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.

Consider a system with N identical particles.

In the *first-quantized theory*,

the wave function is $\Psi(\, \mathbf{r}_1\ \mathbf{r}_2\ \mathbf{r}_3 \ldots \mathbf{r}_N\ ;\ t\,)$

where $\mathbf{r}_i$ = the coordinate vector of particle i .

The goal is to solve the time evolution,

$$i\hbar \frac{\partial \Psi}{\partial t} = H \Psi$$

$$= -\frac{\hbar^2}{2m} \sum_{i=1}^{N} \nabla_i^2 \Psi + \sum_{i<j} v_{ij} \cdot \Psi$$

Or, equivalently, find the energy eigenstates,

$$\Psi(\vec{r}_1\ \vec{r}_2 \ldots \vec{r}_N\ ;\ t) = e^{-iE_n t/\hbar}\ \Phi_n(\vec{r}_1\ \vec{r}_2 \ldots \vec{r}_N)$$

$$E_n \Phi_n = H\, \Phi_n(\vec{r}_1 \ldots \vec{r}_N)$$

The method of quantized fields

/1/ In the second quantized theory we define a ***quantized field*** for the system of particles.
The field obeys a quantum postulate, which is called the *equal-time commutation relations:*

<u>Boson field</u>

$[\ \psi(\mathbf{r})\ ,\ \psi^\dagger(\mathbf{r}')\ ] = \delta^3(\mathbf{r} - \mathbf{r}')$

$[\ \psi(\mathbf{r})\ ,\ \psi(\mathbf{r}')\ ] = 0$

$[\ \psi^\dagger(\mathbf{r})\ ,\ \psi^\dagger(\mathbf{r}')\ ] = 0$

<u>Fermion field</u>

$\{\ \psi(\mathbf{r})\ ,\ \psi^\dagger(\mathbf{r}')\ \} = \delta^3(\mathbf{r} - \mathbf{r}')$

$\{\ \psi(\mathbf{r})\ ,\ \psi(\mathbf{r}')\ \} = 0$

$\{\ \psi^\dagger(\mathbf{r})\ ,\ \psi^\dagger(\mathbf{r}')\ \} = 0$

$[\ A\ ,\ B\ ] = AB - BA$

$\{\ A\ ,\ B\ \} = AB + BA$

/2/ And we define the Hamiltonian operator H and the number operator N_{op} .

The Hamiltonian in the second quantized theory is

$$H = K + \Omega$$

$$K = -\hbar^2/(2m) \int d^3r \;\; \psi^\dagger(\mathbf{r}) \; \nabla^2 \; \psi(\mathbf{r})$$

$$\Omega = \tfrac{1}{2} \int d^3r_1 \int d^3r_2 \;\; \psi^\dagger(\mathbf{r}_1)\, \psi^\dagger(\mathbf{r}_2)\, \boldsymbol{v}_{12}\, \psi(\mathbf{r}_2)\, \psi(\mathbf{r}_1)$$

where again $\boldsymbol{v}_{12} = v(\boldsymbol{r}_1 , \boldsymbol{r}_2)$.

The Number Operator in the second quantized theory is

$$N_{op} = \int d^3r \;\; \psi^\dagger(\mathbf{r})\, \psi(\mathbf{r})$$

and it is a constant in the time evolution.

The Big Theorem

The second quantized theory is equivalent in all predictions to the first quantized theory.

To prove this is not so easy, because the two theories look so different.

$H_{1Q} =$

$$H = -\frac{\hbar^2}{2m}\left(\nabla_1^2 + \nabla_2^2 + \dots + \nabla_N^2\right) + \sum_{i<j} V(\vec{r}_i, \vec{r}_j) \quad \leftarrow \text{sum of } \tfrac{1}{2}N(N-1) \text{ interactions}$$

$H_{2Q} =$

$$H = -\frac{\hbar^2}{2m}\int d^3r\, \psi^\dagger \nabla^2 \psi + \frac{1}{2}\int d^3r_1\, d^3r_2\, \psi^\dagger(r_1)\, \psi^\dagger(r_2)\, V(\vec{r}_1, \vec{r}_2)\, \psi(\vec{r}_2)\, \psi(r_1)$$

The *structures* of the two theories are different. The trick is to prove that the *predictions* are the same.

① The wave function (as defined from the 2nd quantized theory) has the correct exchange symmetry or antisymmetry.

$\Psi (r_1\, r_2 \ldots r_N ; t) \equiv$

$$1/\text{SQRT}(N!)\ \langle 0 |\ \psi(r_1)\, \psi(r_2) \ldots \psi(r_N)\ | t,N \rangle$$

Consider the coordinate exchange,

$$\Psi (r_1 \ldots r_j \ldots r_i \ldots r_N ; t) .$$

- For bosons, all the $\psi(r_k)$ factors commute;

so $\Psi (\ldots r_j \ldots r_i \ldots) = \Psi (\ldots r_i \ldots r_j \ldots)$.

- For fermions, all the $\psi(r_k)$ factors anticommute;

so $\Psi (\ldots r_j \ldots r_i \ldots) = - \Psi (\ldots r_i \ldots r_j \ldots)$;

it takes 2n+1 anticommutations to switch the order.

② *The time-dependent Schroedinger equation has the correct form.*

We define $\Psi(r_1\ r_2 \ldots r_N ; t)$

$= 1/\text{SQRT}(N!)\ \langle 0|\ \psi(r_1)\ \psi(r_2) \ldots \psi(r_N)\ |t,N\rangle$

Now calculate

$i\hbar\,(\partial/\partial t)\,\Psi =$

$= 1/\text{SQRT}(N!)\ \langle 0|\ \psi(r_1)\ \psi(r_2) \ldots \psi(r_N)\ i\hbar\,(\partial/\partial t)|t,N\rangle$

$= H\ |t,N\rangle$

$= 1/\text{SQRT}(N!)\ \langle 0|\ \psi(r_1)\ \psi(r_2) \ldots \psi(r_N)\ H\ |t,N\rangle$

Commute H to the left, commuting H past the $\psi(r_1)$ factors.

Note $\langle 0|H = 0$ *(≡ just the adjoint of* $H\ |0\rangle = 0$ *)*

$i\hbar\,(\partial/\partial t)\,\Psi =$

$= 1/\mathrm{SQRT}(N!)\ \langle 0|\ \psi(\mathbf{r}_1)\,\psi(\mathbf{r}_2)\ \ldots\ \psi(\mathbf{r}_N)\ H\ |t,N\rangle$

Pull H over to the left, repeatedly commuting H past the $\psi(\mathbf{r}_j)$ factors.

Note $\langle 0|H = 0$ *(equiv. to $H\,|0\rangle = 0$).*

Also,

$$\psi(\mathbf{r}_j)\,H = H\,\psi(\mathbf{r}_j) + [\,\psi(\mathbf{r}_j)\,,\,H\,]$$

where

$$[\,\psi(\mathbf{r})\,,\,H\,] = -\hbar^2/(2m)\ \nabla^2\,\psi(\mathbf{r}) + X(\mathbf{r})\,\psi(\mathbf{r})$$

and

$$X(\mathbf{r}) = \int d^3r'\ \psi^\dagger(\mathbf{r}')\,v(\mathbf{r}',\mathbf{r})\,\psi(\mathbf{r}')\ .$$

For each commutation we pick up a term

$$-\hbar^2/(2m)\ \nabla_j^{\,2}\,\psi(\mathbf{r}_j)$$

and a term $X(\mathbf{r}_j)\,\psi(\mathbf{r}_j)$ *$(\propto \psi^\dagger\psi\psi)$*

Now pull the $X(\mathbf{r})$ operators to the left;

Note $\langle 0|X(\mathbf{r}) = 0$.

Also,

$$\psi(\mathbf{r}_j)\,X(\mathbf{r}') = X(\mathbf{r}')\,\psi(\mathbf{r}_j) + [\,\psi(\mathbf{r}_j)\,,\,X(\mathbf{r}')\,]$$

where

$$[\,\psi(\mathbf{r}_j)\,,\,X(\mathbf{r}')\,] = v(\mathbf{r}_j,\mathbf{r}')\,\psi(\mathbf{r}')\,\psi(\mathbf{r}_j)$$

Finally,

$$i\hbar\,(\partial/\partial t)\,\Psi =$$
$$-\hbar^2/(2m)\,(\nabla_1^{\,2} + \nabla_2^{\,2} + \ldots + \nabla_N^{\,2})\Psi$$
$$+ \sum_{i<j} v(\mathbf{r}_i\,,\,\mathbf{r}_j)\,\Psi$$

[QED]

③ *Expansion in single-particle states*

Introduce a complete set of single-particle states

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

Now expand the quantized field in these functions,

$$\psi(\mathbf{r}) = \sum u_\alpha(\mathbf{r})\, c_\alpha \quad \text{and} \quad \psi^\dagger(\mathbf{r}) = \sum u_\alpha^*(\mathbf{r})\, c_\alpha^\dagger$$

Commutators

$$[\, \psi(\mathbf{r}) \,,\, \psi^\dagger(\mathbf{r}') \,]_\mp = \delta^3(\mathbf{r} - \mathbf{r}')$$

$$\Rightarrow [\, c_\alpha \,,\, c_\beta^\dagger \,]_\mp = \delta(\alpha,\beta)$$

That is,

for bosons, $[\, c_\alpha \,,\, c_\beta^\dagger \,] = \delta(\alpha,\beta)$ and $[\, c_\alpha \,,\, c_\beta \,] = 0$;

for fermions, $\{\, c_\alpha \,,\, c_\beta^\dagger \,\} = \delta(\alpha,\beta)$ and $\{\, c_\alpha \,,\, c_\beta \,\} = 0$.

- More precisely,

α = a set of quantum numbers for a single particle;

- $\int u_\alpha^*(\mathbf{r})\, u_\beta(\mathbf{r})\, d^3r = \delta(\alpha,\beta)$
- $c_\alpha = \int u_\alpha^*(\mathbf{r})\, \psi(\mathbf{r})\, d^3r$

We've seen this before!

Something new: *anticommutation* for fermions.

Non-relativistic quantum fields for identical particles

$$\psi(\mathbf{r}) = \sum u_\alpha(\mathbf{r})\, c_\alpha$$

and

$$\psi^\dagger(\mathbf{r}) = \sum u_\alpha^*(\mathbf{r})\, c_\alpha^\dagger$$

where c_α is the annihilation operator for a particle with quantum numbers α
and $c_\alpha^\dagger$ is the creation operator.

The Pauli exclusion principle for fermions,

$$(c_\alpha^\dagger)^2 = 0.$$

Proof: $\{ c_\alpha^\dagger , c_\beta^\dagger \} = 0 = c_\alpha^\dagger c_\beta^\dagger + c_\beta^\dagger c_\alpha^\dagger$;

so for $\beta = \alpha$, $c_\alpha^\dagger c_\alpha^\dagger = 0$.

④ *Matrix elements agree.*

For example, consider 2 identical fermions.

Let $|\alpha\rangle$ = plane wave single-particle state. (momentum $\hbar\alpha$

Calculate $\langle\alpha\beta|T|\gamma\delta\rangle$ and $\langle\alpha\beta|\Omega|\gamma\delta\rangle$.

$$T_{\alpha\beta,\gamma\delta} = \langle\alpha\beta| \underbrace{\int d^3r\, \psi^\dagger(\vec r)\left(\frac{-\hbar^2}{2m}\right)\nabla^2\psi(\vec r)}_{\sum_k \frac{\hbar^2k^2}{2m} c_k^\dagger c_k} \underbrace{|\gamma\delta\rangle}_{c_\gamma^\dagger c_\delta^\dagger|0\rangle}$$

$$= \sum_k \frac{\hbar^2k^2}{2m}\langle 0|c_\beta c_\alpha c_k^\dagger \underbrace{c_k c_\gamma^\dagger}_{=\delta(k,\gamma) - c_\gamma^\dagger c_k} c_\delta^\dagger|0\rangle$$

$$= \sum_k \frac{\hbar^2k^2}{2m}\left\{\delta(k,\gamma)\langle 0|c_\beta c_\alpha c_k^\dagger c_\delta^\dagger|0\rangle - \langle 0|c_\beta c_\alpha c_k^\dagger c_\gamma^\dagger c_k c_\delta^\dagger|0\rangle\right\}$$

$c_k c_\delta^\dagger = \delta(k,\delta) - c_\delta^\dagger c_k$

$= \delta(k,\delta)$ when it acts on $|0\rangle$

$$= \frac{\hbar^2\gamma^2}{2m}\langle 0|c_\beta c_\alpha c_\gamma^\dagger c_\delta^\dagger|0\rangle - \frac{\hbar^2\delta^2}{2m}\langle 0|c_\beta c_\alpha c_\delta^\dagger c_\gamma^\dagger|0\rangle$$

$$= \left(\frac{\hbar^2\gamma^2}{2m} + \frac{\hbar^2\delta^2}{2m}\right)\left(\delta_{\alpha\gamma}\delta_{\beta\delta} - \delta_{\alpha\delta}\delta_{\beta\gamma}\right)$$

which agrees with the 1st quantized theory.

Another Example $\langle \alpha\beta | \Omega | \alpha\beta \rangle$

$$= \langle 0 | c_\beta c_\alpha \frac{1}{2}\int d^3r_1 d^3r_2 v_{12} \; \psi^+(\vec r_1)\, \psi^+(\vec r_2)\, \psi(\vec r_2)\, \underbrace{\psi(\vec r_1)\, c_\alpha^+}\, c_\beta^+ | 0 \rangle$$

$$\underbrace{\psi(\vec r_1) c_\alpha^+} = \{ \psi(\vec r_1), c_\alpha^+ \} - c_\alpha^+ \psi(\vec r_1)$$
$$= u_\alpha(\vec r_1) - c_\alpha^+ \psi(\vec r_1)$$

$$\Omega_{\alpha\beta,\alpha\beta} = \frac{1}{2}\int d^3r_1 d^3r_2 v_{12} \langle 0 | c_\beta c_\alpha \psi^+(\vec r_1) \psi^+(\vec r_2) \underbrace{\psi(\vec r_2) c_\beta^+ | 0 \rangle}_{= u_\beta(\vec r_2) | 0 \rangle} u_\alpha(\vec r_1)$$

+ Other Term

$$= \frac{1}{2}\int d^3r_1 d^3r_2 v_{12} \langle \underbrace{0 | c_\beta c_\alpha \psi^+(\vec r_1) \psi^+(\vec r_2) | 0}\rangle \; u_\alpha(\vec r_1) u_\beta(\vec r_2)$$

+ O.T.

$$\longrightarrow u_\alpha^*(r_1)\, u_\beta^*(r_2) - u_\alpha^*(r_2)\, u_\beta^*(r_1)$$

$$= \int d^3r_1 d^3r_2 v_{12} \{ |u_\alpha(\vec r_1)|^2 |u_\beta(\vec r_2)|^2$$

DIRECT INTERACTION

$$- u_\alpha^*(\vec r_2) u_\alpha(\vec r_1) \; u_\beta^*(\vec r_1) u_\beta(\vec r_2) \}$$

EXCHANGE INTERACTION

(Hartree Fock model)

which agrees with the 1st quantized theory.

One more thing ...

We defined the fermionic operators c_k and c_k † by anticommutators. *Can we still interpret them as annihilation and creation operators?*

Read Mandl and Shaw Section 4.1.

Review the bosonic annihilation and creation operators

- $[\, a_{\mathbf{k}} , a_{\mathbf{k}'}^\dagger \,] = \delta(\mathbf{k},\mathbf{k}')$
  $[\, a_{\mathbf{k}} , a_{\mathbf{k}'} \,] = 0$ and $[\, a_{\mathbf{k}}^\dagger , a_{\mathbf{k}'}^\dagger \,] = 0$
- $N_{op} = \sum a_{\mathbf{k}}^\dagger a_{\mathbf{k}}$
- Therefore

$$[\, N , a_{\mathbf{k}} \,] = a_{\mathbf{k}}^\dagger a_{\mathbf{k}} a_{\mathbf{k}} - a_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} = [\, a_{\mathbf{k}}^\dagger , a_{\mathbf{k}} \,] a_{\mathbf{k}} = - a_{\mathbf{k}}$$

$$\boldsymbol{[\, N , a_{\mathbf{k}} \,] = - a_{\mathbf{k}} \quad \text{and} \quad [\, N , a_{\mathbf{k}}^\dagger \,] = + a_{\mathbf{k}}^\dagger}$$

- *Therefore a_k is an annihilation operator and $a_{\mathbf{k}}$ † is a creation operator.*

$$N_{op}\, a\, |N\rangle = (- a + a N_{op})\, |N\rangle = (N - 1)\, a\, |N\rangle$$

Now consider fermionic operators

- $\{\, c_{\mathbf{k}} , c_{\mathbf{k}'}^\dagger \,\} = \delta(\mathbf{k},\mathbf{k}')$
  $\{\, c_{\mathbf{k}} , c_{\mathbf{k}'} \,\} = 0$ and $\{\, c_{\mathbf{k}}^\dagger , c_{\mathbf{k}'}^\dagger \,\} = 0$
- $N_{op} = \sum c_{\mathbf{k}}^\dagger c_{\mathbf{k}}$
- Therefore

$$[\, N , c_{\mathbf{k}} \,] = c_{\mathbf{k}}^\dagger c_{\mathbf{k}} c_{\mathbf{k}} - c_{\mathbf{k}} c_{\mathbf{k}}^\dagger c_{\mathbf{k}} = - c_{\mathbf{k}} c_{\mathbf{k}}^\dagger c_{\mathbf{k}} = -(1 - c_{\mathbf{k}}^\dagger c_{\mathbf{k}})\, c_{\mathbf{k}} = - c_{\mathbf{k}}$$

$$\boldsymbol{[\, N , c_{\mathbf{k}} \,] = - c_{\mathbf{k}} \quad \text{and} \quad [\, N , c_{\mathbf{k}}^\dagger \,] = + c_{\mathbf{k}}^\dagger}$$

so again c_k is annihilation and c_k † is creation. *(Jordan and Wigner, 1928)*

Homework due Friday, Feb. 3

Problems 11, 12, 13, 14

Problem 15:

In the second quantized theory of 2 identical fermions, calculate

$$\langle 0|\, c_\alpha\, c_\beta\, \psi^\dagger(\mathbf{r}_1)\, \psi^\dagger(\mathbf{r}_2)\, |0\rangle$$

where c_α *is the annihilation operator for a particle with wave function* $u_\alpha(\mathbf{r})$.