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.

3. THE METHOD OF QUANTIZED FIELDS

also called "second quantization"

Consider a system with N identical particles.

In the first-quantized theory,
the wave function is $\Psi(q_1\ q_2\ q_3 \dots q_N ; t)$
where q_i = the coordinates of particle i .
The goal is to solve the time evolution,

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

Or, equivalently, find the energy eigenstates,

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

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

3a - The quantized field operator

/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:*

Boson field

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

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

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

Fermion field

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

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

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

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

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

/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 $\boldsymbol{v}_{12} = \boldsymbol{v}(\boldsymbol{r}_1 - \boldsymbol{r}_2)$.

The Number Operator in the second quantized theory is

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

Note that $\psi(\mathbf{r})$ sort of resembles a wave function. However, it is not a wave function – it is an *operator* in the Fock space.

3b - 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} =

$$H = -\frac{\hbar^2}{2m}\left(\nabla_1^2 + \nabla_2^2 + \dots + \nabla_N^2\right) + \sum_{i<j} V(\vec{r}_i, \vec{r}_j)$$

← sum of $\frac{1}{2}N(N-1)$ 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.

An important little theorem

For the second quantized theory …

$$[\, H , N_{op}] = 0$$

Proof

Consequences

- The number of particles is constant in time.
- An energy eigenstate is simultaneously an eigenstate of the number of particles.
- We can just fix N at the beginning of a calculation, and then forget it.

Proof (for a fermion field)

$$[\, H , N_{op} \,] = [\, T , N_{op} \,] + [\, V , N_{op} \,]$$

Now calculate from the *field anticommutators* …

$$t = -\frac{\hbar^2}{2m} \nabla^2$$

$$[T, N] = \int d^3r \, [\psi^\dagger(\vec{r})\, t \, \psi(\vec{r}), N]$$

$$= \int d^3r \left(\psi^\dagger(\vec{r}) [t\psi, N] + [\psi^\dagger(\vec{r}), N]\, t\psi \right)$$

$$[\psi^\dagger(\vec{r}), N] = \int d^3y \, [\psi^\dagger(\vec{r}), \psi^\dagger(\vec{y})\psi(\vec{y})]$$

$$= \int d^3y \Big(\underbrace{\{\psi^\dagger(\vec{r}), \psi^\dagger(\vec{y})\}}_{0} \psi(\vec{y}) - \psi^\dagger(\vec{y}) \underbrace{\{\psi^\dagger(\vec{r}), \psi(\vec{y})\}}_{\delta^3(\vec{r}-\vec{y})} \Big)$$

$$= -\psi^\dagger(\vec{r})$$

and similarly $[\psi(\vec{r}), N] = \psi(\vec{r})$.

Thus $[T, N] = \int d^3r \left(\psi^\dagger(\vec{r})\, t\, \psi(\vec{r}) - \psi^\dagger(\vec{r})\, t\, \psi(\vec{r}) \right)$

$= 0$

Homework Problem: Show $[\Omega, N_{op}] = 0$.

Result $[H, N] = 0$. QED

The Big Theorem

THEOREM

Define the N-particle wave function from the second quantized theory by

$$\Phi_{EN}(\vec{r}_1\ \vec{r}_2 \ldots \vec{r}_N) = \frac{1}{\sqrt{N!}} \langle 0 | \psi(\vec{r}_1)\, \psi(\vec{r}_2) \ldots \psi(\vec{r}_N) | EN \rangle$$

$|0\rangle$ = the state with $N_{op}|0\rangle = 0$ "Vacuum"

$|EN\rangle$ = the state with $N_{op}|EN\rangle = N\,|EN\rangle$
and $H\,|EN\rangle = E\,|EN\rangle$.

This function obeys the Schroedinger equation of the first quantized theory; i.e.,

$$-\frac{\hbar^2}{2m}\sum_{i=1}^{N} \nabla_i^2\, \Phi_{EN} + \sum_{i<j} v_{ij}\, \Phi_{EN} = E\, \Phi_{EN}(\vec{r}_1 \ldots \vec{r}_N)$$

Because of the commutation [or anticommutation] postulate for the field operator ψ(r) , the wave function $\Phi(r_1\ r_2 \ldots r_N)$ has the correct exchange symmetry [or antisymmetry].

Corollary. The first and second quantized theories have the same energy eigenstates. *(That goes a long way toward proving the big theorem.)*

Proof of the THEOREM

We start with $H\ |E,N\rangle = E\ |E,N\rangle$.

Then

$$E\ \Phi_{EN}\ (\mathbf{r}_1 \ldots \mathbf{r}_N) =$$

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

Remember, $H|0\rangle = 0$; and $\langle 0|H = 0$.

Repeatedly commute H to the left until it acts on $\langle 0|$, at which point the result is 0.

First step: $\psi(r_N)\ H = [\ \psi(r_N)\ , H\ ] + H\ \psi(r_N)$
2nd step: $\psi(r_{N-1})\ H = [\ \psi(r_{N-1})\ , H\ ] + H\ \psi(r_{N-1})$
etc: $\psi(r_j)\ H = [\ \psi(r_j)\ , H\ ] + H\ \psi(r_j)$
last step: $\psi(r_1)\ H = [\ \psi(r_1)\ , H\ ] + H\ \psi(r_1) = [\ \psi(r_1)\ , H\ ]$

Lemma *(you prove it)*

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

where

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

Therefore ….

$$E\,\Phi_{EN} = -\,\hbar^2/(2m)\sum_{j=1}^{N}\nabla_j^{\,2}\,\Phi_{EN}\,(\mathbf{r}_1 \ldots \mathbf{r}_N)$$

$$+\ 1/\text{SQRT}(N!)\sum_{j=1}^{N}\langle 0\,|\,\psi(1)\ldots\psi(j-1)X(j)\psi(j)\ldots\psi(N)\,|\,E,N\rangle$$

Now commute X(j) all the way to the left; note

$\langle 0\,|\,X(j) = 0$ and $[\,\psi(i)\,,\,X(j)\,] = \boldsymbol{v}_{ij}\,\psi(i)\,\psi(j)\,;$

… so the final result is

$$E\,\Phi_{EN} =$$

$$-\,\hbar^2/(2m)\sum\nabla_j^{\,2}\,\Phi_{EN}\,(\mathbf{r}_1 \ldots \mathbf{r}_N)$$

$$+\sum \boldsymbol{v}_{ij}\,\Phi_{EN}\,(\mathbf{r}_1 \ldots \mathbf{r}_N)$$

Q.E.D.

The energy states of the second quantized theory are the same as those of the first quantized theory; and the eigenfunctions are determined by

$$\Phi_{EN}(\vec{r}_1\,\vec{r}_2 \ldots \vec{r}_N) = \frac{1}{\sqrt{N!}}\langle 0\,|\,\psi(\vec{r}_1)\,\psi(\vec{r}_2)\ldots\psi(\vec{r}_N)\,|\,EN\rangle$$

Homework due Friday, Feb. 3

Problem 13.

Prove that $[\Omega, N] = 0$ where Ω is the two-particle interaction potential for identical fermions and N is the total number operator.

Problem 14.

Let $\psi_\alpha(\mathbf{r},t)$ be the *field operator* for spin-½ fermions, in the Heisenberg picture; α = spin coordinate.
Derive the field equation for $\psi(\mathbf{r},t)$ in the form

$$i\hbar\, \partial\psi / \partial t = F[\psi]$$

where $F[\psi]$ is a functional—which may involve derivatives and integrals. Simplify the result as much as possible.
[[Assume that $\tau = -\hbar^2\nabla^2/2m$ and that $v(\mathbf{r_1},\mathbf{r_2})$ is spin independent.]]