6

Non-Relativistic Field Theory

In this Chapter we will discuss the field theory description of non-relativistic systems. The material that we will be presented here is, for the most part, introductory as this topic is covered in depth in many specialized textbooks, such as *Methods of Quantum Field Theory in Statistical Physics* by A. Abrikosov, L. Gorkov and I. Dzyaloshinskii (Prentice-Hall, 1963), *Statistical Mechanics, A Set of lectures* by R. Feynman (Benjamin, 1973) and many others. The discussion of "second quantization" is very standard and is presented her for pedagogical reasons but can be skipped.

6.1 Non-Relativistic Field Theories, Second Quantization and the Many-Body Problem

Let us consider now the problem of a system of N *identical* non-relativistic particles. For the sake of simplicity I will assume that the physical state of *each* particle j is described by its position $\boldsymbol{x}_j$ relative to some reference frame. This case is easy to generalize.

The wave function for this system is $\Psi(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N)$. If the particles are *identical* then the *probability density*, $|\Psi(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N)|^2$, must be invariant (*i.e.,* unchanged) under arbitrary exchanges of the labels that we use to identify (or designate) the particles. In quantum mechanics, the particles do not have well defined trajectories. Only the states of a physical system are well defined. Thus, even though at some initial time t_0 the N particles may be localized at a set of well defined positions $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N$, they will become delocalized as the system evolves. Furthermore the Hamiltonian itself is *invariant* under a permutation of the particle labels. Hence, *permutations* constitute a *symmetry* of a many-particle quantum mechanical system. In other terms, identical particles are indistinguishable in quantum mechanics. In particular, the *probability density* of *any* eigenstate must remain invariant if the labels of any pair of particles are exchanged. If we denote by P_{jk} the operator which exchanges the labels of particles j and k, the wave functions must satisfy

$$P_{jk}\Psi(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_j,\ldots,\boldsymbol{x}_k,\ldots,\boldsymbol{x}_N) = e^{i\phi}\Psi(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_j,\ldots,\boldsymbol{x}_k,\ldots,\boldsymbol{x}_N) \tag{6.1}$$

Under a further exchange operation, the particles return to their initial labels and we recover the original state. This sample argument then requires that $\phi = 0, \pi$ since 2ϕ must not be an observable phase. We then conclude that there are two possibilities: either Ψ is *even* under permutation and $P\Psi = \Psi$, *or* Ψ is *odd* under permutation and $P\Psi = -\Psi$. Systems of identical particles which have wave functions which are *even* under a pairwise permutation of the particle labels are called *bosons*. In the other case, Ψ *odd* under pairwise permutation, they are *Fermions*. It must be stressed that these arguments only show that the requirement that the state prioriΨ be either even or odd is only a *sufficient* condition. It turns out that under special circumstances other options become available and the phase factor ϕ may take values different from 0 or π. These particles are called *anyons*. For the moment the only cases in which they may exist appears to be in situations in which the particles are restricted to move on a line or on a plane. In the case of *relativistic* quantum field theories, the requirement that the states have well defined *statistics* (or *symmetry*) is demanded by a very deep and fundamental theorem which links the *statistics* of the states of the *spin* of the field. This is the *spin-statistics* theorem which we will discuss later on.

6.1.1 Fock Space

We will now discuss a procedure, known as *Second Quantization*, which will enable us to keep track of the symmetry of the states in a simple way. Let us consider now a system of N particles. The wave functions in the coordinate representation are $\Psi(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_N)$ where the labels $\boldsymbol{x}_1,\ldots,\boldsymbol{x}_N$ denote both the coordinates and the spin states of the particles in the state $|\Psi\rangle$. For the sake of definiteness we will discuss physical systems describable by Hamiltonians $\hat{H}$ of the form

$$\hat{H} = -\frac{\hbar^2}{2m}\sum_{j=1}^{N}\bigtriangledown_j^2 + \sum_{j=1}^{N}V(\boldsymbol{x}_j) + g\sum_{j,k}U(\boldsymbol{x}_j-\boldsymbol{x}_k) + \ldots \tag{6.2}$$

Let $\{\phi_n(x)\}$ be the wave functions for a complete set of one-particle states. Then an arbitrary N-particle state can be expanded in a basis which is the tensor product of the one-particle states, namely

$$\Psi(\boldsymbol{x}_1, \dots, \boldsymbol{x}_N) = \sum_{\{nj\}} C(n_1, \dots n_N)\phi_{n1}(\boldsymbol{x}_1) \dots \phi_{nN}(\boldsymbol{x}_N) \tag{6.3}$$

Thus, if Ψ is symmetric (antisymmetric) under an arbitrary exchange $\boldsymbol{x}_j \to \boldsymbol{x}_k$, the coefficients $C(n_1, \dots, n_N)$ must be symmetric (antisymmetric) under the exchange $n_j \leftrightarrow n_k$.

A set of N-particle basis states with well defined permutation symmetry is the properly symmetrized or antisymmetrized tensor product

$$|\Psi_1, \dots \Psi_N\rangle \equiv |\Psi_1\rangle \times |\Psi_2\rangle \times \dots \times |\Psi_N\rangle = \frac{1}{\sqrt{N!}} \sum_P \xi^P |\Psi_{P(1)}\rangle \times \dots \times |\Psi_{P(N)}\rangle \tag{6.4}$$

where the sum runs over the set of all possible permutation P. The weight factor ξ is $+1$ for *bosons* and -1 for fermions. Notice that, for fermions, the N-particle state vanishes if two particles are in the same one-particle state. This is the *exclusion principle.*

The inner product of two N-particle states is

$$\begin{aligned} \langle \chi_1, \dots \chi_N | \psi_1, \dots, \psi_N \rangle &= \frac{1}{N!} \sum_{P,Q} \xi^{P+Q} \langle \chi_{Q(1)} | \psi_{P(1)} \rangle \cdots \langle \chi_{Q(N)} | \psi_{P(1)} \rangle = \\ &= \sum_{P'} \xi^{P'} \langle \chi_1 | \psi_{P(1)} \rangle \cdots \langle \chi_N | \psi_{P(N)} \rangle \end{aligned} \tag{6.5}$$

which is nothing but the *permanent (determinant)* of the matrix $\langle \chi_j | \psi_k \rangle$ for *symmetric (antisymmetric)* states, *i.e.,*

$$\langle \chi_1, \dots \chi_N | \psi_1, \dots \psi_N \rangle = \begin{vmatrix} \langle \chi_1 | \psi_1 \rangle & \dots & \langle \chi_1 | \psi_N \rangle \\ \vdots & & \vdots \\ \langle \chi_N | \psi_1 \rangle & \dots & \langle \chi_N | \psi_N \rangle \end{vmatrix}_\xi \tag{6.6}$$

In the case of antisymmetric states, the inner product is the familiar *Slater determinant.* Let us denote by $\{|\alpha\rangle\}$ the complete set of one-particle states which satisfy

$$\langle \alpha | \beta \rangle = \delta_{\alpha\beta} \qquad \sum_\alpha |\alpha\rangle\langle\alpha| = 1 \tag{6.7}$$

The N-particle states are $\{|\alpha_1, \dots \alpha_N\rangle\}$. Because of the symmetry requirements, the labels α_j can be arranged in the form of a monotonic sequence $\alpha_1 \leq \alpha_2 \leq \dots \leq \alpha_N$ for *bosons*, or in the form of a *strict* monotonic sequence $\alpha_1 < \alpha_2 < \dots < \alpha_N$ for *fermions.* Let n_j be an integer which counts how many particles are in the j-th one-particle state. The *boson* states $|\alpha_1, \ldots \alpha_N\rangle$ must be normalized by a factor of the form

$$\frac{1}{\sqrt{n_1! \ldots n_N!}} |\alpha_1, \ldots, \alpha_N\rangle \qquad (\alpha_1 \leq \alpha_2 \leq \cdots \leq \alpha_N) \tag{6.8}$$

and n_j are non-negative integers. For *fermions* the states are

$$|\alpha_1, \ldots, \alpha_N\rangle \qquad (\alpha_1 < \alpha_2 < \cdots < \alpha_N) \tag{6.9}$$

and $n_j = 0 > 1$. These N-particle states are complete and orthonormal

$$\frac{1}{N!} \sum_{\alpha_1, \ldots, \alpha_N} |\alpha_1, \ldots, \alpha_N\rangle\langle\alpha_1, \ldots, \alpha_N| = \hat{I} \tag{6.10}$$

where the sum over the α's is unrestricted and the operator $\hat{I}$ is the identity operator in the space of N-particle states.

We will now consider the more general problem in which the number of particles N is not fixed a-priori. Rather, we will consider an *enlarged* space of states in which the number of particles is allowed to fluctuate. In the language of Statistical Physics what we are doing is to go from the *Canonical Ensemble* to the *Grand Canonical Ensemble*. Thus, let us denote by $\mathcal{H}_0$ the Hilbert space with no particles, $\mathcal{H}_1$ the Hilbert space with only one particle and, in general, $\mathcal{H}_N$ the Hilbert space for N-particles. The direct sum of these spaces $\mathcal{H}$

$$\mathcal{H} = \mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \cdots \oplus \mathcal{H}_N \oplus \cdots \tag{6.11}$$

is usually called the *Fock space*. An arbitrary state $|\psi\rangle$ in Fock space is the sum over the subspaces $\mathcal{H}_N$,

$$|\psi\rangle = |\psi^{(0)}\rangle + |\psi^{(1)}\rangle + \cdots + |\psi^{(N)}\rangle + \cdots \tag{6.12}$$

The subspace with no particles is a one-dimensional space spanned by the vector $|0\rangle$ which we will call the *vacuum*. The subspaces with well defined number of particles are defined to be orthogonal to each other in the sense that the *inner product* in the *Fock space*

$$\langle\chi|\psi\rangle \equiv \sum_{j=0}^{\infty} \langle\chi^{(j)}|\psi^{(j)}\rangle \tag{6.13}$$

vanishes if $|\chi\rangle$ and $|\psi\rangle$ belong to different subspaces.

6.1.2 Creation and Annihilation Operators

Let $|\phi\rangle$ be an arbitrary *one-particle state*. Let us define the *creation operator* $\hat{a}^\dagger(\phi)$ by its action on an arbitrary state in Fock space

$$\hat{a}^\dagger(\phi)|\psi_1,\ldots,\psi_N\rangle = |\phi,\psi_1,\ldots,\psi_N\rangle \tag{6.14}$$

Clearly, $\hat{a}^\dagger(\phi)$ maps the N-particle state with proper symmetry $|\psi_1,\ldots,\psi_N\rangle$ onto the $N+1$-particle state $|\phi,\psi,\ldots,\psi_N\rangle$, also with proper symmetry . The *destruction* or *annihilation operator* $\hat{a}(\phi)$ is defined to be the *adjoint* of $\hat{a}^\dagger(\phi)$,

$$\langle\chi_1,\ldots,\chi_{N-1}|\hat{a}(\phi)|\psi_1,\ldots,\psi_N\rangle = \langle\psi_1,\ldots,\psi_N|\hat{a}^\dagger(\phi)|\chi_1,\ldots,\chi_{N-1}\rangle^* \tag{6.15}$$

Hence

$$\langle\chi_1,\ldots,\chi_{N-1}|\hat{a}(\phi)|\psi_1,\ldots,\psi_N\rangle = \langle\psi_1,\ldots,\psi_N|\phi,\chi_1,\ldots,\chi_{N-1}\rangle^* = \begin{vmatrix} \langle\psi_1|\phi\rangle & \langle\psi_1|\chi_1\rangle & \cdots & \langle\psi_1|\chi_{N-1}\rangle \\ \vdots & \vdots & & \vdots \\ \langle\psi_N|\phi\rangle & \langle\psi_N|\chi_1\rangle & \cdots & \langle\psi_N|\chi_{N-1}\rangle \end{vmatrix}_\xi^* \tag{6.16}$$

We can now expand the permanent (or determinant) to get

$$\begin{aligned}\langle\chi_1,\ldots,\chi_{N-1}|\hat{a}(\phi)|\psi_1,\ldots,\psi_N\rangle &= \\ &= \sum_{k=1}^{N}\xi^{k-1}\langle\psi_k|\phi\rangle \begin{vmatrix} \langle\psi_1|\chi_1\rangle & \ldots & \langle\psi_1|\chi_{N-1}\rangle \\ \vdots & & \vdots \\ \ldots & (\text{no}\psi_k) & \ldots \\ \langle\psi_N|\chi_1\rangle & \ldots & \langle\psi_N|\chi_{N-1}\rangle \end{vmatrix}_\xi^* \\ &= \sum_{k=1}^{N}\xi^{k-1}\langle\psi_k|\phi\rangle\langle\chi_1,\ldots,\chi_{N-1}|\psi_1,\ldots\hat{\psi}_k\ldots,\psi_N\rangle\end{aligned} \tag{6.17}$$

where $\hat{\psi}_k$ indicates that ψ_k is *absent*. Thus, the destruction operator is given by

$$\hat{a}(\phi)|\psi_1,\ldots,\psi_N\rangle = \sum_{k=1}^{N}\xi^{k-1}\langle\phi|\psi_k\rangle|\psi_1,\ldots,\hat{\psi}_k,\ldots,\psi_N\rangle \tag{6.18}$$

With these definitions, we can easily see that the operators $\hat{a}^\dagger(\phi)$ and $\hat{a}(\phi)$

obey the commutation relations

$$\hat{a}^\dagger(\phi_1)\hat{a}^\dagger(\phi_2) = \xi\, \hat{a}^\dagger(\phi_2)\hat{a}^\dagger(\phi_1) \tag{6.19}$$

Let us introduce the notation

$$\left[\hat{A}, \hat{B}\right]_{-\xi} \equiv \hat{A}\hat{B} - \xi\, \hat{B}\hat{A} \tag{6.20}$$

where $\hat{A}$ and $\hat{B}$ are two arbitrary operators. For $\xi = +1$ (*bosons*) we have the *commutator*

$$\left[\hat{a}^\dagger(\phi_1), \hat{a}^\dagger(\phi_2)\right]_{+1} \equiv \left[\hat{a}^\dagger(\phi_1), \hat{a}^\dagger(\phi_2)\right] = 0 \tag{6.21}$$

while for $\xi = -1$ it is the *anticommutator*

$$\left[\hat{a}^\dagger(\phi_1), \hat{a}^\dagger(\phi_2)\right]_{-1} \equiv \left\{\hat{a}^\dagger(\phi_1), \hat{a}^\dagger(\phi_2)\right\} = 0 \tag{6.22}$$

Similarly for any pair of arbitrary one-particle states $|\phi_1\rangle$ and $|\phi_2\rangle$ we get

$$[\hat{a}(\phi_1), \hat{a}(\phi_2)]_{-\xi} = 0 \tag{6.23}$$

It is also easy to check that the following identity holds

$$\left[\hat{a}(\phi_1), \hat{a}^\dagger(\phi_2)\right]_{-\xi} = \langle\phi_1|\phi_2\rangle \tag{6.24}$$

So far we have not picked any particular representation. Let us consider the occupation number representation in which the states are labelled by the number of particles n_k in the single-particle state k. In this case, we have

$$|n_1, \ldots, n_k, \ldots\rangle \equiv \frac{1}{\sqrt{n_1! n_2! \ldots}} |\overbrace{1\ldots1}^{n1}, \overbrace{2\ldots2}^{n2}\ldots\rangle \tag{6.25}$$

In the case of *bosons*, the n_j's can be any non-negative integer, while for fermions they can only be equal to zero or one. In general we have that if $|\alpha\rangle$ is the αth single-particle state, then

$$\begin{aligned} \hat{a}^\dagger_\alpha|n_1, \ldots, n_\alpha, \ldots\rangle &= \sqrt{n_\alpha + 1}|n_1, \ldots, n_\alpha + 1, \ldots\rangle \\ \hat{a}_\alpha|n_1, \ldots, n_\alpha, \ldots\rangle &= \sqrt{n_\alpha}|n_1, \ldots, n_\alpha - 1, \ldots\rangle \end{aligned} \tag{6.26}$$

Thus for both *fermions* and *bosons*, $\hat{a}_\alpha$ annihilates all states with $n_\alpha = 0$, while for *fermions* $\hat{a}^\dagger_\alpha$ annihilates all states with $n_\alpha = 1$.

The commutation relations are

$$[\hat{a}_\alpha, \hat{a}_\beta] = \left[\hat{a}^\dagger_\alpha, \hat{a}^\dagger_\beta\right] = 0 \qquad \left[\hat{a}_\alpha, \hat{a}^\dagger_\beta\right] = \delta_{\alpha\beta} \tag{6.27}$$

for bosons, and

$$\{\hat{a}_\alpha \hat{a}_\beta\} = \left\{\hat{a}^\dagger_\beta, \hat{a}^\dagger_\beta\right\} = 0 \qquad \left\{\hat{a}_\alpha \hat{a}^\dagger_\beta\right\} = \delta_{\alpha\beta} \tag{6.28}$$

for fermions. Here, $\left\{\hat{A}, \hat{B}\right\}$ is the anticommutator of the operators $\hat{A}$ and $\hat{B}$

$$\left\{\hat{A}, \hat{B}\right\} \equiv \hat{A}\hat{B} + \hat{B}\hat{A} \tag{6.29}$$

If a unitary transformation is performed in the space of one-particle state vectors, then a unitary transformation is *induced* in the space of the operators themselves, *i.e.,* if $|\chi\rangle = \alpha|\psi\rangle + \beta|\phi\rangle$, then

$$\begin{aligned} \hat{a}(\chi) &= \alpha^* \hat{a}(\psi) + \beta^* \hat{a}(\phi) \\ \hat{a}^\dagger(\chi) &= \alpha \hat{a}^\dagger(\psi) + \beta \hat{a}^\dagger(\phi) \end{aligned} \tag{6.30}$$

and we say that $\hat{a}^\dagger(\chi)$ transforms like the *ket* $|\chi\rangle$ while $\hat{a}(\chi)$ transforms like the *bra* $\langle\chi|$.

For example, we can pick as the complete set of one-particle states the momentum states $\{|\boldsymbol{p}\rangle\}$. This is "momentum space". With this choice the commutation relations are

$$\begin{aligned} \left[\hat{a}^\dagger(\boldsymbol{p}), \hat{a}^\dagger(\boldsymbol{q})\right]_{-\xi} &= [\hat{a}(\boldsymbol{p}), \hat{a}(\boldsymbol{q})]_{-\xi} = 0 \\ \left[\hat{a}(\boldsymbol{p}), \hat{a}^\dagger(\boldsymbol{q})\right]_{-\xi} &= (2\pi)^d \delta^d(\boldsymbol{p} - \boldsymbol{q}) \end{aligned} \tag{6.31}$$

where d is the dimensionality of space. In this representation, an N-particle state is

$$|\boldsymbol{p}_1, \ldots, \boldsymbol{p}_N\rangle = \hat{a}^\dagger(\boldsymbol{p}_1) \ldots \hat{a}^\dagger(\boldsymbol{p}_N)|0\rangle \tag{6.32}$$

On the other hand, we can also pick the one-particle states to be eigenstates of the position operators, *i.e.,*

$$|\boldsymbol{x}_1, \ldots \boldsymbol{x}_N\rangle = \hat{a}^\dagger(\boldsymbol{x}_1) \ldots \hat{a}^\dagger(\boldsymbol{x}_N)|0\rangle \tag{6.33}$$

In position space, the operators satisfy

$$\begin{aligned} \left[\hat{a}^\dagger(\boldsymbol{x}_1), \hat{a}^\dagger(\boldsymbol{x}_2)\right]_{-\xi} &= [\hat{a}(\boldsymbol{x}_1), \hat{a}(\boldsymbol{x}_2)]_{-\xi} = 0 \\ \left[\hat{a}(\boldsymbol{x}_1), \hat{a}^\dagger(\boldsymbol{x}_2)\right]_{-\xi} &= \delta^d(\boldsymbol{x}_1 - \boldsymbol{x}_2) \end{aligned} \tag{6.34}$$

This is the position space or coordinate representation. A transformation from position space to momentum space is the Fourier transform

$$|\boldsymbol{p}\rangle = \int d^d x\ |\boldsymbol{x}\rangle\langle\boldsymbol{x}|\boldsymbol{p}\rangle = \int d^d x\ |\boldsymbol{x}\rangle e^{i\boldsymbol{p}\cdot\boldsymbol{x}} \tag{6.35}$$

and, conversely

$$|\boldsymbol{x}\rangle = \int \frac{d^d p}{(2\pi)^d}\ |\boldsymbol{p}\rangle e^{-i\boldsymbol{p}\cdot\boldsymbol{x}} \tag{6.36}$$

Then, the operators themselves obey

$$\begin{aligned} \hat{a}^\dagger(\boldsymbol{p}) &= \int d^d x\ \hat{a}^\dagger(\boldsymbol{x}) e^{i\boldsymbol{p}\cdot\boldsymbol{x}} \\ \hat{a}^\dagger(\boldsymbol{x}) &= \int \frac{d^d p}{(2\pi)^d}\ \hat{a}^\dagger(\boldsymbol{p}) e^{-i\boldsymbol{p}\cdot\boldsymbol{x}} \end{aligned} \tag{6.37}$$

6.1.3 General Operators in Fock Space

Let $A^{(1)}$ be an operator acting on one-particle states. We can always define an *extension* of A acting on any arbitrary state $|\psi\rangle$ of the N-particle Hilbert space as follows:

$$\widehat{A}|\psi\rangle \equiv \sum_{j=1}^{N} |\psi_1\rangle \times \ldots \times A^{(1)}|\psi_j\rangle \times \ldots \times |\psi_N\rangle \tag{6.38}$$

For instance, if the one-particle basis states $\{|\psi_j\rangle\}$ are eigenstates of A with eigenvalues $\{a_j\}$ we get

$$\widehat{A}|\psi\rangle = \left(\sum_{j=1}^{N} a_j\right)|\psi\rangle \tag{6.39}$$

We wish to find an expression for an arbitrary operator A in terms of creation and annihilation operators. Let us first consider the operator $A^{(1)}_{\alpha\beta} = |\alpha\rangle\langle\beta|$ which acts on one-particle states. The operators $A^{(1)}_{\alpha\beta}$ form a basis of the space of operators acting on one-particle states. Then, the N-particle extension of $A_{\alpha\beta}$ is

$$\widehat{A}_{\alpha\beta}|\psi\rangle = \sum_{j=1}^{N} |\psi_1\rangle \times \cdots \times |\alpha\rangle \times \cdots \times |\psi_N\rangle\langle\beta|\psi_j\rangle \tag{6.40}$$

Thus

$$\widehat{A}_{\alpha\beta}|\psi\rangle = \sum_{j=1}^{N} |\psi_1, \dots, \overbrace{\alpha}^{j}, \dots, \psi_N\rangle \; \langle\beta|\psi_j\rangle \tag{6.41}$$

In other words, we can replace the one-particle state $|\psi_j\rangle$ from the basis with the state $|\alpha\rangle$ at the price of a weight factor, the overlap $\langle\beta|\psi_j\rangle$. This operator has a very simple expression in terms of creation and annihilation operators. Indeed,

$$\hat{a}^\dagger(\alpha)\hat{a}(\beta)|\psi\rangle = \sum_{k=1}^{N} \xi^{k-1}\langle\beta|\psi_k\rangle \; |\alpha, \psi_1, \dots, \psi_{k-1}, \psi_{k+1}, \dots, \psi_N\rangle \tag{6.42}$$

We can now use the symmetry of the state to write

$$\xi^{k-1}|\alpha, \psi_1, \dots, \psi_{k-1}, \psi_{k+1}, \dots, \psi_N\rangle = |\psi_1, \dots, \overbrace{\alpha}^{k}, \dots, \psi_N\rangle \tag{6.43}$$

Thus the operator $A_{\alpha\beta}$, the extension of $|\alpha\rangle\langle\beta|$ to the N-particle space, coincides with $\hat{a}^\dagger(\alpha)\hat{a}(\beta)$

$$\widehat{A}_{\alpha\beta} \equiv \hat{a}^\dagger(\alpha)\hat{a}(\beta) \tag{6.44}$$

We can use this result to find the extension for an arbitrary operator $A^{(1)}$ of the form

$$A^{(1)} = \sum_{\alpha,\beta} |\alpha\rangle\langle\alpha|A^{(1)}|\beta\rangle \; \langle\beta| \tag{6.45}$$

we find

$$\widehat{A} = \sum_{\alpha,\beta} \hat{a}^\dagger(\alpha)\hat{a}(\beta)\langle\alpha|A^{(1)}|\beta\rangle \tag{6.46}$$

Hence the coefficients of the expansion are the matrix elements of $A^{(1)}$ between arbitrary one-particle states. We now discuss a few operators of interest.

The Identity Operator

The Identity Operator $\hat{1}$ of the one-particle Hilbert space

$$\hat{1} = \sum_{\alpha} |\alpha\rangle\langle\alpha| \tag{6.47}$$

becomes the *number operator* $\widehat{N}$

$$\widehat{N} = \sum_{\alpha} \hat{a}^\dagger(\alpha)\hat{a}(\alpha) \tag{6.48}$$

In position and in momentum space we find

$$\widehat{N} = \int \frac{d^d p}{(2\pi)^d}\, \hat{a}^\dagger(\boldsymbol{p})\hat{a}(\boldsymbol{p}) = \int d^d x\, \hat{a}^\dagger(\boldsymbol{x})\hat{a}(\boldsymbol{x}) = \int d^d x\, \hat{\rho}(\boldsymbol{x}) \tag{6.49}$$

where $\hat{\rho}(x) = \hat{a}^\dagger(\boldsymbol{x})\hat{a}(\boldsymbol{x})$ is the *particle density operator*.

The Linear Momentum Operator

In the space $\mathcal{H}_1$, the linear momentum operator is

$$\hat{p}_j^{(1)} = \int \frac{d^d p}{(2\pi)^d}\, p_j\, |\boldsymbol{p}\rangle\langle\boldsymbol{p}| = \int d^d x\, |\boldsymbol{x}\rangle\, \frac{\hbar}{i}\partial_j\, \langle\boldsymbol{x}| \tag{6.50}$$

Thus, we get that the total momentum operator $\widehat{P}_j$ is

$$\widehat{P}_j = \int \frac{d^d p}{(2\pi)^d}\, p_j \hat{a}^\dagger(\boldsymbol{p})\hat{a}(\boldsymbol{p}) = \int d^d x\, \hat{a}^\dagger(\boldsymbol{x})\frac{\hbar}{i}\partial_j \hat{a}(\boldsymbol{x}) \tag{6.51}$$

Hamiltonian

The one-particle Hamiltonian $H^{(1)}$

$$H^{(1)} = \frac{\boldsymbol{p}^2}{2m} + V(\boldsymbol{x}) \tag{6.52}$$

has the matrix elements

$$\langle\boldsymbol{x}|H^{(1)}|\boldsymbol{y}\rangle = -\frac{\hbar^2}{2m}\bigtriangledown^2\, \delta^d(\boldsymbol{x}-\boldsymbol{y}) + V(\boldsymbol{x})\delta^d(\boldsymbol{x}-\boldsymbol{y}) \tag{6.53}$$

Thus, in Fock space we get

$$\widehat{H} = \int d^d x\, \hat{a}^\dagger(\boldsymbol{x}) \left(-\frac{\hbar^2}{2m}\bigtriangledown^2 + V(\boldsymbol{x})\right) \hat{a}(\boldsymbol{x}) \tag{6.54}$$

in position space. In momentum space we can define

$$\widetilde{V}(\boldsymbol{q}) = \int d^d x\, V(\boldsymbol{x}) e^{-i\boldsymbol{q}\cdot\boldsymbol{x}} \tag{6.55}$$

the Fourier transform of the potential $V(x)$, and get

$$\widehat{H} = \int \frac{d^d p}{(2\pi)^d}\, \frac{\boldsymbol{p}^2}{2m}\hat{a}^\dagger(\boldsymbol{p})\hat{a}(\boldsymbol{p}) + \int \frac{d^d p}{(2\pi)^d} \int \frac{d^d q}{(2\pi)^d}\, \widetilde{V}(\boldsymbol{q})\hat{a}^\dagger(\boldsymbol{p}+\boldsymbol{q})\hat{a}(\boldsymbol{p}) \tag{6.56}$$

The last term has a very simple physical interpretation. When acting on a one-particle state with well-defined momentum, say $|\boldsymbol{p}\rangle$, the potential term yields another one-particle state with momentum $\boldsymbol{p}+\boldsymbol{q}$, where $\boldsymbol{q}$ is the *momentum transfer*, with amplitude $\tilde{V}(\boldsymbol{q})$. This *process* is usually depicted by the diagram of the following figure.

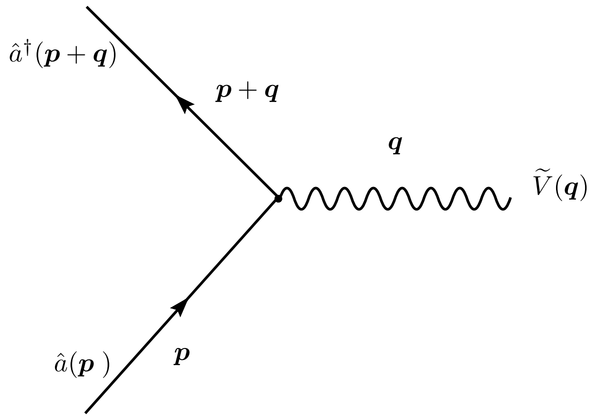

Figure 6.1 One-body scattering.

Two-Body Interactions

A two-particle interaction is a operator $\hat{V}^{(2)}$ which acts on the space of two-particle states $\mathcal{H}_2$, has the form

$$V^{(2)} = \frac{1}{2} \sum_{\alpha,\beta} |\alpha, \beta\rangle V^{(2)}(\alpha, \beta) \langle \alpha, \beta| \tag{6.57}$$

The methods developed above yield an extension of $V^{(2)}$ to Fock space of the form

$$\widehat{V} = \frac{1}{2} \sum_{\alpha,\beta} \hat{a}^\dagger(\alpha) \hat{a}^\dagger(\beta) \hat{a}(\beta) \hat{a}(\alpha)\; V^{(2)}(\alpha, \beta) \tag{6.58}$$

In position space, ignoring spin, we get

$$\begin{aligned} \widehat{V} &= \frac{1}{2} \int d^d x \int d^d y \; \hat{a}^\dagger(\boldsymbol{x})\; \hat{a}^\dagger(\boldsymbol{y})\; \hat{a}(\boldsymbol{y})\; \hat{a}(\boldsymbol{x})\; V^{(2)}(\boldsymbol{x}, \boldsymbol{y}) \\ &\equiv \frac{1}{2} \int d^d x \int d^d y \; \hat{\rho}(\boldsymbol{x}) V^{(2)}\,(\boldsymbol{x}, \boldsymbol{y}) \hat{\rho}(\boldsymbol{y}) + \frac{1}{2} \int d^d x \; V^{(2)}(\boldsymbol{x}, \boldsymbol{x})\; \hat{\rho}(\boldsymbol{x}) \end{aligned} \tag{6.59}$$

while in momentum space we find

$$\widehat{V} = \frac{1}{2} \int \frac{d^d p}{(2\pi)^d} \int \frac{d^d q}{(2\pi)^d} \int \frac{d^d k}{(2\pi)^d} \; \widetilde{V}(\boldsymbol{k})\; \hat{a}^\dagger(\boldsymbol{p}+\boldsymbol{k}) \hat{a}^\dagger(\boldsymbol{q}-\boldsymbol{k}) \hat{a}(\boldsymbol{q}) \hat{a}(\boldsymbol{p}) \tag{6.60}$$

where $\widetilde{V}(\boldsymbol{k})$ is only a function of the momentum transfer $\vec{k}$. This is a consequence of translation invariance. In particular for a Coulomb interaction,

$$V^{(2)}(\boldsymbol{x}, \boldsymbol{y}) = \frac{e^2}{|\boldsymbol{x} - \boldsymbol{y}|} \tag{6.61}$$

for which we have

$$\widetilde{V}(\boldsymbol{k}) = \frac{4\pi e^2}{\boldsymbol{k}^{\,2}} \tag{6.62}$$

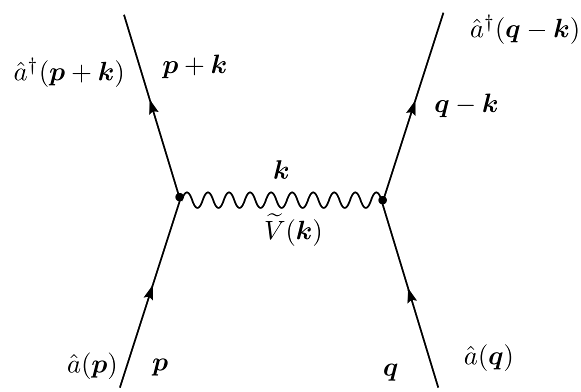

Figure 6.2 Two-body interaction.

6.2 Non-Relativistic Field Theory and Second Quantization

We can now reformulate the problem of an N-particle system as a non-relativistic field theory. The procedure described in the previous section is commonly known as Second Quantization. If the (identical) particles are *bosons*, the operators $\hat{a}(\phi)$ obey *canonical commutation relations*. If the (identical) particles are *Fermions*, the operators $\hat{a}(\phi)$ obey *canonical anti-commutation relations*. In position space, it is customary to represent $\hat{a}^\dagger(\phi)$ by the operator $\hat{\psi}(\boldsymbol{x})$ which obeys the equal-time algebra

$$\begin{aligned} \left[\hat{\psi}(\boldsymbol{x}), \hat{\psi}^\dagger(\boldsymbol{y})\right]_{-\xi} &= \delta^d(\boldsymbol{x} - \boldsymbol{y}) \\ \left[\hat{\psi}(\boldsymbol{x}), \hat{\psi}(\boldsymbol{y})\right]_{-\xi} &= \left[\hat{\psi}^\dagger(\boldsymbol{x}), \hat{\psi}^\dagger(\boldsymbol{y})\right]_{-\xi} = 0 \end{aligned} \tag{6.63}$$

In this framework, the one-particle Schrödinger equation becomes the classical field equation

$$\left[i\hbar\frac{\partial}{\partial t}+\frac{\hbar^2}{2m}\bigtriangledown^2 - V(\boldsymbol{x})\right]\hat{\psi}=0 \tag{6.64}$$

Can we find a Lagrangian density $\mathcal{L}$ from which the one-particle Schrödinger equation follows as its classical equation of motion? The answer is yes and $\mathcal{L}$ is given by

$$\mathcal{L}=i\hbar\psi^\dagger\partial_t\psi-\frac{\hbar^2}{2m}\bigtriangledown\psi^\dagger\cdot\bigtriangledown\psi-V(\boldsymbol{x})\psi^\dagger\psi \tag{6.65}$$

Its Euler-Lagrange equations are

$$\partial_t\frac{\delta\mathcal{L}}{\delta\partial_t\psi^\dagger}=-\bigtriangledown\cdot\frac{\delta\mathcal{L}}{\delta\bigtriangledown\psi^\dagger}+\frac{\delta\mathcal{L}}{\delta\psi^\dagger} \tag{6.66}$$

which are equivalent to the field Equation Eq. 10.17. The canonical momenta Π_ψ and $\Pi_\psi^\dagger$ are

$$\Pi_\psi=\frac{\delta\mathcal{L}}{\delta\partial_t\psi^\dagger}=-i\hbar\psi \tag{6.67}$$

and

$$\Pi_\psi^\dagger=\frac{\delta\mathcal{L}}{\delta\partial_t\psi}=i\hbar\psi^\dagger \tag{6.68}$$

Thus, the (equal-time) canonical commutation relations are

$$\left[\hat{\psi}(\boldsymbol{x}),\hat{\Pi}_\psi(\boldsymbol{y})\right]_{-\xi}=i\hbar\delta(\boldsymbol{x}-\boldsymbol{y}) \tag{6.69}$$

which require that

$$\left[\hat{\psi}(\boldsymbol{x}),\hat{\psi}^\dagger(\boldsymbol{y})\right]_{-\xi}=\delta^d(\boldsymbol{x}-\boldsymbol{y}) \tag{6.70}$$

6.3 Non-Relativistic Fermions at Zero Temperature

The results of the previous sections tell us that the action for non-relativistic fermions (with two-body interactions) is (in $D=d+1$ space-time dimensions)

$$\begin{aligned}S=&\int d^Dx\left[\hat{\psi}^\dagger i\hbar\partial_t\hat{\psi}-\frac{\hbar^2}{2m}\bigtriangledown\hat{\psi}^\dagger\cdot\bigtriangledown\hat{\psi}-V(\boldsymbol{x})\hat{\psi}^\dagger(x)\hat{\psi}(x)\right]\\&-\frac{1}{2}\int d^Dx\int d^Dx'\hat{\psi}^\dagger(x)\hat{\psi}^\dagger(x')U(x-x')\hat{\psi}(x')\hat{\psi}^\dagger(x)\hat{\psi}(x)\end{aligned} \tag{6.71}$$

where $U(x-x')$ represents instantaneous pair-interactions,

$$U(x-x') \equiv U(\boldsymbol{x}-\boldsymbol{x}')\delta(x_0-x_0') \tag{6.72}$$

The Hamiltonian $\hat{H}$ for this system is

$$\begin{aligned}\hat{H} = &\int d^dx\, [\frac{\hbar^2}{2m}\bigtriangledown\hat{\psi}^\dagger\cdot\bigtriangledown\hat{\psi}+V(\boldsymbol{x})\hat{\psi}^\dagger(\boldsymbol{x})\psi(\boldsymbol{x})] \\ &+\frac{1}{2}\int d^dx\int d^dx'\hat{\psi}^\dagger(x)\hat{\psi}^\dagger(x')U(x-x')\hat{\psi}(x')\hat{\psi}(x)\end{aligned} \tag{6.73}$$

For *Fermions* the fields $\hat{\psi}$ and $\hat{\psi}^\dagger$ satisfy equal-time canonical anticommutation relations

$$\{\hat{\psi}(\boldsymbol{x}),\hat{\psi}^\dagger(\boldsymbol{x})\} = \delta(\boldsymbol{x}-\boldsymbol{x}') \tag{6.74}$$

while for *Bosons* they satisfy

$$[\hat{\psi}(\boldsymbol{x}),\hat{\psi}^\dagger(\boldsymbol{x}')] = \delta(\boldsymbol{x}-\boldsymbol{x}') \tag{6.75}$$

In both cases, the Hamiltonian $\hat{H}$ commutes with the total number operator $\hat{N}=\int d^dx\hat{\psi}^\dagger(x)\hat{\psi}(x)$ since $\hat{H}$ conserves the total number of particles. The Fock space picture of the many-body problem is equivalent to the Grand Canonical Ensemble of Statistical Mechanics. Thus, instead of fixing the number of particles we can introduce a Lagrange multiplier μ, the chemical potential, to weigh contributions from different parts of the Fock space. Thus, we define the operator $\tilde{H}$.

$$\widetilde{H} \equiv \widehat{H}-\mu\widehat{N} \tag{6.76}$$

In a Hilbert space with fixed $\hat{N}$ this amounts to a shift of the energy by μN. We will now allow the system to choose the sector of the Fock space but with the requirement that the *average* number of particles $\langle\hat{N}\rangle$ is fixed to be some number $\bar{N}$. In the thermodynamic limit ($N\to\infty$), μ represents the difference of the ground state energies between two sectors with $N+1$ and N particles respectively. The modified Hamiltonian $\widetilde{H}$ is

$$\begin{aligned}\widetilde{H} = &\int d^dx\,\sum_\sigma\hat{\psi}^\dagger_\sigma(\boldsymbol{x})\left(-\frac{\hbar^2}{2m}\bigtriangledown^2+V(\boldsymbol{x})-\mu\right)\hat{\psi}_\sigma(\boldsymbol{x}) \\ &+\frac{1}{2}\int d^dx\int d^dy\,\sum_{\sigma,\sigma'}\hat{\psi}^\dagger_\sigma(\boldsymbol{x})\hat{\psi}^\dagger_{\sigma'}(\boldsymbol{y})U(\boldsymbol{x}-\boldsymbol{y})\hat{\psi}_{\sigma'}(\boldsymbol{y})\hat{\psi}_\sigma(\boldsymbol{x})\end{aligned} \tag{6.77}$$

6.3.1 The Ground State

Let us discuss now the very simple problem of finding the ground state for a system of N spinless *free* fermions. In this case, the pair-potential vanishes and, if the system is isolated, so does the potential $V(\boldsymbol{x})$. In general there will be a complete set of one-particle states $\{|\alpha\rangle\}$ and, in this basis, $\hat{H}$ is

$$\hat{H} = \sum_{\alpha} E_\alpha \hat{a}_\alpha^\dagger a_\alpha \tag{6.78}$$

where the index α labels the one-particle states by increasing order of their single-particle energies

$$E_1 \leq E_2 \leq \cdots \leq E_n \leq \cdots \tag{6.79}$$

Since were are dealing with fermions, we cannot put more than one particle in each state. Thus the state the *lowest* energy is obtained by filling up all the first N single particle states. Let $|\text{gnd}\rangle$ denote this ground state

$$|\text{gnd}\rangle = \prod_{\alpha=1}^{N} \hat{a}_\alpha^\dagger |0\rangle \equiv \hat{a}_1^\dagger \cdots \hat{a}_N^\dagger |0\rangle = |\overbrace{1\ldots 1}^{N}, 00\ldots\rangle \tag{6.80}$$

The energy of this state is E_{gnd} with

$$E_{\text{gnd}} = E_1 + \cdots + E_N \tag{6.81}$$

The energy of the top-most occupied single particle state, E_N, is called the *Fermi energy* of the system and the set of occupied states is called the *filled Fermi sea*.

6.3.2 Excited States

A state like $|\psi\rangle$

$$|\psi\rangle = |\overbrace{1\ldots 1}^{N-1} 010\ldots\rangle \tag{6.82}$$

is an excited state. It is obtained by removing one particle from the single particle state N (thus leaving a *hole* behind) and putting the particle in the unoccupied single particle state $N+1$. This is a state with one *particle-hole pair*, and it has the form

$$|1\ldots 1010\ldots\rangle = \hat{a}_{N+1}^\dagger \hat{a}_N |\text{gnd}\rangle \tag{6.83}$$

The energy of this state is

$$E_\psi = E_1 + \cdots + E_{N-1} + E_{N+1} \tag{6.84}$$

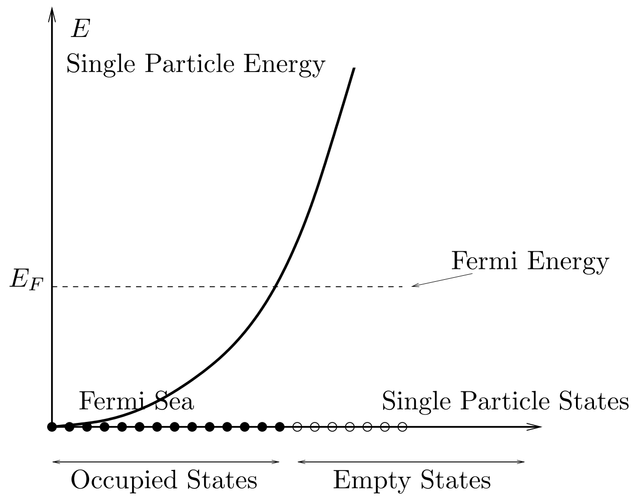

Figure 6.3 The Fermi Sea.

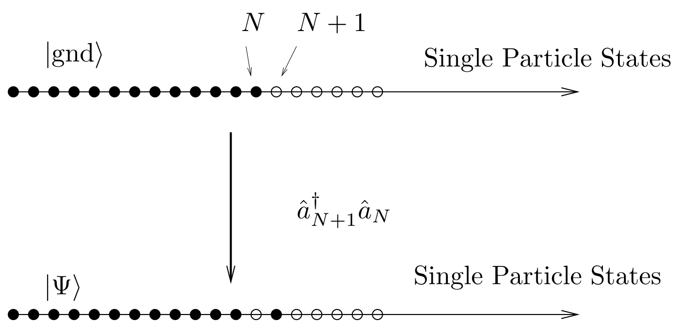

Figure 6.4 An excited (particle-hole) state.

Hence

$$E_\psi = E_{\text{gnd}} + E_{N+1} - E_N \tag{6.85}$$

and, since $E_{N+1} \geq E_N, E_\psi \geq E_{\text{gnd}}$. The *excitation energy* $\varepsilon_\psi = E_\psi - E_{\text{gnd}}$ is

$$\varepsilon_\psi = E_{N+1} - E_N \geq 0 \tag{6.86}$$

6.3.3 Normal Ordering and Particle-Hole transformation: Construction of the Physical Hilbert Space

It is apparent that, instead of using the empty state $|0\rangle$ for reference state, it is physically more reasonable to use instead the filled Fermi sea $|\text{gnd}\rangle$ as the physical reference state or *vacuum state*. Thus this state is a vacuum in the sense of *absence of excitations*. These arguments motivate the introduction of the *particle-hole transformation*.

Let us introduce the fermion operators b_α such that

$$\hat{b}_\alpha = \hat{a}^\dagger_\alpha \qquad \text{for } \alpha \leq N \tag{6.87}$$

Since $\hat{a}^\dagger_\alpha|\text{gnd}\rangle = 0$ (for $\alpha \leq N$) the operators $\hat{b}_\alpha$ *annihilate the ground state* $|\text{gnd}\rangle$, *i.e.,*

$$\hat{b}_\alpha|\text{gnd}\rangle = 0 \tag{6.88}$$

The following anticommutation relations hold

$$\begin{gathered}\{\hat{a}_\alpha, \hat{a}'_\alpha\} = \left\{\hat{a}_\alpha, \hat{b}_\beta\right\} = \left\{\hat{b}_\beta, \hat{b}'_\beta\right\} = \left\{\hat{a}_\alpha, \hat{b}^\dagger_\beta\right\} = 0 \\ \left\{\hat{a}_\alpha, \hat{a}^\dagger_{\alpha'}\right\} = \delta_{\alpha\alpha'}, \qquad \left\{\hat{b}_\beta, \hat{b}^\dagger_{\beta'}\right\} = \delta_{\beta\beta'}\end{gathered} \tag{6.89}$$

where $\alpha, \alpha' > N$ and $\beta, \beta' \leq N$. Thus, relative to the state $|\text{gnd}\rangle$, $\hat{a}^\dagger_\alpha$ and $\hat{b}^\dagger_\beta$ behave like creation operators. An arbitrary excited state has the form

$$|\alpha_1 \ldots \alpha_m, \beta_1 \ldots \beta_n; \text{gnd}\rangle \equiv \hat{a}^\dagger_{\alpha_1} \ldots \hat{a}^\dagger_{\alpha_m} \hat{b}^\dagger_{\beta_1} \ldots \hat{b}^\dagger_{\beta_n}|\text{gnd}\rangle \tag{6.90}$$

This state has m *particles* (in the single-particle states $\alpha_1, \ldots, \alpha_m$) and n *holes* (in the single-particle states $\beta_1, \ldots, \beta_n$). The ground state is annihilated by the operators $\hat{a}_\alpha$ and $\hat{b}_\beta$

$$\hat{a}_\alpha|\text{gnd}\rangle = \hat{b}_\beta|\text{gnd}\rangle = 0 \qquad (\alpha > N \ \beta \leq N) \tag{6.91}$$

The Hamiltonian $\hat{H}$ is normal ordered relative to the *empty state* $|0\rangle$, *i. e.* $\hat{H}|0\rangle = 0$, but is not normal ordered relative to the actual ground state $|\text{gnd}\rangle$. The particle-hole transformation enables us to normal order $\hat{H}$ relative to $|\text{gnd}\rangle$.

$$\widehat{H} = \sum_\alpha E_\alpha \hat{a}^\dagger_\alpha \hat{a}_\alpha = \sum_{\alpha \leq N} E_\alpha + \sum_{\alpha > N} E_\alpha \hat{a}^\dagger_\alpha \hat{a}_\alpha - \sum_{\beta \leq N} E_\beta \hat{b}^\dagger_\beta \hat{b}_\beta \tag{6.92}$$

where the minus sign in the last term reflects the Femi statistics.

Thus

$$\widehat{H} = E_{\text{gnd}} + :\widehat{H}: \tag{6.93}$$

where

$$E_{\text{gnd}} = \sum_{\alpha=1}^{N} E_\alpha \tag{6.94}$$

is the ground state energy, and the normal ordered Hamiltonian is

$$: \widehat{H} := \sum_{\alpha > N} E_\alpha \hat{a}_a^\dagger \hat{a}_\alpha - \sum_{\beta \leq N} \hat{b}_\beta^\dagger \hat{b}_\beta \; E_\beta \tag{6.95}$$

The number operator $\widehat{N}$ is not normal-ordered relative to $|\text{gnd}\rangle$ either. Thus, we write

$$\widehat{N} = \sum_\alpha \hat{a}_\alpha^\dagger \hat{a}_\alpha = N + \sum_{\alpha > N} \hat{a}_\alpha^\dagger a_\alpha - \sum_{\beta \leq N} \hat{b}_\beta^\dagger \hat{b}_\beta \tag{6.96}$$

We see that particles raise the energy while holes reduce it. However, if we deal with Hamiltonians that conserve the particle number $\widehat{N}$ (*i.e.*, $[\widehat{N}, \hat{H}] = 0$) for every particle that is removed a hole must be created. Hence particles and holes can only be created in *pairs*. A particle-hole state $|\alpha, \beta \text{ gnd}\rangle$ is

$$|\alpha, \beta \text{ gnd}\rangle \equiv \hat{a}_\alpha^\dagger \hat{b}_\beta^\dagger |\text{gnd}\rangle \tag{6.97}$$

It is an eigenstate with an energy

$$\begin{aligned} \widehat{H}|\alpha, \beta \text{ gnd}\rangle &= \left(E_{\text{gnd}} + : \widehat{H} :\right) \hat{a}_\alpha^\dagger \hat{b}_\beta^\dagger |\text{gnd}\rangle \\ &= \left(E_{\text{gnd}} + E_\alpha - E_\beta\right) |\alpha, \beta \text{ gnd}\rangle \end{aligned} \tag{6.98}$$

and the excitation energy is $E_\alpha - E_\beta \geq 0$. Hence the ground state is stable to the creation of particle-hole pairs.

This state has exactly N particles since

$$\widehat{N}|\alpha, \beta \text{ gnd}\rangle = (N + 1 - 1)|\alpha, \beta \text{ gnd}\rangle = N|\alpha, \beta \text{ gnd}\rangle \tag{6.99}$$

Let us finally notice that the field operator $\hat{\psi}^\dagger(x)$ in position space is

$$\hat{\psi}^\dagger(\boldsymbol{x}) = \sum_\alpha \langle \boldsymbol{x}|\alpha\rangle \hat{a}_\alpha^\dagger = \sum_{\alpha > N} \phi_\alpha(\boldsymbol{x}) \hat{a}_\alpha^\dagger + \sum_{\beta \leq N} \phi_\beta(\boldsymbol{x}) \hat{b}_\beta \tag{6.100}$$

where $\{\phi_\alpha(\boldsymbol{x})\}$ are the single particle wave functions.

The procedure of normal ordering allows us to define the physical Hilbert space. The physical meaning of this approach becomes more transparent in the *thermodynamic limit* $N \to \infty$ and $V \to \infty$ at *constant density* ρ. In this limit, the space of Hilbert space is the set of states which is obtained by acting with creation and annihilation operators *finitely* on the ground state. The spectrum of states that results from this approach consists on the set of states with *finite* excitation energy. Hilbert spaces which are built on reference states with *macroscopically* different number of particles are effectively *disconnected* from each other. Thus, the normal ordering of a Hamiltonian of a system with an infinite number of degrees of freedom amounts to a choice of the Hilbert space. This restriction becomes of fundamental importance when interactions are taken into account.

6.3.4 The Free Fermi Gas

Let us consider the case of free spin one-half electrons moving in free space. The Hamiltonian for this system is

$$\tilde{H} = \int d^d x \sum_{\sigma=\uparrow,\downarrow} \hat{\psi}^\dagger_\sigma(\boldsymbol{x})[-\frac{\hbar^2}{2m} \bigtriangledown^2 - \mu]\hat{\psi}_\sigma(\boldsymbol{x}) \tag{6.101}$$

where the label $\sigma = \uparrow, \downarrow$ indicates the z-projection of the spin of the electron. The value of the chemical potential μ will be determined once we satisfy that the electron *density* is equal to some fixed value $\bar{\rho}$.

In momentum space, we get

$$\hat{\psi}_\sigma(\boldsymbol{x}) = \int \frac{d^d p}{(2\pi)^d} \; \hat{\psi}_\sigma(\boldsymbol{p}) \; e^{-i\frac{\boldsymbol{p}\cdot\boldsymbol{x}}{\hbar}} \tag{6.102}$$

where the operators $\hat{\psi}_\sigma(\boldsymbol{p})$ and $\hat{\psi}^\dagger_\sigma(\boldsymbol{p})$ satisfy

$$\begin{aligned} \left\{\hat{\psi}_\sigma(\boldsymbol{p}), \hat{\psi}^\dagger_{\sigma'}(\boldsymbol{p})\right\} &= (2\pi)^d \delta_{\sigma\sigma'} \delta^d(\boldsymbol{p} - \boldsymbol{p}') \\ \left\{\hat{\psi}^\dagger_\sigma(\boldsymbol{p}), \hat{\psi}^\dagger_{\sigma'}(\boldsymbol{p})\right\} &= \{\hat{\psi}(\boldsymbol{p}), \hat{\psi}_{\sigma'}(\boldsymbol{p}')\} = 0 \end{aligned} \tag{6.103}$$

The Hamiltonian has the very simple form

$$\tilde{H} = \int \frac{d^d p}{(2\pi)^d} \sum_{\sigma=\hat{\imath},\downarrow} \left(\varepsilon(\boldsymbol{p}) - \mu\right) \hat{\psi}^\dagger_\sigma(\boldsymbol{p})\hat{\psi}_\sigma(\boldsymbol{p}) \tag{6.104}$$

where $\epsilon(\boldsymbol{p})$ is given by

$$\epsilon(\boldsymbol{p}) = \frac{\boldsymbol{p}^2}{2m} \tag{6.105}$$

For this simple case, $\varepsilon(\boldsymbol{p})$ is independent of the spin orientation.

It is convenient to measure the energy relative to the chemical potential (or *Fermi energy*) $\mu = E_F$. The relative energy $E(\boldsymbol{p})$ is

$$E(\boldsymbol{p}) = \varepsilon(\boldsymbol{p}) - \mu \tag{6.106}$$

Hence, $E(\boldsymbol{p})$ is the excitation energy measured from the Fermi energy $E_F = \mu$. The energy $E(\boldsymbol{p})$ does not have a definite sign since there are states with

$\varepsilon(\boldsymbol{p}) > \mu$ as well as states with $\varepsilon(\boldsymbol{p}) < \mu$. Let us define by p_F the value of $|\boldsymbol{p}|$ for which

$$E(p_F) = \varepsilon(p_F) - \mu = 0 \tag{6.107}$$

This is the *Fermi momentum*. Thus, for $|\boldsymbol{p}| < p_F, E(\boldsymbol{p})$ is *negative* while for $|\boldsymbol{p}| > p_F, E(\boldsymbol{p})$ is *positive*.

We can construct the ground state of the system by finding the state with lowest energy at fixed μ. Since $E(\boldsymbol{p})$ is negative for $|\boldsymbol{p}| \leq p_F$, we see that by filling up all of those states we get the *lowest* possible energy. It is then natural to normal order the system relative to a state in which all one-particle states with $|\boldsymbol{p}| \leq p_F$ are occupied. Hence we make the particle-hole transformation

$$\begin{aligned} \hat{b}_\sigma(\boldsymbol{p}) &= \hat{\psi}_\sigma^\dagger(\boldsymbol{p}) \quad \text{for} \quad |\boldsymbol{p}| \leq p_F \\ \hat{a}_\sigma(\boldsymbol{p}) &= \hat{\psi}_\sigma(\boldsymbol{p}) \quad \text{for} \quad |\boldsymbol{p}| > p_F \end{aligned} \tag{6.108}$$

In terms of the operators $\hat{a}_\sigma$ and $\hat{b}_\sigma$, the Hamiltonian is

$$\tilde{H} = \sum_{\sigma=\uparrow,\downarrow} \int \frac{d^d p}{(2\pi)^d} \left[E(\boldsymbol{p})\theta(|\boldsymbol{p}|-p_F)\hat{a}_\sigma^\dagger(\boldsymbol{p})\hat{a}_\sigma(\boldsymbol{p}) + \theta(p_F-|\boldsymbol{p}|)E(\boldsymbol{p})\hat{b}_\sigma(\boldsymbol{p})\hat{b}_\sigma^\dagger(\boldsymbol{p})\right] \tag{6.109}$$

where $\theta(x)$ is the step function

$$\theta(x) = \begin{cases} 1 & x > 0 \\ 0 & x \leq 0 \end{cases} \tag{6.110}$$

Using the anticommutation relations in the last term we get

$$\tilde{H} = \sum_{\sigma=\uparrow,\downarrow} \int \frac{d^d p}{(2\pi)^d} E(\boldsymbol{p})[\theta(|\boldsymbol{p}|-p_F)\hat{a}_\sigma^\dagger(\boldsymbol{p})\hat{a}_\sigma(\boldsymbol{p}) - \theta(p_F-|(\boldsymbol{p})|)\hat{b}_\sigma^\dagger(\boldsymbol{p})\hat{b}_\sigma(\boldsymbol{p})] + \tilde{E}_{\text{gnd}} \tag{6.111}$$

where $\tilde{E}_{\text{gnd}}$, the ground state energy measured from the chemical potential μ, is given by

$$\tilde{E}_{\text{gnd}} = \sum_{\sigma=\uparrow,\downarrow} \int \frac{d^d p}{(2\pi)^d} \theta(p_F - |\boldsymbol{p}|)E(\boldsymbol{p})(2\pi)^d\delta^d(0) = E_{\text{gnd}} - \mu N \tag{6.112}$$

Recall that $(2\pi)^d\delta(0)$ is equal to

$$(2\pi)^d\delta^d(0) = \lim_{\boldsymbol{p}\to 0}(2\pi)^d\delta^d(\boldsymbol{p}) = \lim_{\boldsymbol{p}\to 0}\int d^d x e^{i\boldsymbol{p}\cdot\boldsymbol{x}} = V \tag{6.113}$$

where V is the *volume* of the system. Thus, $\tilde{E}_{\text{gnd}}$ is extensive

$$\tilde{E}_{\text{gnd}} = V\tilde{\varepsilon}_{\text{gnd}} \tag{6.114}$$

and the ground state energy density $\tilde{\varepsilon}_{\text{gnd}}$ is

$$\tilde{\varepsilon}_{\text{gnd}} = 2\int_{|\boldsymbol{p}|\leq p_F} \frac{d^dp}{(2\pi)^d} E(\boldsymbol{p}) = \varepsilon_{\text{gnd}} - \mu\bar{\rho} \tag{6.115}$$

where the factor of 2 comes from the two spin orientations. Putting everything together we get

$$\tilde{\varepsilon}_{\text{gnd}} = 2\int_{|\boldsymbol{p}|\leq p_F} \frac{d^dp}{(2\pi)^d}\left(\frac{\boldsymbol{p}^2}{2m} - \mu\right) = 2\int_0^{p_F} dp\, p^{d-1}\frac{S_d}{(2\pi)^d}\left(\frac{p^2}{2m} - \mu\right) \tag{6.116}$$

where S_d is the area of the d-dimensional hypersphere. Our definitions tell us that the chemical potential is $\mu = \frac{p_F^2}{2m} \equiv E_F$ where E_F, is the Fermi energy. Thus the ground state energy density ε_{gnd} (measured from the empty state) is equal to

$$E_{\text{gnd}} = \frac{1}{m}\frac{S_d}{(2\pi)^d}\int_0^{p_F} dp\, p^{d+1} = \frac{p_F^{d+2}}{m(d+2)}\frac{S_d}{(2\pi)^d} = 2E_F\frac{p_F^d S_d}{(d+2)(2\pi)^d} \tag{6.117}$$

How many particles does this state have? To find that out we need to look at the number operator. The number operator can also be normal-ordered with respect to this state

$$\begin{aligned}\hat{N} &= \int \frac{d^dp}{(2\pi)^d}\sum_{\sigma=\uparrow,\downarrow}\hat{\psi}_\sigma^\dagger(\boldsymbol{p})\hat{\psi}_\sigma(\boldsymbol{p}) = \\ &= \int \frac{d^dp}{(2\pi)^d}\sum_{\sigma=\uparrow,\downarrow}\{\theta(|\boldsymbol{p}| - p_F)\hat{a}_\sigma^\dagger(\boldsymbol{p})\hat{a}_\sigma(\boldsymbol{p}) + \theta(p_F - |\boldsymbol{p}|)\hat{b}_\sigma(\boldsymbol{p})\hat{b}_\sigma^\dagger(\boldsymbol{p})\}\end{aligned} \tag{6.118}$$

Hence, $\hat{N}$ can also be written in the form

$$\hat{N} =: \hat{N}: +N \tag{6.119}$$

where the normal-ordered number operator $:\hat{N}:$ is

$$:\hat{N}:= \int \frac{d^dp}{(2\pi)^d}\sum_{\sigma=\uparrow,\downarrow}[\theta(|\boldsymbol{p}|-p_F)\hat{a}_\sigma^\dagger(\boldsymbol{p})\hat{a}_\sigma(\boldsymbol{p}) - \theta(p_F-|\boldsymbol{p}|)\hat{b}_\sigma^\dagger(\boldsymbol{p})\hat{b}_\sigma(\boldsymbol{p})] \tag{6.120}$$

and N, the number of particles in the reference state $|\text{gnd}\rangle$, is

$$N = \int \frac{d^dp}{(2\pi)^d}\sum_{\sigma=\uparrow,\downarrow}\theta(p_F - |\boldsymbol{p}|)(2\pi)^d\delta^d(0) = \frac{2}{d}p_F^d\frac{S_d}{(2\pi)^d}V \tag{6.121}$$

Therefore, the particle density $\bar{\rho} = \frac{N}{V}$ is

$$\bar{\rho} = \frac{2}{d} \frac{S_d}{(2\pi)^d} p_F^d \tag{6.122}$$

This equation determines the *Fermi momentum* p_F in terms of the density $\bar{\rho}$. Similarly we find that the ground state energy *per particle* is $\frac{E_{\text{gnd}}}{N} = \frac{2d}{d+2} E_F$.

The excited states can be constructed in a similar fashion. The state $|+, \sigma, \boldsymbol{p}\rangle$

$$|+, \sigma, \boldsymbol{p}\rangle = \hat{a}^\dagger_\alpha(\boldsymbol{p})|\text{gnd}\rangle \tag{6.123}$$

is a state which represents an *electron* with spin σ and momentum $\boldsymbol{p}$ while the state $|-, \sigma, \boldsymbol{p}\rangle$

$$|-, \sigma, \boldsymbol{p}\rangle = \hat{b}^\dagger_\sigma(\boldsymbol{p})|\text{gnd}\rangle \tag{6.124}$$

represents a *hole* with spin σ and momentum $\boldsymbol{p}$. From our previous discussion we see that *electrons* have momentum $\boldsymbol{p}$ with $|\boldsymbol{p}| > p_F$ while *holes* have momentum $\boldsymbol{p}$ with $|\boldsymbol{p}| < p_F$. The excitation energy of a one-electron state is $E(\boldsymbol{p}) \geq 0$(for $|\boldsymbol{p}| > p_F$), while the excitation energy of a one-hole state is $-E(\boldsymbol{p}) \geq 0$ (for $|\boldsymbol{p}| < p_F$).

Similarly, an electron-hole *pair* is a state of the form

$$|\sigma\boldsymbol{p}, \sigma'\boldsymbol{p}'\rangle = \hat{a}^\dagger_\sigma(\boldsymbol{p})\hat{b}^\dagger_{\sigma'}(\boldsymbol{p}')|\text{gnd}\rangle \tag{6.125}$$

with $|\boldsymbol{p}| > p_F$ and $|\boldsymbol{p}'| < p_F$. This state has excitation energy $E(\boldsymbol{p}) - E(\boldsymbol{p}')$, which is positive. Hence, states which are obtained from the ground state without changing the density, can only increase the energy. This proves that $|\text{gnd}\rangle$ is indeed the ground state. However, if the density is allowed to change, we can always construct states with energy less than E_{gnd} by creating a number of holes without creating an equal number of particles.