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,

$$i\hbar \frac{\partial \Psi}{\partial t} = H \Psi \quad = H \Psi ( q_1 \cdots q_N ; t )$$

Or, equivalently, find the energy eigenstates,

$$\Psi ( q_1 \cdots q_N ; t ) = e^{-iE_n t/\hbar} \quad \Phi_n ( q_1 \cdots q_N )$$

$$E_n \Phi_n = H \Phi_n \ ( q_1 \cdots q_N ; t )$$

## 1a - The exchange operator

Let $P_{ij}$ be the operator that exchanges the coordinates $q_i$ and $q_j$ ; definition,

$$P_{ij}\,\Phi_n\,(\,q_1 \dots q_i \dots q_j \dots q_N) = \Phi_n\,(\,q_1 \dots q_j \dots q_i \dots q_N)$$

<u>Exchange symmetry of the Hamiltonian</u>

Because the N particles are identical we have

$$P^{-1}\,H\,P = H \qquad \text{(P is short for } P_{ij}.\text{)}$$

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,

$$
\begin{aligned}
P_{ij}\,\Phi_n(q_1 \cdots q_N) &= \Phi_n(q_1 \cdots q_j \cdots q_i \cdots q_N) \\
&= +\,\Phi_n(q_1 \cdots q_i \cdots q_j \cdots q_N)
\end{aligned}
$$

the wavefunction is symmetric under coordinate exchanges (*bosons)*.

■ For identical particles with half-integer spin,

$$
\begin{aligned}
P_{ij}\,\Phi_n(q_1 \cdots q_N) &= -\,\Phi_n(q_1 \cdots q_i \cdots q_j \cdots q_N)
\end{aligned}
$$

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

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

$$\Omega = \sum_{i<j} v_{ij} \quad ; \quad v_{ij} = v(\vec{r}_i , \vec{r}_j)$$

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

The w.f. normalization is

$$(\Phi , \Phi) = \iint \ldots \int \Phi^* \Phi \quad d^3r_1\, d^3r_2 \ldots d^3r_N = 1.$$

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,

$$\{ u_\alpha(r) \ ; \ \alpha = 1\ 2\ 3 \ldots \infty \}$$

$\alpha \equiv$ a set of quantum numbers for one particle;
e.g., $(p_x, p_y, p_z, \text{spin})$
$\exists$ an infinite number of possible states

$$\int u_\alpha^*(\vec{r})\, u_\beta(\vec{r})\, d^3r = \delta_{\alpha\beta}$$

Now consider an N-particle product wave function,

$$u_{\alpha 1}(\mathbf{r_1})\, u_{\alpha 2}(\mathbf{r_2}) \ldots u_{\alpha i}(\mathbf{r_i}) \ \ldots u_{\alpha N}(\mathbf{r_N})$$

i.e., particle # i has quantum numbers $\boldsymbol{\alpha_i}$ .

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

$\{\boldsymbol{\alpha}\} = \{ \alpha\ \alpha\ \alpha \dots \beta\ \beta\ \beta \dots \gamma\ \gamma\ \gamma \dots$ *etc* $\}$

Or, write

$\{\boldsymbol{\alpha}\} = \{ \alpha_1 , \alpha_2 , \alpha_3 , \dots , \alpha_N \}$

The corresponding basis wavefunction is

$$\Phi_{\{\alpha\}}(\vec{r}_1\, \vec{r}_2 \dots \vec{r}_N)$$

$$= \frac{1}{\sqrt{N!}} \sum_P u_{\alpha_1'}(\vec{r}_1)\, u_{\alpha_2'}(\vec{r}_2) \dots u_{\alpha_N'}(\vec{r}_N)$$

where

$$\{ \alpha_1', \alpha_2', \dots, \alpha_N' \} = P\{\alpha_1\, \alpha_2 \dots \alpha_N\}$$

*Orthogonality*

$$(\Phi_{\{\alpha\}}, \Phi_{\{\beta\}}) = 0 \quad \text{if} \quad \{\alpha_1 \dots \alpha_N\} \neq \{\beta_1 \dots \beta_N\}$$

(independent of ordering)

*Normalization*

$$(\Phi_{\{\alpha\}}, \Phi_{\{\alpha\}}) = \prod_\alpha (n_\alpha !) \qquad \text{(bosons)}$$

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

They are not ortho***normal***, but that's OK.

## Examples with N = 2

- $\{\boldsymbol{\alpha}\} = \{\gamma\gamma\}$  $n_\gamma = 2$

$$\Phi_{\{\alpha\}}(\mathbf{r}_1\, \mathbf{r}_2) = \mathrm{SQRT}(2)\, u_\gamma(\mathbf{r}_1)\, u_\gamma(\mathbf{r}_2)$$

- $\{\boldsymbol{\alpha}\} = \{\gamma\delta\}$  $n_\gamma = 1\,,\, n_\delta = 1$

$$\Phi_{\{\alpha\}}(\mathbf{r}_1\, \mathbf{r}_2) = 1/\mathrm{SQRT}(2)\ [u_\gamma(\mathbf{r}_1)\, u_\delta(\mathbf{r}_2) + u_\delta(\mathbf{r}_1)\, u_\gamma(\mathbf{r}_2)\,]$$

| $n_\gamma$ = *occupation number* for state $\gamma$ .

## Examples with N = 3

- $\{\boldsymbol{\alpha}\} = \{\gamma\gamma\gamma\}$  $n_\gamma = 3$

$$\Phi_{\{\alpha\}}(\mathbf{r}_1\, \mathbf{r}_2\, \mathbf{r}_3) = \mathrm{SQRT}(6)\, u_\gamma(\mathbf{r}_1)\, u_\gamma(\mathbf{r}_2)\, u_\gamma(\mathbf{r}_3)$$

- $\{\boldsymbol{\alpha}\} = \{\gamma\gamma\delta\}$  $n_\gamma = 2\,,\, n_\delta = 1$

$$\Phi_{\{\alpha\}}(\mathbf{r}_1\, \mathbf{r}_2\, \mathbf{r}_3) = \mathrm{SQRT}(\tfrac{2}{3})\, [u_\gamma(\mathbf{r}_1)\, u_\gamma(\mathbf{r}_2)\, u_\delta(\mathbf{r}_3) + u_\gamma(\mathbf{r}_1)\, u_\delta(\mathbf{r}_2)\, u_\gamma(\mathbf{r}_3) + u_\delta(\mathbf{r}_1)\, u_\gamma(\mathbf{r}_2)\, u_\gamma(\mathbf{r}_3)\,]$$

- $\{\boldsymbol{\alpha}\} = \{\gamma\delta\lambda\}$  $n_\gamma = 1\,,\, n_\delta = 1\,,\, n_\lambda = 1$

$$\Phi_{\{\alpha\}}(\mathbf{r}_1\, \mathbf{r}_2\, \mathbf{r}_3) = \mathrm{SQRT}(\tfrac{1}{6})$$

✖ *[sum of six orderings]*

## 2c - An example of an N-boson calculation

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

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

$$\langle \Omega \rangle = \frac{1}{2} N(N-1) \int (d^3r)^N \, \Phi^*_{\{\alpha\}} \, v_{12} \, \Phi_{\{\alpha\}}$$

$$= \frac{N(N-1)}{2\,N!} \sum_P \sum_Q \left[ u_{\alpha_1'}(r_1)\, u_{\alpha_2'}(r_2) \ldots u_{\alpha_N'}(r_N) \right] v_{12} \left[ u_{\alpha_1''}(r_1)\, u_{\alpha_2''}(r_2) \ldots u_{\alpha_N''}(r_N) \right]$$

$$= \frac{N(N-1)}{2\,N!} \sum_P \sum_Q \underbrace{\langle \alpha_1' \alpha_2' | v_{12} | \alpha_1'' \alpha_2'' \rangle}_{\text{2 body expression}} \delta(\alpha_3' \alpha_3'') \ldots \delta(\alpha_N' \alpha_N'')$$

$$= \int u^*_{\alpha_1'} u^*_{\alpha_2'} v(r_1, r_2)\, u_{\alpha_1''} u_{\alpha_2''} \, d^3r_1 d^3r_2$$

$$= \frac{N(N-1)}{2N!} \sum_P \Big\{ \langle \alpha_1' \alpha_2' | v_{12} | \alpha_1 \alpha_2 \rangle \quad \text{"direct"}$$
$$+ \langle \alpha_1' \alpha_2' | v_{12} | \alpha_2 \alpha_1 \rangle \Big\} \quad \text{"exchange"}$$

**combinatorial counting**

$$= \frac{N(N-1)}{2N!} (N-2)! \sum_{\alpha,\beta} f_{\alpha\beta} \times \left[ \langle \alpha\beta | v | \alpha\beta \rangle + \langle \alpha\beta | v | \beta\alpha \rangle \right]$$

$$f_{\alpha\beta} = \begin{cases} n_\alpha n_\beta & (\alpha \neq \beta) \\ \frac{1}{2} n_\alpha (n_\alpha - 1) & (\alpha = \beta) \end{cases}$$

$$= \frac{1}{2} \sum_{\alpha\beta} f_{\alpha\beta} \left[ \langle \alpha\beta | v | \alpha\beta \rangle + \langle \alpha\beta | v | \beta\alpha \rangle \right] = \langle \Omega \rangle$$

## 2d - Identical spin - ½ fermions

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

We have a set of occupied states

$$\{\boldsymbol{\alpha}\} = \{ \alpha_1 , \alpha_2 , \alpha_3 , \ \dots \ , \alpha_N \}$$

The corresponding basis wavefunction is

$$\Phi_{\{\alpha\}}(\vec{r}_1\, \vec{r}_2 \dots \vec{r}_N)$$

$$= \frac{1}{\sqrt{N!}} \sum_P \delta_P\, u_{\alpha_1'}(\vec{r}_1)\, u_{\alpha_2'}(\vec{r}_2) \dots u_{\alpha_N'}(\vec{r}_N)$$

where

$$\{ \alpha_1', \alpha_2', \dots, \alpha_N' \} = P\{ \alpha_1\, \alpha_2 \dots \alpha_N \}$$

**$\delta_P$ = signature of P = +1 or −1**

- *The Pauli exclusion principle*

  ***$\Phi$ = 0 unless***

  $\{ \alpha_1 , \alpha_2 , \alpha_3 , \ \dots \ , \alpha_N \}$

  ***are all different.***

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

  ***$n_\alpha$ = 0 (unoccuied)***

  ***or = 1 (occupied).***

- *$\Phi_{\{\alpha\}}(\boldsymbol{r}_1\ \boldsymbol{r}_2\ \boldsymbol{r}_3 \dots\ \boldsymbol{r}_N)$ can be written as a determinant (the Slater determinant)*

Fermions

$$\langle \Omega \rangle = \tfrac{1}{2} \sum_{\alpha\beta} n_\alpha \, n_\beta \; \{ \; \langle \alpha\beta | v | \alpha\beta \rangle - \langle \alpha\beta | v | \beta\alpha \rangle \; \}$$

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 $\mathbf{p}_1$ and $\mathbf{p}_2$.

(a ) Calculate the expectation value of the two-body potential energy $V( \mathbf{x}_1 , \mathbf{x}_2 )$.

(b) Now suppose $V( \mathbf{x}_1 , \mathbf{x}_2 ) = U( \mathbf{x}_1 - \mathbf{x}_2 )$. Express the result of (a) in terms of the Fourier transform of $U(\mathbf{r})$.