

4. Many-particle theory



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4.1 Multi-particle states, bosons and fermions

- ▶ arbitrary single-particle state: $|\psi\rangle = \sum_i c_i |i\rangle$
 - ▶ $\{|i\rangle\}$: complete basis of the single-particle Hilbert space (usually orthonormalized)
 - ▶ continuous spectra: $\sum \rightarrow \int$
 - ▶ basis of the N -particle Hilbert space: $|i_1, i_2, \dots, i_N\rangle \equiv |i_1\rangle_1 |i_2\rangle_2 \dots |i_N\rangle_N$
 - ▶ direct product of single-particle basis states
 - ▶ $|i\rangle_j$: The j^{th} particle is in the state $|i\rangle$.
- general N -particle state: $|\psi\rangle = \sum_{i_1, \dots, i_N} c_{i_1, \dots, i_N} |i_1, \dots, i_N\rangle$



► example: position-space representation

$$|\psi\rangle = \int d^3x_1 \dots \int d^3x_N \psi(\vec{x}_1, \dots, \vec{x}_N) |\vec{x}_1, \dots, \vec{x}_N\rangle$$

$$\Rightarrow \langle \vec{x}_1, \dots, \vec{x}_N | \psi \rangle = \int d^3x'_1 \dots \int d^3x'_N \psi(\vec{x}'_1, \dots, \vec{x}'_N) \langle \vec{x}_1, \dots, \vec{x}_N | \vec{x}'_1, \dots, \vec{x}'_N \rangle$$

$$\begin{aligned} \langle \vec{x}_1, \dots, \vec{x}_N | \vec{x}'_1, \dots, \vec{x}'_N \rangle &= \langle \vec{x}_1 |_1 \dots \langle \vec{x}_N |_N | \vec{x}'_1 \rangle_1 \dots | \vec{x}'_N \rangle_N \\ &= \langle \vec{x}_1 | \vec{x}'_1 \rangle \dots \langle \vec{x}_N | \vec{x}'_N \rangle \\ &= \delta^3(\vec{x}_1 - \vec{x}'_1) \dots \delta^3(\vec{x}_N - \vec{x}'_N) \end{aligned}$$

$$\Rightarrow \langle \vec{x}_1, \dots, \vec{x}_N | \psi \rangle = \psi(\vec{x}_1, \dots, \vec{x}_N) \quad \checkmark$$

► short-hand notation often used in the following:

$$|\psi\rangle = \sum_{\vec{x}_1, \dots, \vec{x}_N} \psi(\vec{x}_1, \dots, \vec{x}_N) |\vec{x}_1, \dots, \vec{x}_N\rangle$$



- ▶ **transposition operator P_{ij} :** interchanges the i^{th} and the j^{th} particle

$$\begin{aligned} P_{ij} |i_1, \dots, i_i, \dots, i_j, \dots, i_N\rangle &= P_{ij} (|i_1\rangle_1 \dots |i_i\rangle_i \dots |i_j\rangle_j \dots |i_N\rangle_N) \\ &= |i_1\rangle_1 \dots |i_j\rangle_j \dots |i_i\rangle_i \dots |i_N\rangle_N \\ &= |i_1\rangle_1 \dots |i_j\rangle_i \dots |i_i\rangle_j \dots |i_N\rangle_N \\ &= |i_1, \dots, i_j, \dots, i_i, \dots, i_N\rangle \end{aligned}$$

- ▶ **position-space representation:**

$$\begin{aligned} P_{ij} |\psi\rangle &= P_{ij} \sum_{\vec{x}_1, \dots, \vec{x}_N} \psi(\dots, \vec{x}_i, \dots, \vec{x}_j, \dots) |\dots, \vec{x}_i, \dots, \vec{x}_j, \dots\rangle \\ &= \sum_{\vec{x}_1, \dots, \vec{x}_N} \psi(\dots, \vec{x}_i, \dots, \vec{x}_j, \dots) |\dots, \vec{x}_j, \dots, \vec{x}_i, \dots\rangle \\ &= \sum_{\vec{x}_1, \dots, \vec{x}_N}^{\vec{x}_i \leftrightarrow \vec{x}_j} \psi(\dots, \vec{x}_j, \dots, \vec{x}_i, \dots) |\dots, \vec{x}_i, \dots, \vec{x}_j, \dots\rangle \end{aligned}$$



$$\begin{aligned} P_{ij} |\psi\rangle &= P_{ij} \sum_{\vec{x}_1, \dots, \vec{x}_N} \psi(\dots, \vec{x}_i, \dots, \vec{x}_j, \dots) |\dots, \vec{x}_i, \dots, \vec{x}_j, \dots\rangle \\ &= \sum_{\vec{x}_1, \dots, \vec{x}_N} \psi(\dots, \vec{x}_j, \dots, \vec{x}_i, \dots) |\dots, \vec{x}_i, \dots, \vec{x}_j, \dots\rangle \end{aligned}$$

→ If $|\psi\rangle$ has the position-space wave function $\psi(\dots, \vec{x}_i, \dots, \vec{x}_j, \dots)$,
then $P_{ij} |\psi\rangle$ has the position-space wave function $\psi(\dots, \vec{x}_j, \dots, \vec{x}_i, \dots)$.

- ▶ $P_{ij}^2 |\psi\rangle = |\psi\rangle \Rightarrow P_{ij}^2 = \mathbb{1} \Rightarrow$ eigenvalues of $P_{ij} = \pm 1$
- ▶ Any permutation $P \in S_N$ of N particles can be obtained as a product of transpositions.

→ notation:

$$(-1)^P = \left\{ \begin{array}{c} +1 \\ -1 \end{array} \right\} \text{ if the number of transpositions is } \left\{ \begin{array}{c} \text{even} \\ \text{odd} \end{array} \right\}.$$



- ▶ Consider:
 - ▶ N **identical** (= indistinguishable) particles
 - ▶ **observable** \leftrightarrow operator \hat{O}
 - ▶ eigenstate $|\psi_\lambda\rangle$ of \hat{O} with eigenvalue λ : $\hat{O}|\psi_\lambda\rangle = \lambda|\psi_\lambda\rangle$
 - ▶ permutation $P \in S_N$, $P|\psi_\lambda\rangle \equiv |P\psi_\lambda\rangle$
- ▶ particles indistinguishable $\Rightarrow \hat{O}|P\psi_\lambda\rangle = \lambda|P\psi_\lambda\rangle$
 $\Leftrightarrow \hat{O}P|\psi_\lambda\rangle = \lambda P|\psi_\lambda\rangle = P\lambda|\psi_\lambda\rangle = P\hat{O}|\psi_\lambda\rangle \Rightarrow [P, \hat{O}] = 0$
 $\Rightarrow \hat{O}$ must be symmetric under exchange of identical particles.
In particular this holds for $\hat{O} = H$.



► **example:**

N electrons in the (static) Coulomb potential V of an atomic nucleus
+ mutual Coulomb repulsion

$$H = \sum_{i=1}^N \frac{\vec{p}_i^2}{2m} + \sum_{i=1}^N V(\vec{x}_i) + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{|\vec{x}_i - \vec{x}_j|},$$

\vec{p}_i, \vec{x}_i : momentum and position operators acting on the i^{th} particle only

→ H is symmetric under exchange of electrons.

► **further properties of permutations of identical particles:**

P is unitary: $P^\dagger = P^{-1} \Rightarrow P^\dagger P = PP^\dagger = 1$

(reminder: $\langle P\phi|\psi\rangle = \langle\phi|P^\dagger|\psi\rangle = \langle\phi|P^\dagger\psi\rangle$)

$$\Rightarrow \langle P\phi|P\psi\rangle = \langle\phi|\psi\rangle$$

Quantum statistics: two classes of particles,
which differ by the symmetry of their many-body states

▶ bosons:

- ▶ integer spin (0, 1, 2, ...)
- ▶ states symmetric under the interchange of two particles:

$$P_{ij}|\psi\rangle = |\psi\rangle \quad \forall i, j \quad \Rightarrow \quad P|\psi\rangle = |\psi\rangle \quad \forall P \in S_N$$

▶ fermions:

- ▶ half-integer spin ($\frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \dots$)
- ▶ states antisymmetric under the interchange of two particles:

$$P_{ij}|\psi\rangle = -|\psi\rangle \quad \forall i, j \quad \Rightarrow \quad P|\psi\rangle = (-1)^P|\psi\rangle \quad \forall P \in S_N$$

⇒ Pauli principle:

States with two or more fermions in the same single-particle state vanish.

- ▶ The relation between spin and statistics can be proven within QFT.

1. two distinguishable spin- $\frac{1}{2}$ particles (e.g., $e^- p$):

- ▶ four basis states of the two-particle system:

$$|\uparrow, \uparrow\rangle \equiv |\uparrow\rangle_e |\uparrow\rangle_p$$

$$|\uparrow, \downarrow\rangle \equiv |\uparrow\rangle_e |\downarrow\rangle_p$$

$$|\downarrow, \uparrow\rangle \equiv |\downarrow\rangle_e |\uparrow\rangle_p$$

$$|\downarrow, \downarrow\rangle \equiv |\downarrow\rangle_e |\downarrow\rangle_p$$

- ▶ alternative basis: states of good total spin $|SM_S\rangle$

$$\left. \begin{aligned} |1, 1\rangle &= |\uparrow, \uparrow\rangle \\ |1, 0\rangle &= \frac{1}{\sqrt{2}} (|\uparrow, \downarrow\rangle + |\downarrow, \uparrow\rangle) \\ |1, -1\rangle &= |\downarrow, \downarrow\rangle \end{aligned} \right\} \text{spin 1 (symmetric)}$$
$$|0, 0\rangle = \frac{1}{\sqrt{2}} (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) \quad \text{spin 0 (antisymmetric)}$$



2. two indistinguishable spin- $\frac{1}{2}$ particles (e.g., $e^- e^-$):

fermions \rightarrow two-particle systems **antisymmetric**

\rightarrow only total spin 0 allowed: $|\psi\rangle = |0, 0\rangle = \frac{1}{\sqrt{2}}(|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle)$

(as long as the particles do not differ by other quantum numbers)

3. two distinguishable spin-1 particles (e.g., $\rho^+ \rho^-$):

$\rightarrow 3^2 = 9$ basis states: $(m_1, m_2) = (1, 1), (1, 0), (1, -1), \dots, (-1, -1)$

▶ alternative basis: $|S = 2, M_S\rangle, |S = 1, M_S\rangle, |S = 0, M_S = 0\rangle$

5 symmetric + 3 antisymm. + 1 symmetric

4. two indistinguishable spin-1 particles (e.g., $\omega\omega$):

bosons \rightarrow 6 **symmetric** basis states,

e.g., $|S = 2, M_S\rangle$ and $|S = 0, M_S = 0\rangle$