

cone, and therefore this assumption violates the principle of causality. This fact generalizes to the theorem that Lorentz covariant field theories for particles with half-integer spin only satisfy the causality principle if these particles are fermions, and for integer spin particles if they are bosons. In short, the connection between spin and statistics is a theorem of relativistic quantum field theory, and among its most important triumphs.

11.2 Second Quantization

In many circumstances the wave function is not a useful construct for treating systems of many interacting particles. It contains an enormous amount of information, and is therefore very difficult to compute with even questionable accuracy. Furthermore, most of this information is only indirectly relevant to the properties of the systems that are of greatest physical interest. To take an example, consider a system of N identical spin 0 bosons and the problem of computing the probability of finding one particle at \mathbf{x} . Because of indistinguishability, it suffices to find the probability of finding the particle nominally called 1 at \mathbf{x} . If we knew the wave function, $\Psi(\mathbf{x}_1\mathbf{x}_2\dots\mathbf{x}_N)$, this probability would be

$$p_1(\mathbf{x}) = \int d\mathbf{x}_2\dots d\mathbf{x}_N |\Psi(\mathbf{x}\mathbf{x}_2\dots\mathbf{x}_N)|^2. \quad (9)$$

A similar formula, using the wave function in momentum space, holds for the probability of finding a particle with a given momentum. If the system has two-body interactions, the kinetic energy can be computed from this momentum distribution, and the energy due to the interactions from the probability of finding two particles at specific positions. The latter is found by integrating the N -particle density over all but two coordinates. In short, the information about higher order correlations is, so to say, thrown out by the integrations that lead to the quantities of physical interest.

It is also clear that if N is large, the probabilities of the preceding paragraph, which pertain to only one or a pair of particles, are insensitive to the value of N . In the terminology of statistical mechanics, these are intensive quantities, having a well-defined thermodynamic limit — the limit in which N and the volume tend to infinity with a finite ratio n , the particle density. And speaking of thermodynamics, for systems with very large N , the ground state (or any pure state) is often only an idealized notion, because most of these systems have excitation thresholds that tend to zero as $N \rightarrow \infty$, so that the zero temperature limit is rather artificial. Hence, such systems are best described by the density matrix for a system in thermal equilibrium.

What is needed, then, is a formalism that focuses on a small number of degrees of freedom, which does not refer explicitly to N , and which can handle mixtures on an equal footing with pure states. This list of desiderata is met by the technique of *second quantization*.¹ This name stems from the fact that in this formalism certain amplitudes that are c-numbers in conventional quantum mechanics are replaced by non-commuting operators, which results in *non-Hermitian field operators*

¹Second quantization for bosons was invented by Dirac and by Jordan and Klein, and for fermions by Jordan and Wigner.

$\psi(\mathbf{x}, t)$ whose equation of motion in the Heisenberg picture looks, superficially, like the ordinary Schrödinger equation (though it is actually nonlinear, whereas the Schrödinger equation is strictly linear).

Above and beyond its technical merits, the formalism of second quantization has a much deeper significance. It provides a vivid and direct mathematical expression of particle-wave duality. As we said, the operator $\psi(\mathbf{x}, t)$ and its relatives satisfy wavelike equations, and in addition, as we shall soon learn, these operators act on variables that are most corpuscular, because they create, destroy and count particles.

(a) Bose-Einstein Statistics

In §10.1 we saw that the free electromagnetic field can be thought of as a gas of non-interacting particles (photons) obeying Bose-Einstein statistics. A stationary state of the electromagnetic field was specified by giving the number of photons having various momenta and helicities. The basic operators that generated the whole Hilbert space, the creation and destruction operators, and the commutation rules between them guaranteed that all the state vectors were symmetric in the individual photon variables. Furthermore, this formulation of electrodynamics had all the desirable features referred to in the introduction to this section. Thus the expressions for the energy and momentum of the field, as well as the dynamical (Maxwell) equations, did not explicitly depend on the number of photons present. We therefore adapt the formalism of creation and destruction operators to our present problem.

The systems of interest to us now differ in certain fundamental ways from the radiation field, however. We are now concerned with particles having a rest mass, and confine ourselves to a nonrelativistic theory; and to systems where the number of particles is a constant of the motion. Thus we shall not deal with observables, such as the electromagnetic field strengths, which do not commute with the number operator.

Consider a system of spin zero bosons of mass m . The extension of the formalism to nonzero spin is straightforward, and will not be spelled out. As in the theory of the electromagnetic field, introduce creation and destruction operators, $a_{\mathbf{p}}^{\dagger}$ and $a_{\mathbf{p}}$, having the commutation rules

$$[a_{\mathbf{p}}, a_{\mathbf{p}'}^{\dagger}] = \delta_{\mathbf{p}\mathbf{p}'}, \quad [a_{\mathbf{p}}, a_{\mathbf{p}'}] = 0. \quad (10)$$

Here the label \mathbf{p} specifies the momentum. We again employ periodic boundary conditions on a cube whose volume will now be called Ω . From these operators we then construct the number operators $N_{\mathbf{p}} = a_{\mathbf{p}}^{\dagger} a_{\mathbf{p}}$, with commutation rules

$$[a_{\mathbf{p}}, N_{\mathbf{p}}] = a_{\mathbf{p}}, \quad [a_{\mathbf{p}}^{\dagger}, N_{\mathbf{p}}] = -a_{\mathbf{p}}^{\dagger}. \quad (11)$$

Define a normalized empty state, or vacuum, $|0\rangle$ by

$$a_{\mathbf{p}}|0\rangle = 0 \quad (12)$$

for all \mathbf{p} . The complete Hilbert space is then built up from $|0\rangle$. The state in which the commuting observables $\{N_{\mathbf{p}}\}$ have the eigenvalues $\{n_{\mathbf{p}}\}$ is given by

$$|\{n_{\mathbf{p}}\}\rangle = \prod_{\mathbf{p}} (n_{\mathbf{p}}!)^{-\frac{1}{2}} (a_{\mathbf{p}}^{\dagger})^{n_{\mathbf{p}}} |0\rangle. \quad (13)$$

These states are obviously symmetric because the $\{a_{\mathbf{p}}^{\pm}\}$ commute with each other. Thus the two-particle state $|\mathbf{p}_1\mathbf{p}_2\rangle \equiv a_{\mathbf{p}_1}^{\dagger} a_{\mathbf{p}_2}^{\dagger} |0\rangle$ satisfies $|\mathbf{p}_1\mathbf{p}_2\rangle = |\mathbf{p}_2\mathbf{p}_1\rangle$.

It is important to understand the difference between the space spanned by the vectors (13), and the Hilbert space of “conventional” quantum mechanics. In the conventional formulation, we specify the total number¹ N' of particles, and the Hilbert space $\mathfrak{H}_{N'}$ only contains state vectors describing N' -body systems. Operators that connect states with different numbers of particles do not arise. The space spanned by the states (13) is far larger, however, and one refers to it as *Fock space*. The Fock space \mathfrak{F} is the sum of all the Hilbert spaces referred to above, i.e., $\mathfrak{F} = \mathfrak{H}_0 \oplus \mathfrak{H}_1 \oplus \mathfrak{H}_2 \oplus \dots$. The operators $a_{\mathbf{p}}$ and $a_{\mathbf{p}}^{\dagger}$ are defined in \mathfrak{F} , though not in the conventional formulation, because they connect vectors in $\mathfrak{H}_{N'}$ and $\mathfrak{H}_{N''}$ with $N' = N'' \pm 1$. When dealing with systems (such as photons or pions) where the number of bosons is not conserved, a description in Fock space is indispensable, because observables (c.g., the field strengths) that are linear Hermitian forms in $a_{\mathbf{p}}$ and $a_{\mathbf{p}}^{\dagger}$ really exist. For systems such as liquid He, such observables do not occur, but the Fock space formulation is almost as indispensable.

All other observables may be constructed from the $a_{\mathbf{p}}$'s. As we are dealing with systems in which the total number of particles is conserved, we are only concerned with observables that are products of equal numbers of creation and destruction operators. The simplest example is the total momentum operator,

$$\mathbf{P} = \sum_{\mathbf{p}} \mathbf{p} a_{\mathbf{p}}^{\dagger} a_{\mathbf{p}}. \quad (14)$$

Equation (13) is an eigenstate of \mathbf{P} with eigenvalue $\sum \mathbf{p} n_{\mathbf{p}}$, whereas $a_{\mathbf{p}}^{\dagger}$ increases the eigenvalue of any eigenstate of \mathbf{P} in the amount \mathbf{p} , and vice versa for $a_{\mathbf{p}}$. If the particles in question do not interact, the Hamiltonian is

$$H = \sum_{\mathbf{p}} \frac{p^2}{2m} a_{\mathbf{p}}^{\dagger} a_{\mathbf{p}}, \quad (15)$$

and the states (13) are eigenstates of H with eigenvalue $\sum (p^2/2m)n_{\mathbf{p}}$.

The momentum representation operators are not sacrosanct. An equally important set of operators are defined by²

$$\psi(\mathbf{x}) = \Omega^{-\frac{1}{2}} \sum_{\mathbf{p}} e^{i\mathbf{p}\cdot\mathbf{x}} a_{\mathbf{p}}, \quad \psi^{\dagger}(\mathbf{x}) = \Omega^{-\frac{1}{2}} \sum_{\mathbf{p}} e^{-i\mathbf{p}\cdot\mathbf{x}} a_{\mathbf{p}}^{\dagger}. \quad (16)$$

These destruction and creation operators are also called *Bose field operators*. Because

$$\Omega^{-1} \int_{\Omega} d\mathbf{x} e^{-i(\mathbf{p}-\mathbf{p}')\cdot\mathbf{x}} = \delta_{\mathbf{p},\mathbf{p}'}, \quad (17)$$

the inverse relations to (16) are

$$a_{\mathbf{p}} = \Omega^{-\frac{1}{2}} \int d\mathbf{x} e^{-i\mathbf{p}\cdot\mathbf{x}} \psi(\mathbf{x}), \quad a_{\mathbf{p}}^{\dagger} = \Omega^{-\frac{1}{2}} \int d\mathbf{x} e^{i\mathbf{p}\cdot\mathbf{x}} \psi^{\dagger}(\mathbf{x}). \quad (18)$$

¹We reserve the symbol N for the number operator [see (23)], and designate its eigenvalues by N' or n .

²In this chapter no confusion between the operators $\psi(\mathbf{x})$ and wave functions should occur, because we will always use the symbols φ and u for the latter.

The completeness relationship,

$$\Omega^{-1} \sum_{\mathbf{p}} e^{i(\mathbf{x}-\mathbf{x}') \cdot \mathbf{p}} = \delta(\mathbf{x} - \mathbf{x}') , \quad (19)$$

then leads to the *basic boson commutation rules*

$$[\psi(\mathbf{x}), \psi^\dagger(\mathbf{x}')] = \delta(\mathbf{x} - \mathbf{x}') . \quad (20)$$

$$[\psi(\mathbf{x}), \psi(\mathbf{x}')] = [\psi^\dagger(\mathbf{x}), \psi^\dagger(\mathbf{x}')] = 0 . \quad (21)$$

The operator for the total number of particles,

$$N = \sum_{\mathbf{p}} a_{\mathbf{p}}^\dagger a_{\mathbf{p}} , \quad (22)$$

can be expressed in terms of ψ and ψ^\dagger by using (18) and (19):

$$N = \int d\mathbf{x} \psi^\dagger(\mathbf{x})\psi(\mathbf{x}) . \quad (23)$$

The commutation rules of N with the field operators then follow from (20) and (21):

$$[\psi(\mathbf{x}), N] = \psi(\mathbf{x}) , \quad [\psi^\dagger(\mathbf{x}), N] = -\psi^\dagger(\mathbf{x}) . \quad (24)$$

Hence if $|N'\rangle$ is an eigenket of N with eigenvalue N' , $\psi(\mathbf{x})|N'\rangle$ has the eigenvalue $N' - 1$ of N , whereas $\psi^\dagger(\mathbf{x})|N'\rangle$ belongs to the eigenvalue $N' + 1$. These facts also follow immediately from the definition of $\psi(\psi^\dagger)$ as a linear form in $a_{\mathbf{p}}(a_{\mathbf{p}}^\dagger)$.

We have already observed that $a_{\mathbf{p}}^\dagger|0\rangle$ is a one-particle state of momentum \mathbf{p} , and that the eigenvalues of $a_{\mathbf{p}}^\dagger a_{\mathbf{p}}$ are integers which were shown to be the number of particles of momentum \mathbf{p} . What are the analogous statements in the position representation? It is tempting, on the basis of (23), to interpret the positive Hermitian operator $\psi^\dagger(\mathbf{x})\psi(\mathbf{x})$ as the number density operator in position space— i.e., to assert that in any state $|\rangle$, $\langle\psi^\dagger(\mathbf{x})\psi(\mathbf{x})\rangle d\mathbf{x}$ is the mean number of particles in the volume element $d\mathbf{x}$ — and to interpret $|\mathbf{x}\rangle \equiv \psi^\dagger(\mathbf{x})|0\rangle$ as the state in which “one particle is at the point \mathbf{x} .” The latter is justified since it implies that the transformation function from $|\mathbf{x}\rangle$ to the one-particle momentum eigenstate $|\mathbf{p}\rangle \equiv a_{\mathbf{p}}^\dagger|0\rangle$ is

$$\langle\mathbf{x}|\mathbf{p}\rangle = \Omega^{-\frac{1}{2}} \langle 0 | \psi(\mathbf{x}) \int d\mathbf{x}' e^{i\mathbf{p} \cdot \mathbf{x}'} \psi^\dagger(\mathbf{x}') | 0 \rangle = \Omega^{-\frac{1}{2}} e^{i\mathbf{p} \cdot \mathbf{x}} , \quad (25)$$

which is correct. Furthermore, the basic commutation rule (14) leads to $\langle\mathbf{x}|\mathbf{x}'\rangle = \delta(\mathbf{x} - \mathbf{x}')$. To verify the interpretation of $\psi^\dagger(\mathbf{x})\psi(\mathbf{x})$ given above, we evaluate the result of applying the operator

$$N_{\Delta\Omega} \equiv \int_{\Delta\Omega} d\mathbf{x} \psi^\dagger(\mathbf{x})\psi(\mathbf{x}) \quad (26)$$

onto the ket $\psi^\dagger(\mathbf{y})|0\rangle$. If \mathbf{y} does not lie in the volume $\Delta\Omega$, $N_{\Delta\Omega}\psi^\dagger(\mathbf{y})|0\rangle = 0$. On the other hand, when \mathbf{y} does lie in $\Delta\Omega$,

$$N_{\Delta\Omega}\psi^\dagger(\mathbf{y})|0\rangle = \int_{\Delta\Omega} d\mathbf{x} \psi^\dagger(\mathbf{x})[\delta(\mathbf{x} - \mathbf{y}) + \psi^\dagger(\mathbf{y})\psi(\mathbf{x})]|0\rangle = \psi^\dagger(\mathbf{y})|0\rangle . \quad (27)$$

Thus $\psi^\dagger(\mathbf{y})|0\rangle$ is an eigenvector of $N_{\Delta\Omega}$ with eigenvalue one when \mathbf{y} lies inside $\Delta\Omega$, and eigenvalue zero when \mathbf{y} lies outside $\Delta\Omega$, no matter how small $\Delta\Omega$ may be. The argument is readily extended to an n -particle state $\prod_{i=1}^n \psi^\dagger(\mathbf{y}_i)|0\rangle$. Upon commuting the destruction operator through to the right, we obtain

$$\begin{aligned} N_{\Delta\Omega} \prod_{i=1}^n \psi^\dagger(\mathbf{y}_i)|0\rangle &= \int_{\Delta\Omega} d\mathbf{x} \psi^\dagger(\mathbf{x}) \sum_{i=1}^n \delta(\mathbf{x} - \mathbf{y}_i) \frac{\delta}{\delta\psi^\dagger(\mathbf{y}_i)} \prod_{j=1}^n \psi^\dagger(\mathbf{y}_j)|0\rangle \\ &= N'_{\Delta\Omega} \prod_{i=1}^n \psi^\dagger(\mathbf{y}_i)|0\rangle, \end{aligned} \quad (28)$$

where $N'_{\Delta\Omega}$ is the number of points in the set $(\mathbf{y}_1, \dots, \mathbf{y}_n)$ that lie inside $\Delta\Omega$. Hence $N_{\Delta\Omega}$ is the operator whose eigenvalues specify the number of particles in the spatial volume $\Delta\Omega$, and the interpretation of the operator $\psi^\dagger(\mathbf{x})\psi(\mathbf{x})$ given above is therefore correct.

Having established that $\prod_{i=1}^n \psi^\dagger(\mathbf{x}_i)|0\rangle$ is an n -particle state in which the particles "are at" the indicated positions, we may now relate these states to the conventional wave functions. Let $\varphi_a(\mathbf{x}_1 \dots \mathbf{x}_n)$ be a normalized and totally symmetric wave function for n -particles. Consider then the ket

$$|\varphi_a\rangle = (n!)^{-\frac{1}{2}} \int d\mathbf{x}_1 \dots d\mathbf{x}_n \varphi_a(\mathbf{x}_1 \dots \mathbf{x}_n) \psi^\dagger(\mathbf{x}_1) \dots \psi^\dagger(\mathbf{x}_n)|0\rangle. \quad (29)$$

We shall show that the factor $(n!)^{-\frac{1}{2}}$ gives the conventional interpretation of $|\varphi_a\rangle$, i.e., that the transformation function to the coordinate representation is the wave function $\varphi_a(\mathbf{x}_1 \dots \mathbf{x}_n)$. For this purpose it suffices to guarantee that

$$\langle \varphi_b | \varphi_a \rangle = \int d\mathbf{x}_1 \dots d\mathbf{x}_n \varphi_b^*(\mathbf{x}_1 \dots \mathbf{x}_n) \varphi_a(\mathbf{x}_1 \dots \mathbf{x}_n), \quad (30)$$

where $|\varphi_b\rangle$ is constructed in the same way as $|\varphi_a\rangle$. In order to evaluate $\langle \varphi_b | \varphi_a \rangle$ we require $\langle \psi(\mathbf{x}'_1) \dots \psi(\mathbf{x}'_n) \psi^\dagger(\mathbf{x}_1) \dots \psi^\dagger(\mathbf{x}_n) \rangle_0$, where $\langle \dots \rangle_0$ is the expectation value in $|0\rangle$. Repeated use of the commutation rules leads to

$$\langle \psi(\mathbf{x}'_1) \dots \psi(\mathbf{x}'_n) \psi^\dagger(\mathbf{x}_1) \dots \psi^\dagger(\mathbf{x}_n) \rangle_0 = \sum_P \delta(\mathbf{x}_1 - \mathbf{x}'_1) \dots \delta(\mathbf{x}_n - \mathbf{x}'_n), \quad (31)$$

where \sum_P is a sum over all $n!$ permutations P of the n vectors $(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n)$; similarly, $\langle a_{k_1} \dots a_{k_n} a_{q_1}^\dagger \dots a_{q_n}^\dagger \rangle = \sum_P \delta_{k_1 q_1} \delta_{k_n q_n}$. Hence

$$\begin{aligned} \langle \varphi_b | \varphi_a \rangle &= (n!)^{-1} \int d\mathbf{x}_1 \dots d\mathbf{x}_n \varphi_b^*(\mathbf{x}_1 \dots \mathbf{x}_n) \sum_P \varphi_a(\mathbf{x}_1 \dots \mathbf{x}_n) \\ &= \int d\mathbf{x}_1 \dots d\mathbf{x}_n \varphi_b^*(\mathbf{x}_1 \dots \mathbf{x}_n) \varphi_a(\mathbf{x}_1 \dots \mathbf{x}_n), \end{aligned} \quad (32)$$

where the last equality is a consequence of the assumed symmetry of $\varphi_{a,b}(\mathbf{x}_1 \dots \mathbf{x}_n)$; *QED*. In the same vein, define normalized and completely symmetric n -particle coordinate space kets by

$$|\mathbf{x}_1 \dots \mathbf{x}_n; n\rangle = (n!)^{-\frac{1}{2}} \psi^\dagger(\mathbf{x}_1) \dots \psi^\dagger(\mathbf{x}_n)|0\rangle. \quad (33)$$

The orthogonality relationship satisfied by these symmetric kets is therefore

$$\langle \mathbf{x}_1 \dots \mathbf{x}_n; n | \mathbf{x}'_1 \dots \mathbf{x}'_n; n \rangle = (n!)^{-1} \sum_P \delta(\mathbf{x}_1 \dots \mathbf{x}'_1) \dots \delta(\mathbf{x}_n - \mathbf{x}'_n), \quad (34)$$

and the coordinate space wave function is indeed

$$\varphi_\alpha(\mathbf{x}_1 \dots \mathbf{x}_n) = \langle \mathbf{x}_1 \dots \mathbf{x}_n; n | \varphi_\alpha \rangle. \quad (35)$$

The effect of applying the field operators onto the kets (33) is readily determined. By inspection we have

$$\psi^\dagger(\mathbf{y}) | \mathbf{x}_1 \dots \mathbf{x}_n; n \rangle = \sqrt{n+1} | \mathbf{y} \mathbf{x}_1 \dots \mathbf{x}_n; n+1 \rangle. \quad (36)$$

Repeated use of the commutation rule leads to the somewhat more complicated result

$$\psi(\mathbf{y}) | \mathbf{x}_1 \dots \mathbf{x}_n; n \rangle = \frac{1}{\sqrt{n}} \sum_{s=1}^n \delta(\mathbf{x}_s - \mathbf{y}) | \mathbf{x}_1 \dots \mathbf{x}_{s-1} \mathbf{x}_{s+1} \dots \mathbf{x}_n; n-1 \rangle. \quad (37)$$

Combining (36) and (37), and recalling that all these kets are symmetric functions of the coordinates, yields

$$\psi^\dagger(\mathbf{y}) \psi(\mathbf{y}') | \mathbf{x}_1 \dots \mathbf{x}_n; n \rangle = \sum_{s=1}^n \delta(\mathbf{x}_s - \mathbf{y}') | \mathbf{x}_1 \dots \mathbf{x}_{s-1} \mathbf{y} \mathbf{x}_{s+1} \dots \mathbf{x}_n; n \rangle. \quad (38)$$

All the equipment required for the construction of arbitrary symmetric observables¹ in terms of the creation and destruction operators is now at hand. Consider the simplest observable, a symmetric sum of one-particle observables (e.g., the linear or angular momenta). In conventional quantum mechanics such an observable for an n -body system is written as

$$F = \sum_{i=1}^n f_i, \quad (39)$$

where f_i acts only on the coordinates of particle i . Let us first define the action of this operator in the Hilbert space \mathfrak{H}_n . If $|\mathbf{x}\rangle_i$ is a position eigenket of particle i , a symmetrized position ket for n particles is given by

$$|\mathbf{x}_1 \dots \mathbf{x}_n\rangle_S = (n!)^{-\frac{1}{2}} \sum_P |\mathbf{x}_1\rangle_1 \dots |\mathbf{x}_n\rangle_n. \quad (40)$$

The kets (40) span the space \mathfrak{H}_n . Applying F to (40) gives

$$\begin{aligned} F |\mathbf{x}_1 \dots \mathbf{x}_n\rangle_S &= (n!)^{-\frac{1}{2}} \sum_P \int d\mathbf{y} |\mathbf{y}\rangle_1 |\mathbf{x}_2\rangle_2 \dots |\mathbf{x}_n\rangle_n \langle \mathbf{y} | f_1 | \mathbf{x}_1 \rangle_1 \\ &+ (n!)^{-\frac{1}{2}} \sum_P \int d\mathbf{y} |\mathbf{x}_1\rangle_1 |\mathbf{y}\rangle_2 \dots |\mathbf{x}_n\rangle_n \langle \mathbf{y} | f_2 | \mathbf{x}_2 \rangle_2 \\ &+ \dots \end{aligned} \quad (41)$$

¹Note that in the second quantization formalism, it is impossible to write down an operator which refers to one specific particle.

The matrix elements ${}_i\langle \mathbf{y} | f_i | \mathbf{x} \rangle_i$ are the same for all i , however, and is written simply as $\langle \mathbf{y} | f | \mathbf{x} \rangle$. Therefore (41) is

$$F|\mathbf{x}_1 \dots \mathbf{x}_n\rangle_S = \sum_{s=1}^n |\mathbf{x}_1 \dots \mathbf{x}_{s-1} \mathbf{y} \mathbf{x}_{s+1} \dots \mathbf{x}_n\rangle \langle \mathbf{y} | f | \mathbf{x}_s \rangle. \quad (42)$$

Our problem is now solved: the Fock space representation of the observable F is

$$F = \int d\mathbf{x} d\mathbf{x}' \psi^\dagger(\mathbf{x}) \langle \mathbf{x} | f | \mathbf{x}' \rangle \psi(\mathbf{x}'). \quad (43)$$

Equation (38) insures that (43) gives the correct result (42) in every n -particle subspace of \mathfrak{F} . An intuitive appreciation for expressions such as F should be acquired. As one sees, the integrand destroys a particle at \mathbf{x}' , and recreates it at \mathbf{x} , with amplitude $\langle \mathbf{x} | f | \mathbf{x}' \rangle$.

More complicated observables can be constructed in a similar fashion. The derivations are straightforward, though tedious. We shall only quote the result for a symmetric sum of two-body operators, such as a two-body interaction, i.e.,

$$G = \sum_{i < j} g_{ij} = \frac{1}{2} \sum_{i \neq j} g_{ij}.$$

Let $\langle \mathbf{x}_1 \mathbf{x}_2 | g | \mathbf{x}'_1 \mathbf{x}'_2 \rangle$ be the coordinate space matrix element of g between *unsymmetrized* two-particle position kets. Then G is expressed as follows:

$$G = \frac{1}{2} \int d\mathbf{x}_1 \dots d\mathbf{x}'_2 \psi^\dagger(\mathbf{x}_1) \psi^\dagger(\mathbf{x}_2) \langle \mathbf{x}_1 \mathbf{x}_2 | g | \mathbf{x}'_1 \mathbf{x}'_2 \rangle \psi(\mathbf{x}'_2) \psi(\mathbf{x}'_1). \quad (44)$$

To give some examples of such operators, consider first the total momentum \mathbf{P} . Define the operator

$$\frac{\partial \psi(\mathbf{x})}{\partial \mathbf{x}} = i \frac{1}{\sqrt{\Omega}} \sum_{\mathbf{p}} \mathbf{p} e^{i\mathbf{p} \cdot \mathbf{x}} a_{\mathbf{p}};$$

then

$$\mathbf{P} = \int d\mathbf{x} \psi^\dagger(\mathbf{x}) \frac{1}{i} \frac{\partial \psi(\mathbf{x})}{\partial \mathbf{x}}. \quad (45)$$

Note the appearance of the familiar expression $(1/i)\partial/\partial\mathbf{x}$. The kinetic energy can, in a similar fashion, be written as

$$K = \frac{1}{2m} \int d\mathbf{x} \frac{\partial \psi^\dagger(\mathbf{x})}{\partial \mathbf{x}} \cdot \frac{\partial \psi(\mathbf{x})}{\partial \mathbf{x}} = -\frac{1}{2m} \int d\mathbf{x} \psi^\dagger(\mathbf{x}) \nabla^2 \psi(\mathbf{x}). \quad (46)$$

The Coulomb energy in a system of particles carrying the charge e is an example of an operator of type G . In this case

$$\langle \mathbf{x}_1 \mathbf{x}_2 | g | \mathbf{x}'_1 \mathbf{x}'_2 \rangle = \frac{e^2 \delta(\mathbf{x}_1 - \mathbf{x}'_1) \delta(\mathbf{x}_2 - \mathbf{x}'_2)}{4\pi |\mathbf{x}_1 - \mathbf{x}_2|} \quad (47)$$

and therefore the Coulomb energy is

$$V_C = \frac{1}{2} e^2 \int \frac{\psi^\dagger(\mathbf{x}_1) \psi^\dagger(\mathbf{x}_2) \psi(\mathbf{x}_2) \psi(\mathbf{x}_1)}{4\pi |\mathbf{x}_1 - \mathbf{x}_2|} d\mathbf{x}_1 d\mathbf{x}_2. \quad (48)$$

Finally, we point out that all of these relations can be written in an infinite variety of ways. Let $\{u_\nu(\mathbf{x})\}$ be any complete orthonormal set of one-particle wave functions, and define the creation and destruction operators b_ν^\dagger and b_ν by

$$b_\nu = \int d\mathbf{x} u_\nu^*(\mathbf{x})\psi(\mathbf{x}), \quad b_\nu^\dagger = \int d\mathbf{x} u_\nu(\mathbf{x})\psi^\dagger(\mathbf{x}). \quad (49)$$

The commutation rules (20) and (21) satisfied by the field operators then lead to

$$[b_\nu, b_{\nu'}^\dagger] = \delta_{\nu\nu'}, \quad [b_\nu, b_{\nu'}] = 0. \quad (50)$$

A unitary transformation from $\{u_\nu(\mathbf{x})\}$ to any other basis will lead to a new set of creation and destruction operators with precisely the same commutation rules. The operators F and G can be also written in terms of b_ν and b_ν^\dagger :

$$F = \sum_{\nu\nu'} b_\nu^\dagger \langle \nu | f | \nu' \rangle b_{\nu'}, \quad (51)$$

$$G = \frac{1}{2} \sum_{[\nu]} b_{\nu_1}^\dagger b_{\nu_2}^\dagger \langle \nu_1 \nu_2 | g | \nu'_1 \nu'_2 \rangle b_{\nu_2} b_{\nu_1}. \quad (52)$$

(b) Fermi-Dirac Statistics

The second quantization formalism must undergo some fundamental changes if it is to apply to a system of indistinguishable fermions because the occupation numbers can only assume the values 0 and 1 if the exclusion principle is to be satisfied.

Consider a system of n fermions. Let $\{|\alpha_\nu\rangle_i\}$ be a complete set of states for particle i , where α_ν stands for any convenient set of four one-particle quantum numbers. These could be the position \mathbf{x} and the projection s of the spin angular momentum on a given axis, or the four familiar quantum numbers used in spectroscopy. Recall from §11.1 that an antisymmetric n -particle state can be written as the determinant

$$|\alpha_{\nu_1} \dots \alpha_{\nu_n}\rangle_A \equiv \frac{1}{\sqrt{n!}} \begin{vmatrix} |\alpha_{\nu_1}\rangle_1 & \dots & |\alpha_{\nu_1}\rangle_n \\ \vdots & & \vdots \\ |\alpha_{\nu_n}\rangle_1 & \dots & |\alpha_{\nu_n}\rangle_n \end{vmatrix}. \quad (53)$$

The set of all such Slater determinants spans the Hilbert space \mathfrak{H}_n for an n -body Fermi system. It is crucial to note that (53) is specified, except for phases, by stating whether the quantum number α_ν occurs or not. These are the only two possibilities, because (53) vanishes if α_ν appears more than once. Hence (53) is specified equally well by an infinite number of yes-no statements.

Let us introduce a vector space, the Fock space \mathfrak{F} , spanned by the states $|\{n_\nu\}\rangle$ specified by the occupation numbers $n_\nu = 0, 1$. There is then a correspondence between the state vectors (53) in \mathfrak{H}_n , and the vectors in \mathfrak{F} :

$$|\alpha_{\nu_1} \dots \alpha_{\nu_n}\rangle_A \Leftrightarrow \pm |n_1, n_2, \dots\rangle, \quad \sum_i n_i = n. \quad (54)$$

The sign ambiguity appears because $|\alpha_{\nu_1} \alpha_{\nu_2} \alpha_{\nu_3} \dots \alpha_{\nu_n}\rangle$ and $|\alpha_{\nu_2} \alpha_{\nu_1} \alpha_{\nu_3} \dots \alpha_{\nu_n}\rangle$ have the same occupation numbers. This ambiguity is removed by the convention that $\nu_1 < \nu_2 < \dots < \nu_n$ in $|\alpha_{\nu_1} \dots \alpha_{\nu_n}\rangle_A$.

One should be quite clear on the meaning of (54). Consider a three-body system where one particle is in each of the states $\alpha_2, \alpha_3, \alpha_5$. Then (54) reads $|\alpha_2\alpha_3\alpha_5\rangle_A \Leftrightarrow |0, 1, 1, 0, 1, 0, 0, \dots\rangle$. That is, whereas the state $|\alpha_{\nu_1} \dots \alpha_{\nu_n}\rangle_A$ is specified by n quantum numbers, the Fock space state requires an infinite set of quantum numbers for its specification. On the other hand, the quantum numbers in the \mathfrak{F} -description can only take on two values, whereas the α_ν will, in general, take on an infinite number of values.

We now introduce operators which work on the states $|\{n_\nu\}\rangle$. Define a pair of operators a_ν^\dagger and a_ν for each possible state $|\alpha_\nu\rangle$, with the algebraic properties

$$\{a_\nu^\dagger, a_{\nu'}\} = \delta_{\nu\nu'} \quad , \quad \{a_\nu, a_{\nu'}\} = 0 \quad , \quad (55)$$

where $\{A, B\} \equiv AB + BA$ is called the anticommutator of A and B . Due to (55), $(a_\nu^\dagger a_\nu)^2 = a_\nu^\dagger a_\nu (1 - a_\nu a_\nu^\dagger)$. But (55) requires

$$(a_\nu)^2 = (a_\nu^\dagger)^2 = 0 \quad , \quad (56)$$

and therefore

$$(a_\nu^\dagger a_\nu)^2 = a_\nu^\dagger a_\nu \quad ; \quad (57)$$

hence the eigenvalues of $a_\nu^\dagger a_\nu$ are zero and one. Define now the number operator N_ν by

$$N_\nu = a_\nu^\dagger a_\nu \quad . \quad (58)$$

Then the eigenvalues of N_ν are the occupation number $n_\nu = 0, 1$ introduced earlier. Furthermore, a simple calculation shows that $[N_\nu, N_{\nu'}] = 0$. The kets $|\{n_\nu\}\rangle$ that span \mathfrak{F} are therefore the simultaneous eigenvectors of the observables $\{N_\nu\}$.

The commutation rules of a_ν^\dagger and a_ν with N_ν are again important. Computations with Fermi operators are facilitated by the identities

$$\begin{aligned} [A, BC] &= \{A, B\}C - B\{A, C\} \quad , \\ [AB, C] &= A\{B, C\} - \{A, C\}B \quad . \end{aligned} \quad (59)$$

With their help we immediately find

$$[a_\nu, N_{\nu'}] = a_\nu \delta_{\nu\nu'} \quad , \quad [a_\nu^\dagger, N_{\nu'}] = -a_\nu^\dagger \delta_{\nu\nu'} \quad . \quad (60)$$

These are precisely the same relations as in the Bose case [see (11)]. Hence a_ν^\dagger and a_ν are, respectively, creation and destruction operators. Conditions (56) and (57), which are built into the basic algebraic rules, assure that these operators cannot construct states that violate the exclusion principle.

As in the Bose case, a basis in \mathfrak{F} is constructed from the empty of vacuum state in which $n_\nu = 0$ for all ν . This state $|0\rangle$ is again defined by $a_\nu|0\rangle = 0$ for all ν . Because

$$\langle a_{\nu_n} \dots a_{\nu_1} a_{\nu_1}^\dagger \dots a_{\nu_n}^\dagger \rangle_0 = 1 \quad ,$$

the kets $a_{\nu_1}^\dagger \dots a_{\nu_n}^\dagger |0\rangle$ are orthonormal. They are explicitly antisymmetric in virtue of (55). If $[a_{\nu_1}^\dagger \dots a_{\nu_n}^\dagger]_C$ stands for the canonical order (where the smallest value of ν stands on the left, etc.), we have the correspondence

$$|\alpha_{\nu_1} \dots \alpha_{\nu_n}\rangle_A \Leftrightarrow [a_{\nu_1}^\dagger \dots a_{\nu_n}^\dagger]_C |0\rangle$$

between "conventional" states $|\rangle_A$ in \mathfrak{H}_n and the vectors in \mathfrak{F} .

The creation and destruction operators in coordinate space may be introduced as in (49). Let $\langle \mathbf{x}s | \alpha_\nu \rangle$ be the one-particle coordinate space wave function for spin projection s , and define the field operators by

$$\psi_s(\mathbf{x}) = \sum_\nu a_\nu \langle \alpha_\nu | \mathbf{x}s \rangle, \quad \psi_s^\dagger(\mathbf{x}) = \sum_\nu \langle \mathbf{x}s | \alpha_\nu \rangle a_\nu^\dagger. \quad (61)$$

Equation (55) then yield *the fermion anticommutation rules*

$$\{\psi_s(\mathbf{x}), \psi_{s'}^\dagger(\mathbf{x}')\} = \delta_{ss'} \delta(\mathbf{x} - \mathbf{x}'), \quad \{\psi_s(\mathbf{x}), \psi_{s'}(\mathbf{x}')\} = 0. \quad (62)$$

These rules imply the equivalent of (31):

$$\langle \psi_{s'_n}(\mathbf{x}'_n) \dots \psi_{s_1}(\mathbf{x}'_1) \psi_{s_1}^\dagger(\mathbf{x}_1) \dots \psi_{s_n}(\mathbf{x}_n) \rangle_0 = \sum_P \epsilon_P \prod_{i=1}^n \delta_{s_i s'_i} \delta(\mathbf{x}_i - \mathbf{x}'_i). \quad (63)$$

where the unprimed (or primed) space *and* spin coordinates must be permuted as a unit, and ϵ_P is the signature of the permutation. Thus for $n = 2$ the right-hand side of (63) reads

$$\delta_{s_1 s'_1} \delta(\mathbf{x}_1 - \mathbf{x}'_1) \delta_{s_2 s'_2} \delta(\mathbf{x}_2 - \mathbf{x}'_2) - \delta_{s_1 s'_2} \delta(\mathbf{x}_1 - \mathbf{x}'_2) \delta_{s_2 s'_1} \delta(\mathbf{x}_2 - \mathbf{x}'_1).$$

If $\varphi_\alpha(\mathbf{x}_1 s_1 \dots \mathbf{x}_n s_n)$ is an n -particle antisymmetric wave function, the ket in \mathfrak{F} corresponding to it is

$$|\varphi_\alpha\rangle = (n!)^{-\frac{1}{2}} \int d\mathbf{x}_1 \dots d\mathbf{x}_n \sum_{s_1 \dots s_n} \varphi_\alpha(\mathbf{x}_1 s_1 \dots \mathbf{x}_n s_n) \psi_{s_1}^\dagger(\mathbf{x}_1) \dots \psi_{s_n}^\dagger(\mathbf{x}_n) |0\rangle. \quad (64)$$

This expression has the same structure as (29). The proof that (64) is the correct prescription will not be given for the present case.

The construction of expressions for symmetric observables proceeds in a manner that differs only in detail from the Bose case; they are left to the reader. The final expressions have precisely the same form as in the Bose case. Thus the generic one-body operator (type F) is

$$F = \sum_{ss'} \int d\mathbf{x} d\mathbf{x}' \psi_s^\dagger(\mathbf{x}) \langle \mathbf{x}s | f | \mathbf{x}'s' \rangle \psi_{s'}(\mathbf{x}'), \quad (65)$$

and the two-body operator G is

$$G = \frac{1}{2} \sum_{s_1 \dots s_2'} \int d\mathbf{x}_1 \dots d^3 x_2' \psi_{s_1}^\dagger(\mathbf{x}_1) \psi_{s_2}^\dagger(\mathbf{x}_2) \langle \mathbf{x}_1 s_1 \mathbf{x}_2 s_2 | g | \mathbf{x}_1' s_1' \mathbf{x}_2' s_2' \rangle \psi_{s_2'}(\mathbf{x}_2') \psi_{s_1'}(\mathbf{x}_1'). \quad (66)$$

The order of the operators $\psi_{s_2'}(\mathbf{x}_2') \psi_{s_1'}(\mathbf{x}_1')$ was immaterial in (44). Not so in the antisymmetric case; one *must* adhere to the order as given in (66). The most important observables are the number operator

$$N = \sum_s \int d\mathbf{x} \psi_s^\dagger(\mathbf{x}) \psi_s(\mathbf{x}); \quad (67)$$

the momentum

$$\mathbf{P} = \sum_s \int d\mathbf{x} \psi_s^\dagger(\mathbf{x}) \frac{1}{i} \frac{\partial \psi_s(\mathbf{x})}{\partial \mathbf{x}}; \quad (68)$$

and the Coulomb energy

$$V_C = \frac{1}{2}e^2 \sum_{ss'} \int dx dx' \frac{\psi_s^\dagger(x)\psi_{s'}^\dagger(x')\psi_{s'}(x')\psi_s(x)}{4\pi|\mathbf{x} - \mathbf{x}'|}. \quad (69)$$

(c) The Equations of Motion

In the Fock space representation the Schrödinger picture is usually inappropriate, because it focuses attention on the intractable many-particle state vector. For this reason the Heisenberg picture will be used. Assuming that the Hamiltonian H is time-independent, we define the Heisenberg observables in the familiar way:

$$\psi(xt) = e^{iHt}\psi(x)e^{-iHt}. \quad (70)$$

The definition (70) applies equally well to the Fermi and Bose field operators, or to the creation and destruction operators in any representation. In (70) we have purposely written the argument of the field operator as x ; this symbol will stand for \mathbf{x} and the spin projection s , and instead of $\sum_s \int dx$, we shall simply write $\int(dx)$ henceforth. Thus the number operator is $\int(dx)\psi^\dagger(x)\psi(x)$ for particles of any spin and either statistics.

The commutation rules between equal-time field operators is unaffected by the unitary transformation (70). For Fermi fields, for example, we still have

$$\{\psi^\dagger(xt), \psi(x't)\} = \delta(x - x'),$$

where $\delta(x - x') \equiv \delta(\mathbf{x} - \mathbf{x}')\delta_{ss'}$. Knowledge of the equal-time algebraic rules therefore suffices to determine the commutator which appears in the equations of motion

$$i\dot{\psi}(xt) = [\psi(xt), H]. \quad (71)$$

Assume that H has the form

$$H = K + U + V, \quad (72)$$

where K is the kinetic energy

$$K = -\frac{1}{2m} \int(dx)\psi^\dagger(x)\nabla^2\psi(x), \quad (73)$$

U is a one-body potential

$$U = \int(dx)(dx')\psi^\dagger(x)\langle x|u|x'\rangle\psi(x') \quad (74)$$

which describes the interaction of the system with any static external fields that may be present, and V is the two-body interaction

$$V = \frac{1}{2} \int(dx_1) \dots (dx'_2)\psi^\dagger(x_1)\psi^\dagger(x_2)\langle x_1x_2|v|x'_1x'_2\rangle\psi(x'_2)\psi(x'_1). \quad (75)$$

Direct calculation gives

$$[\psi(y), V] = \frac{1}{2} \int(dx)(dx'_1)(dx'_2)\psi^\dagger(x)[\langle yx|v|x'_1x'_2\rangle \pm \langle xy|v|x'_1x'_2\rangle]\psi(x'_2)\psi(x'_1), \quad (76)$$

where the plus sign holds for Bose statistics, the minus for Fermi statistics. The exchange term may be rewritten as follows:

$$\pm \int (dx'_1)(dx'_2) \langle xy|v|x'_2x'_1\rangle \psi(x'_1)\psi(x'_2) = \int (dx'_1)(dx'_2) \langle xy|v|x'_2x'_1\rangle \psi(x'_2)\psi(x'_1).$$

But $\langle xy|v|x'_2x'_1\rangle = \langle yx|v|x'_1x'_2\rangle$, and therefore the two terms in (76) give the same contribution. In both statistics, the equations of motion are therefore

$$\begin{aligned} i\dot{\psi}(\mathbf{x}t) = & -\frac{1}{2m}\nabla^2\psi(\mathbf{x}t) + \int \langle \mathbf{x}|u|\mathbf{x}'\rangle \psi(\mathbf{x}'t)(d\mathbf{x}') \\ & + \int \psi^\dagger(\mathbf{x}_2t) \langle \mathbf{x}\mathbf{x}_2|v|x'_1x'_2\rangle \psi(\mathbf{x}'_2t)\psi(\mathbf{x}'_1t)(d\mathbf{x}_2)(d\mathbf{x}'_1)(d\mathbf{x}'_2). \end{aligned} \quad (77)$$

This equation has the canonical form $i\dot{\psi}(\mathbf{x}t) = \delta H/\delta\psi^\dagger(\mathbf{x}t)$.

When u and v are both local and spin independent, the matrix elements are

$$\langle \mathbf{x}|u|\mathbf{x}'\rangle = \delta(\mathbf{x} - \mathbf{x}')U(\mathbf{x}), \quad (78)$$

$$\langle \mathbf{x}_1\mathbf{x}_2|v|x'_1x'_2\rangle = \delta(\mathbf{x}_1 - \mathbf{x}'_1)\delta(\mathbf{x}_2 - \mathbf{x}'_2)v(\mathbf{x}_1 - \mathbf{x}_2). \quad (79)$$

The equation of motion then simplifies to

$$i\dot{\psi}(\mathbf{x}t) = -\frac{1}{2m}\nabla^2\psi(\mathbf{x}t) + U(\mathbf{x})\psi(\mathbf{x}t) + V_{\text{eff}}(\mathbf{x}t)\psi(\mathbf{x}t), \quad (80)$$

where

$$V_{\text{eff}}(\mathbf{x}t) = \int v(\mathbf{x} - \mathbf{x}')n(\mathbf{x}'t)d\mathbf{x}', \quad (81)$$

and

$$n(\mathbf{x}t) = \sum_s \psi_s^\dagger(\mathbf{x}t)\psi_s(\mathbf{x}t) \quad (82)$$

is the number density operator.

There is a rather superficial resemblance between the equation of motion (80) and the Schrödinger equation. However, Schrödinger's equation is linear, whereas (80) is nonlinear because V_{eff} is a functional of ψ . Nevertheless, the field equation has an intuitively simple structure. If we momentarily ignore that $n(\mathbf{x}t)$ is an operator, we see that $V_{\text{eff}}(\mathbf{x}t)$ is the potential energy at \mathbf{x} as computed in the classical manner from the two-body potential $v(\mathbf{x} - \mathbf{x}')$ and the density $n(\mathbf{x}t)$.

The solution of the operator equations of motion is equivalent to solving the Schrödinger equation in each and every subspace $\mathfrak{H}_{N'}$ of \mathfrak{F} . Clearly, that cannot be done if there are interactions between the particles. But the Heisenberg equations do provide equations of motion for the correlation functions. These equations cannot be solved exactly either, of course, but it is far easier to use our intuition in making approximations on correlation functions than on the many particle wave function. Furthermore, the second quantized method handles mixtures and pure states on an equal footing. This is indispensable when dealing with large systems at nonzero temperature.

(d) Distribution Functions

As in classical statistical mechanics, it usually suffices to restrict attention to the behavior of any one particle, or to any pair of particles, with all others being averaged over. This is done by introducing reduced density matrices and distribution functions. Once these are known it is possible to compute the expectation values of the most important symmetric observables.

For this purpose, define the *n-particle distribution matrices*

$$\langle x'_1 | W_1 | x_1 \rangle = \text{Tr } \rho \psi^\dagger(x_1) \psi(x'_1), \quad (83)$$

$$\langle x'_1 x'_2 | W_2 | x_1 x_2 \rangle = \text{Tr } \rho \psi^\dagger(x_1) \psi^\dagger(x_2) \psi(x'_2) \psi(x'_1), \quad (84)$$

etc., where ρ is an arbitrary density matrix defined in \mathfrak{F} , the trace runs over any complete set in \mathfrak{F} , and as before, $x \equiv (\mathbf{x}, s)$. The diagonal elements of the distribution matrices, obtained by setting $x_1 = x'_1$, have a simple significance in coordinate space, and they merit a more compact notation:

$$D_n(x_1 \dots x_n) \equiv \langle x_1 \dots x_n | W_n | x_1 \dots x_n \rangle. \quad (85)$$

Because $D_1(\mathbf{x}s) = \text{Tr } \rho \psi_s^\dagger(\mathbf{x}) \psi_s(\mathbf{x})$, it is clear that $D_1(\mathbf{x}s)$ is the density at \mathbf{x} of particles having spin projection s . The off-diagonal elements of W_1 also have physical significance, because the momentum distribution, defined as the number of particles having momentum \mathbf{p} and spin projection s , is

$$\text{Tr } \rho a_{\mathbf{p}s}^\dagger a_{\mathbf{p}s} = \frac{1}{\Omega} \int d\mathbf{x} d\mathbf{x}' e^{-i\mathbf{p} \cdot (\mathbf{x} - \mathbf{x}')} \langle \mathbf{x}s | W_1 | \mathbf{x}'s \rangle. \quad (86)$$

Thus W_1 incorporates both the coordinate space and momentum space densities. More generally, for an n -particle state W_n is the Wigner distribution, apart from normalization (recall §2.2(d)). As for W_1 , it is normalized as follows:

$$\int d\mathbf{x} D_1(\mathbf{x}) = \langle N \rangle = \bar{N}. \quad (87)$$

The *pair distribution function*, $D_2(x_1, x_2)$, is of great importance. From the basic commutation rules it follows that

$$\psi^\dagger(x_1) \psi^\dagger(x_2) \psi(x'_2) \psi(x'_1) = \psi^\dagger(x_1) \psi(x'_1) \psi^\dagger(x_2) \psi(x'_2) - \delta(x_2 - x'_2) \psi^\dagger(x_1) \psi(x'_1) \quad (88)$$

for both Bose and Fermi statistics. Therefore

$$\int dx_1 dx_2 D_2(x_1, x_2) = \langle N^2 \rangle - \langle N \rangle. \quad (89)$$

For a system with many particles, not to mention the thermodynamic limit, $\langle N \rangle$ is negligible, and $\langle N^2 \rangle - \langle N \rangle^2$. In these circumstances, therefore

$$P(x_1, x_2) = \langle N \rangle^{-2} D_2(x_1, x_2) \quad (90)$$

is a joint probability distribution for any pair.

When the density matrix ρ is invariant under spatial symmetries, these are reflected in the distribution matrices. For example, neglecting gravity, a fluid in thermal equilibrium is spatially homogeneous and isotropic except in the vicinity of

boundaries. Then $D_2(x_1x_2)$ depends only on the coordinate difference $|\mathbf{x}_1 - \mathbf{x}_2|$, unless \mathbf{x}_1 and/or \mathbf{x}_2 is near a boundary. Results of this type are consequences of symmetry assumptions about the ensemble of states. For instance, assume that ρ is translation invariant, i.e. $[\rho, \mathbf{P}] = 0$. The momentum operator generates translations:

$$\psi_s(\mathbf{x} - \mathbf{a}) = e^{i\mathbf{P} \cdot \mathbf{a}} \psi_s(\mathbf{x}) e^{-i\mathbf{P} \cdot \mathbf{a}}. \quad (91)$$

The same transformation law applies to any operator $A(\mathbf{x})$, such as $\psi_s^\dagger(\mathbf{x})\psi_{s'}(\mathbf{x})$, constructed from the operators ψ and ψ^\dagger at the point \mathbf{x} . Furthermore,

$$\text{Tr } \rho A(\mathbf{x})B(\mathbf{x}') = \text{Tr } \rho e^{i\mathbf{P} \cdot \mathbf{x}} A(0) e^{-i\mathbf{P} \cdot (\mathbf{x} - \mathbf{x}')} B(0) e^{-i\mathbf{P} \cdot \mathbf{x}'}. \quad (92)$$

Then $\text{Tr } XY = \text{Tr } YX$ and $[\mathbf{P}, \rho] = 0$ produce

$$\text{Tr } \rho A(\mathbf{x})B(\mathbf{x}') = \text{Tr } \rho A(\mathbf{x} - \mathbf{x}')B(0). \quad (93)$$

As a consequence, the distribution matrices W_n are only functions of the coordinate differences if ρ is invariant under translations.

If ρ is rotationally invariant, there are further simplifications. Should spin-orbit forces be negligibly weak, ρ is invariant under orbital and spin rotations separately, and it then follows that $[\rho, \mathbf{L}] = [\rho, \mathbf{S}] = 0$. In this case,

$$\langle \mathbf{x}_1 s_1 \dots \mathbf{x}_n s_n | W_n | \mathbf{x}'_1 s'_1 \dots \mathbf{x}'_n s'_n \rangle$$

is a function of the absolute value of the coordinate differences, and vanishes unless

$$\sum_{m=1}^n s_m = \sum_{m=1}^n s'_m.$$

When ρ is invariant under translations, the momentum representation offers many advantages. Define

$$\begin{aligned} \langle \mathbf{p}_1 \dots \mathbf{p}_n | \tilde{W}_n | \mathbf{p}'_1 \dots \mathbf{p}'_n \rangle &\equiv \Omega^{-n} \int d\mathbf{x}_1 \dots d\mathbf{x}'_n e^{-i(\mathbf{p}_1 \cdot \mathbf{x}_1 + \dots + \mathbf{p}_n \cdot \mathbf{x}_n)} \\ &\quad \times \langle \mathbf{x}_1 \dots \mathbf{x}_n | W_n | \mathbf{x}'_1 \dots \mathbf{x}'_n \rangle e^{i(\mathbf{p}'_1 \cdot \mathbf{x}'_1 + \dots + \mathbf{p}'_n \cdot \mathbf{x}'_n)} \\ &= \text{Tr } \rho a_{\mathbf{p}'_1}^\dagger \dots a_{\mathbf{p}'_n}^\dagger a_{\mathbf{p}_n} \dots a_{\mathbf{p}_1}; \end{aligned} \quad (94)$$

then translation invariance implies that \tilde{W}_n vanishes unless

$$\sum_{m=1}^n \mathbf{p}_m = \sum_{m=1}^n \mathbf{p}'_m.$$