CHAPTER 1. SECOND QUANTIZATION

Review of Section 1:

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

for fermions / for bosons

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

$$[\, c_i \,, c^{*} \,]_{\pm} = \delta_{ij}$$

- In Chapter 1, F&W explain the basic theory:
  - Start from the many-particle Schroedinger equation ("1st quantized") ;
  - Introduce creation and annihilation operators for bosons and fermions ("2nd quantized") ;
  - Section 2: Introduce the *field operator* $\Psi_{\propto}(x)$.
- In Chapter 3, F&W will explain how to use this theory to do calculations for many-particle systems.
- Today: Summarize the general principles of NRQFT.

Section 2:

- define the ***field operator*** for these "particles"; (in fact, we already did this)
- figure out the defining equations of the field; (i.e., the commutation relations)
- and, what is the Hamiltonian?

Field operators $\hat{\Psi}(\vec{x})$ and $\hat{\Psi}^{\dagger}(\vec{x})$

They depend on the coordinates (space & spin)

I'm suppressing that.

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

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

in terms of a complete set of basis functions $\psi_{E_i}(\vec{x})$; but $\Psi(\vec{x})$ does not depend on the choice of basis functions. I.e., we could expand in different basis functions $\longrightarrow$ same field.

## The quantum field

- The field operator $\Psi_\alpha(\mathbf{x})$ annihilates a particle at position $\mathbf{x}$.

> ★ $\alpha$ is the spin component.
> ★ For spin 0 bosons there is no $\alpha$
> ★ For spin-½ fermions, $\Psi_\alpha(\mathbf{x})$ is a 2-component operator ; $\alpha$ = +1 (or -1) for the upper (or lower) component.

The adjoint field operator $\Psi_\alpha^\dagger(\mathbf{x})$ creates a particle at $\mathbf{x}$.

- The actions of $\Psi_\alpha(\mathbf{x})$ and $\Psi_\alpha^\dagger(\mathbf{x})$ in the Hilbert space are based on postulated commutation relations (for bosons) or anti-commutation relations (for fermions).

For spin 0 bosons,

$$[\Psi(\vec{x}), \Psi^\dagger(\vec{y})] = \delta^3(\vec{x}-\vec{y})$$
$$[\Psi(\vec{x}), \Psi(\vec{y})] = 0 \qquad [A,B] = AB - BA$$

For spin ½ fermions,

$$\{\Psi_\alpha(\vec{x}), \Psi_\beta^\dagger(\vec{y})\} = \delta^3(\vec{x}-\vec{y})\,\delta_{\alpha\beta}$$
$$\{\Psi_\alpha(\vec{x}), \Psi_\beta(\vec{y})\} = 0 \qquad \{A,B\} = AB + BA$$

Note:

for bosons, $\Psi(\vec{x})\,\Psi(\vec{y}) = \Psi(\vec{y})\,\Psi(\vec{x})$

for fermions, $\Psi_\alpha(\vec{x})\,\Psi_\beta(\vec{y}) = -\Psi_\beta(\vec{y})\,\Psi_\alpha(\vec{x})$

> In Chapter 3 we'll introduce "particles and holes"; then $\Psi$ can annihilate a particle or create a hole; and $\Psi^\dagger$ can create a particle or annihilate a hole.
> In relativistic QFT, $\Psi$ can annihilate an electron or create a positron.

■ The Hamiltonian operator for spin-½ particles is

$$H = \int d^3x\, \psi^\dagger_\alpha(\vec{x})\, T_{\alpha\beta}(\vec{x})\, \psi_\beta(\vec{x}) + \frac{1}{2}\int d^3x\, d^3x'\, \psi^\dagger_\alpha(\vec{x})\, \psi^\dagger_{\alpha'}(\vec{x}')\, V_{\alpha\alpha'\beta\beta'}(\vec{x},\vec{x}')\, \psi_{\beta'}(\vec{x}')\, \psi_\beta(\vec{x})$$

where

$$T_{\alpha\beta}(\vec{x}) = \underbrace{\delta_{\alpha\beta}\left(-\frac{\hbar^2\nabla^2}{2m}\right)}_{\text{KINETIC ENERGY}} + \underbrace{U_{\alpha\beta}(\vec{x})}_{\text{SINGLE PARTICLE POTENTIAL ENERGY W/ SPIN DEPENDENCE}}$$

$$V_{\alpha\alpha'\beta\beta'}(\vec{x},\vec{x}') = V_0(\vec{x}-\vec{x}')\,\delta_{\alpha\beta}\,\delta_{\alpha'\beta'} + V_3(\vec{x}-\vec{x}')\,\vec{\sigma}_{\alpha\beta}\cdot\vec{\sigma}_{\alpha'\beta'}$$

TWO PARTICLE INTERACTION W/ POSSIBLE SPIN DEPENDENCE

If Ψ(x) were the Schroedinger wave function of a particle then the first term would be the expectation value of the kinetic energy;
the second term would be the expectation value of V in a two-particle wave function;

but Ψ(x) is not the Schroedinger wave function of a particle—it is the quantum field operator.

The theory based on these postulates (NRQFT) implies the equations of N-particle Schroedinger wave mechanics.

Define the Schroedinger wave function

$$\Phi_\alpha(x_1 \cdots x_N; t) = \langle 0 | e^{iHt/\hbar} \hat{\psi}(x_1) \cdots \hat{\psi}(x_N) \, e^{-iHt/\hbar} | \alpha \rangle$$

and show that this obeys the time-dependent Schroedinger equation.

$$i\hbar \frac{\partial}{\partial t} \Phi_\alpha = H_N \Phi_\alpha$$

where $H_N = \sum_{k=1}^{N} T_k + \frac{1}{2} {\sum_{k,l}}' V(x_k, x_l)$

- In field theory, the *number density operator* is

$$n(\vec{x}) = \psi_\alpha^\dagger(\vec{x})\,\psi_\alpha(\vec{x})$$

where the sum over α from -1 to +1 is implied. Repeated spin indices are summed by convention.

and the *total number operator* is

$$N = \int \psi_\alpha^\dagger(\vec{x})\,\psi_\alpha(\vec{x})\,d^3x$$

Compare 3 formulations

| | no. density operator | number operator |
|---|---|---|
| 1st quantized | $\sum_{k=1}^{N} \delta^3(\vec{x}-\vec{x}_k)$ | $N$ |
| 2nd quantized | $\sum_{i=1}^{\infty}\sum_{j=1}^{\infty} \psi_i^*(\vec{x})\,\psi_j(\vec{x})\,c_i^\dagger c_j$ | $\sum_{i=1}^{\infty} c_i^\dagger c_i$ |
| Q.F.T. | $\Psi^\dagger(\vec{x})\,\Psi(\vec{x})$ | $\int \Psi^\dagger(\vec{x})\,\Psi(\vec{x})\,d^3x$ |

# A crucial theorem of NRQFT

$$[H, N] = 0$$

Proof (for a fermion field)

$$[H, N] = [T, N] + [V, N]$$

Rewrite in terms of field anticommutators

$$[T, N] = \int d^3x \, [\psi^\dagger(x) T_x \psi(x), N]$$
$$= \int d^3x \, \{ \psi^\dagger [T\psi, N] + [\psi^\dagger, N] T\psi \}$$

$$[\psi^\dagger, N] = \int d^3y \, [\psi^\dagger(x), \psi^\dagger(y)\psi(y)]$$
$$= \int d^3y \, \{ \underbrace{\{\psi^\dagger(x), \psi^\dagger(y)\}}_{0} \psi(y) - \psi^\dagger(y) \underbrace{\{\psi^\dagger(x), \psi(y)\}}_{\delta^3(x-y)} \}$$
$$= -\psi^\dagger(x)$$

Similarly, $[\psi(x), N] = \psi(x)$

Thus

$$[T, N] = \int d^3x \, \{ \psi^\dagger(x) T\psi(x) - \psi^\dagger(x) T\psi(x) \}$$
$$= 0.$$

Homework Problem : $[V, N] = 0$.

Thus $[H, N] = 0$

# $[\,H\,,N\,] = 0$

Corollary #1

The energy eigenstates are also particle number eigenstates.

Proof: Commuting operators have common eigenstates.

Corollary #2

The total number of particles is constant in time.

Proof: H is the generator of translation in time.

## Consider N = 0

In NRQFT, the state with no particles is just empty space. (RQFT is different!)

$|\,0\,>$ has $H\,|\,0\,> = 0$ and $N\,|\,0\,> = 0$.

## Consider N = 1

An energy eigenstate with N = 1 and energy E is $|\,E,1\,>$ .

Define the Schroedinger wave function for this state,

$$\varphi_\alpha(\mathbf{x}) = <0\,|\;\Psi_\alpha(\mathbf{x})\;|\,E,1> .$$

$$\langle 0|\;\underbrace{\psi_\alpha H - H\psi_\alpha}\,|1\rangle = E\,\langle 0|\psi_\alpha|1\rangle = E\,\varphi_\alpha$$

$$[\psi_\alpha, H] = [\psi_\alpha, \textstyle\int \psi_\beta^\dagger T \psi_\beta]$$

$$= \underbrace{\{\psi_\alpha, \psi_\beta^\dagger\}}_{=\,\delta_{\alpha\beta}\,\delta^3(x-x')} T\psi_\beta - \psi_\beta^\dagger \underbrace{\{\psi_\alpha, T\psi_\beta\}}_{=\,0}$$

$$= T\psi_\alpha = -\frac{\hbar^2}{2m}\nabla^2\psi_\alpha + U\psi_\alpha$$

$$\therefore\; E\,\varphi_\alpha = -\frac{\hbar^2}{2m}\nabla^2\varphi_\alpha + U\varphi_\alpha \quad \text{as expected}$$

## Consider N = 2

An energy eigenstate with N = 2 and energy E is $|E,2>$ .

Define the Schroedinger wave function for this state,

$$\varphi_{\alpha 1\, \alpha 2}(\mathbf{x_1}, \mathbf{x_2}) = < 0 |\ \Psi_{\alpha 1}(\mathbf{x_1})\, \Psi_{\alpha 2}(\mathbf{x_2})\ | E,2 >$$

<u>Theorem 1.</u>

$\varphi_{\alpha 1\, \alpha 2}(x_1,x_2)$ is antisymmetric under exchange of particle coordinates.
(obvious because $\{\psi,\psi\} = 0$ .)

<u>Theorem 2.</u>

$\varphi_{\alpha 1\, \alpha 2}(x_1,x_2)$ obeys the 2-particle Schroedinger equation.

## Consider arbitrary N

$$\Phi(x_1 \ldots x_N) = \langle 0 | \psi(x_1) \ldots \psi(x_N) | E, N \rangle$$

energy eigenstate with N particles

$$\Rightarrow$$

$$E\,\Phi = -\frac{\hbar^2}{2m} \sum_{k=1}^{N} \nabla_k^2 \Phi + \sum_{k=1}^{N} U(\vec{x}_k)\,\Phi$$
$$+ \sum_{\substack{\text{pairs}\\(k,\ell)}} V_2(x_k, x_\ell)\,\Phi$$

## Field operators and wave functions

What is an electron?

Is it a particle or a wave?

We could ask the same questions for photons. In electromagnetism, the field **A**($\mathbf{x}$) is a quantum operator, which annihilates and creates photons.

The answer for electrons is the same, from quantum field theory:

There is an electron field $\Psi(\mathbf{x})$, and the electron is the ***quantum**** of the field.

$\Psi(\mathbf{x})$ annihilates an electron ***at x***;

$\Psi^{\dagger}(\mathbf{x})$ creates an electron ***at x***.

OK; then what is the "wave function"?

Dirac provided the answer.

For a single particle in the state with quantum numbers E, the wave function is

$$\varphi_E(\mathbf{x}) = \langle \text{vacuum} \,|\, \Psi(\mathbf{x}) \,|\, \mathbf{E} \rangle$$

where $|\,\mathbf{E}\rangle = c_E^{\dagger}\,|\,\text{vacuum}\rangle$ ;

$$c_E^{\dagger} = \int \Psi^{\dagger}(\mathbf{x})\, \varphi_E(\mathbf{x})\, d^3x \,.$$

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All of this is just formal theory.

What can we actually calculate from it?

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**quantum = single excitation*

Homework due Friday, Feb. 5

**Problem 14.**

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

**Problem 15.**

Let $\Psi(x,t)$ be the field operator for a spin-½ fermion, in the Heisenberg picture. Derive the field equation for $\Psi(x,t)$, 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 $T(x) = -\hbar^2 \nabla^2 / 2m$ and that $V(x_1,x_2)$ is spin independent.]]