Finishing Chapter 1

Review of Chapter 1 and Preview of Chapter 3

Chapter 1 : second quantization

Chapter 3 : methods of nonrelativistic quantum field theory (NRQFT)

In Chapter 1, F&W derive the equations of NRQFT: Start from the many-particle Schroedinger equation (1st quantized) ; introduce second quantization, i.e., creation and annihilation operators; define the field operator $\psi_\alpha(\mathbf{x})$.

Today I'll do the opposite: Start from the equations of NRQFT as postulates; then derive the many-particle Schroedinger equation.

The postulates of NRQFT

(as deduced from chapter 1)

■ The states are elements of an abstract Hilbert space, called "Fock space".

Let $\{\psi_E(x) : E = E_1\ E_2\ E_3 \ldots E_i \ldots E_\infty\}$ be a complete set of single particle wave functions, where E_i = a set of s.p. quantum numbers .
The basis states for Fock space are the occupation number states
$| n_1\ n_2\ n_3 \ldots n_i \ldots n_\infty >$

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

α is the spin component.
For spin 0 bosons there is no α.
For spin-½ fermions, ψ(x) is a 2-component operator ; α = +½ (or -½) 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,

$$[\hat{\psi}(\vec{x}), \hat{\psi}(\vec{y})] = 0 \quad \text{where } [A,B] = AB - BA$$

$$[\hat{\psi}^\dagger(\vec{x}), \hat{\psi}^\dagger(\vec{y})] = 0$$

$$[\hat{\psi}(\vec{x}), \hat{\psi}^\dagger(\vec{y})] = \delta^3(\vec{x}-\vec{y})$$

For spin ½ fermions,

$$\{\hat{\psi}_\alpha(\vec{x}), \hat{\psi}_\beta(\vec{y})\} = 0 \quad \text{where } \{A,B\} = AB + BA$$

$$\{\hat{\psi}_\alpha^\dagger(\vec{x}), \hat{\psi}_\beta^\dagger(\vec{y})\} = 0$$

$$\{\hat{\psi}_\alpha(\vec{x}), \hat{\psi}_\beta^\dagger(\vec{y})\} = \delta_{\alpha\beta}\, \delta^3(\vec{x}-\vec{y})$$

Note:

$$\text{for bosons} \quad \hat{\psi}(x)\hat{\psi}(y) = \hat{\psi}(y)\hat{\psi}(x)$$

$$\text{for fermions} \quad \hat{\psi}_\alpha(x)\hat{\psi}_\beta(y) = -\hat{\psi}_\beta(y)\hat{\psi}_\alpha(x)$$

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

■ The number density operator is

n(x) = $$\hat{n}(\vec{x}) = \hat{\psi}^{\dagger}_{\alpha}(\vec{x})\,\hat{\psi}_{\alpha}(\vec{x})$$

sum over alpha from -½ to +½ is implied. Repeated spin indices are summed by convention.

and the total number operator is

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

■ The Hamiltonian operator is

$$\hat{H} = \int d^3x\ \hat{\psi}^{\dagger}_{\alpha}(\vec{x})\,T_{\alpha\beta}\,\hat{\psi}_{\beta}(x)$$

$$+\ \frac{1}{2}\int d^3x\, d^3x'\ \hat{\psi}^{\dagger}_{\alpha}(x)\,\hat{\psi}^{\dagger}_{\alpha'}(x')\,V_{\alpha\alpha';\beta\beta'}(\vec{x},\vec{x}')\,\hat{\psi}_{\beta'}(x')\,\hat{\psi}_{\beta}(x)$$

where

$$T^{(x)}_{\alpha\beta} = \delta_{\alpha\beta}\left(\frac{-\hbar^2\nabla_x^2}{2m}\right) + v_{\alpha\beta}(x)$$

kinetic energy

single particle potential energy; usually $v_{\alpha\beta} = 0$.

and

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

= 2 particle interaction potential

To Prove: that the theory based on these postulates (NRQFT) implies the equations of N-particle Schroedinger wave mechanics.

Theorem $[\hat{H}, \hat{N}] = 0$

Proof (for a fermion field)
Prove it using the anticommutators.

$$[\hat{H}, \hat{N}] = [\hat{T}, \hat{N}] + [\hat{V}, \hat{N}]$$

$$[\hat{T}, \hat{N}] = \int d^3x \, [\hat{\psi}^{+}_{\alpha}(x) T_{\alpha\beta} \hat{\psi}_{\beta}(x), \hat{N}]$$

$$[AB, C] = A[B,C] + [A,C]B$$
$$= ABC - ACB + ACB - CAB \checkmark$$

$$= \int d^3x \{ \psi^{+}_{\alpha} [T_{\alpha\beta}\psi_{\beta}, N] + [\psi^{+}_{\alpha}, N] T_{\alpha\beta}\psi_{\beta} \}$$

$$[\psi^{+}_{\alpha}, N] = \int d^3y \, [\psi^{+}_{\alpha}(x), \psi^{+}_{\gamma}(y)\psi_{\gamma}(y)]$$

$$[D, EF] = \{D,E\}F - E\{D,F\}$$
$$= DEF + EDF - EDF - EFD \checkmark$$

$$[\psi^{+}_{\alpha}, N] = \int d^3y \{ 0 \, \psi_{\gamma}(y) - \psi^{+}_{\gamma}(y) \delta_{\alpha\gamma} \delta^3(x-y) \}$$
$$= -\psi^{+}_{\alpha}(x)$$

Also....

$$[T_{\alpha\beta}\psi_{\beta}, N] = T_{\alpha\beta}[\psi_{\beta}, N]$$
$$= T_{\alpha\beta}[N^{+}, \psi^{+}_{\beta}]^{+} \quad \text{because } (AB)^{+} = B^{+}A^{+}$$
$$= T_{\alpha\beta}(- - \psi^{+}_{\beta}(x))^{+} \quad \text{because } N^{+} = N$$
$$= T_{\alpha\beta}\psi_{\beta}(x) \quad \text{because } (\psi^{+})^{+} = \psi$$

Thus $[\hat{T}, \hat{N}] = \int d^3x \{ \psi^{+}_{\alpha} T_{\alpha\beta}\psi_{\beta} - \psi^{+}_{\alpha} T_{\alpha\beta}\psi_{\beta} \}$
$= 0$

Similarly (H.W. problem 3) $[\hat{V}, \hat{N}] = 0$

Thus $[\hat{H}, \hat{N}] = 0$.

Corollary

The energy eigenstates are also particle number eigenstates.

Proof

Because $[\hat{H}, \hat{N}] = 0$. Q.E.D.

$\therefore$ Let $\hat{H}|E,N\rangle = E|E,N\rangle$

and $\hat{N}|E,N\rangle = N|E,N\rangle$

Note $[\hat{H}, \hat{N}]|E,N\rangle = (EN - NE)|E,N\rangle$
$= 0$

Consider N = 0

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

$|0\rangle$ has $H|0\rangle = 0$ and $N|0\rangle = 0$.

Consider N = 1

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

Define the Schroedinger wave function for this state,

$$\varphi_\alpha(\mathbf{x}) = \langle 0|\ \psi_\alpha(\mathbf{x})\ |E,1\rangle.$$

Theorem. $\varphi_\alpha(\mathbf{x})$ obeys the Schroedinger equation.

Proof.

$$\phi_\alpha(\vec{x}) = \langle 0 | \hat{\psi}_\alpha(\vec{x}) | E, 1 \rangle$$

$$E\,\phi_\alpha(\vec{x}) = \langle 0 | \hat{\psi}_\alpha(\vec{x})\, \hat{H}\, | E, 1 \rangle$$

$$= \langle 0 | \hat{\psi}_\alpha(\vec{x}) [\hat{T} + \hat{V}] | E, 1 \rangle$$

- The $\hat{T}$ part

$$= \langle 0 | [\hat{\psi}_\alpha(\vec{x}), \hat{T}] + \hat{T}\,\hat{\psi}_\alpha(\vec{x}) | E, 1 \rangle$$

$\langle 0 | \hat{T} = 0$ because
$\hat{T} | 0 \rangle = 0$ {or $\langle 0 | \psi^+ = 0$
because $\psi | 0 \rangle = 0$

$$[\hat{\psi}_\alpha(x), \hat{T}] = \int d^3y\, [\hat{\psi}_\alpha(x), \hat{\psi}^+_\beta T_{\beta\gamma} \hat{\psi}_\gamma(y)]$$

$$= \int d^3y \{ \{\hat{\psi}_\alpha(x), \hat{\psi}^+_\beta(y)\} T_{\beta\gamma} \hat{\psi}_\gamma$$

$$- \psi^+_\beta \{\hat{\psi}_\alpha, T_{\beta\gamma} \hat{\psi}_\gamma\}]$$

$[A, BC] = \{A, B\}C - B\{A, C\}$

$$= T_{\alpha\gamma}\, \hat{\psi}_\gamma(x)$$

Thus

$$\langle 0 | [\hat{\psi}_\alpha(x), \hat{T}] | E, 1 \rangle = \langle 0 | T_{\alpha\gamma}\, \hat{\psi}_\gamma(x) | E, 1 \rangle$$

$$= T_{\alpha\gamma}\, \phi_\gamma(x)$$

$\sum_\beta$ is implied

$$= -\frac{\hbar^2 \nabla^2}{2m} \phi_\alpha(x) + V_{\alpha\beta}(x)\, \phi_\beta(x)$$

- The $\hat{V}$ part

$$\langle 0 | \hat{\psi}_\alpha(x)\, \hat{V} | E, 1 \rangle$$

$$= \langle 0 | [\psi_\alpha(x), \hat{V}] + \hat{V}\, \psi_\alpha | E, 1 \rangle$$

This gives 0 because
$\langle 0 | \psi^+_\beta = 0$
(because $\psi_\beta | 0 \rangle = 0$)

Now calculate

$$[\psi_\alpha(x), \hat{V}] = \int d^3y\, d^3y' \, [\psi_\alpha(x),\ \psi^+_{\beta(y)}\psi^+_{\gamma(y)} V\ \psi_{\gamma'(y')}\psi_{\beta'(y)}]$$

$V_{\beta\gamma,\beta'\gamma'}(y,y')$

$$= \int d^3y\, d^3y' \ V_{\beta\gamma\,\beta'\gamma'}(\vec{y},\vec{y}') \ [\underset{(x)}{\psi},\ \underset{(y)}{\psi^+}\underset{(y')}{\psi^+}\ \underset{(y')}{\psi}\underset{(y)}{\psi}]$$

suppress the spin indices

$$[\overset{x}{\psi},\ \overset{y}{\psi^+}\overset{y'}{\psi^+}\overset{y'}{\psi}\overset{y}{\psi}]$$

$$= \underbrace{[\underset{x}{\psi}, \psi^+\psi^+]}_{\{\underset{x}{\psi}, \underset{y}{\psi^+}\}\underset{y'}{\psi^+} - \underset{y}{\psi^+}\{\underset{x}{\psi}, \underset{y'}{\psi^+}\}}\psi\psi + \psi^+\psi^+\underbrace{[\underset{x}{\psi}, \psi\psi]}_{0 \text{ because } \{\psi,\psi\}}$$

$$= \delta^3(x-y)\,\psi^+(y') - \delta^3(x-y')\,\psi^+(y)$$

But $\langle 0|\,\psi^+(\xi) = 0$

because $\psi(\xi)\,|0\rangle = 0$.

So the $\hat{V}$ part is 0.

Result

$$E\,\phi_\alpha(\vec{x}) = \frac{-\hbar^2\nabla^2}{2m}\phi_\alpha(\vec{x}) + U_{\alpha\beta}(\vec{x})\,\varphi_\beta(x),$$

which is just the Schrodinger equation for a single particle.

Q.E.D. for N = 1

Consider N = 2

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

Define the Schroedinger wave function for this state,

$$\varphi_{\alpha 1\ \alpha 2}(\mathbf{x}_1, \mathbf{x}_2) = \langle 0|\ \psi_{\alpha 1}(\mathbf{x}_1)\ \psi_{\alpha 2}(\mathbf{x}_2)\ |E,2\rangle$$

<u>Theorem.</u>

$\varphi_{\alpha 1\ \alpha 2}(x_1,x_2)$ is antisymmetric.

<u>Proof.</u>

$$\phi_{\alpha_2 \alpha_1}(x_2\, x_1) = \langle 0|\ \underbrace{\hat{\psi}_{\alpha_2}(x_2)\ \hat{\psi}_{\alpha_1}(x_1)}_{= -\psi_{\alpha_1}(x_1)\,\psi_{\alpha_2}(x_2)}\ |E;2\rangle$$

$$= -\ \phi_{\alpha_1 \alpha_2}(x_1\, x_2)$$

Q.E.D.

<u>Theorem.</u>

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

<u>Proof.</u>

$$E\,\phi_{\alpha_1 \alpha_2}(\vec{x}_1 \vec{x}_2) = \langle 0|\ \hat{\psi}_{\alpha_1}(\vec{x}_1)\ \hat{\psi}_{\alpha_2}(\vec{x}_2)\ (\hat{T}+\hat{V})\ |E;2\rangle$$

- The $\hat{T}$ part

$$\langle 0|\ \hat{\psi}_{\alpha_1}(\vec{x}_1)\ \hat{\psi}_{\alpha_2}(\vec{x}_2)\ \hat{T}\ |E;2\rangle$$

$$= \langle 0|\ [\hat{\psi}_{\alpha_1}(x_1)\ \hat{\psi}_{\alpha_2}(x_2),\ \hat{T}]\ |E;2\rangle$$

because $\langle 0|\hat{T} = 0$

because $\langle 0|\psi^{+}(x) = 0.$

$$\left[\hat{\psi}_{\alpha_1}(x_1)\,\hat{\psi}_{\alpha_2}(x_2),\ \hat{T}\right]$$

$$= \hat{\psi}_{\alpha_1}(x_1)\left[\hat{\psi}_{\alpha_2}(x_2),\hat{T}\right] + \left[\hat{\psi}_{\alpha_1}(x_1),\hat{T}\right]\hat{\psi}_{\alpha_2}(x_2)$$

$$= \hat{\psi}_{\alpha_1}(x_1)\ T_{\alpha_2\gamma}(x_2)\,\hat{\psi}_{\gamma}(x_2)$$

$$+\ T_{\alpha_1\gamma}(x_1)\ \hat{\psi}_{\gamma}(x_1)\ \hat{\psi}_{\alpha_2}(x_2)$$

$\therefore$

$$\langle 0|\ \hat{\psi}_{\alpha_1}(x_1)\,\hat{\psi}_{\alpha_2}(x_2)\,\hat{T}\,|E;2\rangle$$

$$= T_{\alpha_1\gamma}(x_1)\,\phi_{\gamma\alpha_2}(x_1x_2) + T_{\alpha_2\gamma}(x_2)\,\phi_{\alpha_1\gamma}(x_1x_2)$$

$$= \left(-\frac{\hbar^2\nabla_1^2}{2m} - \frac{\hbar^2\nabla_2^2}{2m}\right)\phi_{\alpha_1\alpha_2}(x_1x_2)$$

$$+\ v_{\alpha_1\beta}(x_1)\,\phi_{\beta\alpha_2}(x_1x_2) + v_{\alpha_2\beta}(x_2)\,\phi_{\alpha_1\beta}(x_1x_2)$$

+ The $\hat{V}$ part

$= \langle 0 | \hat{\Psi}_{\alpha_1}(x_1) \hat{\Psi}_{\alpha_2}(x_2) \hat{V} | E; 2\rangle$

$= \langle 0 | [\Psi_{\alpha_1}(x_1) \Psi_{\alpha_2}(x_2), V] | E; 2\rangle$

$= \langle 0 | \Psi_{\alpha_1}(x_1) [\Psi_{\alpha_2}(x_2), V]$

$+ [\Psi_{\alpha_1}(x_1), V] \Psi_{\alpha_2}(x_2) | E; 2\rangle$

$$[\Psi_\alpha(x), V] = \frac{1}{2}\int d^3y\, d^3y' \left[\Psi_\alpha(x), \Psi^+_{(y)} \Psi^+_{(y')} V_{(y,y')} \Psi_{(y')} \Psi_{(y)}\right]$$

$$= \frac{1}{2}\int d^3y\, d^3y'\, V(yy') \{ \delta^3(x-y) \Psi^+(y') \Psi(y') \Psi(y)$$

$$- \delta^3(x-y') \Psi^+(y) \Psi(y') \Psi(y) \}$$

$\langle 0 | \hat{\Psi}_\alpha(x_1) \hat{\Psi}_{\alpha_2} \hat{V} | E; 2\rangle$

$= \langle 0 | \Psi(x_1) \frac{1}{2}\int d^3y'\, V(x_2 y') \Psi^+(y') \Psi(y') \Psi(x_2)$

$+ \Psi(x_1)(\frac{-1}{2}) \int d^3y\, V(y x_2) \Psi^+(y) \Psi(x_2) \Psi(y)$

$+ \frac{1}{2}\int d^3y'\, V(x_1 y') \Psi^+(y') \Psi(y') \Psi(x_1) \quad \Psi(x_2)$

$+ (-\frac{1}{2})\int d^3y\, V(y x_2) \Psi^+(y) \Psi(x_1) \Psi(y) \quad \Psi(x_2)$

$| E; 2\rangle$

Note

$\langle 0 | \Psi(x_1) \Psi^+(y') = \delta^3(x_1 - y') \langle 0 |$ etc

$\langle 0 |$

$= \frac{1}{2} V(x_2 x_1) \Psi(x_1) \Psi(x_2) - \frac{1}{2} V(x_1 x_2) \Psi(x_2) \Psi(x_1)$

$+ 0 + 0 \; | E; 2\rangle$

$= V(x_1 x_2)\, \Phi_{\alpha_1 \alpha_2}(x_1 x_2)$

Restoring the spin indices

$$E\,\phi_{\alpha_1\alpha_2}(x_1 x_2) = \frac{-\hbar^2}{2m}(\nabla_1^2+\nabla_2^2)\,\phi_{\alpha_1\alpha_2}(x_1 x_2)$$

$$+\; U_{\alpha_1\beta}(x_1)\,\phi_{\beta\alpha_2}(x_1 x_2) + U_{\alpha_2\beta}(x_2)\,\phi_{\alpha_1\beta}(x_1 x_2)$$

$$+\; V_{\alpha_1\alpha_2\beta_1\beta_2}(x_1 x_2)\,\phi_{\beta_1\beta_2}(x_1 x_2)$$

and this is just the 2-particle Schroedinger equation. / Q.E.D. for $N=2$ /

Consider arbitrary N

Arbitrary N

$$\phi(x_1 x_2 \ldots x_N) = \langle 0|\,\hat{\psi}^+(x_1)\,\hat{\psi}^+(x_2)\ldots\hat{\psi}^+(x_N)\,|E;N\rangle$$

$$E\phi = \frac{-\hbar^2}{2m}\sum_{k=1}^{N}\nabla_k^2\,\phi + \sum_{k=1}^{N} U(x_k)\,\phi$$

$$+ \sum_{\substack{\text{pairs}\\(k,\ell)}} V(x_k x_\ell)\,\phi$$

the Schroedinger equation for N particles.

Q.E.D. for arbitrary N