

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.

$$\begin{array}{c|cc} & \text{qubit}_B & \\ & |0\rangle & |1\rangle \\ \hline \text{qubit}_A & |0\rangle & |00\rangle \quad |01\rangle \\ & |1\rangle & |10\rangle \quad |11\rangle \end{array} \quad (1)$$

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

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

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

$$\begin{pmatrix} \psi_{00} & \psi_{01} \\ \psi_{10} & \psi_{11} \end{pmatrix}. \quad (3)$$

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

$$\begin{pmatrix} \psi_{00} \\ \psi_{01} \\ \psi_{10} \\ \psi_{11} \end{pmatrix} \rightarrow \begin{pmatrix} \psi_0 \\ \psi_1 \\ \psi_2 \\ \psi_3 \end{pmatrix}. \quad (4)$$

We can relabel the index $\psi_{\alpha\beta} \rightarrow \psi_i$ 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, $\mathbb{C}^{2 \times 2} \rightarrow \mathbb{C}^4$.
- In **vector representation**, the ket vector $|00\rangle$ is a **tensor product** of $|0\rangle_A$ and $|0\rangle_B$,

$$|00\rangle = |0\rangle_A \otimes |0\rangle_B \doteq \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}. \quad (5)$$

Similarly,

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

$$|10\rangle = |1\rangle_A \otimes |0\rangle_B \doteq \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad (6)$$

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

■ From Two to Many

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

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

$$\alpha = \alpha_1 \alpha_2 \dots \alpha_N \text{ for } \alpha_i \in \{0, 1\}, \quad (7)$$

and defined by the tensor product of single-qubit states

$$|\alpha\rangle := |\alpha_1\rangle \otimes |\alpha_2\rangle \otimes \dots \otimes |\alpha_N\rangle. \quad (8)$$

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

$$|\Psi\rangle = \sum_{\alpha} \Psi_{\alpha} |\alpha\rangle. \quad (9)$$

The coefficients Ψ_{α} form a $\mathbb{C}^{2 \times 2 \times \dots \times 2}$ *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 i th 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** $|\alpha\rangle$ ($\alpha = 1, 2, \dots, D$).
- The **many-body Hilbert space** of N *distinct* particles will be D^N dimensional, spanned by the **many-body basis states**

$$|\alpha\rangle \equiv |\alpha_1\rangle \otimes |\alpha_2\rangle \otimes \dots \otimes |\alpha_N\rangle, \quad (10)$$

where $\alpha_i = 1, 2, \dots, D$ labels the state of the i th particle.

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

$$|\Psi\rangle = \sum_{\alpha} \Psi_{\alpha} |\alpha\rangle. \quad (11)$$

The coefficient Ψ_{α} is also called the **many-body wave function**.

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

$$p(\alpha | \Psi) = |\langle \alpha | \Psi \rangle|^2 = |\Psi_{\alpha}|^2. \quad (12)$$

■ 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$
<div style="border: 1px solid black; padding: 2px; display: inline-block;"> the 1st particle on $\alpha_1\rangle$ the 2nd particle in $\alpha_2\rangle$ </div>	<div style="border: 1px solid black; padding: 2px; display: inline-block;"> the 1st particle on $\alpha_2\rangle$ the 2nd particle in $\alpha_1\rangle$ </div>

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.

$$p(\alpha_1 \alpha_2 | \Psi) = p(\alpha_2 \alpha_1 | \Psi) \quad (13)$$

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

$$\hat{\mathcal{P}}_\pi |\alpha\rangle = |\alpha_\pi\rangle \equiv |\alpha_{\pi(1)}\rangle \otimes |\alpha_{\pi(2)}\rangle \otimes \dots \otimes |\alpha_{\pi(N)}\rangle. \quad (14)$$

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

$$123 \xrightarrow{\pi} 132 \quad (15)$$

is a permutation in S_3 , defined by $\pi(1) = 1$, $\pi(2) = 3$, $\pi(3) = 2$.

- α_π denotes a new **sequence** obtained from the sequence α by permuting its elements by π . For example,

$$\alpha = \alpha_1 \alpha_2 \alpha_3 \xrightarrow{\pi} \alpha_\pi = \alpha_1 \alpha_3 \alpha_2. \quad (16)$$

- $\hat{\mathcal{P}}_\pi$ denotes the **operator** that take the state $|\alpha\rangle$ to $|\alpha_\pi\rangle$ for all α , which implements the permutation of particles.

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

$$\forall \pi \in S_N : p(\alpha | \Psi) = p(\alpha_\pi | \Psi) \quad (17)$$

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

$$\forall \pi \in S_N : |\Psi_\alpha|^2 = |\Psi_{\alpha_\pi}|^2. \quad (18)$$

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

$$\Psi_\alpha = e^{i\varphi} \Psi_{\alpha_\pi}. \quad (19)$$

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 \Rightarrow **bosons**

$$\Psi_\alpha = \Psi_{\alpha_\pi}, \quad (20)$$

- **antisymmetric** (sign) representation \Rightarrow **fermions**

$$\Psi_\alpha = (-)^\pi \Psi_{\alpha_\pi}, \quad (21)$$

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

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

Take the S_3 group for example:

$$\begin{aligned} 123 &\xrightarrow{\pi} 123 \ 231 \ 312 \ 321 \ 213 \ 132 \\ (-)^{\pi} &= +1 \ +1 \ +1 \ -1 \ -1 \ -1 \end{aligned} \quad (23)$$

■ 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 $|\alpha\rangle$, we can pick out the **basis states** for the *bosonic* and *fermionic* subspaces:

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

$$\hat{S}|\alpha\rangle = \sum_{\pi \in S_N} \hat{P}_\pi |\alpha\rangle = \sum_{\pi \in S_N} |\alpha_\pi\rangle. \quad (24)$$

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

$$\hat{A}|\alpha\rangle = \sum_{\pi \in S_N} (-)^\pi \hat{P}_\pi |\alpha\rangle = \sum_{\pi \in S_N} (-)^\pi |\alpha_\pi\rangle. \quad (25)$$

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

- **Bosonic** states (unnormalized):

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

- **Fermionic** states (unnormalized):

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

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):

$$\mathcal{D} = D^N, \quad (28)$$

- the **bosonic** subspace:

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

- the **fermionic** subspace:

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

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

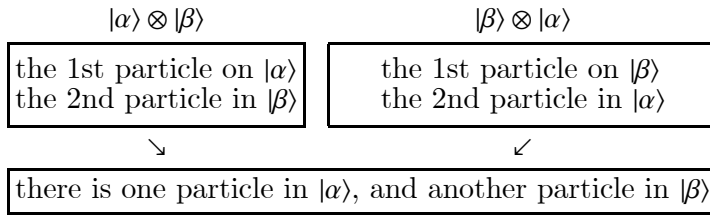
■ Fock Space

■ 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:



The new description does not require the labeling of particles \Rightarrow no redundant or unphysical basis state \Rightarrow 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 $\alpha = 1, 2, \dots, D$)

$$|\mathbf{n}\rangle \equiv |n_1, n_2, \dots, n_\alpha, \dots, n_D\rangle, \quad (31)$$

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

$$n_\alpha = \begin{cases} 0, 1, 2, 3, \dots & \text{bosons,} \\ 0, 1 & \text{fermions.} \end{cases} \quad (32)$$

- 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 $|\mathbf{n}\rangle$ 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*,

$$|\Psi\rangle = \sum_n \Psi_n |n\rangle. \quad (33)$$

■ 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

$$|0\rangle \equiv |\dots, 0, \dots\rangle \quad (34)$$

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

$$|0\rangle_B = |0\rangle_F = 1. \quad (35)$$

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

$$|n_\alpha\rangle = |\dots, 0, n_\alpha, 0, \dots\rangle \quad (36)$$

In terms of the first-quantized states

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

- 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,

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

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

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

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

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

- for **bosons**,

$$|\mathbf{n}\rangle_B = \left(\frac{\prod_\alpha n_\alpha!}{N!} \right)^{1/2} \hat{S}_\alpha |\alpha\rangle^{\otimes n_\alpha}. \quad (40)$$

- for **fermions**,

$$|\mathbf{n}\rangle_F = \frac{1}{\sqrt{N!}} \hat{\mathcal{A}}_\alpha |\alpha\rangle^{\otimes n_\alpha}. \quad (41)$$

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

$$\hat{S} = \sum_{\pi \in S_N} \hat{\mathcal{P}}_\pi, \quad \hat{\mathcal{A}} = \sum_{\pi \in S_N} (-1)^\pi \hat{\mathcal{P}}_\pi, \quad (42)$$

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 1 be the *tensor identity* (meaning that $|\alpha\rangle \otimes 1 = 1 \otimes |\alpha\rangle = |\alpha\rangle$).
- 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 $a, b \in \mathbb{C}$)

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

- Vacuum property

$$\begin{aligned} |\alpha\rangle \triangleright_{\pm} 1 &= |\alpha\rangle, \\ |\alpha\rangle \triangleleft_{\pm} 1 &= 0. \end{aligned} \quad (44)$$

- Recursive relation

$$\begin{aligned} |\alpha\rangle \triangleright_{\pm} |\beta\rangle \otimes |\Psi\rangle &= |\alpha\rangle \otimes |\beta\rangle \otimes |\Psi\rangle \pm |\beta\rangle \otimes (|\alpha\rangle \triangleright_{\pm} |\Psi\rangle), \\ |\alpha\rangle \triangleleft_{\pm} |\beta\rangle \otimes |\Psi\rangle &= \langle\alpha | \beta\rangle |\Psi\rangle \pm |\beta\rangle \otimes (|\alpha\rangle \triangleleft_{\pm} |\Psi\rangle). \end{aligned} \quad (45)$$

- $\langle\alpha | \beta\rangle = \delta_{\alpha\beta}$ 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 $n_{\alpha} \rightarrow n_{\alpha} + 1$. It acts on a N -particle first-quantized state $|\Psi\rangle$ as

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

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

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

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

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

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

**Exc
1**

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

- Especially, when acting on the vacuum state

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

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

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

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

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

□ Generic Fock States

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

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

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

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

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

- $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$ 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}_α^\dagger adds a fermion to the single-particle state $|\alpha\rangle$, *increasing* the occupation number by one $n_\alpha \rightarrow n_\alpha + 1$ (while $n_\alpha = 0$). It acts on a N -particle first-quantized state $|\Psi\rangle$ as

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

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}_α removes a fermion from the single-particle state $|\alpha\rangle$, *reducing* the occupation number by one $n_\alpha \rightarrow n_\alpha - 1$ (while $n_\alpha = 1$). It acts on a N -particle first-quantized state $|\Psi\rangle$ as

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

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)

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

Exc 2

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

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

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

meaning that $\hat{c}_\alpha^\dagger \hat{c}_\alpha$ 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

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

□ Generic Fock States

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

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

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

$$\{\hat{c}_\alpha^\dagger, \hat{c}_\beta^\dagger\} = \{\hat{c}_\alpha, \hat{c}_\beta\} = 0, \quad \{\hat{c}_\alpha, \hat{c}_\beta^\dagger\} = \delta_{\alpha\beta}. \quad (60)$$

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

- $\{\hat{A}, \hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}$ 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}

$$\hat{H} |E_k\rangle = E_k |E_k\rangle, \quad (61)$$

- 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} ,

$$\langle O \rangle = \sum_k \langle E_k | \hat{O} | E_k \rangle p_k. \quad (62)$$

- $\langle E_k | \hat{O} | E_k \rangle$ - 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 k th 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

$$S[p] = - \sum_k p_k \ln p_k. \quad (63)$$

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

$$\langle H \rangle = \sum_k \langle E_k | \hat{H} | E_k \rangle p_k = \sum_k E_k p_k = E. \quad (64)$$

The problem to solve is

$$\max_p S[p] = - \sum_k p_k \ln p_k,$$

subject to :

$$\begin{aligned} \sum_k p_k &= 1, \\ \sum_k E_k p_k &= E. \end{aligned} \quad (65)$$

The solution is simple

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

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

$$\hat{H} = \epsilon_\alpha \hat{b}_\alpha^\dagger \hat{b}_\alpha. \quad (68)$$

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

$$\hat{H} |n_\alpha\rangle = \epsilon_\alpha n_\alpha |n_\alpha\rangle, \quad (69)$$

with eigen energies

$$E_{n_\alpha} = \epsilon_\alpha n_\alpha. \quad (70)$$

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

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

with a partition function given by

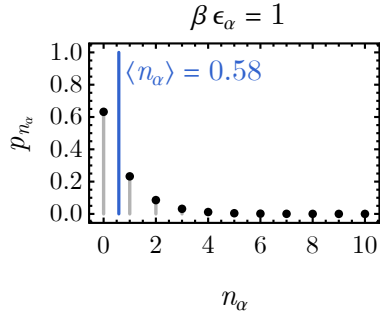
$$Z = \sum_{n_\alpha=0}^{\infty} e^{-\beta \epsilon_\alpha n_\alpha} = \frac{1}{1 - e^{-\beta \epsilon_\alpha}}. \quad (72)$$

Exc
4

Evaluate the summation in Eq. (72).

Put together

$$p_{n_\alpha} = (1 - e^{-\beta \epsilon_\alpha}) e^{-\beta \epsilon_\alpha n_\alpha}. \quad (73)$$



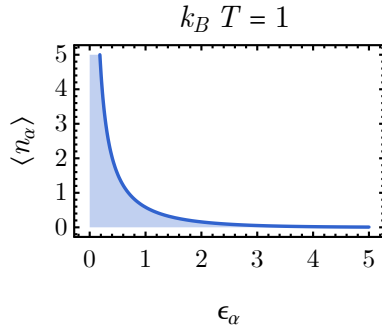
Based on the probability distribution Eq. (73), one can compute the **average boson number**

$$\langle n_\alpha \rangle = \sum_{n_\alpha=0}^{\infty} n_\alpha p_{n_\alpha} = \frac{1}{e^{\beta \epsilon_\alpha} - 1}. \quad (74)$$

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.

$$\hat{H} = \sum_{\alpha} \epsilon_{\alpha} \hat{b}_{\alpha}^{\dagger} \hat{b}_{\alpha}. \quad (75)$$

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

$$\mathbf{n} = n_1, n_2, \dots, n_D, \quad (76)$$

where $n_{\alpha} = 0, 1, 2, \dots$ for bosons.

- Eigensystem:

$$\hat{H} |\mathbf{n}\rangle = E_{\mathbf{n}} |\mathbf{n}\rangle, \quad (77)$$

with eigen energies

$$E_{\mathbf{n}} = \sum_{\alpha} \epsilon_{\alpha} n_{\alpha}. \quad (78)$$

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

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

meaning that

$$p_{\mathbf{n}} = \prod_{\alpha} p_{n_{\alpha}}, \quad (80)$$

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

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

$$\langle n_{\alpha} \rangle = \frac{1}{e^{\beta \epsilon_{\alpha}} - 1}. \quad (81)$$

- The average *total* boson number

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

- The average *total* energy

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

■ 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

$$\hat{H} = \epsilon_{\alpha} \hat{c}_{\alpha}^{\dagger} \hat{c}_{\alpha}. \quad (84)$$

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

$$\hat{H} |n_\alpha\rangle = \epsilon_\alpha n_\alpha |n_\alpha\rangle, \quad (85)$$

with eigen energies

$$E_{n_\alpha} = \epsilon_\alpha n_\alpha. \quad (86)$$

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

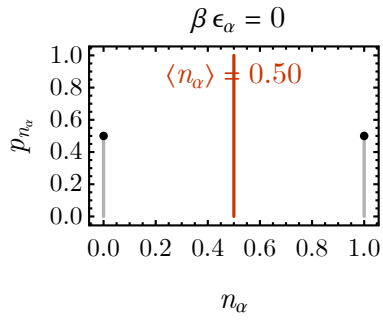
$$p_{n_\alpha} = \frac{1}{Z} e^{-\beta E_{n_\alpha}} = \frac{1}{Z} e^{-\beta \epsilon_\alpha n_\alpha}, \quad (87)$$

with a partition function given by

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

Put together

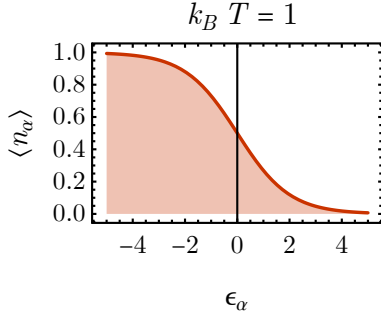
$$p_{n_\alpha} = \frac{e^{-\beta \epsilon_\alpha n_\alpha}}{1 + e^{-\beta \epsilon_\alpha}} = \begin{cases} \frac{1}{e^{-\beta \epsilon_\alpha} + 1} & n_\alpha = 0, \\ \frac{1}{e^{\beta \epsilon_\alpha} + 1} & n_\alpha = 1. \end{cases} \quad (89)$$



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

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

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.

$$\hat{H} = \sum_{\alpha} \epsilon_{\alpha} \hat{c}_{\alpha}^{\dagger} \hat{c}_{\alpha}. \quad (91)$$

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

$$\mathbf{n} = n_1, n_2, \dots, n_D, \quad (92)$$

where $n_{\alpha} = 0, 1$ for fermions.

- Eigensystem:

$$\hat{H} |\mathbf{n}\rangle = E_{\mathbf{n}} |\mathbf{n}\rangle, \quad (93)$$

with eigen energies

$$E_{\mathbf{n}} = \sum_{\alpha} \epsilon_{\alpha} n_{\alpha}. \quad (94)$$

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

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

meaning that

$$p_{\mathbf{n}} = \prod_{\alpha} p_{n_{\alpha}}, \quad (96)$$

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

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

$$\langle n_\alpha \rangle = \frac{1}{e^{\beta \epsilon_\alpha} + 1}. \quad (97)$$

- The average *total* fermion number

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

- The average *total* energy

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