \\ \hat{a}^\dagger = \frac{1}{\sqrt{2}}\, (\hat{x} - i\, \hat{p}) \end{cases}, \quad \begin{cases} \hat{x} = \frac{1}{\sqrt{2}}\, \left(\hat{a} + \hat{a}^\dagger\right) \\ \hat{p} = \frac{1}{\sqrt{2}\, i}\, \left(\hat{a} - \hat{a}^\dagger\right) \end{cases}. \tag{73}$$

  They satisfies the commutation relation

$$[\hat{x}, \hat{p}] = i\, \mathbb{1} \Leftrightarrow \left[\hat{a}, \hat{a}^\dagger\right] = \mathbb{1}. \tag{74}$$

- Number operator

$$\hat{n} = \hat{a}^\dagger\, \hat{a}. \tag{75}$$

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

$$\begin{aligned} \hat{a}\, |n\rangle &= \sqrt{n}\; |n-1\rangle, \\ \hat{a}^\dagger\, |n\rangle &= \sqrt{n+1}\; |n+1\rangle. \end{aligned} \tag{76}$$

- Hamiltonian

$$\hat{H} = \frac{1}{2}\, \hbar\, \omega \left(\hat{p}^2 + \hat{x}^2\right) = \hbar\, \omega \left(\hat{n} + \frac{\mathbb{1}}{2}\right). \tag{77}$$

  - Eigen energies

$$E_n = \hbar\, \omega \left(n + \frac{1}{2}\right). \tag{78}$$

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

$$|n\rangle = \frac{1}{\sqrt{n!}}\, (\hat{a}^\dagger)^n\, |0\rangle. \tag{79}$$

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 $\hat{\boldsymbol{J}} = \left(\hat{J}_1, \hat{J}_2, \hat{J}_3\right)$, satisfying the following commutation relation

$$\boxed{\left[\hat{J}_a, \hat{J}_b\right] = i\,\epsilon_{abc}\,\hat{J}_c.} \tag{80}$$

- ϵ_{abc} is the Levi-Civita symbol: the sign of the abc permutation.
- Equivalently, in vector form, $\hat{\boldsymbol{J}} \times \hat{\boldsymbol{J}} = i\,\hat{\boldsymbol{J}}$.

Examples:

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

$$\boxed{\hat{\boldsymbol{L}} = \hat{\boldsymbol{x}} \times \hat{\boldsymbol{p}}.} \tag{81}$$

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

$$\left[\hat{L}_a, \hat{L}_b\right] = i\,\epsilon_{abc}\,\hat{L}_c. \tag{82}$$

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

$$\boxed{\hat{\boldsymbol{S}} = \frac{1}{2}\,\hat{\boldsymbol{\sigma}}.} \tag{83}$$

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

$$\left[\hat{S}_a, \hat{S}_b\right] = i\,\epsilon_{abc}\,\hat{S}_c. \tag{84}$$

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** $\hat{\boldsymbol{J}}^2 = \hat{\boldsymbol{J}} \cdot \hat{\boldsymbol{J}}$,

$$\boxed{\hat{\boldsymbol{J}}^2 = \hat{J}_1^2 + \hat{J}_2^2 + \hat{J}_3^2.} \tag{85}$$

- $\hat{\boldsymbol{J}}^2$ is Hermitian.
- By Eq. (80), one can verify that (for $a = 1, 2, 3$)

$$\left[\hat{\boldsymbol{J}}^2, \hat{J}_a\right] = 0. \tag{86}$$

Exc 6 Prove Eq. (86).

Raising and Lowering Operators

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

$$\boxed{\hat{J}_\pm = \hat{J}_1 \pm i\, \hat{J}_2.} \tag{87}$$

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

By definition Eq. (87), one can prove the following relations (for $l = 0, 1, 2, \ldots$)

$$\hat{J}_3\, \hat{J}_\pm^l = \hat{J}_\pm^l\left(\hat{J}_3 \pm l\right). \tag{88}$$

$$\hat{J}_\mp^{l+1}\, \hat{J}_\pm^{l+1} = \hat{J}_\mp^l\, \hat{J}_\pm^l\left(\hat{\boldsymbol{J}}^2 - \left(\hat{J}_3 \pm l\right)\left(\hat{J}_3 \pm (l+1)\right)\right). \tag{89}$$

Exc 7 Prove Eq. (88).

Exc 8 Prove Eq. (89).

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

$$\begin{aligned} \hat{\boldsymbol{J}}^2\, |j,m\rangle &= \lambda_j\, |j,m\rangle, \\ \hat{J}_3\, |j,m\rangle &= \lambda_m\, |j,m\rangle, \end{aligned} \tag{90}$$

- 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.

General Principles

Any operator $\hat{O}$ must satisfy the following consistency conditions.

- **Eigen condition**

$$\begin{aligned}&\langle j,m|\, f\left(\hat{\boldsymbol{J}}^2, \hat{J}_3\right) \hat{O}\, |j,m\rangle \\ &= \langle j,m|\, \hat{O}\, f\left(\hat{\boldsymbol{J}}^2, \hat{J}_3\right) |j,m\rangle \\ &= f\left(\lambda_j, \lambda_m\right) \langle j,m|\, \hat{O}\, |j,m\rangle,\end{aligned} \tag{91}$$

for any function f. In particular, it implies

$$\boxed{\langle j,m|\left[\hat{\boldsymbol{J}}^2, \hat{O}\right] |j,m\rangle = \langle j,m|\left[\hat{J}_3, \hat{O}\right] |j,m\rangle = 0.} \tag{92}$$

- **Positivity constraint**

$$\boxed{\langle j,m|\, \hat{O}^\dagger\, \hat{O}\, |j,m\rangle \geq 0.} \tag{93}$$

Angular Momentum Quantization

The goal is to estimate the expectation value of $\hat{J}_\mp^l\, \hat{J}_\pm^{l'}$ on the common eigen state $|j,m\rangle$ for general l and l', i.e. $\langle j,m|\, \hat{J}_\mp^l\, \hat{J}_\pm^{l'}\, |j,m\rangle$, satisfying all the consistency conditions.
Using Eq. (88), it can be shown that

$$\left[\hat{J}_3, \hat{J}_\mp^l\, \hat{J}_\pm^{l'}\right] = \mp(l - l')\, \hat{J}_\mp^l\, \hat{J}_\pm^{l'}, \tag{94}$$

Exc 9 | Prove Eq. (94) using Eq. (88).

which implies

$$\langle j,m|\left[\hat{J}_3, \hat{J}_\mp^l\, \hat{J}_\pm^{l'}\right] |j,m\rangle = \mp(l - l')\, \langle j,m|\, \hat{J}_\mp^l\, \hat{J}_\pm^{l'}\, |j,m\rangle. \tag{96}$$

On the other hand, apply Eq. (92) with $\hat{O} = \hat{J}_\mp^l\, \hat{J}_\pm^{l'}$,

$$(l - l')\, \langle j,m|\, \hat{J}_\mp^l\, \hat{J}_\pm^{l'}\, |j,m\rangle = 0. \tag{97}$$

- If $l \neq l'$, we must have $\langle j,m|\, \hat{J}_\mp^l\, \hat{J}_\pm^{l'}\, |j,m\rangle = 0$.

- If $l = l'$, Eq. (97) is automatically satisfied, and there is no restriction on $\langle j,m|\, \hat{J}_{\mp}^{l}\, \hat{J}_{\pm}^{l'}\, |j,m\rangle$. Its value remains to be determined, and can be defined as

$$A_{j,m}^{\pm,l} := \langle j,m|\, \hat{J}_{\mp}^{l}\, \hat{J}_{\pm}^{l}\, |j,m\rangle. \tag{98}$$

To determine $A_{j,m}^{\pm,l}$, start with Eq. (89) and use the eigen condition Eq. (91) ⇒ recurrent equation:

$$A_{j,m}^{\pm,l+1} = \big(\lambda_j - (\lambda_m \pm l)\,(\lambda_m \pm (l+1))\big)\, A_{j,m}^{\pm,l}. \tag{99}$$

Exc 10 Derive Eq. (99) using Eq. (89).

Given that $A_{j,m}^{\pm,0} = \langle j,m|j,m\rangle = 1$, the solution of Eq. (99) is

$$A_{j,m}^{\pm,l} = \prod_{k=0}^{l-1}\big(\lambda_j - (\lambda_m \pm k)\,(\lambda_m \pm (k+1))\big). \tag{100}$$

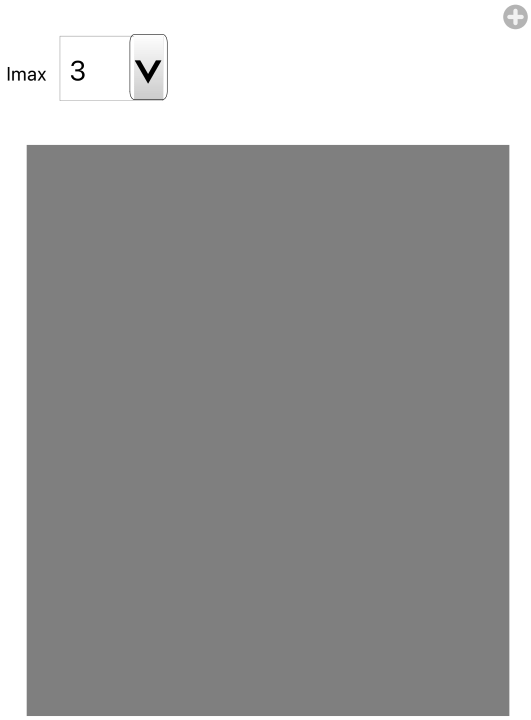
Finally, the positivity constraint Eq. (93) for $\hat{O} = \hat{J}_{\pm}^{l}$ requires

$$A_{j,m}^{\pm,l} = \langle j,m|\, \hat{J}_{\mp}^{l}\, \hat{J}_{\pm}^{l}\, |j,m\rangle \geq 0, \tag{101}$$

which gives a series of inequalities (for $l = 1, 2, \ldots$)

$$\prod_{k=0}^{l-1}\big(\lambda_j - (\lambda_m \pm k)\,(\lambda_m \pm (k+1))\big) \geq 0. \tag{102}$$

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

$$\boxed{\begin{array}{ll} \lambda_j = j(j+1) & \text{for } j = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots \\ \lambda_m = m & \text{for } m = -j, -j+1, \ldots, j-1, j \end{array}} \tag{103}$$

- For **orbital** angular momentum j takes *integer* values.
  For **spin** angular momentum j can also be *half-integers*.
- The eigen equations in Eq. (90) become

$$\begin{aligned} \hat{\boldsymbol{J}}^2 \, |j,m\rangle &= j(j+1) \, |j,m\rangle, \\ \hat{J}_3 \, |j,m\rangle &= m \, |j,m\rangle. \end{aligned} \tag{104}$$

- The expectation value reads

$$\langle j,m| \, \hat{J}_\mp^{\,l} \, \hat{J}_\pm^{\,l'} \, |j,m\rangle = \begin{cases} 0 & \text{if } l \neq l' \\ \prod_{k=0}^{l-1} (j(j+1) - (m \pm k)\,(m \pm (k+1))) & \text{if } l = l' \end{cases}. \tag{105}$$

▪ Operator Representation

From Eq. (88) with $l = 1$, $\hat{J}_3 \, \hat{J}_\pm = \hat{J}_\pm\left(\hat{J}_3 \pm 1\right)$ we have

$$\begin{aligned} \hat{J}_3 \, \hat{J}_\pm \, |j,m\rangle &= \hat{J}_\pm\left(\hat{J}_3 \pm 1\right) |j,m\rangle \\ &= (m \pm 1) \, \hat{J}_\pm \, |j,m\rangle \end{aligned} \tag{106}$$

$\Rightarrow$ 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 $(m \pm 1)$ $\Rightarrow$ $\hat{J}_\pm |j,m\rangle$ is just the $|j,m\pm1\rangle$ state (up to overall coefficient)

$$\hat{J}_\pm |j,m\rangle = c^\pm_{j,m} |j,m\pm1\rangle. \tag{107}$$

To determine the coefficient $c^\pm_{j,m}$, use Eq. (105) with $l = l' = 1$

$$\langle j,m| \hat{J}_\mp \hat{J}_\pm |j,m\rangle = j(j+1) - m(m \pm 1). \tag{108}$$

On the other hand

$$\langle j,m| \hat{J}_\mp \hat{J}_\pm |j,m\rangle = \left(c^\pm_{j,m}\right)^2 \langle j,m\pm1|j,m\pm1\rangle = \left(c^\pm_{j,m}\right)^2. \tag{109}$$

Combining Eq. (108) and Eq. (109), $c^\pm_{j,m}$ can be solved

$$c^\pm_{j,m} = \sqrt{j(j+1) - m(m \pm 1)}\,. \tag{110}$$

In conclusion, we have obtained the following representations for angular momentum operators (from Eq. (104) and Eq. (107))

$$\boxed{\begin{aligned} &\hat{\boldsymbol{J}}^2 |j,\, m\rangle = j(j+1) |j,\, m\rangle, \\ &\hat{J}_3 |j,\, m\rangle = m |j,\, m\rangle, \\ &\hat{J}_\pm |j,\, m\rangle = \sqrt{j(j+1) - m(m \pm 1)}\, |j,\, m \pm 1\rangle. \end{aligned}} \tag{111}$$

Induction implies that all basis states can be

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

$$|j,\, m\rangle = \left(\frac{(j-m)!}{(2\,j)!\,(j+m)!}\right)^{1/2} \hat{J}_+^{j+m} |j,\, -j\rangle, \tag{112}$$

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

$$|j,\, m\rangle = \left(\frac{(j+m)!}{(2\,j)!\,(j-m)!}\right)^{1/2} \hat{J}_-^{j-m} |j,\, j\rangle. \tag{113}$$

This is just like the Harmonic oscillator.

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

$$\begin{aligned} \frac{\hat{J}_+}{\sqrt{2\,j}} |j,\, -j+n\rangle &= \sqrt{n+1}\, |j,\, -j+n+1\rangle + O\left(j^{-1/2}\right), \\ \frac{\hat{J}_-}{\sqrt{2\,j}} |j,\, -j+n\rangle &= \sqrt{n}\, |j,\, -j+n-1\rangle + O\left(j^{-1/2}\right). \end{aligned} \tag{114}$$

Under the following correspondence

$$\begin{aligned}&|j, -j+n\rangle \to |n\rangle,\\&(2\,j)^{-1/2}\,\hat{J}_- \to a,\ \ (2\,j)^{-1/2}\,\hat{J}_+ \to a^\dagger,\end{aligned}\tag{115}$$

the boson creation/annihilation algebra Eq. (72) 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

$$\hat{\boldsymbol{J}} \times \hat{\boldsymbol{J}} = i\,\hat{\boldsymbol{J}}.\tag{116}$$

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

- The total angular momentum operator

$$\hat{\boldsymbol{J}}^2 = \hat{J}_1^2 + \hat{J}_2^2 + \hat{J}_3^2.\tag{117}$$

- The raising and lowering operators

$$\hat{J}_\pm = \hat{J}_1 \pm i\,\hat{J}_2.\tag{118}$$

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

$$\begin{aligned}&\hat{\boldsymbol{J}}^2\,|j, m\rangle = j(j+1)\,|j, m\rangle,\\&\hat{J}_3\,|j, m\rangle = m\,|j, m\rangle,\\&\hat{J}_\pm\,|j, m\rangle = \sqrt{j(j+1) - m(m\pm 1)}\,\,|j, m\pm 1\rangle,\end{aligned}\tag{119}$$

where

$$\begin{aligned}&j = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots,\\&m = -j, -j+1, \ldots, j-1, j.\end{aligned}\tag{120}$$