Chapter 1 : SECOND QUANTIZATION

Review

$$H = \sum_{ij} c_i^+ < i\,|T|\,j > c_j + \sum_{ij} c_i^+ c_j^+ < ij\,|V|\,kl > \; c_l\, c_k$$

$$[c_i\,, c_j]_{\pm} = [c_i^+\,, c_j^+\,]_{\pm} = 0$$

$[c_i\,, c_j^{\,+}]_{\pm} = \delta_{ij}$ for fermions / for bosons

2. FIELDS

So far we have written the N-particle theory in terms of some complete set of single-particle states.

The ***s.p.*** wave functions are denoted by $\psi_E(x)$ where x = a set of coordinates for one particle, and E = a set of quantum numbers for one particle.

The annihilation and creation operators, e.g., denoted by c_i and $c_j^{\,\dagger}$, annihilate or create a particle in the state ψ_{Ei} or ψ_{Ej} , respectively.

But we could choose a different set of ***s.p.*** states, which would result in a different set of wave functions and quantum numbers; *but it is still the same theory* — just a different basis.

Now we define a ***quantized field*** for the particles, such that the the theory no longer depends on any specific set of ***s.p.*** states.

We have the theory written in terms of a specific set of single particle states.

$$H = \sum_{ij} c_i^+ < i\,|T|\,j > c_j$$
$$+ \sum_{ij} c_i^+ c_j^+ < ij\,|V|\,kl > \; c_l\, c_k$$

$$[c_i\,, c_j]_\pm = [c_i^+\,, c_j^+]_\pm \;= 0$$

$[c_i\,, c_j^{\,+}]_\pm \;= \delta_{ij}$ for fermions / for bosons

Now…

- define the ***field operator*** for these "particles";
- figure out the defining equations of the field (i.e., commutations relations);
- and, what is the Hamiltonian?

Now define field operators, $\hat{\psi}(\vec{x})$ and $\hat{\psi}^+(\vec{x})$, which are independent of the choice of s.p. states, but depend on the coordinate.

$$\hat{\psi}(\vec{x}) = \sum_{i=1}^{\infty} \psi_{E_i}(\vec{x})\, c_i$$

$$\hat{\psi}^+(\vec{x}) = \sum_{i=1}^{\infty} \psi^+_{E_i}(\vec{x})\, c_i^+$$

Commutation relations

$$\left\{ \begin{matrix} \text{upper case} \\ \text{lower case} \end{matrix} \right\} = \left\{ \begin{matrix} \text{bosons} \\ \text{fermions} \end{matrix} \right\}$$

$$\left[\hat{\Psi}(\vec{x}), \hat{\Psi}(\vec{x}')\right]_\pm = \sum_i \sum_j \psi_{E_i}(\vec{x})\, \psi_{E_j}(\vec{x}') \underbrace{[c_i, c_j]_\pm}_{0}$$

$$= 0$$

and

$$\left[\hat{\Psi}(\vec{x}), \hat{\Psi}^\dagger(\vec{x}')\right]_\pm = \sum_i \sum_j \psi_{E_i}(\vec{x})\, \psi^\dagger_{E_j}(\vec{x}') \underbrace{[c_i, c_j^\dagger]_\pm}_{\delta_{ij}}$$

$$= \sum_i \psi_{E_i}(\vec{x})\, \psi^\dagger_{E_i}(\vec{x}')$$

$$= \delta^3(\vec{x} - \vec{x}')$$ ← by completeness of the single-particle states

The Hamiltonian in field theory

We have, in second quantization

$$\hat{H} = \sum_{ij} \langle i | T | j \rangle\, c_i^\dagger c_j$$

$$+ \frac{1}{2} \sum_{ijkl} \langle ij | V | kl \rangle\, c_i^\dagger c_j^\dagger c_l c_k$$

Compare

$$\int \hat{\Psi}^\dagger(\vec{x})\, T(\vec{x})\, \hat{\Psi}(\vec{x})\, (d\tau)$$

$$= \sum_i \sum_j c_i^\dagger \int \psi^\dagger_{E_i}(\vec{x})\, T(\vec{x})\, \psi_{j}(\vec{x})\, (d^3\tau)\, c_j$$

$$= \sum_{ij} \langle i | T | j \rangle\, c_i^\dagger c_j$$

And

$$\iint \hat{\Psi}^\dagger(\vec{x})\, \hat{\Psi}^\dagger(\vec{x}')\, V(\vec{x}, \vec{x}')\, \hat{\Psi}(\vec{x}')\, \hat{\Psi}(\vec{x})\, (d\tau)(d\tau')$$

$$= \sum_{ijkl} c_i^\dagger c_j^\dagger \iint \psi^\dagger_{E_i}(x)\, \psi^\dagger_{E_j}(x')\, V(x, x')\, \psi_{E_l}(x')\, \psi_{E_k}(x)\, (d\tau)(d\tau')\; c_l c_k$$

$$= \sum_{ijkl} \langle ij | V | kl \rangle\, c_i^\dagger c_j^\dagger c_l c_k$$

So, in terms of field operators,

$$\hat{H} = \int \hat{\Psi}^{+}(\vec{x})\, T(\vec{x})\, \Psi(\vec{x})\, (d\tau)$$
$$+ \frac{1}{2} \iint \hat{\Psi}^{+}(\vec{x})\, \hat{\Psi}^{+}(\vec{x}')\, V(x,x')\, \hat{\Psi}(x')\, \hat{\Psi}(x)\, (d\tau)(d\tau')$$

looks like the 1^{st} quantized Hamiltonian!!
But it's different, because have
$$\left[\hat{\Psi}(\vec{x}),\ \hat{\Psi}^{+}(\vec{x}')\right]_{\pm} = \delta^3(\vec{x}-\vec{x}').$$
$\hat{\Psi}(\vec{x})$ is an operator that annihilates a particle, and $\hat{\Psi}^{+}(\vec{x})$ creates a particle.

One body operators

Consider $\quad J = \sum_{k=1}^{N} J(\vec{x}_k)$,

a general one-body operator in first-quantized form.

In second quantized form,
$$J = \sum_{r,s} \langle r|J|s\rangle\, c_r^{+} c_s .$$
In field theoretic form
$$\hat{J} = \int d^3x\ \hat{\Psi}^{+}(\vec{x})\, J(\vec{x})\, \hat{\Psi}(\vec{x}).$$

For example, the number density is
$$n(\vec{x}) = \sum_{k=1}^{N} \delta^3(\vec{x}-\vec{x}_k) \qquad \text{first quantized}$$
or $$\hat{n}(\vec{x}) = \hat{\Psi}^{+}(\vec{x})\, \hat{\Psi}(\vec{x}) \qquad \text{second quantized}$$
The number operator is
$$\hat{N} = \int \hat{n}(\vec{x})\, d^3x = \int \hat{\Psi}^{+}(\vec{x})\, \hat{\Psi}(\vec{x})\, d^3x .$$
(first quantized: $N = N$; second quantized: $N = \sum_{i=1}^{\infty} c_i^{+} c_i$)

Field operators and wave functions

What is an electron?

particle or wave?

The answer from quantum field theory: there is an electron *field* $\psi(x)$, and the electron is the quantum* of the field.

$\psi(x)$ annihilates an electron;
$\psi^{+}(x)$ creates an electron.

*quantum = single excitation

But then what is the "wave function"?

Dirac provided the answer.
For a single particle in the state with quantum numbers E,

$$\psi_E(x) = \langle x \mid E \rangle$$

where $| E \rangle = c_E^{+} | \text{vacuum} \rangle$;

$$c_E^{+} = \int \psi^{+}(x)\, \psi_E(x)\, d\tau \, .$$

All of this is just formal theory.
What can we actually calculate from it?