Next topic:
QUANTUM FIELD THEORY AND MANY PARTICLE SYSTEMS

Think of many applications …

References:
Fetter and Walecka,
Quantum Theory of Many-Particle Systems (famous primary text; not obsolete, but old fashioned)

E. G. Harris,
A Pedestrian Approach to Quantum Field Theory (pedestrian; somewhat obsolete)

We don't have time to cover the field at the depth of Fetter and Walecka.
We'll study some essential ideas:
Chapters 1, 3, 4 ?

Chapter 1 : SECOND QUANTIZATION
1. The Schroedinger equation in first and second quantization
   a. Bosons
   b. Many particle Hilbert space
   c. Fermions
2. Fields
3. Example : Degenerate electron gas

SECTION 1 : THE SCHROEDINGER EQUATION IN FIRST AND SECOND QUANTIZATION

Start with

$$H = \sum_{k=1}^{N} T_k + \tfrac{1}{2} \sum'^{N}_{k,l=1} V(x_k, x_l) \; ;$$

Note $\sum'$: the prime means $l \neq k$.

N particles; interacting with each other by a 2-particle interaction $V(x_1, x_2)$.

The essential goal of quantum mechanics is to solve the Schroedinger equation,

$$i\hbar \, \partial\Psi / \partial t = H \, \Psi$$

where

$$\Psi = \Psi(x_1, x_2, x_3, \ldots, x_N \; ; t) \; .$$

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The first quantized theory

$$H = \sum_{k=1}^{N} T_k + \frac{1}{2} \sum_{k,\ell=1}^{N}{}' V(x_k, x_\ell)$$

$$T_k = -\frac{\hbar^2}{2m} \nabla_k^2 + U(x_k) \quad \text{"one-body operator"}$$

$$V(x_k, x_\ell) = \text{interaction energy} \quad \text{"two-body operator"}$$

Notations

- .*Index k labels one of the N particles;* the set of k values is $\{k\} = \{1\,2\,3 \dots k \dots N\}$.

- .x_k *is a complete set of coordinates for particle k*; for example, for an electron, $x_k = (x_k, y_k, z_k, \xi_k)$.
  Cartesian coords.;   spin coord.;
  $\in (0,L)$ $\in (1,-1)$

To Solve: $i\hbar\, \partial\Psi / \partial t = H\, \Psi$
where $\Psi = \Psi(x_1\, x_2\, x_3 \dots x_k \dots x_N)$

Introduce a complete set of time-independent single-particle wave functions

Single - particle states

$$\Psi_E(x) \quad \begin{cases} x = \text{coordinates} \\ E = \text{quantum numbers} \end{cases}$$

For example, for an electron in a box,

$$E = (p_x, p_y, p_z, S_z)$$

$$\Psi_E(x) = \frac{1}{\sqrt{\Omega}} e^{i\vec{p}\cdot\vec{x}/\hbar} \, u$$

$$\vec{p} = \frac{2\pi\hbar}{L} \vec{n} \quad (P.B.C.) \quad \text{and} \quad u = \binom{1}{0} \text{ or } \binom{0}{1}$$

<u>Completeness:</u> We can expand the N-particle wave function as a product of single-particle wave functions __

$$\Psi(x_1, x_2, x_3 \cdots x_N; t)$$
$$= \sum_{E_1'} \sum_{E_2'} \cdots \sum_{E_N'} C(E_1' E_2' \cdots E_N'; t)$$
$$\times \prod_{k=1}^{N} \psi_{E_k'}(x_k)$$

Or,
$$\Psi(\{x\}; t) = \sum_{\{E'\}} C(\{E'\}; t) \prod_{k=1}^{N} \psi_{E_k'}(x_k)$$

By the orthonormality of the s.-p. states __

$$C(\{E\}; t) = \int \prod_{k=1}^{N} \psi_{E_k}^{\dagger}(x_k) \, \Psi(\{x\}; t) \, d\tau_k$$
$$d\tau_k = d^3 x_k \sum_{s_k}$$

Interpretation: $|C(\{E\}; t)|^2 =$ the probability that the particles have quantum numbers $\{ E_1 \, E_2 \ldots E_k \ldots E_N \}$

Normalization relations

$$\int \Phi^{\dagger} \Psi \prod_{k=1}^{N} d\tau_k = 1$$
$$\sum_{\{E\}} |C(\{E\}; t)|^2 = 1$$

The Schroedinger equation for C({E};t)

$$i\hbar \frac{\partial}{\partial t} C = \sum_{k=1}^{N} \sum_{W} \langle E_k | T | W \rangle \, C(E_1 \cdots W \cdots E_N; t)$$
— position k

$$+ \frac{1}{2} \sum_{k,\ell=1}^{N}{}' \sum_{W} \sum_{W'} \langle E_k E_\ell | V | W W' \rangle$$
$$C(E_1 \cdots W \cdots W' \cdots E_N; t)$$
— positions k and ℓ

$$\langle E_k | T | W \rangle = \text{a single particle matrix element}$$
$$\langle E_k E_\ell | V | W W' \rangle = \text{a 2-particle matrix element}$$

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So far, this is simple.

But now comes the hard part:

Assume that the N particles are ***identical particles.***

Identical particles are indistinguishable.

I.e., the N-body wave function cannot tell which particle (k) has a particular set of quantum numbers (E_i).

$\therefore \Psi^+\Psi$ must be invariant under any interchange of coordinates, $x_k \leftrightarrow x_l$.

1a.   BOSONS

$\Psi(x_1 \dots x_N ; t)$ must be *symmetric* with respect to interchange of any two coordinates;   i.e.,

$$\Psi(\dots x_k \dots x_l \dots ; t) = + \Psi(\dots x_l \dots x_k \dots ; t)$$

Then also,

$$C(\dots E_i \dots E_j \dots ; t) = + C(\dots E_j \dots E_i \dots ; t)$$

Understand the notation:
k, l, … are particle labels; all are different;
$k \in \{1, 2, 3, \dots, N\}$;
i, j, … = s.-p. state labels; some might be the same; $i \in \{1, 2, 3, \dots, \infty\}$;

The space of occupation numbers (Fock space)

$C(E_1, E_2, E_3, \dots, E_N)$ could depend on 3N quantum numbers (ignore spin; set spin = 0 since they are bosons);

e.g., $\{ \mathbf{p_1}, \mathbf{p_2}, \mathbf{p_3}, \dots, \mathbf{p_N})$

where $\mathbf{p_k} = (p_{kx}, p_{ky}, p_{kz})$.

But C could depend on as few as 3 quantum numbers,

$\{ \mathbf{p_1}, \mathbf{p_1}, \mathbf{p_1}, \dots, \mathbf{p_1} \}$ *for bosons!*

i.e., all the particles have the same quantum numbers.

In fact, by the exchange symmetry of the N-particle wave function, *C is completely determined by the list of occupation numbers.*

Imagine that all possible s.p. states can be listed in some order,
$\{ E_1, E_2, E_3, \dots, E_k, \dots \dots \dots \}$
                    "standard order"

(this is an *infinite* list).

Define occupation numbers :
n_i = the number of particles in the state $|E_i\rangle$.

So, for a *basis state* Ψ, the set of occupation numbers is
$\{ n_1, n_2, n_3, \dots, n_i, \dots \dots \dots \}$

For each i, $n_i \in \{ 0, 1, 2, 3, \dots, N \}$;
and there is a crucial *restriction* ,

$$\sum_i n_i = N .$$

Then $C(E_1, E_2, E_3, \dots, E_N) = \hat{C}(n_1, n_2, n_3, \dots)$ because different orderings are equal.

$C(\{E\}\,;\,t)$ is symmetric w.r.t. any exchanges in the list
$$\{E\} \equiv \{E_1, E_2, E_3, \dots, E_N\}$$

$\hat{C}(\{n\}\,;\,t)$ has no symmetry property; $\{n\}$ is in the standard order; and there is a restriction, $\sum_i n_i = N$.

<u>The interpretation of $\underline{\hat{C}}(\{n\}\,;\,t)$</u>

We have

$\hat{C}(n_1, n_2, n_3, \dots) = C(E_1, E_2, E_3, \dots, E_N)$; the right-hand side is invariant w.r.t. all permutations of the list
$\{E_1, E_2, E_3, \dots, E_N\}$;

"symmetry of the wavefunction"

<u>Probabilities and normalizations</u>
We have

$$\int \Phi^{\dagger} \Phi \prod_{k=1}^{N} d\tau_k = 1$$
$$\sum_{\{E\}} |C(\{E\}\,;t)|^2 = 1$$

But $\sum_{\{n\}} |\hat{C}(\{n\},t)|^2$ is not 1.

So $\hat{C}$ is not a probability amplitude.

The probability amplitude for occupation numbers $\{n\}$ is

$$f_N(\{n\},t) = \mathrm{Sqrt}[\,N!/\prod n_i!\,]\,\hat{C}(\{n\},t)$$

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The probability amplitude for the list of occupation numbers is

$$f_N\,(\,\{n\}\,;t\,) = \,(\,N!\;/\;\prod_i n_i!\,)^{\frac{1}{2}}\;\;\hat{C}\,(\,\{n\}\,;t\,)\,.$$

$N!\;/\;(\prod_i n_i!)\;$ = the number of distinguishable
permutations of $\{E\}$ when the list
of occupation numbers is $\{n\}$.

Normalization:

$$\sideset{}{'}\sum_{\{n\}}|\,f_N\,(\,\{n\}\,;t\,)|^{\,2}\;=\;1$$

(Σ' : prime implies
the restriction $\sum n_i = N$)

Example. Consider N = 2.

- ❖ Both in the same state ;
  - ➢ N! / (∏ n_i!) = 2! / 2! = 1
  - ➢ $\Psi(x_1, x_2) = \psi_\alpha(x_1) \psi_\alpha(x_2)$
  - ➢ $C(E_\alpha, E_\alpha) = 1$

- ❖ Two in different states ;
  - ➢ N! / (∏ n_i!) = 2! / (1! 1!) = 2
  - ➢ $\Psi(x_1, x_2) =$
    $1/\sqrt{2} [\psi_\alpha(x_1) \psi_\beta(x_2) + \psi_\beta(x_1) \psi_\alpha(x_2)]$
  - ➢ $C(E_\alpha, E_\beta) = 1/\sqrt{2}$, $C(E_\beta, E_\alpha) = 1/\sqrt{2}$
  - ➢ $\hat{C}(\{1,1\}) = 1/\sqrt{2}$, $f_2(\{1,1\}) = 1$

Example. Consider N=3.

- ❖ All three in the same state ;
  - ➢ $\psi_\alpha(x_1) \psi_\alpha(x_2) \psi_\alpha(x_3)$
  - ➢ $f_3(\{3,0,0,0....\}) = 1$

- ❖ All three in different states ;

  $1/\sqrt{6}$ [
  $\psi_\alpha(x_1) \psi_\beta(x_2) \psi_\gamma(x_3) + \psi_\gamma(x_1)\psi_\alpha(x_2) \psi_\beta(x_3)$
  $+ \psi_\beta(x_1) \psi_\gamma(x_2) \psi_\alpha(x_3) + \psi_\beta(x_1) \psi_\alpha(x_2) \psi_\gamma(x_3)$
  $+ \psi_\gamma(x_1) \psi_\beta(x_2) \psi_\alpha(x_3) + \psi_\alpha(x_1) \psi_\gamma(x_2) \psi_\beta(x_3)$
  ]

  $f_3(\{1,1,1,0,0,0,0....\}) = 1$

The most general state with N particles (bosons!) :

- .The state would be a superposition of states
    with different occupation numbers;

- .but *each component* would have to have $\sum n_i = N$.

- .Thus, the *basis states* for the N-particle Hilbert space
  are

$$\Phi_N(\,\{n\}\,;\{x\}\,) =$$

$$\text{Sqrt}[\,\prod n_i!\ /N!\,]\ \sum_P\ \psi_{E1}(x_1)\,\psi_{E2}(x_2)\,...\,\psi_{EN}(x_N)$$

Homework due Friday, February 5 …

Problem 11.

Three identical bosons are in a harmonic oscillator potential. The total energy is $9/2\ \hbar\omega$. What is the most that you can say about the 3-particle wave function, $\Psi(\,x_1\,,\,x_2\,,\,x_3\,)$.

Problem 12.

Consider two identical bosons (spin = 0) 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 $V(\mathbf{x_1}\,,\,\mathbf{x_2})$.

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