6. Second Quantization and Quantum Field Theory

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6.0. Preliminary

Second quantization is an indispensable tool for the study of systems with variable numbers of particles. Some notable examples of the latter are

1. High energy scattering and decay processes.
2. Relativistic systems.
3. Many body systems (not necessarily relativistic).

The term 1st quantization refers to the *physical fact* that certain classically continuous quantities, such as energy and angular momentum, can take on only discrete values in the quantum regime. In a purely mathematical sense, 2nd quantization is simply a transformation to the number representation so that all dynamical properties of the system can be obtained by counting the numbers of the 1-particle states being occupied at each instance of time. Here, the “quantization” refers to the discreteness of the counting. However, a more physical interpretation is to take 2nd quantization as adopting the *viewpoint* that all quantum processes can be described in terms of the exchange of real or virtual particles. For example, the electromagnetic interaction can be described in terms of the exchange of real or virtual photons.

The technique is particular useful when dealing with systems near their ground states. In which case, the problem is reduced to the study of only a few weakly interacting “quasi-particles”, or “elementary excitations”, so that standard perturbation techniques can be applied. Thus, the art is in the identification of a “ground” state that

1. can be described in known, preferably simple, mathematical terms.
2. contains as much of the interactions as possible.

6.1. The Occupation Number Representation

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6.1.1. Many Body System

Consider a system of N identical particles. Let $\{ |k\rangle \}$ be a set of complete, orthonormal, 1-particle states that satisfy the boundary conditions of the system. Using particle labels as subscripts, the set $\{ |k_1\rangle \otimes \cdots \otimes |k_N\rangle \}$ of all direct products of N 1-particle states is an orthonormal basis for the system.

Owing to the uncertainty principle, identical particles in quantum mechanics are **indistinguishable**. This means the state $|\cdots, k_i, \cdots, k_j, \cdots\rangle$ in which particles i and j are in states k_i and k_j , respectively, is equivalent to state $|\cdots, k_j, \cdots, k_i, \cdots\rangle$ obtained by interchanging the particles i and j. Thus,

$$|\cdots, k_i, \cdots, k_j, \cdots\rangle = \alpha |\cdots, k_j, \cdots, k_i, \cdots\rangle \qquad \forall\, i, j$$

where α is some complex number. Obviously, exchanging the same pair of particles twice brings back the original state so that

$$\alpha^2 = 1 \quad \Rightarrow \quad \alpha = \pm 1$$

Particles with $\alpha = +1$ ($\alpha = -1$) are called **bosons** (**fermions**) since they obey **Bose-Einstein** (**Fermi-Dirac**) **statistics**. It was found experimentally that all particles with integer and half-integer spins are bosons and fermions, respectively. According to the **spin-statistics theorem** in quantum field theory, the reason for this association is causality [see Chap 7]. In terms of the 1-particle basis, we can write

$$|k_1, \cdots, k_N\rangle = C_{\pm} \sum_P (\pm)^P |k_{P(1)}\rangle \otimes \cdots \otimes |k_{P(N)}\rangle \qquad \text{for} \quad \begin{matrix} bosons \\ fermions \end{matrix}$$

where P denotes a permutation

$$(1, \cdots, N) \to P(1, \cdots, N) = [P(1), \cdots, P(N)]$$

with

$$(\pm)^P = \begin{cases} +1 \\ -1 \end{cases} \quad \text{if } P \text{ consists of an } \begin{matrix} even \\ odd \end{matrix} \text{ number of transpositions (exchanges)}$$

The orthonormality of $\{ |k\rangle \}$ can be used to show that

1. Normalization of $\left| k_1, \cdots, k_N \right\rangle$ gives $C_\pm = \sqrt{\dfrac{\prod_j n_j !}{N!}}$, where n_j is the number of particles in state k_j and j runs through the distinct states in $k_1, \cdots, k_N$ so that $N = \sum_j n_j$. Note that for fermions, $n_j = 0,1$.

2. $\left| k_1, \cdots, k_N \right\rangle$ is orthonormal in the sense that

$$\left\langle k_1, \cdots, k_N \,\middle|\, k_1', \cdots, k_{N'}' \right\rangle = \delta_{\{k_1,\cdots,k_N\},\{k_1',\cdots,k_{N'}'\}} \tag{6.1}$$

where

$$\delta_{\{k_1,\cdots,k_N\},\{k_1',\cdots,k_{N'}'\}} = \begin{cases} 1 & \text{if} \quad \{k_1,\cdots,k_N\} = P\{k_1',\cdots,k_{N'}'\} \\ 0 & \quad otherwise \end{cases}$$

Note that 2 states with $N \neq N'$ are always orthogonal.

6.1.2. Number Representation: States

Consider a set of complete, orthonormal 1-particle (1-P) basis. For the sake of clarity, we shall assume the quantum numbers to be discrete. (Results for the continuous case can be obtained by some limiting procedure). To begin, we arrange the 1-P states by some rule into a unique sequence $\alpha = 0,1,2,\cdots$ of monotonically increasing energy so that $|0\rangle$ is always the 1-P ground state. For example, the one electron spinless states $|nlm\rangle$ in a hydrogenic atom can be arranged as $|0\rangle = |100\rangle$, $|1\rangle = |11-1\rangle$, $|2\rangle = |110\rangle$, $|3\rangle = |111\rangle$, … .

The basis in the number (*n*-) representation consists of all the eigenstates of the number operator $\hat{n}_\alpha$:

$$\hat{n}_\alpha |n_0, n_1, \cdots, n_\alpha, \cdots\rangle = n_\alpha |n_0, n_1, \cdots, n_\alpha, \cdots\rangle$$

where n_α is the number of particles in the 1-particle state $|\alpha\rangle$. We shall assume orthonormality:

$$\langle n_0, n_1, \cdots, n_\alpha, \cdots | n_0', n_1', \cdots, n_\alpha', \cdots\rangle = \delta_{n_0 n_0'} \delta_{n_1 n_1'} \cdots \delta_{n_\alpha n_\alpha'} \cdots \qquad (6.2)$$

Completeness of the basis means the state vector of the system can be written as

$$\begin{aligned} |\Psi(t)\rangle &= \sum_{n_0, n_1, \cdots, n_\alpha, \cdots} |n_0, n_1, \cdots, n_\alpha, \cdots\rangle \langle n_0, n_1, \cdots, n_\alpha, \cdots | \Psi(t)\rangle \\ &= \sum_{n_0, n_1, \cdots, n_\alpha, \cdots} |n_0, n_1, \cdots, n_\alpha, \cdots\rangle \, \Psi_{n_0, n_1, \cdots, n_\alpha, \cdots}(t) \qquad (6.3) \end{aligned}$$

6.1.3. Creation and Annihilation Operators

The conjugate variables in the n-representation are the annihilation operators $\hat{a}_\alpha$ and the creation operators $\hat{a}_\alpha^+$. By definition

$$\hat{n}_\alpha = \hat{a}_\alpha^+ \hat{a}_\alpha \qquad \hat{a}_\alpha^+ = \left(\hat{a}_\alpha\right)^+$$

$$\hat{n}_\alpha \left|n_0, n_1, \cdots, n_\alpha, \cdots\right\rangle = n_\alpha \left|n_0, n_1, \cdots, n_\alpha, \cdots\right\rangle$$

$$\hat{a}_\alpha \left|n_0, n_1, \cdots, n_\alpha, \cdots\right\rangle = A\left(n_\alpha\right)\left|n_0, n_1, \cdots, n_\alpha - 1, \cdots\right\rangle$$

$$\hat{a}_\alpha^+ \left|n_0, n_1, \cdots, n_\alpha, \cdots\right\rangle = C\left(n_\alpha\right)\left|n_0, n_1, \cdots, n_\alpha + 1, \cdots\right\rangle$$

where $A(n_\alpha)$ and $C(n_\alpha)$ are normalization constants to be determined. Thus,

$$n_\alpha = \left\langle n_0, n_1, \cdots, n_\alpha, \cdots\right| \hat{a}_\alpha^+ \hat{a}_\alpha \left|n_0, n_1, \cdots, n_\alpha, \cdots\right\rangle$$

$$= \left|A\left(n_\alpha\right)\right|^2 \left\langle n_0, n_1, \cdots, n_\alpha - 1, \cdots \middle| n_0, n_1, \cdots, n_\alpha - 1, \cdots\right\rangle$$

$$= \left|A\left(n_\alpha\right)\right|^2$$

Assuming A to be real, we have

$$A\left(n_a\right) = \sqrt{n_\alpha}$$

Similarly,

$$\left\langle n_0, n_1, \cdots, n_\alpha, \cdots\right| \hat{a}_\alpha \hat{a}_\alpha^+ \left|n_0, n_1, \cdots, n_\alpha, \cdots\right\rangle = \left|C\left(n_\alpha\right)\right|^2$$

$$= A\left(n_\alpha + 1\right) C\left(n_\alpha\right)$$

Assuming C to be real, we have

either $\quad C\left(n_\alpha\right) = 0$

or $\quad C\left(n_a\right) = A\left(n_\alpha + 1\right) = \sqrt{n_\alpha + 1}$

For bosons, there is no upper limit to n_α. Therefore, $C\left(n_\alpha\right) \neq 0$ for all n_α and

$$\hat{a}_\alpha \left|n_0, n_1, \cdots, n_\alpha, \cdots\right\rangle = \sqrt{n_\alpha} \left|n_0, n_1, \cdots, n_\alpha - 1, \cdots\right\rangle$$

$$\hat{a}_\alpha^+ \left| n_0, n_1, \cdots, n_\alpha, \cdots \right\rangle = \sqrt{n_\alpha + 1} \left| n_0, n_1, \cdots, n_\alpha + 1, \cdots \right\rangle$$

For fermions, the antisymmetry means $n_\alpha = 0,1$. Thus, $C(0) = 1$ and $C(1) = 0$ and we can write

$$\hat{a}_\alpha \left| n_0, n_1, \cdots, n_\alpha, \cdots \right\rangle = (-)^{S_\alpha} \left| \, n_0, n_1, \cdots, n_{\alpha-1} \right\rangle \otimes \hat{a}_\alpha \left| \, n_\alpha \right\rangle \otimes \left| \, n_{\alpha+1}, \cdots \right\rangle$$

where $S_\alpha = \sum_{\beta=0}^{\alpha-1} n_\alpha$ counts the transpositions required to move $\hat{a}_\alpha$ to the proper position.

$$\hat{a}_\alpha \left| n_0, n_1, \cdots, n_\alpha, \cdots \right\rangle = (-)^{S_\alpha} \sqrt{n_\alpha} \left| n_0, n_1, \cdots, n_\alpha - 1, \cdots \right\rangle$$

$$\begin{aligned}
\hat{a}_\alpha^+ \left| n_0, n_1, \cdots, n_\alpha, \cdots \right\rangle &= (-)^{S_\alpha} \sqrt{1 - n_\alpha} \left| n_0, n_1, \cdots, n_\alpha + 1, \cdots \right\rangle \\
&= (-)^{S_\alpha} \sqrt{1 - n_\alpha} \left| n_0, n_1, \cdots, 1 - n_\alpha, \cdots \right\rangle \\
&= (-)^{S_\alpha} (1 - n_\alpha) \left| n_0, n_1, \cdots, n_\alpha + 1, \cdots \right\rangle
\end{aligned}$$

where the various expressions for $\hat{a}_\alpha^+$ all made use of the fact that $n_\alpha = 0,1$.

Finally, we mention that the completeness of the basis $\left| n_0, n_1, \cdots, n_\alpha, \cdots \right\rangle$ is with respect to the Fock space, i.e., all many particle states that can be constructed from the 1-P states. However, there exists many particle states that cannot be constructed in this manner. The most notorious example is the BCS superconducting state, which is a condensate (in momentum space) of Cooper pairs.

6.1.4. Commutation Relations

Before proceeding further, we must establish a way for exchange symmetries to be built into $|n_0, n_1, \cdots, n_\alpha, \cdots\rangle$. To this end, we define

$$|n_0, n_1, \cdots, n_\alpha, \cdots\rangle = \cdots \frac{\left(\hat{a}_\alpha^+\right)^{n_\alpha}}{\prod_{m=0}^{n_\alpha - 1} C(m)} \cdots \frac{\left(\hat{a}_1^+\right)^{n_1}}{\prod_{m=0}^{n_1 - 1} C(m)} \cdots \frac{\left(\hat{a}_0^+\right)^{n_0}}{\prod_{m=0}^{n_0 - 1} C(m)} |\Phi\rangle$$

where $|\Phi\rangle = |0, 0, \cdots\rangle$ is the "vacuum". Note that for fermions, $n_\alpha = 0,1$ so that $\prod_{m=0}^{n_\alpha - 1} C(m) = 1$ for all n_α. The set of all $|n_0, n_1, \cdots, n_\alpha, \cdots\rangle$ thus generated is called the **Fock space**. It is straightforward to check that the exchange symmetries are established by requiring

$$\left[\hat{a}_\alpha^+ , \hat{a}_\beta^+\right]_\mp = 0$$

where the upper and lower signs are for bosons and fermions, respectively. Also,

$$[a, b]_\mp \equiv ab \mp ba$$

Note that the anticommutator $[\ ,\ ]_+$ is often written as $\{\ ,\ \}$. Using $\hat{a}_\alpha^+ = \left(\hat{a}_\alpha\right)^+$, we have

$$\left[\hat{a}_\alpha , \hat{a}_\beta\right]_\mp = 0$$

Also,

$$\langle \cdots, n_\alpha - 1, \cdots, n_\beta + 1, \cdots | \left(\hat{a}_\alpha \hat{a}_\beta^+ \mp \hat{a}_\beta^+ \hat{a}_\alpha\right) | \cdots, n_\alpha, \cdots, n_\beta, \cdots \rangle$$

$$= \begin{cases} \sqrt{n_\alpha (1 \pm n_\beta)} \mp \sqrt{n_\alpha (1 \pm n_\beta)} = 0 & \text{for } \alpha \neq \beta \\ \sqrt{(1 \pm n_\alpha)(1 \pm n_\alpha)} \mp n_\alpha = 1 & \alpha = \beta \end{cases}$$

$\Rightarrow$

$$\left[\hat{a}_\alpha , \hat{a}_\beta^+\right]_\mp = \delta_{\alpha\beta}$$

6.1.5. Number Representation: Operators

Consider a 1-P operator $A(\mathbf{p},\mathbf{x})$. Given the complete orthonormal basis $\{|\alpha\rangle\}$, we can write

$$A(\mathbf{p},\mathbf{x}) = \sum_{\alpha\beta} |\alpha\rangle\langle\alpha|A|\beta\rangle\langle\beta| \quad = \sum_{\alpha\beta} A_{\alpha\beta}|\alpha\rangle\langle\beta|$$

where the matrix elements $A_{\alpha\beta} = \langle\alpha|A|\beta\rangle$ are numbers. Using $|\alpha\rangle = \hat{a}_\alpha^+|\Phi\rangle$,

where $|\Phi\rangle$ is the vacuum, we can write

$$\hat{A} = \sum_{\alpha\beta} A_{\alpha\beta}\hat{a}_\alpha^+|\Phi\rangle\,\langle\Phi|\hat{a}_\beta$$

Note that the vacuum projector $|\Phi\rangle\langle\Phi|$ serves to confine $\hat{A}$ to the 1-particle

subspace, i.e., $\langle\Psi|\hat{A}|\Theta\rangle = 0$ if the number of particles in either Φ or Θ is not one.

By removing this restriction, we obtain the desired many body version

$$\hat{A} = \sum_{\alpha\beta}\langle\alpha|A|\beta\rangle\;\hat{a}_\alpha^+\,\hat{a}_\beta$$

Next, we consider the 2-P potential

$$V = \frac{1}{2}\sum_{i\neq j=1}^{N} V\left(\mathbf{x}_i\,,\mathbf{x}_j\right) = \sum_{i>j=1}^{N} V\left(\mathbf{x}_i\,,\mathbf{x}_j\right)$$

Given the complete orthonormal 1-P basis $\{|\alpha\rangle\}$, a basis vector for the 2-P Hilbert space is

$$|\alpha\rangle_1 \otimes |\beta\rangle_2 \equiv |\alpha\rangle_1|\beta\rangle_2 \equiv |\alpha_1\,\beta_2\,\rangle$$

where, to avoid ambiguity, we have used subscript to indicate the particle occupying the state. Taking the hermitian conjugate, we obtain the adjoint basis vector

$$\left(|\alpha\rangle_1 \otimes |\beta\rangle_2\right)^+ = {}_2\langle\beta|\otimes{}_1\langle\alpha| \quad \equiv {}_2\langle\beta|_1\langle\alpha| \equiv \langle\alpha_1\,\beta_2|$$

where the order of the factors is to be noted with care. Using the completeness condition

$$I = \sum_{\alpha,\beta}|\alpha\rangle_1|\beta\rangle_2\,{}_2\langle\beta|_1\langle\alpha| \quad = \sum_{\alpha,\beta}|\alpha_1\,\beta_2\,\rangle\langle\alpha_1\,\beta_2|$$

we can write the 2-P potential (1^{st} quantized) operator as

$$V = \frac{1}{2}\sum_{\alpha\beta\gamma\delta} |\alpha\rangle_1 |\beta\rangle_2 \, {}_2\langle\beta|_1\langle\alpha|V|\gamma\rangle_1 |\delta\rangle_2 \, {}_2\langle\delta|_1\langle\gamma|$$

$$= \frac{1}{2}\sum_{\alpha\beta\gamma\delta} |\alpha_1\beta_2\rangle\langle\alpha_1\beta_2|V|\gamma_1\delta_2\rangle\langle\gamma_1\delta_2|$$

Using

$$|\alpha_1\, \beta_2\,\rangle = |\alpha\rangle_1 |\beta\rangle_2 \quad = \hat{a}_\alpha^+ \, \hat{a}_\beta^+ |\Phi\rangle$$

$$\langle\gamma_1\, \delta_2| = {}_2\langle\delta|_1\langle\gamma| \quad = \left(|\gamma\rangle_1 |\delta\rangle_2\right)^+ \quad = \left(\hat{a}_\gamma^+ \, \hat{a}_\delta^+ |\Phi\rangle\right)^+ = \langle\Phi|\hat{a}_\delta \, \hat{a}_\gamma$$

we can write the 2nd quantized version of V as

$$\hat{V} = \frac{1}{2}\sum_{\alpha\beta\gamma\delta} \hat{a}_\alpha^+ \hat{a}_\beta^+ |\Phi\rangle \, \langle\alpha\beta|V|\gamma\delta\rangle\langle\Phi|\hat{a}_\delta \, \hat{a}_\gamma$$

where

$$\langle\alpha\beta|V|\gamma\delta\rangle = \int d^3\mathbf{x}_1 \int d^3\mathbf{x}_2 \; \phi_\alpha^*(\mathbf{x}_1)\phi_\beta^*(\mathbf{x}_2) V(\mathbf{x}_1, \mathbf{x}_2)\, \phi_\delta(\mathbf{x}_2)\phi_\gamma(\mathbf{x}_1)$$

As before, the vacuum projector $|\Phi\rangle\langle\Phi|$ serves to confine $\hat{V}$ to the 2-particle subspace. Removing this restriction then gives

$$\hat{V} = \frac{1}{2}\sum_{\alpha\beta\gamma\delta} \langle\alpha\beta|V|\gamma\delta\rangle \; \hat{a}_\alpha^+ \, \hat{a}_\beta^+ \, \hat{a}_\delta \, \hat{a}_\gamma \qquad \text{(a)}$$

Note that α,γ and β,δ refer to the particle at $\mathbf{x}_1$ and $\mathbf{x}_2$, respectively. Thus, in eq(a), the first and last operators refer to particle 1.

6.1.6. Summary

For the ease of reference, we list below the salient results of the *n*-representation (upper and lower signs are for bosons and fermions, respectively):

$$\hat{n}_\alpha = \hat{a}_\alpha^+ \hat{a}_\alpha$$

$$\left[\hat{a}_\alpha , \hat{a}_\beta\right]_\mp = \left[\hat{a}_\alpha^+ , \hat{a}_\beta^+\right]_\mp = 0$$

$$\left[\hat{a}_\alpha , \hat{a}_\beta^+\right]_\mp = \delta_{\alpha\beta} \quad \xrightarrow[\text{continuous}]{} \quad \delta(\alpha - \beta)$$

$$\hat{n}_\alpha \left|n_0, n_1, \cdots, n_\alpha, \cdots\right\rangle = n_\alpha \left|n_0, n_1, \cdots, n_\alpha, \cdots\right\rangle$$

$$\hat{a}_\alpha \left|n_0, n_1, \cdots, n_\alpha, \cdots\right\rangle = (\pm)^{S_\alpha} \sqrt{n_\alpha} \left|n_0, n_1, \cdots, n_\alpha, \cdots\right\rangle \qquad S_\alpha = \sum_{\beta=0}^{\alpha-1} n_\alpha$$

$$\hat{a}_\alpha^+ \left|n_0, n_1, \cdots, n_\alpha, \cdots\right\rangle = (\pm)^{S_\alpha} \sqrt{1 \pm n_\alpha} \left|n_0, n_1, \cdots, n_\alpha, \cdots\right\rangle$$

$$\left\langle n_0, n_1, \cdots, n_\alpha, \cdots \middle| n_0', n_1', \cdots, n_\alpha', \cdots\right\rangle = \delta_{n_0 n_0'} \delta_{n_1 n_1'} \cdots \delta_{n_\alpha n_\alpha'} \cdots$$

1-P operator: $\hat{A} = \sum_{\alpha\beta} \langle \alpha | A | \beta \rangle \; \hat{a}_\alpha^+ \hat{a}_\beta$

2-P operator: $\hat{V} = \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | V | \gamma\delta \rangle \; \hat{a}_\alpha^+ \hat{a}_\beta^+ \hat{a}_\delta \hat{a}_\gamma$

6.2. Field Operators and Observables

Henceforth, we shall take the 1-P states to be momentum eigenstaes. For spinless particles, we have $\alpha = \mathbf{k} = \dfrac{\mathbf{p}}{\hbar}$. Since **k** is continuous, the orthonormality and completeness take the form

$$\langle \mathbf{k} | \mathbf{k}' \rangle = \delta(\mathbf{k} - \mathbf{k}') \qquad \int d^3k \, |\mathbf{k}\rangle\langle\mathbf{k}| = 1$$

with

$$\langle \mathbf{x} | \mathbf{x}' \rangle = \delta(\mathbf{x} - \mathbf{x}') \qquad \int d^3r \, |\mathbf{x}\rangle\langle\mathbf{x}| = 1$$

$$\phi_{\mathbf{k}}(\mathbf{x}) = \langle \mathbf{x} | \mathbf{k} \rangle = \frac{1}{(2\pi)^{3/2}} e^{i\mathbf{k}\cdot\mathbf{x}}$$

Thus, the wave function for a single particle in state $|\Psi(t)\rangle$ can be written as

$$\Psi(\mathbf{x},t) = \langle \mathbf{x} | \Psi(t) \rangle = \int d^3k \langle \mathbf{x} | \mathbf{k} \rangle \langle \mathbf{k} | \Psi(t) \rangle = \int \frac{d^3k}{(2\pi)^{3/2}} e^{i\mathbf{k}\cdot\mathbf{x}} \langle \mathbf{k} | \Psi(t) \rangle$$

$$= \int \frac{d^3k}{(2\pi)^{3/2}} e^{i\mathbf{k}\cdot\mathbf{x}} \langle 0 | \hat{a}(\mathbf{k}) | \Psi(t) \rangle \tag{6.12}$$

where we've used

$$\langle \mathbf{k} | = (|\mathbf{k}\rangle)^+ = \left[\hat{a}^+(\mathbf{k}) |0\rangle \right]^+ = \langle 0 | \hat{a}(\mathbf{k})$$

The **field operators** are defined in the Schrodinger picture by

$$\hat{\psi}(\mathbf{x}) = \sum_\alpha \langle \mathbf{x} | \alpha \rangle \hat{a}_\alpha = \sum_\alpha \phi_\alpha(\mathbf{x}) \hat{a}_\alpha$$

$$\hat{\psi}^+(\mathbf{x}) = \sum_\alpha \langle \alpha | \mathbf{x} \rangle \hat{a}^+_\alpha = \sum_\alpha \phi^*_\alpha(\mathbf{x}) \hat{a}^+_\alpha$$

In the momentum basis, they become

$$\hat{\psi}(\mathbf{x}) = \int d^3k \, \phi_{\mathbf{k}}(\mathbf{x}) \hat{a}(\mathbf{k}) = \int \frac{d^3k}{(2\pi)^{3/2}} e^{i\mathbf{k}\cdot\mathbf{x}} \hat{a}(\mathbf{k}) \tag{6.13}$$

$$\hat{\psi}^+(\mathbf{x}) = \int d^3k \, \phi^*_{\mathbf{k}}(\mathbf{x}) \hat{a}^+(\mathbf{k}) = \int \frac{d^3k}{(2\pi)^{3/2}} e^{-i\mathbf{k}\cdot\mathbf{x}} \hat{a}^+(\mathbf{k}) \tag{6.14}$$

The corresponding commutation relations are

$$\left[\hat{\psi}(\mathbf{x}),\hat{\psi}(\mathbf{x}')\right]_{\mp}=\sum_{\alpha\beta}\langle\mathbf{x}|\alpha\rangle\langle\mathbf{x}'|\beta\rangle\left[\hat{a}_{\alpha},\hat{a}_{\beta}\right]_{\mp}=0$$

$$\left[\hat{\psi}^{+}(\mathbf{x}),\hat{\psi}^{+}(\mathbf{x}')\right]_{\mp}=\sum_{\alpha\beta}\langle\alpha|\mathbf{x}\rangle\langle\beta|\mathbf{x}'\rangle\left[\hat{a}_{\alpha}^{+},\hat{a}_{\beta}^{+}\right]_{\mp}=0 \qquad (6.15)$$

$$\left[\hat{\psi}(\mathbf{x}),\hat{\psi}^{+}(\mathbf{x}')\right]_{\mp}=\sum_{\alpha\beta}\langle\mathbf{x}|\alpha\rangle\langle\beta|\mathbf{x}'\rangle\left[\hat{a}_{\alpha},\hat{a}_{\beta}^{+}\right]_{\mp}=\sum_{\alpha}\langle\mathbf{x}|\alpha\rangle\langle\alpha|\mathbf{x}'\rangle$$

$$=\langle\mathbf{x}|\mathbf{x}'\rangle=\delta(\mathbf{x}-\mathbf{x}') \qquad (6.16)$$

Consider the operator

$$\hat{\rho}(\mathbf{x})=\hat{\psi}^{+}(\mathbf{x})\,\hat{\psi}(\mathbf{x})$$

we have

$$\int d^3x\,\hat{\rho}(\mathbf{x})=\int d^3x\;\hat{\psi}^{+}(\mathbf{x})\,\hat{\psi}(\mathbf{x})$$

$$=\int d^3x\int\frac{d^3k}{(2\pi)^{3/2}}\int\frac{d^3k'}{(2\pi)^{3/2}}\,e^{-i\mathbf{k}\cdot\mathbf{x}}\,\hat{a}^{+}(\mathbf{k})e^{i\mathbf{k}'\cdot\mathbf{x}}\;\hat{a}(\mathbf{k}')$$

$$=\int\frac{d^3k}{(2\pi)^{3/2}}\int\frac{d^3k'}{(2\pi)^{3/2}}\;\hat{a}^{+}(\mathbf{k})\,\hat{a}(\mathbf{k}')\,(2\pi)^3\,\delta(\mathbf{k}-\mathbf{k}')$$

$$=\int d^3k\,\hat{a}^{+}(\mathbf{k})\,\hat{a}(\mathbf{k})=\int d^3k\,\hat{n}(\mathbf{k})=N$$

where N is the total number of particles. Hence, $\hat{\rho}(\mathbf{x})$ is the number density operator at $\mathbf{x}$. The 2nd quantized forms discussed in §6.1.5 can be rewritten in terms of the field operators.

1-P operator:

$$\hat{A}=\int d^3k\int d^3k'\langle\mathbf{k}|A(\mathbf{x},\mathbf{p})|\mathbf{k}'\rangle\,\hat{a}^{+}(\mathbf{k})\,\hat{a}(\mathbf{k}')$$

$$=\int d^3x\;\hat{\psi}^{+}(\mathbf{x})\;A\left(\mathbf{x},-\frac{\hbar}{i}\nabla\right)\hat{\psi}(\mathbf{x})$$

2-P operator:

$$\hat{V}=\frac{1}{2}\int d^3k_1\int d^3k_2\int d^3k_3\int d^3k_4\,\langle\mathbf{k}_1\mathbf{k}_2|V(\mathbf{x},\mathbf{x}')|\mathbf{k}_3\mathbf{k}_4\rangle\,\hat{a}^{+}(\mathbf{k}_1)\,\hat{a}^{+}(\mathbf{k}_2)\,\hat{a}(\mathbf{k}_4)\,\hat{a}(\mathbf{k}_3)$$

$$=\frac{1}{2}\int d^3x\int d^3x'\;\hat{\psi}^{+}(\mathbf{x})\,\hat{\psi}^{+}(\mathbf{x}')\,V(\mathbf{x},\mathbf{x}')\,\hat{\psi}(\mathbf{x}')\,\hat{\psi}(\mathbf{x}) \qquad (6.21)$$

6.2.a. Field Operators and Observables

Note: *This section is the same as §6.2 but with different normalization.*

Henceforth, we shall take the 1-P states to be momentum eigenstaes. For spinless particles, we have $\alpha = \mathbf{k} = \frac{\mathbf{p}}{\hbar}$. Since **k** is continuous, the orthonormality and completeness take the form

$$\langle \mathbf{k} | \mathbf{k}' \rangle = (2\pi)^3 \delta(\mathbf{k} - \mathbf{k}') \qquad \int \frac{d^3k}{(2\pi)^3} |\mathbf{k}\rangle\langle\mathbf{k}| = 1$$

with

$$\langle \mathbf{x} | \mathbf{x}' \rangle = \delta(\mathbf{x} - \mathbf{x}') \qquad \int d^3x\, |\mathbf{x}\rangle\langle\mathbf{x}| = 1$$

$$\phi_{\mathbf{k}}(\mathbf{x}) = \langle \mathbf{x} | \mathbf{k} \rangle = e^{i\mathbf{k}\cdot\mathbf{x}}$$

Thus, the wave function for a single particle in state $|\Psi(t)\rangle$ can be written as

$$\Psi(\mathbf{x},t) = \langle \mathbf{x} | \Psi(t) \rangle = \int \frac{d^3k}{(2\pi)^3} \langle \mathbf{x} | \mathbf{k} \rangle \langle \mathbf{k} | \Psi(t) \rangle = \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{x}} \langle \mathbf{k} | \Psi(t) \rangle$$

$$= \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{x}} \langle 0 | \hat{a}(\mathbf{k}) | \Psi(t) \rangle \qquad (6.12)$$

where we've used

$$\langle \mathbf{k} | = (|\mathbf{k}\rangle)^+ = [\hat{a}^+(\mathbf{k})|0\rangle]^+ = \langle 0 | \hat{a}(\mathbf{k})$$

The **field operators** are defined in the Schrodinger picture by

$$\hat{\psi}(\mathbf{x}) = \sum_\alpha \langle \mathbf{x} | \alpha \rangle \hat{a}_\alpha = \sum_\alpha \phi_\alpha(\mathbf{x}) \hat{a}_\alpha$$

$$\hat{\psi}^+(\mathbf{x}) = \sum_\alpha \langle \alpha | \mathbf{x} \rangle \hat{a}_\alpha^+ = \sum_\alpha \phi_\alpha^*(\mathbf{x}) \hat{a}_\alpha^+$$

In the momentum basis, they become

$$\hat{\psi}(\mathbf{x}) = \int \frac{d^3k}{(2\pi)^3} \phi_{\mathbf{k}}(\mathbf{x}) \hat{a}(\mathbf{k}) = \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{x}} \hat{a}(\mathbf{k}) \qquad (6.13)$$

$$\hat{\psi}^+(\mathbf{x}) = \int \frac{d^3k}{(2\pi)^3} \phi_{\mathbf{k}}^*(\mathbf{x}) \hat{a}^+(\mathbf{k}) = \int \frac{d^3k}{(2\pi)^3} e^{-i\mathbf{k}\cdot\mathbf{x}} \hat{a}^+(\mathbf{k}) \qquad (6.14)$$

The corresponding commutation relations are

$$\left[\hat{\psi}(\mathbf{x}), \hat{\psi}(\mathbf{x}')\right]_{\mp} = \sum_{\alpha\beta} \langle \mathbf{x}|\alpha\rangle\langle \mathbf{x}'|\beta\rangle \; \left[\hat{a}_\alpha \,,\, \hat{a}_\beta\right]_{\mp} = 0$$

$$\left[\hat{\psi}^+(\mathbf{x}), \hat{\psi}^+(\mathbf{x}')\right]_{\mp} = \sum_{\alpha\beta} \langle \alpha|\mathbf{x}\rangle\langle \beta|\mathbf{x}'\rangle \; \left[\hat{a}^+_\alpha \,,\, \hat{a}^+_\beta\right]_{\mp} = 0 \qquad (6.15)$$

$$\left[\hat{\psi}(\mathbf{x}), \hat{\psi}^+(\mathbf{x}')\right]_{\mp} = \sum_{\alpha\beta} \langle \mathbf{x}|\alpha\rangle\langle \beta|\mathbf{x}'\rangle \quad \left[\hat{a}_\alpha \,,\, \hat{a}^+_\beta\right]_{\mp} = \sum_{\alpha} \langle \mathbf{x}|\alpha\rangle\langle \alpha|\mathbf{x}'\rangle$$

$$= \langle \mathbf{x}|\mathbf{x}'\rangle = \delta(\mathbf{x}-\mathbf{x}') \qquad (6.16)$$

Consider the operator

$$\hat{\rho}(\mathbf{x}) = \hat{\psi}^+(\mathbf{x})\, \hat{\psi}(\mathbf{x})$$

we have

$$\int d^3x\, \hat{\rho}(\mathbf{x}) = \int d^3x \;\; \hat{\psi}^+(\mathbf{x})\, \hat{\psi}(\mathbf{x})$$

$$= \int d^3x \int \frac{d^3k}{(2\pi)^3} \int \frac{d^3k'}{(2\pi)^3}\, e^{-i\mathbf{k}\cdot\mathbf{x}}\, \hat{a}^+(\mathbf{k})\, e^{i\mathbf{k}'\cdot\mathbf{x}} \;\; \hat{a}(\mathbf{k}')$$

$$= \int \frac{d^3k}{(2\pi)^3} \int \frac{d^3k'}{(2\pi)^3} \;\; \hat{a}^+(\mathbf{k})\, \hat{a}(\mathbf{k}')\, (2\pi)^3\, \delta(\mathbf{k}-\mathbf{k}')$$

$$= \int \frac{d^3k}{(2\pi)^3}\, \hat{a}^+(\mathbf{k})\, \hat{a}(\mathbf{k}) = \int \frac{d^3k}{(2\pi)^3}\, \hat{n}(\mathbf{k}) = N$$

where N is the total number of particles. Hence, $\hat{\rho}(\mathbf{x})$ is the number density operator at **x**. The 2[nd] quantized forms discussed in §6.1.5 can be rewritten in terms of the field operators.

1-P operator:

$$\hat{A} = \int \frac{d^3k}{(2\pi)^3} \int \frac{d^3k'}{(2\pi)^3} \langle \mathbf{k}|A(\mathbf{x},\mathbf{p})|\mathbf{k}'\rangle\, \hat{a}^+(\mathbf{k})\, \hat{a}(\mathbf{k}')$$

$$= \int d^3x \;\; \hat{\psi}^+(\mathbf{x})\; A\!\left(\mathbf{x}, \frac{\hbar}{i}\nabla\right) \hat{\psi}(\mathbf{x})$$

2-P operator:

$$\hat{V} = \frac{1}{2} \int \frac{d^3k_1}{(2\pi)^3} \int \frac{d^3k_2}{(2\pi)^3} \int \frac{d^3k_3}{(2\pi)^3} \int \frac{d^3k_4}{(2\pi)^3} \langle \mathbf{k}_1\mathbf{k}_2|V(\mathbf{x},\mathbf{x}')|\mathbf{k}_3\mathbf{k}_4\rangle$$

$$\times \hat{a}^{+}(\mathbf{k}_1)\, \hat{a}^{+}(\mathbf{k}_2)\, \hat{a}(\mathbf{k}_4)\, \hat{a}(\mathbf{k}_3)$$

$$= \frac{1}{2}\int d^3x \int d^3x'\, \hat{\psi}^{+}(\mathbf{x})\, \hat{\psi}^{+}(\mathbf{x}')\, V(\mathbf{x},\mathbf{x}')\, \hat{\psi}(\mathbf{x}')\, \hat{\psi}(\mathbf{x}) \qquad (6.21)$$

6.3. Equation of Motion and Lagrangian Formalism for Field Operators

6.3.1. Equation of Motion
6.3.2. Lagrangian

6.3.1. Equation of Motion

Field operators in the Heisenberg picture are defined by eq(5.35) as

$$\hat{\psi}(\mathbf{x},t) = \exp\left(\frac{i}{\hbar}\hat{H}\,t\right)\hat{\psi}(\mathbf{x})\exp\left(-\frac{i}{\hbar}\hat{H}\,t\right) \tag{6.22}$$

$$\hat{\psi}^{+}(\mathbf{x},t) = \exp\left(\frac{i}{\hbar}\hat{H}\,t\right)\hat{\psi}^{+}(\mathbf{x})\exp\left(-\frac{i}{\hbar}\hat{H}\,t\right)$$

Similarly,

$$\hat{H}(\mathbf{p},\mathbf{x},t) = \exp\left(\frac{i}{\hbar}\hat{H}\,t\right)\hat{H}(\mathbf{p},\mathbf{x})\exp\left(-\frac{i}{\hbar}\hat{H}\,t\right) = \hat{H}(\mathbf{p},\mathbf{x})$$

In general, commutation relations in the Heisenberg picture take on simple forms only when the operators are at the same time. For example, it is easy to verify the following **equal time commutation relations**:

$$\left[\hat{\psi}(\mathbf{x},t),\hat{\psi}(\mathbf{x}',t)\right]_{\mp} = \left[\hat{\psi}^{+}(\mathbf{x},t),\hat{\psi}^{+}(\mathbf{x}',t)\right]_{\mp} = 0$$

$$\left[\hat{\psi}(\mathbf{x},t),\hat{\psi}^{+}(\mathbf{x}',t)\right]_{\mp} = \delta(\mathbf{x}-\mathbf{x}')$$

For a system of particles subject to an external potential U and mutual 2-body interaction potential V, the hamiltonian can be written as

$$\hat{H} = \int d^3x\,\hat{\psi}^{+}(\mathbf{x},t)\left(-\frac{\hbar^2}{2m}\nabla^2 + U(\mathbf{x})\right)\hat{\psi}(\mathbf{x},t)$$

$$+\frac{1}{2}\int d^3x\int d^3x'\,\hat{\psi}^{+}(\mathbf{x},t)\hat{\psi}^{+}(\mathbf{x}',t)V(\mathbf{x},\mathbf{x}')\hat{\psi}(\mathbf{x}',t)\hat{\psi}(\mathbf{x},t)$$

The commutators in the equation of motion [see (5.36)]

$$i\hbar\frac{\partial}{\partial t}\hat{\psi}(\mathbf{x},t) = \left[\hat{\psi}(\mathbf{x},t),\hat{H}\right]$$

can be evaluated using

$$[a,bc] = abc - bca = abc \mp bac \pm bac - bca = [a,b]_{\mp}\,c \pm b\,[a,c]_{\mp}$$

$$[ab,c] = abc - cab = abc \mp acb \pm acb - cab = a[b,c]_{\mp} \pm [a,c]_{\mp}\,b$$

Thus,

$$\left[\hat{\psi}(\mathbf{x},t),\hat{\psi}^{+}(\mathbf{x}',t)\hat{\psi}(\mathbf{x}',t)\right]_{\mp}$$

$$= \left[\hat{\psi}(\mathbf{x},t),\hat{\psi}^{+}(\mathbf{x}',t)\right]_{\mp}\hat{\psi}(\mathbf{x}',t) \pm \hat{\psi}^{+}(\mathbf{x}',t)\left[\hat{\psi}(\mathbf{x},t),\hat{\psi}(\mathbf{x}',t)\right]_{\mp}$$

$$= \delta(\mathbf{x}-\mathbf{x}')\,\hat{\psi}(\mathbf{x}',t)$$

$$
\begin{aligned}
&\left[\hat{\psi}(\mathbf{x},t),\hat{\psi}^{+}(\mathbf{x}',t)\hat{\psi}^{+}(\mathbf{x}'',t)\right]_{\mp}\\
&=\left[\hat{\psi}(\mathbf{x},t),\hat{\psi}^{+}(\mathbf{x}',t)\right]_{\mp}\hat{\psi}^{+}(\mathbf{x}'',t)\pm\hat{\psi}^{+}(\mathbf{x}',t)\left[\hat{\psi}(\mathbf{x},t),\hat{\psi}^{+}(\mathbf{x}'',t)\right]_{\mp}\\
&=\delta(\mathbf{x}-\mathbf{x}')\hat{\psi}^{+}(\mathbf{x}'',t)\pm\delta(\mathbf{x}-\mathbf{x}'')\hat{\psi}^{+}(\mathbf{x}',t)
\end{aligned}
$$

so that, with a little arrangement, we have

$$
\begin{aligned}
i\hbar\frac{\partial}{\partial t}\hat{\psi}(\mathbf{x},t)&=\left(-\frac{\hbar^2}{2m}\nabla^2+U(\mathbf{x})\right)\hat{\psi}(\mathbf{x},t)\\
&\quad+\int d^3x'\;\hat{\psi}^{+}(\mathbf{x}',t)V(\mathbf{x},\mathbf{x}')\hat{\psi}(\mathbf{x}',t)\hat{\psi}(\mathbf{x},t)
\end{aligned}
\tag{6.24}
$$

6.3.2. Lagrangian

The equation of motion (6.24) can of course be derived from a suitable Lagrangian using the principle of least action. Now, in a variational calculation, operators and functions behave identically except that operators need not commute. Hence, the technique can be demonstrated by the derivation of the Schrodinger equation for wavefunctions. By carefully maintaining the order of all quantities, we obtain results that are valid for field operators.

An action that gives rise to the time-dependent 1-P Schrodinger equation is

$$S = \int dt \int d^3x \, \psi^*(\mathbf{x},t) \left(i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \nabla^2 - U \right) \psi(\mathbf{x},t) \qquad (6.25)$$

$$= \int dt \int d^3x \, \mathcal{L}$$

Since ψ is a complex function, each $\psi(\mathbf{x})$ represents 2 degrees of freedom. The corresponding independent variables may be chosen to be $\mathrm{Re}\,\psi$ and $\mathrm{Im}\,\psi$. However, a more manageable choice is ψ and ψ^*. [Note, ψ^* can be calculated from ψ only after the real axis is chosen. Until then, ψ and ψ^* are independent.]

Variation on ψ^* gives

$$\frac{\partial \mathcal{L}}{\partial(\partial_t \psi^*)} = 0 \qquad \frac{\partial \mathcal{L}}{\partial(\partial_j \psi^*)} = 0$$

$$\frac{\partial \mathcal{L}}{\partial \psi^*} = \left(i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \nabla^2 - U \right) \psi$$

Thus, the Euler-Lagrange equation

$$\frac{\partial \mathcal{L}}{\partial \psi^*} - \partial_t \frac{\partial \mathcal{L}}{\partial(\partial_t \psi^*)} - \partial_j \frac{\partial \mathcal{L}}{\partial(\partial_j \psi^*)} = 0$$

becomes

$$i\hbar \frac{\partial \psi}{\partial t} = \left(-\frac{\hbar^2}{2m} \nabla^2 + U \right) \psi$$

which is the desired Schrodinger equation.

Variation on ψ gives

$$\frac{\partial \mathcal{L}}{\partial(\partial_t \psi)} = i\hbar \psi^*$$

$$\frac{\partial \mathcal{L}}{\partial(\partial_j \psi)} = -\frac{\hbar^2}{2m}\partial_j \psi^* \qquad \text{[integration by part performed]}$$

$$\frac{\partial \mathcal{L}}{\partial \psi} = -U\psi^*$$

$$\Rightarrow \qquad -U\psi^* - i\hbar \partial_t \psi^* + \frac{\hbar^2}{2m}\partial_j \partial_j \psi^* = 0$$

or
$$-i\hbar \frac{\partial \psi^*}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + U\right)\psi^*$$

The generalized momentum conjugate to ψ is

$$\Pi = \frac{\partial \mathcal{L}}{\partial(\partial_t \psi)} = i\hbar \psi^* \qquad (6.26)$$

But the momentum conjugate to ψ^* vanishes identically. The Hamiltonian density is

$$\mathcal{H} = \Pi\, \partial_t \psi - \mathcal{L} \quad = \psi^* \left(-\frac{\hbar^2}{2m}\nabla^2 + U\right)\psi$$

so that the Hamiltonian becomes

$$H = \int d^3x\, \psi^* \left(-\frac{\hbar^2}{2m}\nabla^2 + U\right)\psi \qquad (6.27)$$

In the 2nd quantization, the wavefunctions ψ and ψ^* are replaced by the field operators $\hat{\psi}$ and $\hat{\psi}^+$. On the other hand, if we treat (6.25) as the action for a classical field and apply the quantization rule to the conjugate variables $\psi(\mathbf{x},t)$ and $\Pi(\mathbf{x},t)$ so that

$$\left[\hat{\psi}(\mathbf{x},t), \hat{\Pi}(\mathbf{x}',t)\right]_{\mp} = i\hbar \delta(\mathbf{x}-\mathbf{x}')$$

we recover the commutation relation (6.16). Thus, 2nd quantization is equivalent to quantizing a classical field; hence the name **quantum field theory**. Obviously, nothing new was gained in the derivation of the Schrodinger equation. However, new physics may be expected when the procedure is applied to other classical fields such as the electromagnetic fields.

6.4. Second Quantization for Fermions