This note is mostly based on the appendix of the lecture note of Prof. Mila

§ Indistinguishability of identicle particles

* Second quantization is a useful language to deal with identical particles

1) The wave function should be symmetric or antisymmetric under the exchange of two particles:

$$\psi(x_1, x_2) = e^{i\alpha}\psi(x_2, x_1)$$

$$\Longrightarrow \psi(x_1, x_2) = e^{i\alpha}\psi(x_2, x_1) = e^{2i\alpha}\psi(x_1, x_2)$$

So $e^{2i\alpha} = 1 \Longrightarrow e^{i\alpha} = \pm 1$

+1 : boson -1 : fermion

2) Restriction to the wave function ; Fock space

Denote by $\{|\lambda_i\rangle\}$ a basis of one-particle wave function ($\psi_{\lambda_i}(x)$)

- Boson

  symmetric wave function

$$\frac{1}{\sqrt{C}}\sum_P |P(\lambda_1)\rangle_1 \otimes |P(\lambda_2)\rangle_2 \otimes \cdots \otimes |P(\lambda_N)\rangle_N$$

$$\psi(x_1, \cdots, x_N) = \frac{1}{\sqrt{C}}\sum_P \psi_{P(\lambda_1)}(x_1)\cdots\psi_{P(\lambda_N)}(x_N)$$

If there are 2 or more equal indicies, then permutations involving those terms are only counted once

e.g. 3 particles using ψ_1 twice & ψ_2 once:

$\psi_1(x_1)\psi_1(x_2)\psi_2(x_3) + \psi_1(x_1)\psi_1(x_3)\psi_2(x_2) + \psi_1(x_2)\psi_1(x_3)\psi_2(x_1)$

$\Longrightarrow$ It is an interesting mathematical problem to show that $C = \frac{N!}{N_1!\,N_2!\cdots N_k!}$

\# permutations

* e.g. two particles

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|\lambda_1\rangle_1 \otimes |\lambda_2\rangle_2 + |\lambda_2\rangle_1 \otimes |\lambda_1\rangle_2\right)$$

- Fermion

  Slater determinant:

$$\psi(x_1, \cdots, x_N) = \frac{1}{\sqrt{N!}}\begin{vmatrix} \psi_{\lambda_1}(x_1) & \psi_{\lambda_1}(x_2) & \cdots & \psi_{\lambda_1}(x_N) \\ \psi_{\lambda_2}(x_1) & \psi_{\lambda_2}(x_2) & \cdots & \psi_{\lambda_2}(x_N) \\ \vdots & \vdots & & \vdots \\ \psi_{\lambda_N}(x_1) & \psi_{\lambda_N}(x_2) & \cdots & \psi_{\lambda_N}(x_N) \end{vmatrix} = \frac{1}{\sqrt{N!}}\sum_P (-1)^P P\{|\lambda_1\rangle_1 \otimes |\lambda_2\rangle_2 \otimes \cdots \otimes |\lambda_N\rangle_N\}$$

* e.g. two particles

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|\lambda_1\rangle_1 \otimes |\lambda_2\rangle_2 - |\lambda_2\rangle_1 \otimes |\lambda_1\rangle_2\right) \text{ or } |\psi\rangle = \frac{1}{\sqrt{2}}\left(-|\lambda_1\rangle_1 \otimes |\lambda_2\rangle_2 + |\lambda_2\rangle_1 \otimes |\lambda_1\rangle_2\right)$$

It is worthwhile to point out that Slate Det can pick up a minus sign, so once the order of the quantum status $\lambda_1, \cdots, \lambda_N$ is set at the beginning, we shall never change it from later on.

- For system of identicle particles, it suffices to only specify how many particles there are on each level (eigenstate):

$$|\Psi\rangle \equiv |\underset{\lambda_1}{N_1}, \underset{\lambda_2}{N_2}, \cdots, \underset{\lambda_M}{N_M}\rangle.$$

As long as $\{N_i\}$ is fixed, there is no more room to play around.

* For fermionic systems, $N_i = 0, 1$. If two fermions are at the same level, the Slater determinant immediately becomes 0.

All possible $|N_1, \cdots, N_M\rangle$ span a huge Hilbert space called Fock space.

§ Harmonic oscillator

(optional)

(As the inspiration for introducing creation and annihilation operator)

(See the last)

§ Creation and destruction operators in Fock space

Given a single particle basis $\{|\lambda_i\rangle\}$, we construct the basis of Fock space as

$$|N_1, N_2, \cdots, N_M\rangle$$

Let's define creation and destruction operator by explicitly write down the matrix elements:

* For fermions, the addition should be understood as modulo 2

$1 + 1 = 0 \mod 2$

$1 + 0 = 1 \mod 2$

$0 + 0 = 0 \mod 2$

$$\begin{cases} \langle N_1, \cdots, N_i+1, \cdots, N_M | a_i^\dagger | N_1, \cdots, N_i, \cdots, N_M\rangle = \sqrt{N_i+1} \\ \langle N_i, \cdots, N_i, \cdots, N_M | a_i | N_1, \cdots, N_i+1, \cdots, N_M\rangle = \sqrt{N_i+1} \\ 0 \quad \text{otherwise} \end{cases}$$

Equivalently, $a_i^\dagger |\cdots, N_i, \cdots\rangle = \sqrt{N_i+1}\, |\cdots, N_i+1, \cdots\rangle$ creation

$a_i |\cdots, N_i, \cdots\rangle = \sqrt{N_i}\, |\cdots, N_i-1, \cdots\rangle$ destruction

① Commutation relation — boson

— Different levels $i \neq j$

$$\begin{cases} a_i a_j |\cdots, N_i, \cdots, N_j, \cdots\rangle = \sqrt{N_i N_j}\, |\cdots, N_i-1, \cdots, N_j-1, \cdots\rangle \\ a_j a_i |\cdots, N_i, \cdots, N_j, \cdots\rangle = \sqrt{N_i N_j}\, |\cdots, N_i-1, \cdots, N_j-1, \cdots\rangle \\ \qquad \Longrightarrow [a_i, a_j] = 0 \end{cases}$$

$$\begin{cases} a_i a_j^\dagger |\cdots, N_i, \cdots, N_j, \cdots\rangle = \sqrt{N_i (N_j+1)}\, |\cdots, N_i-1, \cdots, N_j+1, \cdots\rangle \\ a_j^\dagger a_i \quad \text{same} \\ \qquad \Longrightarrow [a_i, a_j^\dagger] = 0 \end{cases}$$

— Same level i

$$\begin{cases} a_i a_i^\dagger |\cdots, N_i, \cdots\rangle = (N_i+1) |\cdots, N_i, \cdots\rangle \\ a_i^\dagger a_i |\cdots, N_i, \cdots\rangle = N_i |\cdots, N_i, \cdots\rangle \\ \qquad \Longrightarrow [a_i, a_i^\dagger] = 1 \end{cases}$$

In short, $[a_i, a_j] = [a_i^\dagger, a_j^\dagger] = 0$

$$[a_i, a_j^\dagger] = \delta_{ij}$$

② Anticommutation — fermion

The situation for fermions is a bit more complicated.

For simplicity, let's consider only 2 levels.

First note that

$C_1^\dagger |0, 0\rangle = |1, 0\rangle = |\lambda_1\rangle$, $\quad C_1 C_1 = C_1^\dagger C_1^\dagger = 0$

$N_1 = 0$ or 1

— What is the wavefunction after we put another fermion at λ_2,

i.e. what is $C_2^\dagger C_1^\dagger |0,0\rangle$?

Two options
$$\begin{cases} \frac{1}{\sqrt{2}}\left(|\lambda_1\rangle_1 |\lambda_2\rangle_2 - |\lambda_2\rangle_1 \otimes |\lambda_1\rangle_2\right) \\ \quad \text{or} \\ \frac{1}{\sqrt{2}}\left(|\lambda_2\rangle_1 |\lambda_1\rangle_2 - |\lambda_1\rangle_1 \otimes |\lambda_2\rangle_2\right) \end{cases}$$

For bosons, only one possibility:
$$\frac{1}{\sqrt{2}}\left(|\lambda_1\rangle_1 |\lambda_2\rangle_2 + |\lambda_2\rangle_1 |\lambda_1\rangle_2\right)$$

Let's choose the first one as the fixed rule of adding fermions:
$$C_1^\dagger |0,0\rangle = |1,0\rangle \equiv |\lambda_1\rangle$$
$$C_2^\dagger C_1^\dagger |0,0\rangle = |1,1\rangle \equiv \frac{1}{\sqrt{2}}\left(|\lambda_1\rangle_1 |\lambda_2\rangle_2 - |\lambda_2\rangle_1 |\lambda_1\rangle_2\right)$$

Then, what is $C_1^\dagger C_2^\dagger |0,0\rangle$?
$$C_2^\dagger |0,0\rangle \longrightarrow |\lambda_2\rangle$$
$$C_1^\dagger C_2^\dagger |0,0\rangle \longrightarrow \frac{1}{\sqrt{2}}\left(|\lambda_2\rangle_1 |\lambda_1\rangle_2 - |\lambda_1\rangle_1 |\lambda_2\rangle_2\right) = -|1,1\rangle \ !$$

Therefore, $C_1^\dagger C_2^\dagger = -C_2^\dagger C_1^\dagger$, or $\{C_1^\dagger, C_2^\dagger\} = 0$ anticommutation !

— $C_1 C_1^\dagger + C_1^\dagger C_1$?
$$\langle 0| C_1 C_1^\dagger + C_1^\dagger C_1 |0\rangle = \langle 1| C_1 C_1^\dagger + C_1^\dagger C_1 |1\rangle = 1$$
$$\langle 0| C_1 C_1^\dagger + C_1^\dagger C_1 |1\rangle = \langle 1| C_1 C_1^\dagger + C_1^\dagger C_1 |0\rangle = 0$$
$$\Longrightarrow \{C_1, C_1^\dagger\} = 1$$

— $C_1 C_2^\dagger + C_2^\dagger C_1$?
$$C_1 C_2^\dagger |1,0\rangle = C_1 C_2^\dagger C_1^\dagger |0,0\rangle = -C_1 C_1^\dagger C_2^\dagger |0,0\rangle = -(1 - C_1^\dagger C_1) C_2^\dagger |0,0\rangle = -C_2^\dagger |$$
$$C_2^\dagger C_1 |1,0\rangle = C_2^\dagger C_1 C_1^\dagger |0,0\rangle = C_2^\dagger (1 - C_1^\dagger C_1) |0,0\rangle = C_2^\dagger |0,0\rangle$$
$$\Longrightarrow \{C_1, C_2^\dagger\} = 0$$

In short, $\{C_i, C_j\} = \{C_i^\dagger, C_j^\dagger\} = 0$
$$\{C_i, C_j^\dagger\} = \delta_{ij}$$

§ Physical operators in second quantization

$*$ Change of basis

$\{|i\rangle\} \longrightarrow \{|\mu\rangle\}$

$$a_i^\dagger|0\rangle = |i\rangle = \sum_\mu |\mu\rangle\langle\mu|i\rangle = \sum_\mu \langle\mu|i\rangle a_\mu^\dagger|0\rangle$$

$$\Rightarrow a_i^\dagger = \sum_\mu \langle\mu|i\rangle a_\mu^\dagger \quad \& \quad a_i = \sum_\mu \langle i|\mu\rangle a_\mu$$

- One-body operators $\hat{F}^{(1)} = \sum_i \hat{f}_i$ or $= \sum_i \mathbb{1}_1 \otimes \cdots \otimes \hat{f}_i \otimes \cdots \otimes \mathbb{1}_N$ more precisely. i denotes each particle

Let's suppose $\hat{f}$ is diagonalised by $\{|\lambda_j\rangle\}$: $\hat{f} = \sum_{\lambda_j} \lambda_j |\lambda_j\rangle\langle\lambda_j|$, then we find that

$$\langle N_1', \dots, N_M'|\hat{F}_1|N_1, \dots, N_M\rangle = \sum_i \langle N_1', \dots, N_M'|\mathbb{1}_1 \otimes \cdots \otimes \hat{f}_i \otimes \cdots \otimes \mathbb{1}_N|N_1, \dots, N_M\rangle$$

in the basis of $\{|\lambda\rangle\}$

$$= \sum_{j=1}^{k} N_j \lambda_j \langle N_1', \dots, N_M'|N_1, \dots, N_M\rangle$$

$$= \sum_{j=1}^{k} \langle N_1', \dots, N_M'|\lambda_j \hat{N}_j|N_1, \dots, N_M\rangle$$

$$\Rightarrow \hat{F}_1 = \sum_j \lambda_j \hat{N}_j = \sum_j \langle\lambda_j|\hat{f}|\lambda_j\rangle \hat{a}^\dagger_{\lambda_j} \hat{a}_{\lambda_j}$$

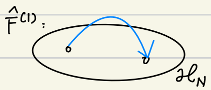
By changing to a general basis $\{|\mu\rangle\}$, we obtain

$$\hat{F}^{(1)} = \sum_{\mu,\nu} \langle\mu|\hat{f}|\nu\rangle \hat{a}_\mu^\dagger \hat{a}_\nu$$

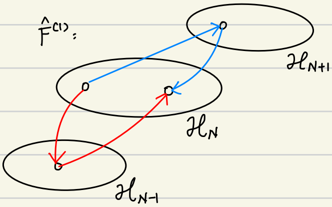
- One can also derive the expression for two-body operators (with some more tedious calculations):

$$\hat{F}^{(2)} = \sum_{\mu\nu} \sum_{\mu'\nu'} \langle\mu\nu|\hat{f}^{(2)}|\mu'\nu'\rangle a_\mu^\dagger a_\nu^\dagger a_{\mu'} a_{\nu'}$$

$*$ First quantization



Second quantization



§ Harmonic oscillator

— Another way to introduce creation & destruction operators

$H = \frac{\omega}{2}(X^2 + P^2)$, $[X, P] = i$ (set $\hbar = 1$)

- Define $\begin{cases} a := \frac{1}{\sqrt{2}}(X + iP) \\ a^\dagger := \frac{1}{\sqrt{2}}(X - iP) \end{cases} \iff \begin{cases} X = \frac{1}{\sqrt{2}}(a + a^\dagger) \\ P = \frac{1}{i\sqrt{2}}(a - a^\dagger) \end{cases}$

and the commutation relation followed is then

$$[a, a^\dagger] = \frac{1}{\sqrt{2}}[X + iP, X - iP] = \frac{1}{\sqrt{2}}(-i[X, P] + i[P, X]) = 1.$$

Besides, we can also check that

$$a^\dagger a = \frac{1}{2}(X - iP)(X + iP) = \frac{1}{2}(X^2 + P^2 + i[X, P]) = \frac{1}{2}(X^2 + P^2 - 1)$$

Therefore, we can rewrite the Hamiltonian as

$$H = \hbar\omega(a^\dagger a + \frac{1}{2})$$

- The structure of the Hilbert space

Let's define an Hermitian operator $N := a^\dagger a$, and write its eigenfunction as $N|\nu\rangle = \nu|\nu\rangle$

We can have the following observations:

1) $\nu \geq 0$, since

$$\nu = \langle\nu|N|\nu\rangle = \| a|\nu\rangle \|^2 \geq 0$$

2) if $\nu = 0$, then $\| a|\nu\rangle \|^2 = 0 \implies a|\nu\rangle = 0$

3) Let's calculate

$$Na|\nu\rangle = a^\dagger a a|\nu\rangle = (-[a, a^\dagger] + a a^\dagger) a|\nu\rangle$$

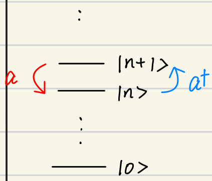
$$= -a|\nu\rangle + a\underbrace{a^\dagger a}_{N}|\nu\rangle = (\nu - 1)a|\nu\rangle$$

Hence, $a|\nu\rangle$ is also an eigenstate with the eigenvalue $\nu - 1$.

$\implies$ ν can only be integer

From now on, we write it as n

Similarly, we can also find that $a^\dagger|n\rangle$ is also an eigenstate of N, with the eigenvalue $n+1$



Finally, let's determine the coefficient C_n

$$\begin{cases} a|n\rangle = C_{n-1}|n-1\rangle \\ a^\dagger|n\rangle = C_{n+1}|n+1\rangle \end{cases}$$

$$|C_{n+1}|^2 = \langle n|a a^\dagger|n\rangle = \langle n|(a^\dagger a+1)|n\rangle = n+1$$

$$\Longrightarrow C_{n+1} = \sqrt{n+1}, \quad \text{similarly } C_{n-1} = \sqrt{n}$$

In conclusion, $\begin{cases} a^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle \\ a|n\rangle = \sqrt{n}\,|n-1\rangle \end{cases}$, and we can generate all the basis by $|n\rangle = \frac{1}{\sqrt{n!}}(a^\dagger)^n|0\rangle$.