130B Quantum Physics

Part III. Quantum Statistics

Introduction

▪ Tensors are Vectors

▪ From One to Two

Each **qubit** has *two* basis states $|0\rangle$ and $|1\rangle$, spanning a 2-dimensional single-qubit Hilbert space.
$\Rightarrow$ *two* qubits together have *four* basis states, spanning a 4-dimensional two-qubit Hilbert space.

$$\begin{array}{cc|cc} & & \multicolumn{2}{c}{\text{qubit}_B} \\ & & |0\rangle & |1\rangle \\ \hline \text{qubit}_A & |0\rangle & |00\rangle & |01\rangle \\ & |1\rangle & |10\rangle & |11\rangle \end{array} \tag{1}$$

- A generic **two-qubit quantum state** will be a linear superposition of these basis states

  $$|\psi\rangle = \psi_{00}\,|00\rangle + \psi_{01}\,|01\rangle + \psi_{10}\,|10\rangle + \psi_{11}\,|11\rangle, \tag{2}$$

  where the *coefficients* $\psi_{\alpha\beta}$ is most naturally arranged as a 2×2 array (a matrix) like

  $$\begin{pmatrix} \psi_{00} & \psi_{01} \\ \psi_{10} & \psi_{11} \end{pmatrix}. \tag{3}$$

- However, it makes no difference to rearrange them in a vector

  $$\begin{pmatrix} \psi_{00} \\ \psi_{01} \\ \psi_{10} \\ \psi_{11} \end{pmatrix} \to \begin{pmatrix} \psi_{0} \\ \psi_{1} \\ \psi_{2} \\ \psi_{3} \end{pmatrix}. \tag{4}$$

  We can relabel the index $\psi_{\alpha\beta} \to \psi_i$ by converting each binary string $\alpha\beta$ to an integer i (e.g. through the binary number encoding).

  - A matrix can be viewed as a vector by *flattening*. Here, $\mathbb{C}^{2\times 2} \to \mathbb{C}^4$.

- In **vector representation**, the ket vector $|00\rangle$ is a **tensor product** of $|0\rangle_A$ and $|0\rangle_B$,

$$|00\rangle = |0\rangle_A \otimes |0\rangle_B \doteq \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ \hline 0 \\ 0 \end{pmatrix}. \tag{5}$$

Similarly,

$$|01\rangle = |0\rangle_A \otimes |1\rangle_B \doteq \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ \hline 0 \\ 0 \end{pmatrix},$$

$$|10\rangle = |1\rangle_A \otimes |0\rangle_B \doteq \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \hline 1 \\ 0 \end{pmatrix}, \tag{6}$$

$$|11\rangle = |1\rangle_A \otimes |1\rangle_B \doteq \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \hline 0 \\ 1 \end{pmatrix}.$$

From Two to Many

N qubits together have 2^N basis states, spanning a 2^N-dimensional Hilbert space.

- Each basis state $|\boldsymbol{\alpha}\rangle$ is labeled by a bit string $\boldsymbol{\alpha} \in \{0, 1\}^{\times N}$,

$$\boldsymbol{\alpha} = \alpha_1\, \alpha_2 \ldots \alpha_N \quad \text{for } \alpha_i \in \{0, 1\}, \tag{7}$$

and defined by the tensor product of single-qubit states

$$|\boldsymbol{\alpha}\rangle := |\alpha_1\rangle \otimes |\alpha_2\rangle \otimes \ldots \otimes |\alpha_N\rangle. \tag{8}$$

- A generic N-qubit state will be a linear combination of all multi-qubit basis states

$$|\Psi\rangle = \sum_{\boldsymbol{\alpha}} \Psi_{\boldsymbol{\alpha}}\, |\boldsymbol{\alpha}\rangle. \tag{9}$$

The coefficients $\Psi_{\boldsymbol{\alpha}}$ form a $\mathbb{C}^{2\times 2\times \ldots \times 2}$ *tensor*, but can also be viewed as a $\mathbb{C}^{2^N}$ *vector* by flattening. In this sense, tensors are vectors: many-body quantum states can also be described by ket vectors (with pre-defined tensor structure).

Quantum Many-Body States

Overview

Quantum many-body states describe the quantum system of many entities (particles). Depending on whether the particles are *distinguishable*, quantum many-body systems can be divided into two classes:

- **Distinct** particles: spins, qubits ...
- **Identical** particles: bosons, fermions ...

▪ Distinct Particles

Distinct particles can be *labeled*, such that we can specify the state of each particle, e.g. "the ith particle is in the α_i state".

- Suppose the **single-particle Hilbert space** is D dimensional, spanned by a set of orthonormal **single-particle basis states** $|\alpha\rangle$ ($\alpha = 1, 2, \ldots, D$).
- The **many-body Hilbert space** of N *distinct* particles will be D^N dimensional, spanned by the **many-body basis states**

$$\boxed{|\boldsymbol{\alpha}\rangle \equiv |\alpha_1\rangle \otimes |\alpha_2\rangle \otimes \ldots \otimes |\alpha_N\rangle,} \tag{10}$$

  where $\alpha_i = 1, 2, \ldots, D$ labels the state of the ith particle.

- A generic **many-body state** is a linear superposition of these basis states

$$\boxed{|\Psi\rangle = \sum_{\boldsymbol{\alpha}} \Psi_{\boldsymbol{\alpha}} |\boldsymbol{\alpha}\rangle.} \tag{11}$$

  The coefficient $\Psi_{\boldsymbol{\alpha}}$ is also called the **many-body wave function**.

- The **probability** to find the many-body system in a specific state $|\boldsymbol{\alpha}\rangle$ is given by

$$\boxed{p(\boldsymbol{\alpha} \mid \Psi) = |\langle\boldsymbol{\alpha}|\Psi\rangle|^2 = |\Psi_{\boldsymbol{\alpha}}|^2.} \tag{12}$$

▪ Identical Particles

Identical particles does not admit a labeling. Suppose we have a system of two particles, the following states are indistinguishable if we can not tell which particle is the 1st and which is the 2nd.

$\|\alpha_1\rangle \otimes \|\alpha_2\rangle$	$\|\alpha_2\rangle \otimes \|\alpha_1\rangle$
the 1st particle in $\|\alpha_1\rangle$ the 2nd particle in $\|\alpha_2\rangle$	the 1st particle in $\|\alpha_2\rangle$ the 2nd particle in $\|\alpha_1\rangle$

This means that it will be equally likely to observe the system in $|\alpha_1\,\alpha_2\rangle$ state as in $|\alpha_2\,\alpha_1\rangle$ state, i.e.

$$p(\alpha_1\,\alpha_2 \mid \Psi) = p(\alpha_2\,\alpha_1 \mid \Psi) \tag{13}$$

Generalize to N particles, we introduce the **permutation operator** $\hat{\mathcal{P}}_\pi$ associated with each permutation $\pi \in S_N$, and denote the permuted state as

$$\boxed{\hat{\mathcal{P}}_\pi\, |\boldsymbol{\alpha}\rangle = |\boldsymbol{\alpha}_\pi\rangle \equiv |\alpha_{\pi(1)}\rangle \otimes |\alpha_{\pi(2)}\rangle \otimes \ldots \otimes |\alpha_{\pi(N)}\rangle.} \tag{14}$$

- Each **permutation** $\pi \in S_N$ is a *bijective* (*invertible*) map from N objects to themselves. For example,

  $$123 \overset{\pi}{\to} 132 \tag{15}$$

  is a permutation in S_3, defined by $\pi(1) = 1$, $\pi(2) = 3$, $\pi(3) = 2$.
- $\boldsymbol{\alpha}_\pi$ denotes a new **sequence** obtained from the sequence $\boldsymbol{\alpha}$ by permuting its elements by π. For example,

  $$\boldsymbol{\alpha} = \alpha_1\, \alpha_2\, \alpha_3 \overset{\pi}{\to} \boldsymbol{\alpha}_\pi = \alpha_1\, \alpha_3\, \alpha_2. \tag{16}$$
- $\hat{\mathcal{P}}_\pi$ denotes the **operator** that take the state $|\boldsymbol{\alpha}\rangle$ to $|\boldsymbol{\alpha}_\pi\rangle$ for all $\boldsymbol{\alpha}$, which implements the permutation of particles.

The requirement of identical particles imposes a **permutation symmetry** to the *probability*, as a generalization of Eq. (13),

$$\forall\, \pi \in S_N : p(\boldsymbol{\alpha} \,|\, \Psi) = p(\boldsymbol{\alpha}_\pi \,|\, \Psi) \tag{17}$$

which, according to Eq. (12), is also a permutation symmetry of the *many-body wave function*,

$$\forall\, \pi \in S_N : |\Psi_{\boldsymbol{\alpha}}|^2 = |\Psi_{\boldsymbol{\alpha}_\pi}|^2. \tag{18}$$

The wave function can only change up to an *overall phase factor* under symmetry transformation,

$$\Psi_{\boldsymbol{\alpha}} = e^{i\,\varphi}\, \Psi_{\boldsymbol{\alpha}_\pi}. \tag{19}$$

It realizes a **one-dimensional representation** of the **permutation group**. Mathematical fact: there are only *two* 1-dim representations of any permutation group,

- **symmetric** (trivial) representation ⇒ **bosons**

  $$\boxed{\Psi_{\boldsymbol{\alpha}} = \Psi_{\boldsymbol{\alpha}_\pi},} \tag{20}$$
- **antisymmetric** (sign) representation ⇒ **fermions**

  $$\boxed{\Psi_{\boldsymbol{\alpha}} = (-)^\pi\, \Psi_{\boldsymbol{\alpha}_\pi},} \tag{21}$$

  where $(-)^\pi$ denotes the **permutation sign** of π

  $$(-)^\pi = \begin{cases} +1 & \text{if } \pi \text{ contains even number of exchanges,} \\ -1 & \text{if } \pi \text{ contains odd number of exchanges.} \end{cases} \tag{22}$$

  Take the S_3 group for example:

  $$\begin{array}{ccccccc} 123 & \overset{\pi}{\to} & 123 & 231 & 312 & 321 & 213 & 132 \\ (-)^\pi & = & +1 & +1 & +1 & -1 & -1 & -1 \end{array} \tag{23}$$

Bosonic and Fermionic States

The *bosonic* and *fermionic* many-body states only span a *subspace* of the many-body Hilbert space (of distinct particles). Starting from a generic basis state $|\boldsymbol{\alpha}\rangle$, we can pick out the **basis states** for the *bosonic* and *fermionic* subspaces:

- Construct **bosonic** states by **symmetrization**

$$\boxed{\hat{\mathcal{S}}\,|\boldsymbol{\alpha}\rangle = \sum_{\pi\in S_N} \hat{\mathcal{P}}_\pi\,|\boldsymbol{\alpha}\rangle = \sum_{\pi\in S_N} |\boldsymbol{\alpha}_\pi\rangle.} \tag{24}$$

- Construct **fermionic** states by **antisymmetrization**

$$\boxed{\hat{\mathcal{A}}\,|\boldsymbol{\alpha}\rangle = \sum_{\pi\in S_N} (-)^\pi\,\hat{\mathcal{P}}_\pi\,|\boldsymbol{\alpha}\rangle = \sum_{\pi\in S_N} (-)^\pi\,|\boldsymbol{\alpha}_\pi\rangle.} \tag{25}$$

Examples: consider a two-particle ($N = 2$) system.

- **Bosonic** states (unnormalized):

$$\begin{aligned} &\hat{\mathcal{S}}\,|\alpha\rangle\otimes|\beta\rangle = |\alpha\rangle\otimes|\beta\rangle + |\beta\rangle\otimes|\alpha\rangle,\ \text{(assuming } \alpha\neq\beta) \\ &\hat{\mathcal{S}}\,|\alpha\rangle\otimes|\alpha\rangle = |\alpha\rangle\otimes|\alpha\rangle. \end{aligned} \tag{26}$$

- **Fermionic** states (unnormalized):

$$\begin{aligned} &\hat{\mathcal{A}}\,|\alpha\rangle\otimes|\beta\rangle = |\alpha\rangle\otimes|\beta\rangle - |\beta\rangle\otimes|\alpha\rangle,\ \text{(assuming } \alpha\neq\beta) \\ &\hat{\mathcal{A}}\,|\alpha\rangle\otimes|\alpha\rangle = 0 \ \Rightarrow\ \text{no such fermionic state.} \end{aligned} \tag{27}$$

Pauli exclusion principle: two (or more) identical fermions can not occupy the same state simultaneously.

For N particles, the Hilbert space dimension of

- the full space (of distinct particles):

$$\mathcal{D} = D^N, \tag{28}$$

- the **bosonic** subspace:

$$\mathcal{D}_B = \frac{(N + D - 1)!}{N!\,(D-1)!}, \tag{29}$$

- the **fermionic** subspace:

$$\mathcal{D}_F = \frac{D!}{N!\,(D-N)!}. \tag{30}$$

It turns out that $\mathcal{D}_B + \mathcal{D}_F \leq \mathcal{D}$ (for $N > 1$) $\Rightarrow$ the remaining basis states in the many-body Hilbert space are *unphysical* (for identical particles).

Question: Is there a better way to organize the many-body Hilbert space, such that all states in the space are physical?

Second Quantization

Fock Space

Fock States and Fock Space

Sometimes, *conceptual problems* in physics arise from the inappropriate *language* we used. There are two different ways to describe many-body states:

- In **first-quantization**, we ask: *Which particle is in which state*?
- In **second-quantization**, we ask: *How many particles are there in every state*?

The first question is inappropriate for *identical* particles: it is impossible to tell which particle is which in the first place. We need a new language:

$$\begin{array}{ccc}
|\alpha\rangle \otimes |\beta\rangle & & |\beta\rangle \otimes |\alpha\rangle \\
\boxed{\begin{array}{l}\text{the 1st particle in } |\alpha\rangle \\ \text{the 2nd particle in } |\beta\rangle\end{array}} & & \boxed{\begin{array}{l}\text{the 1st particle in } |\beta\rangle \\ \text{the 2nd particle in } |\alpha\rangle\end{array}} \\
\searrow & & \swarrow \\
\multicolumn{3}{l}{\boxed{\text{there is one particle in } |\alpha\rangle\text{, and another particle in } |\beta\rangle}}
\end{array}$$

The new description does not require the labeling of particles ⇒ no redundant or unphysical basis state ⇒ hence a concise and precise description.

- Each **basis state** in the many-body Hilbert space is labeled by a set of **occupation numbers** n_α (for $\alpha = 1, 2, \ldots, D$)

  $$\boxed{|\boldsymbol{n}\rangle \equiv |n_1, n_2, \ldots, n_\alpha, \ldots, n_D\rangle,} \tag{31}$$

  meaning that there are n_α particles in the state $|\alpha\rangle$.

  $$n_\alpha = \begin{cases} 0, 1, 2, 3, \ldots & \text{bosons,} \\ 0, 1 & \text{fermions.} \end{cases} \tag{32}$$

  - For **bosons**, n_α can be any non-negative integer.
  - For **fermions**, n_α can only take 0 or 1, due to the *Pauli exclusion principle*.
  - The occupation numbers n_α sum up to the total number of particles, i.e. $\sum_\alpha n_\alpha = N$.
- The states $|\boldsymbol{n}\rangle$ are also known as **Fock states**.
- All Fock states form a complete set of basis for the many-body Hilbert space, or the **Fock space**.
- Any generic **second-quantized** many-body state is a linear combination of *Fock states*,

$$\boxed{|\Psi\rangle = \sum_{\boldsymbol{n}} \Psi_{\boldsymbol{n}}\, |\boldsymbol{n}\rangle.} \tag{33}$$

▪ Representation of Fock States

The **first-** and the **second-quantization** formalisms can both provide *legitimate* description of identical particles. (The first-quantization is just awkward to use, but it is still valid.)

Every *Fock state* has a **first-quantized representation**.

- The Fock state with all occupation numbers to be zero is called the **vacuum state**, denoted as

$$|\mathbf{0}\rangle \equiv |\ldots, 0, \ldots\rangle \tag{34}$$

  It corresponds to the *tensor product unit* in the first-quantization, which can be written as

$$|\mathbf{0}\rangle_B = |\mathbf{0}\rangle_F = \mathit{1}. \tag{35}$$

  We use a subscript B/F to indicate whether the Fock state is **bosonic** (B) or **fermionic** (F). For vacuum state, there is no difference between them.

- The Fock state with only one *non-zero* occupation number is a **single-mode Fock state**, denoted as

$$|n_\alpha\rangle = |\ldots, 0, n_\alpha, 0, \ldots\rangle \tag{36}$$

  In terms of the first-quantized states

$$\begin{aligned}
|1_\alpha\rangle_B &= |1_\alpha\rangle_F = |\alpha\rangle,\\
|2_\alpha\rangle_B &= |\alpha\rangle \otimes |\alpha\rangle,\\
|3_\alpha\rangle_B &= |\alpha\rangle \otimes |\alpha\rangle \otimes |\alpha\rangle,\\
|n_\alpha\rangle_B &= \underbrace{|\alpha\rangle \otimes |\alpha\rangle \otimes \ldots \otimes |\alpha\rangle}_{n_\alpha \text{ factors}} \equiv |\alpha\rangle^{\otimes n_\alpha}.
\end{aligned} \tag{37}$$

- For **multi-mode Fock states** (meaning more than one single-particle state $|\alpha\rangle$ is involved), the first-quantized state will involve appropriate symmetrization depending on the particle statistics. For example,

$$\begin{aligned}
\left|1_\alpha, 1_\beta\right\rangle_B &= \frac{1}{\sqrt{2}}\,(|\alpha\rangle \otimes |\beta\rangle + |\beta\rangle \otimes |\alpha\rangle),\\
\left|1_\alpha, 1_\beta\right\rangle_F &= \frac{1}{\sqrt{2}}\,(|\alpha\rangle \otimes |\beta\rangle - |\beta\rangle \otimes |\alpha\rangle).
\end{aligned} \tag{38}$$

  Note the difference between bosonic and fermionic Fock states (even if their occupation numbers are the same). Here are more examples

$$\left|2_\alpha, 1_\beta\right\rangle_B = \frac{1}{\sqrt{3}}\,(|\alpha\rangle \otimes |\alpha\rangle \otimes |\beta\rangle + |\alpha\rangle \otimes |\beta\rangle \otimes |\alpha\rangle + |\beta\rangle \otimes |\alpha\rangle \otimes |\alpha\rangle),$$

$$\left|1_\alpha, 1_\beta, 1_\gamma\right\rangle_F = \frac{1}{\sqrt{6}} \left(|\alpha\rangle \otimes |\beta\rangle \otimes |\gamma\rangle + |\beta\rangle \otimes |\gamma\rangle \otimes |\alpha\rangle + \right.$$
$$\left. |\gamma\rangle \otimes |\alpha\rangle \otimes |\beta\rangle - |\gamma\rangle \otimes |\beta\rangle \otimes |\alpha\rangle - |\beta\rangle \otimes |\alpha\rangle \otimes |\gamma\rangle - |\alpha\rangle \otimes |\gamma\rangle \otimes |\beta\rangle\right).$$

Ok, you get the idea. In general, the Fock state can be represented as (labeled by a set of occupation numbers $\boldsymbol{n} = \{n_\alpha\}_{\alpha=1}^D$)

- for **bosons**,

$$\boxed{|\boldsymbol{n}\rangle_B = \left(\frac{\prod_\alpha n_\alpha!}{N!}\right)^{1/2} \hat{\mathcal{S}} \bigotimes_\alpha |\alpha\rangle^{\otimes n_\alpha}.} \tag{40}$$

- for **fermions**,

$$\boxed{|\boldsymbol{n}\rangle_F = \frac{1}{\sqrt{N!}} \hat{\mathcal{A}} \bigotimes_\alpha |\alpha\rangle^{\otimes n_\alpha}.} \tag{41}$$

$\hat{\mathcal{S}}$ and $\hat{\mathcal{A}}$ are symmetrization and antisymmetrization operators

$$\hat{\mathcal{S}} = \sum_{\pi \in S_N} \hat{\mathcal{P}}_\pi, \ \hat{\mathcal{A}} = \sum_{\pi \in S_N} (-)^\pi \hat{\mathcal{P}}_\pi, \tag{42}$$

as introduced in Eq. (24) and Eq. (25).

Creation and Annihilation Operators

State Insertion and Deletion

The **creation** and **annihilation operators** are introduced to *create* and *annihilate* particles in the quantum many-body system, as indicated by their names. The first step towards defining them is to understand how to *insert* and *delete* a single-particle state from the first-quantized state in a *symmetric* (or *antisymmetric*) manner.

Let us first declare some notations:

- Let $|\alpha\rangle$, $|\beta\rangle$ be single-particle states.
- Let $\mathit{1}$ be the *tensor identity* (meaning that $|\alpha\rangle \otimes \mathit{1} = \mathit{1} \otimes |\alpha\rangle = |\alpha\rangle$).
- Let $|\Psi\rangle$, $|\Phi\rangle$ be generic *first-quantized states* as in Eq. (11).

Now we define the **insertion operator** $\triangleright_\pm$ and **deletion operator** $\triangleleft_\pm$ by the following rules:

- Linearity (for $a, b \in \mathbb{C}$)

$$\begin{aligned} |\alpha\rangle \triangleright_\pm (a\,|\Psi\rangle + b\,|\Phi\rangle) &= a\,|\alpha\rangle \triangleright_\pm |\Psi\rangle + b\,|\alpha\rangle \triangleright_\pm |\Phi\rangle, \\ |\alpha\rangle \triangleleft_\pm (a\,|\Psi\rangle + b\,|\Phi\rangle) &= a\,|\alpha\rangle \triangleleft_\pm |\Psi\rangle + b\,|\alpha\rangle \triangleleft_\pm |\Phi\rangle. \end{aligned} \tag{43}$$

- Vacuum property

$$|\alpha\rangle \triangleright_{\pm} \mathit{1} = |\alpha\rangle, \\ |\alpha\rangle \triangleleft_{\pm} \mathit{1} = 0. \tag{44}$$

- Recursive relation

$$|\alpha\rangle \triangleright_{\pm} |\beta\rangle \otimes |\Psi\rangle = |\alpha\rangle \otimes |\beta\rangle \otimes |\Psi\rangle \pm |\beta\rangle \otimes (|\alpha\rangle \triangleright_{\pm} |\Psi\rangle), \\ |\alpha\rangle \triangleleft_{\pm} |\beta\rangle \otimes |\Psi\rangle = \langle \alpha \mid \beta\rangle |\Psi\rangle \pm |\beta\rangle \otimes (|\alpha\rangle \triangleleft_{\pm} |\Psi\rangle). \tag{45}$$

  - $\langle \alpha \mid \beta \rangle = \delta_{\alpha\beta}$ if $|\alpha\rangle$ and $|\beta\rangle$ are orthonormal basis states.
  - The subscript $\pm$ of the insertion or deletion operators indicates whether symmetrization (+) or antisymmetrization (−) is implemented.

■ Boson Creation and Annihilation

The **boson creation operator** $\hat{b}_\alpha^\dagger$ *adds* a boson to the single-particle state $|\alpha\rangle$, *increasing* the occupation number by one $n_\alpha \to n_\alpha + 1$. It acts on a N-particle first-quantized state $|\Psi\rangle$ as

$$\boxed{\hat{b}_\alpha^\dagger |\Psi\rangle = \frac{1}{\sqrt{N+1}} |\alpha\rangle \triangleright_{+} |\Psi\rangle,} \tag{46}$$

where $|\alpha\rangle \triangleright_{+}$ *inserts* the single-particle state $|\alpha\rangle$ to $N+1$ possible insertion positions *symmetrically*.

The **boson annihilation operator** $\hat{b}_\alpha$ *removes* a boson from the single-particle state $|\alpha\rangle$, *reducing* the occupation number by one $n_\alpha \to n_\alpha - 1$ (while $n_\alpha > 0$). It acts on a N-particle first-quantized state $|\Psi\rangle$ as

$$\boxed{\hat{b}_\alpha |\Psi\rangle = \frac{1}{\sqrt{N}} |\alpha\rangle \triangleleft_{+} |\Psi\rangle,} \tag{47}$$

where $|\alpha\rangle \triangleleft_{+}$ *removes* the single-particle state $|\alpha\rangle$ from N possible deletion positions *symmetrically*.

▫ Single-Mode Fock States

Based on these definitions, we can show that the creation and annihilation operators acting on single-mode Fock states as

$$\boxed{\begin{aligned} \hat{b}_\alpha^\dagger |n_\alpha\rangle &= \sqrt{n_\alpha + 1}\; |n_\alpha + 1\rangle, \\ \hat{b}_\alpha |n_\alpha\rangle &= \sqrt{n_\alpha}\; |n_\alpha - 1\rangle. \end{aligned}} \tag{48}$$

Exc 1 Prove Eq. (48) by definitions in Eq. (46) and Eq. (47).

- Especially, when acting on the vacuum state

$$\begin{aligned} &\hat{b}_\alpha^\dagger \left|0_\alpha\right\rangle = \left|1_\alpha\right\rangle, \\ &\hat{b}_\alpha \left|0_\alpha\right\rangle = 0. \end{aligned} \tag{49}$$

- Using Eq. (48), we can show that

$$\boxed{\hat{b}_\alpha^\dagger\, \hat{b}_\alpha \left|n_\alpha\right\rangle = n_\alpha \left|n_\alpha\right\rangle,} \tag{50}$$

  meaning that $\hat{b}_\alpha^\dagger\, \hat{b}_\alpha$ is the **boson number operator** of the $|\alpha\rangle$ state.

All the single-mode Fock state can be constructed by the boson creation operator from the vacuum state

$$\boxed{\left|n_\alpha\right\rangle = \frac{1}{\sqrt{n_\alpha!}} \left(\hat{b}_\alpha^\dagger\right)^{n_\alpha} \left|0_\alpha\right\rangle.} \tag{51}$$

Generic Fock States

The above result can be generalized to any Fock state of bosons

$$\boxed{\begin{aligned} &\hat{b}_\alpha^\dagger \left|\ldots, n_\beta, n_\alpha, n_\gamma, \ldots\right\rangle_B = \sqrt{n_\alpha + 1} \left|\ldots, n_\beta, n_\alpha + 1, n_\gamma, \ldots\right\rangle_B, \\ &\hat{b}_\alpha \left|\ldots, n_\beta, n_\alpha, n_\gamma, \ldots\right\rangle_B = \sqrt{n_\alpha} \left|\ldots, n_\beta, n_\alpha - 1, n_\gamma, \ldots\right\rangle_B. \end{aligned}} \tag{52}$$

These two equations can be considered as the **defining properties** of boson creation and annihilation operators.

Operator Identities

Eq. (52) implies the following operator identities

$$\boxed{\left[\hat{b}_\alpha^\dagger, \hat{b}_\beta^\dagger\right] = \left[\hat{b}_\alpha, \hat{b}_\beta\right] = 0, \; \left[\hat{b}_\alpha, \hat{b}_\beta^\dagger\right] = \delta_{\alpha\beta}.} \tag{53}$$

These relations can be considered as the **algebraic definition** of boson creation and annihilation operators.

- $\left[\hat{A}, \hat{B}\right] = \hat{A}\,\hat{B} - \hat{B}\,\hat{A}$ denotes the **commutator**.
- The algebraic relation in Eq. (53) is identical to that of the creating and annihilation operators in *harmonic oscillator*, therefore, the *elementary excitations* of harmonic oscillator are indeed *bosons*.

Fermion Creation and Annihilation

The **fermion creation operator** $\hat{c}_\alpha^\dagger$ *adds* a fermion to the single-particle state $|\alpha\rangle$, *increasing* the occupation number by one $n_\alpha \to n_\alpha + 1$ (while $n_\alpha = 0$). It acts on a N-particle first-quantized state $|\Psi\rangle$ as

$$\hat{c}_\alpha^\dagger |\Psi\rangle = \frac{1}{\sqrt{N+1}} |\alpha\rangle \triangleright_- |\Psi\rangle, \tag{54}$$

where $|\alpha\rangle \triangleright_-$ *inserts* the single-particle state $|\alpha\rangle$ to $N+1$ possible insertion positions *anti-symmetrically.*

The **fermion annihilation operator** $\hat{c}_\alpha$ *removes* a fermion from the single-particle state $|\alpha\rangle$, *reducing* the occupation number by one $n_\alpha \to n_\alpha - 1$ (while $n_\alpha = 1$). It acts on a N-particle first-quantized state $|\Psi\rangle$ as

$$\hat{c}_\alpha |\Psi\rangle = \frac{1}{\sqrt{N}} |\alpha\rangle \triangleleft_- |\Psi\rangle, \tag{55}$$

where $|\alpha\rangle \triangleleft_-$ *removes* the single-particle state $|\alpha\rangle$ from N possible deletion positions *anti-symmetrically.*

▫ Single-Mode Fock States

Based on these definitions, we can show that the creation and annihilation operators acting on single-mode Fock states as

Thus we conclude (note that $n_\alpha = 0, 1$ only take two values)

$$\begin{aligned} \hat{c}_\alpha^\dagger |n_\alpha\rangle &= \sqrt{1-n_\alpha}\, |1-n_\alpha\rangle, \\ \hat{c}_\alpha |n_\alpha\rangle &= \sqrt{n_\alpha}\, |1-n_\alpha\rangle. \end{aligned} \tag{56}$$

Exc 2 | Prove Eq. (56) by definitions in Eq. (54) and Eq. (55).

- Using Eq. (56), we can show that

$$\hat{c}_\alpha^\dagger \hat{c}_\alpha |n_\alpha\rangle = n_\alpha |n_\alpha\rangle, \tag{57}$$

meaning that $c_\alpha^\dagger c_\alpha$ is the **fermion number operator** of the $|\alpha\rangle$ state.

All the single-mode Fock state can be constructed by the boson creation operator from the vacuum state

$$|n_\alpha\rangle = (\hat{c}_\alpha^\dagger)^{n_\alpha} |0_\alpha\rangle. \tag{58}$$

▫ Generic Fock States

The above result can be generalized to any Fock state of bosons

$$\begin{aligned} \hat{c}_\alpha^\dagger \left|\ldots, n_\beta, n_\alpha, n_\gamma, \ldots\right\rangle_F &= (-)^{\sum_{\beta<\alpha} n_\beta} \sqrt{1-n_\alpha}\, \left|\ldots, n_\beta, 1-n_\alpha, n_\gamma, \ldots\right\rangle_F, \\ \hat{c}_\alpha \left|\ldots, n_\beta, n_\alpha, n_\gamma, \ldots\right\rangle_F &= (-)^{\sum_{\beta<\alpha} n_\beta} \sqrt{n_\alpha}\, \left|\ldots, n_\beta, 1-n_\alpha, n_\gamma, \ldots\right\rangle_F. \end{aligned} \tag{59}$$

These two equations can be considered as the **defining properties** of fermion creation and annihilation operators.

- **Operator Identities**

Eq. (59) implies the following operator identities

$$\left\{\hat{c}_\alpha^\dagger,\ \hat{c}_\beta^\dagger\right\} = \left\{\hat{c}_\alpha,\ \hat{c}_\beta\right\} = 0,\ \left\{\hat{c}_\alpha,\ \hat{c}_\beta^\dagger\right\} = \delta_{\alpha\beta}. \tag{60}$$

These relations can be considered as the **algebraic definition** of fermion creation and annihilation operators.

- $\left\{\hat{A},\ \hat{B}\right\} = \hat{A}\,\hat{B} + \hat{B}\,\hat{A}$ denotes the **anti-commutator**.

Quantum Statistical Physics

General Principles

Connecting Micro and Macro

Statistical physics is an important branch of physics that studies the statistical relationship between the **microscopic states** of a many-body system and its **macroscopic properties**.

- At the **microscopic** level: physical systems are described by **quantum mechanics** in terms of a Hamiltonian operator $\hat{H}$

$$\hat{H}\,|E_k\rangle = E_k\,|E_k\rangle, \tag{61}$$

  - E_k - the possible energy that the system can take,
  - $|E_k\rangle$ - the corresponding quantum state of the system,
  - k - an index that labels the eigenstates.

- At the **macroscopic** level: we are interested in the *expectation value* of physical observables $\hat{O}$,

$$\langle O\rangle = \sum_k \langle E_k|\,\hat{O}\,|E_k\rangle\,p_k. \tag{62}$$

  - $\langle E_k|\,\hat{O}\,|E_k\rangle$ - the expectation value of $\hat{O}$ when the system is in the particular state $|E_k\rangle$ with energy E_k.
  - p_k - the **probability** for the system to be in the kth eigenstate $|E_k\rangle$ (of energy E_k) in the thermal ensemble.

- The ensemble is a *classical* probabilistic *mixture* of *quantum* pure states $|E_k\rangle$ (not a quantum superposition of them), called a **mixed state ensemble**.
- A mixed state ensemble can be specified by a set of pure state basis $|E_k\rangle$ together with a probability distribution p_k.

To connect micro and macro, what is missing is the knowledge about p_k.

Therefore, the central goal of statistical physics is to infer the **mixed state distribution** p_k in an unbiased manner.

Principle of Maximum Entropy

Without any assumption, it seems that p_k can be assigned arbitrarily. However, the **principle of maximum entropy** tells us the only unbiased assignment of p_k is such that maximized the **entropy** of the probability distribution

$$\boxed{S[p] = -\sum_k p_k \ln p_k.} \tag{63}$$

Consider a **canonical ensemble** --- a statistical ensemble whose *average energy* is known

$$\langle H\rangle = \sum_k \langle E_k|\,\hat{H}\,|E_k\rangle\, p_k = \sum_k E_k\, p_k = E. \tag{64}$$

The problem to solve is

$$\begin{aligned}
&\max_p S[p] = -\sum_k p_k \ln p_k,\\
&\text{subject to:}\\
&\sum_k p_k = 1,\\
&\sum_k E_k\, p_k = E.
\end{aligned} \tag{65}$$

The solution is simple

$$\boxed{\begin{aligned}
p_k &= \frac{1}{Z}\, e^{-\beta E_k},\\
Z &= \sum_k e^{-\beta E_k}.
\end{aligned}} \tag{66}$$

Exc 3 Solve the constrained optimization problem Eq. (65) to show Eq. (66).

This result is known as the **Boltzmann distribution**.

- The probability for the system to stay in a lower energy level is exponentially higher.

- $\beta = 1 / k_B\, T$ is the inverse of the **temperature** T (and k_B is the Boltzmann constant). It will be adjusted to meet the average energy condition.
- Z is the normalization coefficient for the probability distribution, also called the **partition function**.

Bose-Einstein Statistics

Single-Mode Problem

Consider a **single-particle mode** labeled by α. Assuming every **boson** in that mode has an **single-particle energy** ϵ_α, the Hamiltonian of this many-body system reads

$$\boxed{\hat{H} = \epsilon_\alpha\, \hat{b}_\alpha^\dagger\, \hat{b}_\alpha.} \tag{68}$$

- Eigensystem: eigenstates are labeled by $n_\alpha = 0, 1, 2, \ldots$,

$$\hat{H}\,|n_\alpha\rangle = \epsilon_\alpha\, n_\alpha\, |n_\alpha\rangle, \tag{69}$$

with eigen energies

$$E_{n_\alpha} = \epsilon_\alpha\, n_\alpha. \tag{70}$$

According to Eq. (66), the random variable n_α follows the Boltzmann distribution

$$p_{n_\alpha} = \frac{1}{Z}\, e^{-\beta\, E_{n_\alpha}} = \frac{1}{Z}\, e^{-\beta\, \epsilon_\alpha\, n_\alpha}, \tag{71}$$

with a partition function given by

$$Z = \sum_{n_\alpha=0}^{\infty} e^{-\beta\, \epsilon_\alpha\, n_\alpha} = \frac{1}{1 - e^{-\beta\, \epsilon_\alpha}}. \tag{72}$$

Exc 4 Evaluate the summation in Eq. (72).

Put together

$$\boxed{p_{n_\alpha} = \left(1 - e^{-\beta\, \epsilon_\alpha}\right) e^{-\beta\, \epsilon_\alpha\, n_\alpha}.} \tag{73}$$

Based on the probability distribution Eq. (73), one can compute the **average boson number**

$$\boxed{\langle n_\alpha \rangle = \sum_{n_\alpha=0}^{\infty} n_\alpha \, p_{n_\alpha} = \frac{1}{e^{\beta \, \epsilon_\alpha} - 1}.} \tag{74}$$

Exc 5 | Evaluate the summation in Eq. (74).

This is also known as the **Bose-Einstein distribution**.

▪ Multi-Mode Generalization

A many-body system typically has *multiple modes* for particles to occupy. A generic **free-boson Hamiltonian** must sum over the contribution like Eq. (68) from different modes.

$$\boxed{\hat{H} = \sum_\alpha \epsilon_\alpha \, \hat{b}_\alpha^\dagger \, \hat{b}_\alpha.} \tag{75}$$

- $\alpha = 1, 2, \ldots, D$ is the mode index, labeling **single-particle states** in the system.

- **Many-body states** are labeled by a sequence of **occupation numbers**

$$\boldsymbol{n} = n_1, n_2, \ldots, n_D, \tag{76}$$

where $n_\alpha = 0, 1, 2, \ldots$ for bosons.

- Eigensystem:

$$\hat{H}\,|\boldsymbol{n}\rangle = E_{\boldsymbol{n}}\,|\boldsymbol{n}\rangle, \tag{77}$$

with eigen energies

$$E_{\boldsymbol{n}} = \sum_\alpha \epsilon_\alpha\, n_\alpha. \tag{78}$$

Boltzmann distribution can be *factorized*, as random fluctuation of occupation number n_α on each mode is independent from each other.

$$p_{\boldsymbol{n}} \propto e^{-\beta E_n} = \exp\left(-\beta \sum_\alpha \epsilon_\alpha\, n_\alpha\right) = \prod_\alpha e^{-\beta\,\epsilon_\alpha\, n_\alpha}, \tag{79}$$

meaning that

$$\boxed{p_{\boldsymbol{n}} = \prod_\alpha p_{n_\alpha},} \tag{80}$$

with p_{n_α} given by Eq. (73). Therefore, the conclusion of the single-mode problem follows:

- The **Bose-Einstein distribution**, see Eq. (74),

$$\boxed{\langle n_\alpha\rangle = \frac{1}{e^{\beta\,\epsilon_\alpha} - 1}.} \tag{81}$$

- The average *total* boson number

$$\langle N\rangle = \sum_\alpha \langle n_\alpha\rangle = \sum_\alpha \frac{1}{e^{\beta\,\epsilon_\alpha} - 1}. \tag{82}$$

- The average *total* energy

$$\langle H\rangle = \sum_\alpha \epsilon_\alpha\,\langle n_\alpha\rangle = \sum_\alpha \frac{\epsilon_\alpha}{e^{\beta\,\epsilon_\alpha} - 1}. \tag{83}$$

Fermi-Dirac Statistics

Single-Mode Problem

Consider a **single-particle mode** labeled by α. Assuming every **fermion** in that mode has an **single-particle energy** ϵ_α, the Hamiltonian of this many-body system reads

$$\boxed{\hat{H} = \epsilon_\alpha\, \hat{c}_\alpha^\dagger\, \hat{c}_\alpha.} \tag{84}$$

- Eigensystem: eigenstates are labeled by $n_\alpha = 0, 1$ (Pauli exclusion principle forbid n_α to go greater than 1 for fermions),

$$\hat{H}\,|n_\alpha\rangle = \epsilon_\alpha\, n_\alpha\, |n_\alpha\rangle, \tag{85}$$

with eigen energies

$$E_{n_\alpha} = \epsilon_\alpha\, n_\alpha. \tag{86}$$

According to Eq. (66), the random variable n_α follows the Boltzmann distribution

$$p_{n_\alpha} = \frac{1}{Z}\, e^{-\beta\, E_{n_\alpha}} = \frac{1}{Z}\, e^{-\beta\, \epsilon_\alpha\, n_\alpha}, \tag{87}$$

with a partition function given by

$$Z = \sum_{n_\alpha = 0,1} e^{-\beta\, \epsilon_\alpha\, n_\alpha} = 1 + e^{-\beta\, \epsilon_\alpha}. \tag{88}$$

Put together

$$\boxed{p_{n_\alpha} = \frac{e^{-\beta\, \epsilon_\alpha\, n_\alpha}}{1 + e^{-\beta\, \epsilon_\alpha}} = \begin{cases} \frac{1}{e^{-\beta\, \epsilon_\alpha} + 1} & n_\alpha = 0, \\ \frac{1}{e^{\beta\, \epsilon_\alpha} + 1} & n_\alpha = 1. \end{cases}} \tag{89}$$

Based on the probability distribution Eq. (89), one can compute the **average fermion number**

$$\boxed{\langle n_\alpha \rangle = \sum_{n_\alpha = 0,1} n_\alpha\, p_{n_\alpha} = \frac{1}{e^{\beta\, \epsilon_\alpha} + 1}.} \tag{90}$$

This is also known as the **Fermi-Dirac distribution**.

▪ Multi-Mode Generalization

A many-body system typically has *multiple modes* for particles to occupy. A generic **free-fermion Hamiltonian** must sum over the contribution like Eq. (84) from different modes.

$$\boxed{\hat{H} = \sum_\alpha \epsilon_\alpha \, \hat{c}_\alpha^\dagger \, \hat{c}_\alpha.} \tag{91}$$

- $\alpha = 1, 2, \ldots, D$ is the mode index, labeling **single-particle states** in the system.
- **Many-body states** are labeled by a sequence of **occupation numbers**

  $$\boldsymbol{n} = n_1, n_2, \ldots, n_D, \tag{92}$$

  where $n_\alpha = 0, 1$ for fermions.
- Eigensystem:

  $$\hat{H} \, |\boldsymbol{n}\rangle = E_{\boldsymbol{n}} \, |\boldsymbol{n}\rangle, \tag{93}$$

  with eigen energies

  $$E_{\boldsymbol{n}} = \sum_\alpha \epsilon_\alpha \, n_\alpha. \tag{94}$$

Boltzmann distribution can be *factorized*, as random fluctuation of occupation number n_α on each mode is independent from each other.

$$p_{\boldsymbol{n}} \propto e^{-\beta \, E_{\boldsymbol{n}}} = \exp\left(-\beta \sum_\alpha \epsilon_\alpha \, n_\alpha\right) = \prod_\alpha e^{-\beta \, \epsilon_\alpha \, n_\alpha}, \tag{95}$$

meaning that

$$\boxed{p_{\boldsymbol{n}} = \prod_\alpha p_{n_\alpha},} \tag{96}$$

with p_{n_α} given by Eq. (89). Therefore, the conclusion of the single-mode problem follows:

- The **Fermi-Dirac distribution**, see Eq. (90),

$$\boxed{\langle n_\alpha \rangle = \frac{1}{e^{\beta \epsilon_\alpha} + 1}\,.} \tag{97}$$

- The average *total* fermion number

$$\langle N \rangle = \sum_\alpha \langle n_\alpha \rangle = \sum_\alpha \frac{1}{e^{\beta \epsilon_\alpha} + 1}\,. \tag{98}$$

- The average *total* energy

$$\langle H \rangle = \sum_\alpha \epsilon_\alpha \langle n_\alpha \rangle = \sum_\alpha \frac{\epsilon_\alpha}{e^{\beta \epsilon_\alpha} + 1}\,. \tag{99}$$