Lect 1: Description of many body states

§: First quantization v.s. the second quantization

Classic mechanics $\{x, p\}_{\text{Possion}} = 1 \xrightarrow[\text{firist quantization}]{\text{Quantum}} [x, p] = i\hbar$; wavefunction $\psi(x)$ is still an ordinary function.

Drawbacks of the first quantization:

① difficult to use for many-body systems

$$H = \sum_{i=1,\cdots N} h(r_i) + \frac{1}{2} \sum_{1<i,j<N} V(r_i - r_j)$$

$$i\frac{\partial}{\partial t} \Psi(r_1, \cdots r_N, t) = H(r_1, \cdots r_N, t)\, \Psi(r_1, \cdots r_N, t)$$

② the statistics of indistinguish particles is not imposed on H, but on $\Psi(r_1, \cdots r_N)$. We need to constrain $\Psi(r_1 \cdots r_N)$ to be symmetric function (anti-symmetric) for exchanging $r_i \leftrightarrow r_j$ for boson (ferimon) systems.

In other words, statistics is not explicit.

③ particle number is conserved, which can not be generalized to systems with particle number variation, say, quantum electrodyamic, ...

$\boxed{\text{Solution: Second quantization!}}$ ← quantization of wavefunction $\psi(x) \longrightarrow \hat{\psi}(x)$.

§ warm up: creation & annihilation operators

a simple example of harmonic oscillator

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2} m\omega^2 x^2 \longrightarrow \text{characteristic length } l = \sqrt{\frac{\hbar}{m\omega}}$$

$$a = \frac{1}{\sqrt{2}}\left[\frac{x}{l} + i l p\right], \quad a^\dagger = \left[\frac{x}{l} - i l p\right] \leftarrow$$ creation & annihilation of phonons

$$[a, a^\dagger] = 1, \quad \text{and} \quad H = \hbar\omega\,[a^\dagger a + \tfrac{1}{2}]$$

the eigenstates of the oscillator can be expressed as $|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}}|0\rangle$

where $|0\rangle$ is the ground state satisfying $a|0\rangle = 0$

ex: ① $\langle x|0\rangle = \frac{1}{\sqrt{\pi^{1/2} l}}\, e^{-\frac{x^2}{2l^2}}$

② $a^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle$, $a|n\rangle = \sqrt{n}\,|n-1\rangle$, $a^\dagger a\,|n\rangle = n|n\rangle$

§ Bose statistics and Fermi statistics in the first quantization

Suppose we have a set of complete and normalized basis of single particle wavefunctions $\psi_1, \psi_2, \cdots$, we can use them to construct the basis for many-body states.

For bosons, let us consider the state with total number of N and the partition (N_1 particles in ψ_1, N_2 particles in ψ_2, $\cdots$,).

Write · $\underbrace{\psi_1(x_1) \cdots \psi_1(x_{n_1})}_{N_1}\, \psi_2(x_{n_1+1}) \cdots \psi_2(x_{n_1+n_2}), \cdots \underbrace{\psi_k(\ ) \cdots \psi_k(x_N)}_{N_k}$

however, such a state is NOT allowed, we need to symmetrize it

$$\Psi_{N_1\cdots N_k}(x_1\cdots x_N)=\left(\frac{N!}{N_1!\cdots N_k!}\right)^{1/2}\sum P\{\underbrace{\psi_1(x_1)\cdots\psi_1(x_{N_1})}_{N_1}\cdots\underbrace{\{\psi_k\cdots\psi(x_N)}_{N_k}\}$$

permutation

But for fermions

each state can only hold one particle. The set of basis can be represented as

$$\Psi_{\{l_{i1},\cdots l_{iN}\}}(x_1\cdots x_N)=\frac{1}{\sqrt{N!}}\sum_P(-)^P P[\psi_{i_1}(x_1)\psi_{i_2}(x_2)\cdots\psi_{iN}(x_N)]$$

the states of $i_1,\cdots i_N$ are occupied

-1 for odd permutation

$+1$ for even permutation

☆ Examples: let us consider a two-particle system, with the single particle basis of $\psi_1,\psi_2\cdots\psi_n\cdots$

For bosons: the two particle wavefunction basis:

$$\psi_1(x_1)\psi_1(x_2)\ ;\ \psi_2(x_1)\psi_2(x_2)\ ;\ \cdots\ ;\ \psi_k(x_1)\psi_k(x_2)\ ;\ \cdots\cdots$$

$$\frac{1}{\sqrt{2}}\{\psi_i(x_1)\psi_j(x_2)+\psi_i(x_2)\psi_j(x_1)\},\ \text{where } (1\le i<j\cdots)$$

For fermions:
$$\frac{1}{\sqrt{2}}\{\psi_i(x_1)\psi_j(x_2)-\psi_i(x_2)\psi_j(x_1)\}=\frac{1}{\sqrt{2}}\begin{vmatrix}\psi_1(x_1) & \psi_2(x_1)\\ \psi_1(x_2) & \psi_2(x_2)\end{vmatrix}$$

where $(1\le i<j)$

Slater determinate

EX: ~~Emulate~~ enumerate all the basis for 3-particle states of bosons and fermions.

§ Particle number occupation representation — Fock space

In the above section, we have set the basis for many-body bosonic/fermion systems. This set of many-body states is characterized by the eigenstates of particle number operators $\hat{n}_1, \hat{n}_2 \cdots$ for the single particle states $\psi_1, \psi_2 \cdots$. Creation / annilation operators connect different Hilbert space with diffierent total particle numbers.

For bosonic systems, the basis of

$$\Psi_{N_1 N_2 \cdots N_k \cdots}(x_1, x_2 \cdots x_N) = \sqrt{\frac{N_1! \cdots N_k! \cdots}{N!}} \sum P\{\underbrace{(\psi_1(x_1) \cdots \psi_1(x_{N_1}))}_{N_1}\underbrace{(\psi_2(x_{N_1+1}) \cdots)}_{N_2} \cdots \underbrace{(\cdots \psi_k(x_N))}_{N_k}\overbrace{}^{\cdots}\}$$

coordinate representation

in the particle number occupation reprensention, it is represented as.

$$|N_1 N_2 \cdots N_k \cdots \rangle .$$

* key point: because of the indistinguishbility of particles, the occupation number distribution completely determines the many-body quantum state. We do NOT care which particle is in a specified state.

An arbitary state of bosons (N-body) can be expanded as

$$\Psi(x_1 \cdots x_N) = \sum_{N_1 N_2 \cdots} \Psi_{N_1 N_2 \cdots}(x_1 x_2 \cdots x_N)\, C(N_1 N_2 \cdots)$$

or $\boxed{|\Psi\rangle = \sum_{N_1 N_2 \cdots} C(N_1 N_2 \cdots) |N_1 N_2 \cdots\rangle}$ where $C(N_1 N_2 \cdots) = \begin{cases} 0, & \text{if } \sum_i N_i \neq N \\ \langle \Psi_{N_1 N_2 \cdots} | \Psi \rangle & \text{if } \sum_i N_i = N \end{cases}$

we can also define the inner product of two general wave functions.

$$\langle \psi_A | \psi_B \rangle = \sum_{N_1 N_2 \cdots} C_A^*(N_1 N_2, \cdots) C_B(N_1 N_2 \cdots).$$

The orthangonality and completeness of $|N_1 N_2 \cdots\rangle$

$$\boxed{\begin{aligned} &\langle N_1 N_2 \cdots | N_1' N_2' \cdots \rangle = \delta_{N_1 N_1'} \delta_{N_2 N_2'} \cdots \delta_{N_k N_k'} \cdots, \\ &\sum_{N_1 N_2 \cdots} |N_1 N_2 \cdots\rangle\langle N_1 N_2 \cdots| = I \end{aligned}}$$

Define creation / annihilation operators

$$\hat{n}_i |N_1 N_2 \cdots\rangle = N_i |N_1 N_2 \cdots\rangle, \text{ where } \hat{n}_i^\dagger = n_i, \ [n_i, n_j] = 0$$

we define operators for each single particle state

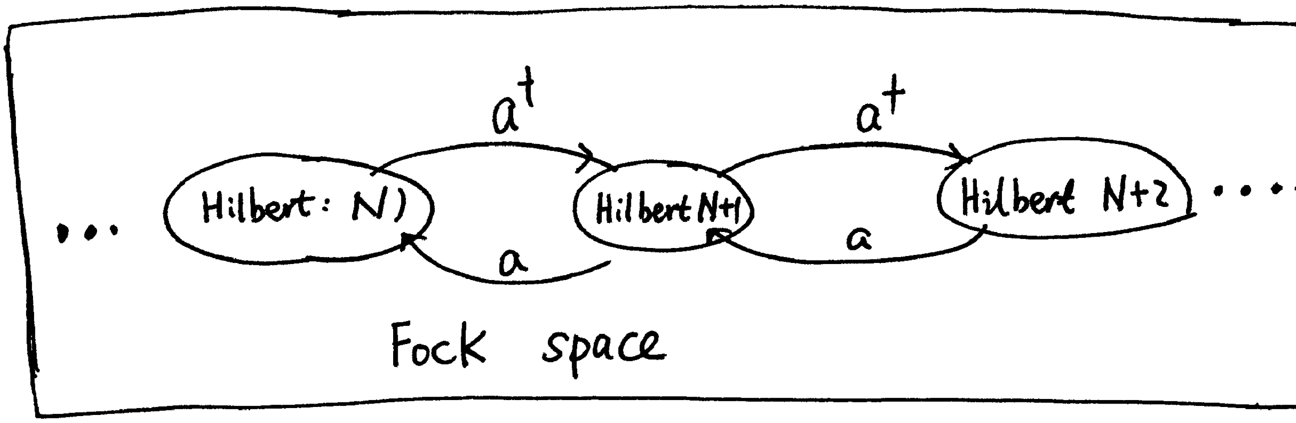
$$\boxed{\begin{aligned} &a_i = \sum_{N_1 N_2 \cdots} \sqrt{N_i} \ |N_1 N_2 \cdots (N_i - 1) \cdots\rangle\langle N_1 \cdots N_i \cdots|, \\ &a_i^\dagger = \sum_{N_1 N_2 \cdots} \sqrt{N_i + 1} \ |N_1 N_2 \cdots N_i + 1, \cdots\rangle\langle N_1 \cdots N_i \cdots|, \end{aligned}}$$

Ex: 1. Check $a_i | N_1 N_2 \cdots N_i \cdots\rangle = \sqrt{N_i} \ |N_1 N_2 \cdots, N_i - 1, \cdots\rangle$

$a_i^\dagger | N_1 N_2 \cdots N_i \cdots\rangle = \sqrt{N_i + 1} \ |N_1 N_2 \cdots N_i + 1, \cdots\rangle$

2. $[a_i, a_j^\dagger] = \delta_{ij}, \quad [a_i, a_j] = [a_i^\dagger a_j^\dagger] = 0$

3. $|N_1 N_2 \cdots\rangle = \frac{(a_1^\dagger)^{N_1}}{\sqrt{N_1!}} \frac{(a_2^\dagger)^{N_2}}{\sqrt{N_2!}} \cdots \ |00 \cdots 0\rangle$ ← the vaccum state.



1 Even when we deal with non-relativistic systems in which particle number N is fixed, it is much more convenient to first extend to Fock space to allow particle numble change. When we deal with relativistic field theory, Fock space is necessary. Similar stories occur before. For example, we prefer to use grand canonical ensemble rather than canonical esemble even though particle number is actually conserved. When we do a complicated real integral, we use complex-plane for loop integral.

> The key lesson here is: in many situations, a more general problem is easier. In order to solve a specified problem, we first generalize it, and then solve it.

In a Chinese idom, "if you want to capture sth, first let it escape".

欲擒故纵.

§ Fock space. creation/annilation operators for fermions

Again we define the many-body basis for fermions with occupation numbers $|N_1 N_2 \cdots\rangle$, but N_i can only be zero or one! The definition of the many-body basis has a sign ambiguity. If we exchang one pair, we have $\psi \to -\psi$. Say, in the first quantization Representation.

$$\psi_{\substack{N_1 N_2 \cdots \\ \cdots N_{\ell-1} N_\ell \cdots}}(x_1, x_2 \cdots x_N) = (-)^{N_{\ell-1} N_\ell} \Psi_{N_1 N_2 \cdots N_\ell N_{\ell-1} \cdots}(x_1, x_2, \cdots x_N \cdots)$$

★ if both $\psi_{\ell-1}$ and ψ_ℓ are occupied.

★ here we exchange the sequence of the single-particle basis $\psi_{\ell-1} \leftrightarrow \psi_\ell$, the effect ~~is~~ also results in a "$-$" sign.

$\boxed{\text{we need to specify the ordering of the single particle basis.}}$

Furthermore, we have

$$\psi_{N_1 N_2 \cdots N_{\ell-1} N_\ell \cdots}(x_1 x_2 \cdots x_N) = \underbrace{(-)^{N_\ell \sum_{j=1}^{\ell-1} N_j}}_{\text{the sign ambiguity}} \psi_{N_\ell N_1 N_2 \cdots}(x_1 x_2 \cdots)$$

in the particle number occupation representation

$$|N_1 N_2 \cdots N_{\ell-1} N_\ell \cdots\rangle = (-)^{N_\ell N_{\ell-1}} |N_1 N_2 \cdots N_\ell N_{\ell-1} \cdots\rangle$$

$$= (-)^{N_\ell \sum_{j=1}^{\ell-1} N_j} |N_\ell N_1 N_2 \cdots \cdots\rangle$$

orthangonality $\quad \langle N_1 N_2 \cdots | N_1' N_2' \cdots\rangle = \delta_{N_1 N_1'} \delta_{N_2 N_2'} \cdots$

Completness $\quad \sum_{N_1 N_2 \cdots} |N_1 N_2 \cdots\rangle\langle N_1 N_2 \cdots| = I$