Advanced Quantum Mechanics

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Many Particle Systems; Second Quantization

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Identical Particles; Bosons, Fermions

Experimental observation: Two type of particles

- **Bosons** whose states are totally symmetric
- **Fermions** whose states are totally antisymmetric

- Wave function of N identical particles

$$\Psi = \Psi(1, \cdots, N), \qquad i \equiv \boldsymbol{x}_i, \sigma_i$$

- The Hamiltonian of N identical particles

$$H = H(1, 2, \cdots, N)$$

Permutation operator

Definition: The permutation operator interchanges two particle i and j

$$P_{ij}\Psi(1\cdots,i,\cdots,j,\cdots,N)=\Psi(1\cdots,j,\cdots,i,\cdots,N)$$

Question: What is the relation between $\Psi(1\cdots,j,\cdots,i,\cdots,N)$ and $\Psi(1\cdots,i,\cdots,j,\cdots,N)$

$$\longrightarrow P_{ij}\Psi_{S/A}(1\cdots,i,\cdots,j,\cdots,N)=\pm\Psi_{S/A}(1\cdots,i,\cdots,j,\cdots,N)$$

S=**S**ymmetric and A=**A**ntisymmetric

- A system including N (identical) bosons is described by $\psi_S(1,\cdots,N)$
- A system including N (identical) fermions is described by $\psi_A(1,\cdots,N)$

Example

- Consider $\hat{H}$, being the Hamiltonian of a particle, described by $|\lambda\rangle$
$$\hat{H}|\lambda\rangle = \epsilon_\lambda|\lambda\rangle$$
- $|\lambda\rangle$ is a one-particle state
- Consider two identical particles [(B) or (F)]
- **Question:** What is the two-body state of these two particles?
- For bosons:
$$|\lambda_1, \lambda_2\rangle_B = \frac{1}{\sqrt{2}}\left(|\lambda_1\rangle_{(1)} \otimes |\lambda_2\rangle_{(2)} + |\lambda_2\rangle_{(1)} \otimes |\lambda_1\rangle_{(2)}\right)$$
- For fermions:
$$\begin{aligned} |\lambda_1, \lambda_2\rangle_F &= \frac{1}{\sqrt{2}}\left(|\lambda_1\rangle_{(1)} \otimes |\lambda_2\rangle_{(2)} - |\lambda_2\rangle_{(1)} \otimes |\lambda_1\rangle_{(2)}\right) \\ &= \frac{1}{\sqrt{2}}\det\begin{vmatrix} |\lambda_1\rangle_{(1)} & |\lambda_2\rangle_{(1)} \\ |\lambda_1\rangle_{(2)} & |\lambda_2\rangle_{(2)} \end{vmatrix} \end{aligned}$$

In general:

$$|\lambda_1, \lambda_2\rangle_{B/F} = \frac{1}{\sqrt{2}} \left(|\lambda_1\rangle_{(1)} \otimes |\lambda_2\rangle_{(2)} + \zeta |\lambda_2\rangle_{(1)} \otimes |\lambda_1\rangle_{(2)} \right)$$

$\zeta = +1$ for bosons and $\zeta = -1$ for fermions

- A two particle state in x- space:

$$\psi_{B/F}(x_1, x_2) = \frac{1}{\sqrt{2}} \left(\langle x_1|\lambda_1\rangle\langle x_2|\lambda_2\rangle + \zeta \langle x_1|\lambda_2\rangle\langle x_2|\lambda_1\rangle \right)$$

Question:

$$\psi_{B/F}\left(x_1, \cdots, x_N\right) \qquad \text{or} \qquad |\lambda_1, \lambda_2, \cdots, \lambda_N\rangle_{B/F}$$

Many particle systems $\rightarrow\rightarrow\rightarrow$

N-boson system

- Single particle state $|\lambda\rangle \in \mathcal{E}_1$
- $\mathcal{E}_1$ is the one boson Hilbert space
- **N-bosons:** Product space $\mathcal{E}_N = \mathcal{E}_1^{(1)} \otimes \mathcal{E}_1^{(2)} \otimes \cdots \otimes \mathcal{E}_1^{(N)}$

- Let $|\lambda_1\rangle_{(1)} \in \mathcal{E}_1^{(1)}$ denote the single particle state of particle 1 being in the state $|\lambda_1\rangle$ etc
- The **basis of the *N*-boson system** is given by

$$|\lambda_1, \cdots, \lambda_\alpha, \cdots, \lambda_N\rangle \equiv |\lambda_1\rangle_{(1)} \otimes \cdots \otimes |\lambda_\alpha\rangle_{(\alpha)} \otimes \cdots \otimes |\lambda_N\rangle_{(N)}$$

$\longrightarrow$ $|\lambda_\alpha\rangle_{(\alpha)}$ means particle α is in the state $|\lambda_\alpha\rangle \in \mathcal{E}_1^{(\alpha)}$

Symmetrization of N-boson system

- Define **totally symmetrized state**

$$
\begin{aligned}
|\lambda_1, \cdots, \lambda_N\rangle_+ &\equiv S_+|\lambda_1, \cdots, \lambda_N\rangle \\
&\equiv \frac{1}{\sqrt{N!}} \sum_{P \in S_N} (+1)^P P|\lambda_1, \cdots, \lambda_N\rangle \\
&= \frac{1}{\sqrt{N!}} \sum_{P \in S_N} |\lambda_{P(1)}\rangle_{(1)} \otimes \cdots \otimes |\lambda_{P(N)}\rangle_{(N)}
\end{aligned}
$$

- $|\lambda_1, \cdots, \lambda_N\rangle_+ \in \mathcal{E}_N^{(s)} \subset \mathcal{E}_N$

Properties of the symmetrized N-particle state

Completeness:

- The set of symmetized states is complete

$$\sum_{\lambda_1,\cdots,\lambda_N} |\lambda_1,\cdots,\lambda_N\rangle_{++}\langle\lambda_1,\cdots,\lambda_N| = 1 \in \mathcal{E}_N^{(s)}$$

Orthonormality:

!!! $|\lambda_1,\cdots,\lambda_N\rangle_+$ is **not** normalized

Because it can happen that $|\lambda_1,\cdots,\lambda_N\rangle_+$ contains single particle states occuring more than once.

Example:

$$
\begin{aligned}
&|\lambda_1 \lambda_1 \lambda_1 \lambda_4 \cdots \lambda_i \cdots \lambda_N\rangle \\
&= \underbrace{|\lambda_1\rangle_{(1)} \otimes |\lambda_1\rangle_{(2)} \otimes |\lambda_1\rangle_{(3)}}_{|\lambda_1\rangle \text{ occurs } n_1=3 \text{ times}} \otimes |\lambda_4\rangle_{(4)} \otimes \cdots \otimes |\lambda_i\rangle_{(i)} \otimes \cdots |\lambda_N\rangle_{(N)}
\end{aligned}
$$

- We thus have:

$$(n_1, n_2, n_3, n_4, n_5 \cdots, n_i, \cdots) = (3, 0, 0, 1, 1, \cdots, 1, \cdots)$$

- Assume: $|\lambda_\alpha\rangle$ occurs n_α times ($\alpha = 1, 2, \cdots, N$)
- We know $|\lambda_1, \cdots, \lambda_N\rangle_+$ contains a total of $N!$ terms, of which $\frac{N!}{n_1!\cdots n_N!}$ are different, each of these terms occurs with a multiplicity of $n_1!n_2!\cdots$

- Then

$$_+\langle\lambda_1, \cdots, \lambda_N|\lambda_1, \cdots, \lambda_N\rangle_+ = n_1!n_2!\cdots$$

- Hence, the normalized Bose basis function

$$\left(\frac{1}{n_1!n_2!\cdots}\right)^{1/2} |\lambda_1, \cdots, \lambda_N\rangle_+$$

Occupation numbers:

- n_α are the **occupation numbers**, i.e., n_α is the number of times the state $|\lambda_\alpha\rangle$ occurs

  Previous example:

$$(n_1, n_2, n_3, n_4, n_5 \cdots, n_\alpha, \cdots) = (3, 0, 0, 1, 1, \cdots, 1, \cdots)$$

- **Alternative formulation:** We use

$$|n_1, n_2, \cdots, n_\alpha, \cdots\rangle \equiv \left(\frac{1}{n_1! n_2! \cdots}\right)^{1/2} |\lambda_1, \cdots, \lambda_N\rangle_+$$

  with $n_\alpha = 0, 1, \cdots$ being the number of particles in the state $|\lambda_\alpha\rangle$ and $\sum_\alpha n_\alpha = N$

Properties:

- The states $|n_1, n_2, \cdots\rangle$ form a complete set of totally symmetric orthonormal N-particle states

- **Orthonormality**

$$\langle n_1, n_2, \cdots | n'_1, n'_2, \cdots \rangle = \delta_{n_1 n'_1} \delta_{n_2 n'_2} \cdots = \prod_{i=1}^{N} \delta_{n_i, n'_i}$$

- **Completeness**

$$\sum_{n_1, n_2, \cdots} |n_1, n_2, \cdots\rangle\langle n_1, n_2, \cdots| = \mathbf{1}$$

- Any desired symmetric N-particle state can be constructed by a linear superposition of these states

The many-boson system; The “big” picture

The extended space where these states are defined is given by the **direct sum** of

- ▸ a space with no particles (vacuum $|0\rangle$)
- $\oplus$ a space with one particle
- $\oplus$ a space with two particles
- $\oplus$ $\cdots$

$$\mathcal{E} = \mathcal{E}_0 \oplus \mathcal{E}_1 \oplus \mathcal{E}_2^{(s)} \oplus \mathcal{E}_3^{(s)} \oplus \cdots$$

Fock space

Creation and annihilation operators

- We define **creation** and **annihilation** operators, which lead from the space of N-particle states to spaces of $N \pm 1$-particle states $\mathcal{E}_N \to \mathcal{E}_{N\pm1}$:
  - Creation

$$a_i^\dagger|\cdots, n_i, \cdots\rangle = \sqrt{n_i + 1}|\cdots, n_i + 1, \cdots\rangle$$

  - Annihilation

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

$$a_i|\cdots, n_i = 0, \cdots\rangle = 0$$

Commutation relations for bosons

$$[a_i, a_j] = 0, \qquad [a_i^\dagger, a_j^\dagger] = 0, \qquad [a_i, a_j^\dagger] = \delta_{ij}$$

Proof: $\cdots$

$$\begin{aligned}(a_i a_i^\dagger - a_i^\dagger a_i)|\cdots, n_i, \cdots\rangle &= \left(\sqrt{(n_i+1)^2} - \sqrt{n_i^2}\right)|\cdots, n_i, \cdots\rangle \\ &= |\cdots, n_i, \cdots\rangle \qquad \square\end{aligned}$$

Constructing many particle state:

- Ground state $\equiv$ Vacuum state

$$|\mathbf{0}\rangle = |0, 0, 0, \cdots\rangle$$

- Single-particle state: $a_i^\dagger|0\rangle$
- Two-particle state: $(a_i^\dagger)^2|0\rangle, a_i^\dagger a_j^\dagger, \cdots$
- $\cdots$
- The general **many-boson state**

$$|n_1, n_2, \cdots\rangle = \frac{1}{\sqrt{n_1!}\sqrt{n_2!}\cdots}\left(a_1^\dagger\right)^{n_1}\left(a_2^\dagger\right)^{n_2}\cdots|\mathbf{0}\rangle$$

The particle (occupation) number operator

$$\hat{n}_i = a_i^\dagger a_i$$

The many particle state $|\cdots, n_i, \cdots\rangle$ is the eigenfunction of $\hat{n}_i$

$$\hat{n}_i|\cdots, n_i, \cdots\rangle = n_i|\cdots, n_i, \cdots\rangle$$

The corresponding eigenvalue n_i is the number of particles in the state i

The operator for the total number of particles $\hat{N} = \sum_i \hat{n}_i$, so that

$$\hat{N}|n_1, n_2, \cdots\rangle = \left(\sum_i n_i\right)|n_1, n_2, \cdots\rangle$$

N-fermion system; Slater determinant

- Define **totally anti-symmetric state**

$$
\begin{aligned}
|\lambda_1, \cdots, \lambda_N\rangle_- &\equiv S_-|\lambda_1, \cdots, \lambda_N\rangle \\
&= \frac{1}{\sqrt{N!}} \sum_{P \in S_N} (-1)^P P|\lambda_1, \cdots, \lambda_N\rangle \\
&= \frac{1}{\sqrt{N!}} \det \begin{pmatrix} |\lambda_1\rangle_1 & |\lambda_1\rangle_2 & \cdots & |\lambda_1\rangle_N \\ \ldots & \ldots & \vdots & \ldots \\ |\lambda_N\rangle_1 & |\lambda_N\rangle_2 & \cdots & |\lambda_N\rangle_N \end{pmatrix} \\
|\lambda_1, \cdots, \lambda_N\rangle_- &\in \mathcal{E}_N^{(A)} \subset \mathcal{E}_N
\end{aligned}
$$

- **Note:** If any of the single particle states in the above expression are the same, the result will be zero
  $\rightarrow$ **Pauli exclusion principle:**
  Two identical fermions are not allowed to occupy the same state

Occupation numbers:

- Characterize the states by specifying their **occupation numbers** (only 0 and 1)

$$|n_1, n_2, \cdots\rangle, \qquad n_i = 0, 1 \ \ \forall i$$

- **Fock space:**
  $|\mathbf{0}\rangle +$ single-particle states + two-particle states $+ \cdots$ with

$$\langle n_1, n_2, \cdots | n_1', n_2', \cdots \rangle = \delta_{n_1, n_1'} \delta_{n_2, n_2'} \cdots$$

and

$$\sum_{n_1, n_2, \cdots = 0}^{1} |n_1, n_2, \cdots\rangle\langle n_1, n_2, \cdots| = 1$$

Creation and annihilation operators for fermions:

a and $a^\dagger$ for fermions are defined such that

- by applying them twice to a fermionic state the result is zero and
- we have to take the order in which they are applied into account

Creation and annihilation operators for fermions:

Use:

$$|\lambda_1, \lambda_2, \cdots, \lambda_N\rangle_- = -|\lambda_2, \lambda_1, \cdots, \lambda_N\rangle_-$$

and $a^\dagger_{\lambda_\alpha}|\mathbf{0}\rangle = |\lambda_\alpha\rangle$. We thus have

$$\begin{aligned}
\underbrace{a^\dagger_{\lambda_1} a^\dagger_{\lambda_2}} a^\dagger_{\lambda_3} \cdots a^\dagger_{\lambda_N}|\mathbf{0}\rangle &= |\lambda_1, \lambda_2, \lambda_3, \cdots, \lambda_N\rangle_- \\
&= -|\lambda_2, \lambda_1, \lambda_3, \cdots, \lambda_N\rangle_- \\
&= -\underbrace{a^\dagger_{\lambda_2} a^\dagger_{\lambda_1}} a^\dagger_{\lambda_3} \cdots a^\dagger_{\lambda_N}|\mathbf{0}\rangle
\end{aligned}$$

We thus have:

$$\boxed{\{a^\dagger_i, a^\dagger_j\} = 0}$$

- As a result: $(a_i^\dagger)^2 = 0$

  and therefore no double occupancy of state i is allowed
- $\Longrightarrow$

$$|n_1, n_2, \cdots\rangle = (a_1^\dagger)^{n_1}(a_2^\dagger)^{n_2}\cdots|0\rangle, \quad n_i = 0, 1, \quad \forall i = 1, 2, \cdots$$

and

$$\begin{aligned} a_i^\dagger|\cdots, n_i, \cdots\rangle &= (1-n_i)(-1)^{\sum_{j<i} n_j}|\cdots, n_i+1, \cdots\rangle \\ a_i|\cdots, n_i, \cdots\rangle &= n_i(-1)^{\sum_{j<i} n_j}|\cdots, n_i-1, \cdots\rangle \end{aligned}$$

Claim: $\{a_i, a_i^\dagger\} = 1$ [anti-commutator]

Proof:

$$
\begin{aligned}
a_i a_i^\dagger |\cdots, n_i, \cdots\rangle &= (1-n_i)(-1)^{\sum_{j<i} n_j} a_i |\cdots, n_i+1, \cdots\rangle \\
&= (1-n_i)(n_i+1)\underbrace{[(-1)^{\cdots}]^2}_{=1}|\cdots, n_i, \cdots\rangle \\
&= (1-n_i^2)|\cdots, n_i, \cdots\rangle \\
&= (1-n_i)|\cdots, n_i, \cdots\rangle \\
a_i^\dagger a_i |\cdots, n_i, \cdots\rangle &= n_i(-1)^{\sum_{j<i} n_j} a_i^\dagger |\cdots, n_i-1, \cdots\rangle \\
&= n_i(1-n_i+1)\underbrace{[(-1)^{\cdots}]^2}_{=1}|\cdots, n_i, \cdots\rangle \\
&= \underbrace{n_i(2-n_i)}_{=2n_i-n_i^2=2n_i-n_i=n_i} |\cdots, n_i, \cdots\rangle = n_i|\cdots, n_i, \cdots\rangle
\end{aligned}
$$

We thus arrive at

$$\left(a_i a_i^\dagger + a_i^\dagger a_i\right)|\cdots, n_i, \cdots\rangle = |\cdots, n_i, \cdots\rangle \Rightarrow \{a_i, a_i^\dagger\} = 1 \quad \text{q.e.d.}$$

Anti-commutation relations for fermions

$$\{a_i, a_j\} = 0, \qquad \{a_i, a_j^\dagger\} = 0, \qquad \{a_i, a_j^\dagger\} = \delta_{ij}$$