Next topic: Quantum Field Theories for Quantum Many-Particle Systems; or "Second Quantization"

Outline
1) Bosons and Fermions
2) N-particle wave functions ("first quantization")
3) The method of quantized fields ("second quantization")

Motivation
- Quantum field theory can be used as a mathematical technique for describing many-particle systems with identical particles.
- There are many applications:
  - atomic physics – many electron atoms
  - nuclear physics – many protons and neutrons
  - condensed matter physics – many atoms in quantum statistical mechanics; superfluids, metals, etc.
- This topic is not in Mandl and Shaw
- There are whole books devoted to this topic. I'm using Huang, Appendix A.
1. BOSONS AND FERMIONS

Consider a system with \( N \) identical particles.

The wave function is \( \Psi(q_1, q_2, q_3, \ldots, q_N; t) \)

where \( q_i = \) the coordinates of particle \( i \).

The goal is to solve the time evolution,

\[
i\hbar \frac{\partial \Psi}{\partial t} = H \Psi = H \Psi(q_1, \ldots, q_N; t)
\]

Or, equivalently, find the energy eigenstates,

\[
\Psi(q_1, \ldots, q_N; t) = e^{-iE_n t / \hbar} \Phi_n(q_1, \ldots, q_N)
\]

\[
E_n \Phi_n = H \Phi_n(q_1, \ldots, q_N; t)
\]
1a - The exchange operator
Let $P_{ij}$ be the operator that exchanges the coordinates $q_i$ and $q_j$; definition,
\[ P_{ij} \Phi_n(q_1 \ldots q_i \ldots q_j \ldots q_N) = \Phi_n(q_1 \ldots q_j \ldots q_i \ldots q_N) \]

Exchange symmetry of the Hamiltonian
Because the $N$ particles are identical we have
\[ P^{-1} H P = H \]
so
\[ H (P \Phi_n) = P H \Phi_n = P E_n \Phi_n = E_n (P \Phi_n) \]

$P \Phi_n$ is an energy eigenfunction with the same energy.

The postulate of identical particles
$\Rightarrow \quad (P \Phi_n) = \lambda \Phi_n$

Now, $P^2 = 1$; therefore, $\lambda^2 = 1$; that is,
- either $\lambda = +1$ (bosons)
- or $\lambda = -1$ (fermions)
Symmetry or antisymmetry of the wave function

The "spin-statistics theorem"

- For identical particles with integer spin,

\[ P_{ij} \Phi_n (q_1, \ldots, q_N) = \Phi_n (q_1, \ldots, q_2', \ldots, q_i', \ldots, q_N) = 1 \Phi_n (q_1, \ldots, q_2, \ldots, q_i, \ldots, q_N) \]

the wavefunction is symmetric under coordinate exchanges (bosons).

- For identical particles with half-integer spin,

\[ P_{ij} \Phi_n (q_1, \ldots, q_N) = - \Phi_n (q_1, \ldots, q_2', \ldots, q_i', \ldots, q_N) \]

the wavefunction is antisymmetric under coordinate exchanges (fermions).
2./ N-PARTICLE WAVE FUNCTIONS
2a - The N-particle system

Let's define the N-particle system in more detail. The Hamiltonian is \( H = K + \Omega \) where

\[
K = -\frac{\hbar^2}{2m} \left( \nabla_1^2 + \nabla_2^2 + \ldots + \nabla_N^2 \right)
\]

\[
\Omega = \sum_{i<j} \nu_{ij} \quad ; \quad \nu_{ij} = \nu \left( r_i, r_j \right)
\]

To solve: \( H\Phi = E\Phi( \mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \ldots, \mathbf{r}_N ) \)

The w.f. normalization is

\[
(\Phi, \Phi) = \int \ldots \int \Phi^* \Phi \; d^3r_1 \; d^3r_2 \ldots d^3r_N = 1.
\]

E.g., we might use a finite volume \( V \), with periodic boundary conditions, and finally let \( V \to \infty \).
2b - Product wave functions
First, introduce a complete set of orthonormal single-particle wave functions,
\[ \{ u_\alpha(r) ; \alpha = 1 \ 2 \ 3 \ \ldots \ \infty \} \]

Now consider an N-particle product wave function,
\[ u_{\alpha_1}(r_1) u_{\alpha_2}(r_2) \ldots u_{\alpha_i}(r_i) \ldots u_{\alpha_N}(r_N) \]
i.e., particle # i has quantum numbers \( \alpha_i \).

But that is neither exchange symmetric (for bosons) nor antisymmetric (for fermions).

So we need to do something better.
Identical spin-0 bosons
The basis wavefunctions must be **symmetrized products**.

We have a set of occupied states
\[ \{ \alpha \} = \{ \alpha \, \alpha \, \alpha \, \ldots \, \beta \, \beta \, \ldots \, \gamma \, \gamma \, \ldots \, \text{etc} \} \]

Or, write
\[ \{ \alpha \} = \{ \alpha_1, \alpha_2, \alpha_3, \ldots, \alpha_N \} \]

The corresponding basis wavefunction is
\[
\Phi_\{\alpha\} (\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N) \\
= \frac{1}{N!} \sum_P u_{\alpha_1}(\vec{r}_1) u_{\alpha_2}(\vec{r}_2) \ldots u_{\alpha_N}(\vec{r}_N) \\
\]

where
\[ \{ \alpha_1', \alpha_2', \ldots, \alpha_N' \} = P \{ \alpha_1, \alpha_2, \ldots, \alpha_N \} \]

**Orthogonality**
\[
(\Phi_{\{\alpha\}}, \Phi_{\{\beta\}}) = 0 \quad \text{if} \quad \{\alpha_1, \ldots, \alpha_N\} \neq \{\beta_1, \ldots, \beta_N\} \\
\text{(independent of ordering)}
\]

**Normalization**
\[
(\Phi_{\{\alpha\}}, \Phi_{\{\alpha\}}) = \frac{1}{\alpha!} (\alpha_N!) \\
\quad \text{(bosons)}
\]

i.e., the \( \Phi_{\{\alpha\}} \) are not normalized, that's OK.

They are not ortho**normal**, but that's OK.
Examples with $N = 2$

- $\{\alpha\} = \{\gamma\gamma\}$  \hspace{1cm} $n_\gamma = 2$
  \[ \Phi_{\{\alpha\}}(\mathbf{r}_1 \mathbf{r}_2) = \text{SQRT}(2) \, u_\gamma(\mathbf{r}_1) \, u_\gamma(\mathbf{r}_2) \]

- $\{\alpha\} = \{\gamma\delta\}$  \hspace{1cm} $n_\gamma = 1, n_\delta = 1$
  \[ \Phi_{\{\alpha\}}(\mathbf{r}_1 \mathbf{r}_2) = 1/\text{SQRT}(2) \]
  \[ \left[ u_\gamma(\mathbf{r}_1) \, u_\delta(\mathbf{r}_2) + u_\delta(\mathbf{r}_1) \, u_\gamma(\mathbf{r}_2) \right] \]

$|n_\gamma = \text{occupation number for state } \gamma|$

Examples with $N = 3$

- $\{\alpha\} = \{\gamma\gamma\gamma\}$  \hspace{1cm} $n_\gamma = 3$
  \[ \Phi_{\{\alpha\}}(\mathbf{r}_1 \mathbf{r}_2 \mathbf{r}_3) = \text{SQRT}(6) \, u_\gamma(\mathbf{r}_1) \, u_\gamma(\mathbf{r}_2) \, u_\gamma(\mathbf{r}_3) \]

- $\{\alpha\} = \{\gamma\gamma\delta\}$  \hspace{1cm} $n_\gamma = 2, n_\delta = 1$
  \[ \Phi_{\{\alpha\}}(\mathbf{r}_1 \mathbf{r}_2 \mathbf{r}_3) = \text{SQRT}(\frac{2}{3}) \]
  \[ \left[ u_\gamma(\mathbf{r}_1) \, u_\gamma(\mathbf{r}_2) \, u_\delta(\mathbf{r}_3) + u_\gamma(\mathbf{r}_1) \, u_\delta(\mathbf{r}_2) \, u_\gamma(\mathbf{r}_3) + u_\delta(\mathbf{r}_1) \, u_\gamma(\mathbf{r}_2) \, u_\gamma(\mathbf{r}_3) \right] \]

- $\{\alpha\} = \{\gamma\delta\lambda\}$  \hspace{1cm} $n_\gamma = 1, n_\delta = 1, n_\lambda = 1$
  \[ \Phi_{\{\alpha\}}(\mathbf{r}_1 \mathbf{r}_2 \mathbf{r}_3) = \text{SQRT}(\frac{1}{6}) \]
  \[ \times \left[ \text{sum of six orderings} \right] \]
2c - An example of an N-boson calculation

Calculate $\langle \Omega \rangle = (\Phi_{\{\alpha\}}, \Omega \Phi_{\{\alpha\}})$ where $\Omega = \text{the two-particle interactions}$

$$\Omega = \sum_{i < j} \nu_{ij}.$$

**Combinatorial counting**

$$2 \text{body expression} = \int \Phi_{\alpha_1}^\dagger \Phi_{\alpha_2}^\dagger \nu_{\alpha_1 \alpha_2} \nu_{\alpha_2 \alpha_1} d^3p_1 d^3p_2$$
2d - Identical spin - $\frac{1}{2}$ fermions

The basis wavefunctions must be **antisymmetrized products**.

We have a set of occupied states

$\{ \alpha \} = \{ \alpha_1, \alpha_2, \alpha_3, \ldots, \alpha_N \}$

The corresponding basis wavefunction is

$$
\Phi \{ \alpha \} (\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) = \frac{1}{\sqrt{N!}} \sum_P \delta_P \psi_{\alpha_1}(\mathbf{r}_1) \psi_{\alpha_2}(\mathbf{r}_2) \ldots \psi_{\alpha_N}(\mathbf{r}_N)
$$

where

$$
\delta_P = \text{signature of } P = +1 \text{ or } -1
$$

- **The Pauli exclusion principle**

  $$
  \Phi = 0 \text{ unless } \{ \alpha_1, \alpha_2, \alpha_3, \ldots, \alpha_N \} \text{ are all different.}
  $$

- **Occupation numbers can only be 0 or 1.**

  $$
  n_{\alpha} = 0 \text{ (unoccupied)} \text{ or } = 1 \text{ (occupied)}. 
  $$

- **$\Phi_{\{\alpha\}} (r_1, r_2, r_3 \ldots r_N)$ can be written as a determinant (the Slater determinant)**
Fermions

\[ \langle \Omega \rangle = \frac{1}{2} \sum_{\alpha \beta} n_\alpha n_\beta \left\{ \langle \alpha \beta | V | \alpha \beta \rangle \right. \\
\left. - \langle \alpha \beta | V | \beta \alpha \rangle \right\} \]

direct and exchange terms

Recall the Hartree-Fock wavefunction.
Homework Problems due Friday February 3

Problem 11.

Three identical spin-0 bosons are in a harmonic oscillator potential. The total energy is $9/2 \hbar \omega$. From this information alone, write an expression for the 3-particle wave function, $\Psi(x_1, x_2, x_3)$?

Problem 12.

Consider two identical spin-0 bosons moving in free space, and interacting with each other. Approximate the 2-particle wave function by products of free waves with momenta $p_1$ and $p_2$.

(a) Calculate the expectation value of the two-body potential energy $V(x_1, x_2)$.

(b) Now suppose $V(x_1, x_2) = U(x_1 - x_2)$. Express the result of (a) in terms of the Fourier transform of $U(r)$. 