Chapter 4
MANY PARTICLE SYSTEMS

The postulates of quantum mechanics outlined in previous chapters include no restrictions as to the kind of systems to which they are intended to apply. Thus, although we have considered numerous examples drawn from the quantum mechanics of a single particle, the postulates themselves are intended to apply to all quantum systems, including those containing more than one and possibly very many particles.

Thus, the only real obstacle to our immediate application of the postulates to a system of many (possibly interacting) particles is that we have till now avoided the question of what the linear vector space, the state vector, and the operators of a many-particle quantum mechanical system look like. The construction of such a space turns out to be fairly straightforward, but it involves the forming a certain kind of methematical product of different linear vector spaces, referred to as a **direct** or **tensor product**. Indeed, the basic principle underlying the construction of the state spaces of many-particle quantum mechanical systems can be succinctly stated as follows:

> The state vector $|\psi\rangle$ of a system of N particles is an element of the direct product space
> $$S^{(N)} = S(1) \otimes S(2) \otimes \cdots \otimes S(N)$$
> formed from the N single-particle spaces associated with each particle.

To understand this principle we need to explore the structure of such direct product spaces. This exploration forms the focus of the next section, after which we will return to the subject of many particle quantum mechanical systems.

4.1 The Direct Product of Linear Vector Spaces

Let S_1 and S_2 be two independent quantum mechanical state spaces, of dimension N_1 and N_2, respectively (either or both of which may be infinite). Each space might represent that of a single particle, or they may be more complicated spaces, each associated with a few or many particles, but it is assumed that the degrees of mechanical freedom represented by one space are independent of those represented by the other. We distinguish states in each space by superscripts. Thus, e.g., $|\psi\rangle^{(1)}$ represents a state in S_1 and $|\phi\rangle^{(2)}$ a state of S_2. To describe the combined system we now define a new vector space

$$S_{12} = S_1 \otimes S_2 \tag{4.1}$$

of dimension $N_{12} = N_1 \times N_2$ which we refer to as the direct or tensor product of S_1 and S_2. Some of the elements of S_{12} are referred to as direct or tensor product *states*, and are

formed as a direct product of states from each space. In other words, from each pair of states $|\psi\rangle^{(1)} \in S_1$ and $|\phi\rangle^{(2)} \in S_2$ we can construct an element

$$|\psi, \phi\rangle \equiv |\psi\rangle^{(1)} \otimes |\phi\rangle^{(2)} = |\psi\rangle^{(1)}|\phi\rangle^{(2)} \in S_{12} \tag{4.2}$$

of S_{12}, in which, as we have indicated, a simple juxtaposition of elements defines the tensor product state when there is no possibility of ambiguous interpretation. By definition, then, the state $|\psi, \phi\rangle$ represents that state of the combined system in which subsystem 1 is definitely in state $|\psi\rangle^{(1)}$ and subsystem 2 is in state $|\phi\rangle^{(2)}$. The linear vector space S_{12} , which is intended to describe the combined system, consists precisely of *all such direct product states as well as all possible linear combinations of those states.* This direct product of states is assumed to be commutative in the trivial sense that there is nothing special about taking the elements in the reverse order, i.e.,

$$|\psi, \phi\rangle \equiv |\psi\rangle^{(1)}|\phi\rangle^{(2)} = |\phi\rangle^{(2)}|\psi\rangle^{(1)} \tag{4.3}$$

except that in the abbreviated notation on the left hand side we agree to chose a distinct ordering of the spaces once and for all and thus associate the first symbol in the list with that part of the state arising from S_1 and the second symbol for that part of the state arising from S_2. In the decoupled form on the right, however, we are free to move the two kets from each space past each other whenever it is convenient. The tensor product is also assumed to be linearly distributive in the sense that if $|\psi\rangle^{(1)} = \alpha|\xi\rangle^{(1)} + \beta|\eta\rangle^{(1)}$, then

$$|\psi, \phi\rangle \equiv |\psi\rangle^{(1)}|\phi\rangle^{(2)} = [\alpha|\xi\rangle^{(1)} + \beta|\eta\rangle^{(1)}]|\phi\rangle^{(2)} = \alpha|\xi, \phi\rangle + \beta|\eta, \phi\rangle, \tag{4.4}$$

and similarly for kets $|\phi\rangle^{(2)}$ which are linear combinations in S_2. It is important to emphasize that there are many states in the space S_{12} that are *not* direct product states, although (by construction) any state in the product space can be written as a linear combination of such states. On the other hand, for any given linear combination

$$|\psi\rangle = \alpha|\xi, \phi\rangle + \beta|\eta, \chi\rangle \tag{4.5}$$

of product states, there may or may not be other states in S_1 and S_2 which allow $|\psi\rangle$ to be "factored" into a single direct product of states from each space. If no such factorization exists, then the state is said to be an **entangled state** of the combined system. Under such circumstances neither subsystem can be described independently by its own state vector, without consideration of the state of the other. Generally, such entanglements arise as a result of interactions between the component degrees of freedom of each space. The space combined space S_{12} consists of all possible direct product states as well as all possible entangled states.

We denote by $\langle\psi, \phi|$ the bra of the dual space $S_{12}^* = S_1^* \otimes S_2^*$ adjoint to the ket $|\psi, \phi\rangle$. Thus, the combined symbol ψ, ϕ labeling the state is untouched by the adjoint process:

$$[|\psi, \phi\rangle]^+ = [|\psi\rangle^{(1)}|\phi\rangle^{(2)}]^+ = [\langle\psi|^{(1)}\langle\phi|^{(2)}] = \langle\psi, \phi|. \tag{4.6}$$

Inner products taken between elements of the direct product space are obtained by straightforward linear extension of inner products in each factor space, with the stipulation that it is only possible to take inner products between those factors in the same space, i.e.,

$$\begin{aligned} \langle\psi, \phi|\eta, \xi\rangle &= \left(\langle\psi|^{(1)}\langle\phi|^{(2)}\right)\left(|\eta\rangle^{(1)}|\xi\rangle^{(2)}\right) \\ &= \langle\psi|\eta\rangle^{(1)}\langle\phi|\xi\rangle^{(2)}. \end{aligned} \tag{4.7}$$

Thus, kets and bras in one space commute past those of the other to form a bracket with members of their own space. Since any state is expressible as a linear combination of product states, this completely specifies the inner product in the combined space.

Basis vectors for the product space S_{12} can be constructed from basis vectors in the factor spaces S_1 and S_2. Specifically, if the states $\{|\phi_i\rangle^{(1)}\}$ form a discrete ONB for S_1 and the states $\{|\chi_j\rangle^{(2)}\}$ form a discrete ONB for S_2, then the set of $N_1 \times N_2$ product states $\{|\phi_i, \chi_j\rangle\}$ form an ONB for the tensor product space S_{12}. We write:

$$\langle \phi_i, \chi_j | \phi_{i'}, \chi_{j'} \rangle = \delta_{i,i'} \delta_{j,j'} \tag{4.8}$$

$$\sum_{i,j} |\phi_i, \chi_j\rangle\langle \phi_i, \chi_j| = 1 \tag{4.9}$$

to denote the orthonormality and completeness of the product basis in S_{12}. Any state in the system can be expanded in such a basis in the usual way, i.e.,

$$|\psi\rangle = \sum_{i,j} |\phi_i, \chi_j\rangle\langle \phi_i, \chi_j|\psi\rangle = \sum_{i,j} \psi_{ij} |\phi_i, \chi_j\rangle. \tag{4.10}$$

Similar relations hold for direct product bases formed form continuous ONB's in S_1 and

S_2. Thus, if $\{|\xi\rangle^{(1)}\}$ and $\{|\chi\rangle^{(1)}\}$ form continuous ONB's for the two (infinite dimensional) factor spaces then the product space is spanned by the basis vectors $|\xi, \chi\rangle$, for which we can write

$$\langle \xi, \chi | \xi', \chi\prime \rangle = \delta(\xi - \xi')\delta(\chi - \chi') \tag{4.11}$$

$$\int d\xi \int d\chi \; |\xi, \chi\rangle\langle \xi, \chi| = 1 \tag{4.12}$$

$$|\psi\rangle = \int d\xi \int d\chi \; |\xi, \chi\rangle\langle \xi, \chi|\psi\rangle = \sum_{i,j} \psi(\xi, \chi) |\xi, \chi\rangle. \tag{4.13}$$

Finally, we can also form direct product bases using a discrete basis for one space and a continuous basis for the other.
Note, that by unitary transformation in the product space it is generally possible to produce bases which are not the direct products of bases in the factor spaces (i.e., ONB's formed at least partially from entangled states). Note also, that we have implicitly defined operators in the product space through the last relation.

More generally, operators in S_{12} are formed from linear combinations of (what else) the direct product of operators from each space. That is, for every pair of linear operators A of S_1 and B of S_2 we associate an operator $AB = A \otimes B$ which acts in S_{12} in such a way that each operator acts only on that part of the product state with which it is associated. Thus,

$$AB|\psi, \chi\rangle = \left(A|\psi\rangle^{(1)}\right)\left(B|\chi\rangle^{(2)}\right) = |\psi_A, \chi_B\rangle. \tag{4.14}$$

Every operator in the individual factor spaces has a natural extension into the product space, since it can be multiplied by the identity operator of the other space; i.e., the extension of the operator $A^{(1)}$ of S_1 into S_{12} is the operator

$$A^{(12)} = A^{(1)} \otimes \mathbf{1}^{(2)}, \tag{4.15}$$

where $\mathbf{1}^{(2)}$ is the identity operator in S_2. Often we will drop the superscripts, since the symbol A represents the same physical observable in S_1 and in S_{12} (but is generally undefined in S_2). Identical constructions hold for the extension of operators of S_2. Clearly, $\mathbf{1}^{(12)} = \mathbf{1}^{(1)} \otimes \mathbf{1}^{(2)} = \mathbf{1}^{(1)}\mathbf{1}^{(2)}$. Again, as with direct product states, the order of the factors is not important, so that *operators of one factor space always commute with operators of the other*, while operators from the *same* space retain the commutation relations that they had in the original space This implies, for example, that if $A|a\rangle^{(1)} = a|a\rangle^{(1)}$ and $B|b\rangle^{(2)} = b|b\rangle^{(2)}$, then

$$AB|a,b\rangle = BA|a,b\rangle = \left(A|a\rangle^{(1)}\right)\left(B|b\rangle^{(2)}\right) = ab|a,b\rangle \tag{4.16}$$

so that the eigenstates of a product of operators from different spaces are simply products of the eigenstates of the factors.

As with the states, a *general* linear operator in S_{12} can be expressed as a linear combination of direct product operators, but *need not* be factorizeable into such a product itself. A simple example is the sum or difference of two operators, one from each space; again if $A|a\rangle^{(1)} = a|a\rangle^{(1)}$ and $B|b\rangle^{(2)} = b|b\rangle^{(2)}$, then

$$(A \pm B)|a,b\rangle = (a \pm b)|a,b\rangle. \tag{4.17}$$

In general any operator can be expanded in terms of an ONB for the product space in the usual way, e.g.,

$$H = \sum_{i,j}\sum_{i',j'} |\phi_i,\chi_j\rangle H_{ij,i'j'}\langle\phi_{i'},\chi_{j'}|, \tag{4.18}$$

where $H_{ij,i'j'} = \langle\phi_i,\chi_j|H|\phi_{i'},\chi_{j'}\rangle$. Note that if $H = AB$ is a product of operators from each space, then the matrix elements representing H in any direct product basis is just the product of the matrix elements of each operator as defined in the factor spaces, i.e.,

$$\langle\phi_i,\chi_j|H|\phi_{i'},\chi_{j'}\rangle = \langle\phi_i,\chi_j|AB|\phi_{i'},\chi_{j'}\rangle = \langle\phi_i|A|\phi_{i'}\rangle\langle\chi_j|B|\chi_{j'}\rangle$$

The resulting $N_1 \times N_2$ dimensional matrix in S_{12} is then said to be the direct or tensor product of the matrices representing A in S_1 and B in S_2.

Finally we note that this definition of direct product spaces is easily extensible to treat multiple factor spaces. Thus, e.g., if S_1, S_2, and S_3 are three independent quantum mechanical state spaces, then we can take the 3-fold direct product of states $|\psi\rangle^{(1)} \in S_1$ and $|\phi\rangle^{(2)} \in S_2$, and $|\chi\rangle^{(3)} \in S_3$ to construct elements $|\psi,\phi,\chi\rangle = |\psi\rangle^{(1)}|\phi\rangle^{(2)}|\chi\rangle^{(3)}$ of the direct product space

$$S_{123} = S_1 \otimes S_2 \otimes S_3$$

with inner products

$$\langle\psi',\phi',\chi'|\psi,\phi,\chi\rangle = \langle\psi'|\psi\rangle^{(1)}\langle\phi'|\phi\rangle^{(2)}\langle\chi'|\chi\rangle^{(2)}$$

and operators

$$ABC|\psi,\phi,\chi\rangle = |\psi_A,\phi_B,\chi_C\rangle.$$

4.1.1 Motion in 3 *Dimensions Treated as a Direct Product of Vector Spaces*

To make these formal definitions more concrete we consider a few examples. Consider, e.g., our familiar example of a single spinless quantum particle moving in 3 dimensions. It turns out that this space can be written as the direct product

$$S_{3D} = S_x \otimes S_y \otimes S_x. \tag{4.19}$$

of 3 spaces S_i, each of which is isomorphic to the space of a particle moving along one cartesian dimension. In each of the factor spaces we have a basis of position states and relevant operators, e.g., in S_x we have the basis states, $\{|x\rangle\}$ and operators $X, K_x, P_x, \cdots$, in S_y the basis states $\{|y\rangle\}$ and operators $Y, K_y, P_y, \cdots$, and similarly for S_z. In the direct product space S_{3D} we can then form, according to the rules outlined in the last section, the basis states

$$|\vec{r}\rangle = |x, y, z\rangle = |x\rangle \otimes |y\rangle \otimes |z\rangle \tag{4.20}$$

each of which is labeled by the 3 cartesian coordinates of the position vector $\vec{r}$ of R^3. Any state in this space can be expanded in terms of this basis

$$|\psi\rangle = \int dx\, dy\, dz\ |x, y, z\rangle\langle x, y, z|\psi\rangle = \int dx\, dy\, dz\ \psi(x, y, z)\ |x, y, z\rangle, \tag{4.21}$$

or in more compact notation

$$|\psi\rangle = \int d^3r\ |\vec{r}\rangle\langle\vec{r}|\psi\rangle = \int d^3r\ \psi(\vec{r})|\vec{r}\rangle. \tag{4.22}$$

Thus, the state $|\psi\rangle$ is represented in this basis by a wave function $\psi(\vec{r}) = \psi(x, y, z)$ of 3 variables. Note that by forming the space as the direct product, the individual components of the position operator X_i automatically are presumed to commute with one another, since they derive from different factor spaces. Indeed, it follows that the canonical commutation relations

$$[X_i, X_j] = 0 = [P_i, P_j] \tag{4.23}$$

$$[X_i, P_j] = i\hbar\delta_{i,j} \tag{4.24}$$

are automatically obeyed due to the rule for extending operators into the product space. The action of the individual components of the position operator and momentum operators also follow from the properties of the direct product space, i.e.,

$$X|x, y, z\rangle = X|x\rangle\mathbf{1}_y|y\rangle\mathbf{1}_z|z\rangle = x|x, y, z\rangle \tag{4.25}$$

$$P_x|\psi\rangle = -i\hbar \int d^3r\ \frac{\partial\psi(\vec{r})}{\partial x}|\vec{r}\rangle \tag{4.26}$$

and so on.

In a similar fashion it is easily verified that all other properties of the space S_{3D} of a single particle moving in 3 dimensions follow entirely from the properties of the tensor product of 3 one-dimensional factor spaces. Of course, in this example, it is merely a question of mathematical convenience whether we view S_3 in this way or not.

4.1.2 The State Space of Spin-1/2 Particles

Another situation in which the concept of a direct product space becomes valuable is in treating the internal, or spin degrees of freedom of quantum mechanical particles. It is a well-established experimental fact that the quantum state of most fundamental particles is not completely specified by properties related either to their spatial coordinates or to their linear momentum. In general, each quantum particle possesses an internal structure characterized by a vector observable $\vec{S}$, the components of which transform under rotations like the components of angular momentum. The particle is said to possess "spin degrees of freedom". For the constituents of atoms, i.e., electrons, neutrons, protons, and other spin-1/2 particles, the internal state of each particle can be represented as a superposition of two linearly independent eigenvectors of an operator S_z whose eigenvalues $s = \pm 1/2$ (in units of $\hbar$) characterize the projection of their spin angular momentum vectors $\vec{S}$ onto some fixed quantization axis (usually taken by convention to be the z axis). A particle whose internal state is the eigenstate with $s = 1/2$ is said to be spin up, with $s = -1/2$, spin down.

The main point of this digression, of course, is that the state space of a spin-1/2 particle can be represented as direct product

$$S_{\text{spin-1/2}} = S_{\text{spatial}} \otimes S_{\text{spin}}$$

of a quantum space S_{spatial} describing the particle's spatial state (which is spanned, e.g., by an infinite set of position eigenstates $|\vec{r}\rangle$), and a two-dimensional quantum space S_{spin} describing the particle's internal structure. This internal space is spanned by the eigenstates $|s\rangle$ of the Cartesian component S_z of its spin observable $\vec{S}$, with eigenvalues $s = \pm 1/2$. The direct product of these two sets of basis states from each factor space then generates the direct product states

$$|\vec{r}, s\rangle = |\vec{r}\rangle \otimes |s\rangle,$$

which satisfy the obvious orthonormality and completeness relations

$$\sum_{s=\pm 1/2} \int d^3r \; |\vec{r}, s\rangle\langle\vec{r}, s| = 1 \qquad\qquad \langle\vec{r}', s'|\vec{r}, s\rangle = \delta(\vec{r} - \vec{r}')\delta_{s,s'}.$$

An arbitrary state of a spin-1/2 particle can then be expanded in this basis in the form

$$|\psi\rangle = \sum_{s=\pm 1/2} \int d^3r \; \psi_s(\vec{r})|\vec{r}, s\rangle = \int d^3r \; [\psi_+(\vec{r})|\vec{r}, 1/2\rangle + \psi_-(\vec{r})|\vec{r}, -1/2\rangle]$$

and thus requires a two component wave function (or spinor). In other words, to specify the state of the system we must provide two seprate complex-valued functions $\psi_+(\vec{r})$ and $\psi_-(\vec{r})$, with $|\psi_+(\vec{r})|^2$ describing the probability density to find the particle spin-up at $\vec{r}$ and $|\psi_-(\vec{r})|^2$ describing the density to find the particle spin-down at $\vec{r}$. Note that, by construction, all spin related operators ($\vec{S}, S_z, S^2$, etc.) automatically commute with all spatial related operators ($\vec{R}, \vec{K}, \vec{P}$, etc.).

Thus, the concept of a direct product space arises in many different situtations in quantum mechanics and when properly identified as such can help to elucidate the structure of the underlying state space.

4.2 The State Space of Many Particle Systems

We are now in a position to return to the topic that motivated our interest in direct product spaces in the first place, namely, the construction of quantum states of many

particle systems. The guiding principle has already been state, i.e., that the state vector of a system of N particles is an element of the direct product space formed from the N single-particle spaces associated with each particle.

Thus, as the simplest example, consider a collection of N spinless particles each moving in one-dimension, along the x-axis, say (e.g., a set of particles confined to a quantum wire). The αth particle of this system is itself associated with a single particle state space $S(\alpha)$ that is spanned by a set of basis vectors $\{|x_\alpha\rangle\}$, and is associated with the standard set of operators $X_\alpha, K_\alpha, P_\alpha$, etc. The combined space $S^{(N)}$ of all N particles in this system is then the N-fold direct product

$$S^{(N)} = S(1) \otimes S(2) \otimes \cdots \otimes S(N) \tag{4.27}$$

of the individual single-particle spaces, and so is spanned by the basis vectors formed from the position eigenstates of each particle, i.e., we can construct the direct product basis

$$|x_1, \ldots, x_N\rangle = |x_1\rangle^{(1)} \otimes |x_2\rangle^{(2)} \ldots \otimes |x_N\rangle^{(N)}. \tag{4.28}$$

In terms of this basis an arbitrary N-particle quantum state of the system can be expanded in the form

$$\begin{aligned} |\psi\rangle &= \int dx_1 \ldots dx_N \; |x_1, \ldots, x_N\rangle\langle x_1, \ldots, x_N|\psi\rangle \\ &= \int dx_1 \ldots dx_N \; \psi(x_1, \ldots, x_N) \; |x_1, \ldots, x_N\rangle. \end{aligned} \tag{4.29}$$

Thus, the quantum mechanical description involves a wave function $\psi(x_1, \ldots, x_N)$ which is a function of the position coordinates of all particles in the system. This space is clearly isomorphic to that of a single particle moving in N dimensions, but the interpretation is different. For a single particle in N dimensions the quantity $\psi(x_1, \ldots, x_N)$ represents the amplitude that a position measurement of the particle will find it located at the point $\vec{r}$ having the associated cartesian coordinates $x_1, \ldots, x_N$. For N particles moving in one dimension, the quantity $\psi(x_1, \ldots, x_N)$ represents the amplitude that a simultaneous position measurement of *all* the particles will find the first at x_1, the second at x_2, and so on.

The extension to particles moving in higher dimensions is straightforward. Thus, for example, the state space of N spinless particles moving in 3 dimensions is the tensor product of the N single particle spaces $S(\alpha)$ each describing a single particle moving in 3 dimensions. The αth such space is now spanned by a set of basis vectors $\{|\vec{r}_\alpha\rangle\}$, and is associated with the standard set of vector operators $\vec{R}_\alpha, \vec{K}_\alpha, \vec{P}_\alpha$, etc. We can now expand an arbitrary state of the combined system

$$\begin{aligned} |\psi\rangle &= \int d^3r_1 \ldots d^3r_N \; |\vec{r}_1, \ldots, \vec{r}_N\rangle\langle\vec{r}_1, \ldots, \vec{r}_N|\psi\rangle \\ &= \int d^3r_1 \ldots d^3r_N \; \psi(\vec{r}_1, \ldots, \vec{r}_N) \; |\vec{r}_1, \ldots, \vec{r}_N\rangle. \end{aligned} \tag{4.30}$$

in the direct product basis $\{|\vec{r}_1, \ldots, \vec{r}_N\rangle\}$ of position localized states, each of which describes a distinct configuration of the N particles. The wave function is then a function of the N position vectors $\vec{r}_\alpha$ of all of the particles (or of the $3N$ cartesian components thereof). A little reflection shows that the mathematical description of N particles moving

in 3 dimensions is mathematically equivalent, both classically and quantum mechanically, to a single particle moving in space of $3N$ dimensions.

Before discussing other properties of many-particle systems, it is worth pointing out that our choice of the position representation in the examples presented above is arbitrary. The state of a system of N spinless particles moving in 3 dimensions may also be expanded in the ONB of momentum eigenstates

$$|\psi\rangle = \int d^3k_1 \dots d^3k_N \, |\vec{k}_1, \dots, \vec{k}_N\rangle\langle\vec{k}_1, \dots, \vec{k}_N|\psi\rangle$$

$$= \int d^3k_1 \dots d^3k_N \, \psi(\vec{k}_1, \dots, \vec{k}_N) \, |\vec{k}_1, \dots, \vec{k}_N\rangle,$$

or in any other complete direct product basis. In addition, it should be noted that the rules associated with forming a direct product space ensure that all operators associated with a given particle automatically commute with all the operators associated with any other particle.

4.3 Evolution of Many Particle Systems

The evolution of a many particle quantum system is, as the basic postulates assert, governed through the Schrödinger equation

$$i\hbar\frac{d}{dt}|\psi\rangle = H|\psi\rangle \tag{4.31}$$

where H represents the Hamiltonian operator describing the total energy of the many particle system. For a system of N particles, the Hamiltonian can often be written in the form

$$H = \sum_{\alpha=1}^{N} \frac{P_\alpha^2}{2m_\alpha} + V(\vec{R}_1, \vec{R}_2, \dots, R_N). \tag{4.32}$$

As for conservative single particle systems, the evolution of the system is most easily described in terms of the eigenstates of H, i.e., the solutions to the energy eigenvalue equation

$$H|\phi_E\rangle = E|\phi_E\rangle. \tag{4.33}$$

Projecting this expression onto the position representation leads to a partial differential equation

$$\sum_{\alpha=1}^{N} \frac{-\hbar^2}{2m_\alpha}\nabla_\alpha^2\phi_E + V(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N)\phi_E = E\phi_E \tag{4.34}$$

for the many particle eigenfunctions $\phi_E(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N)$. When N is greater than two this equation is (except in special cases) analytically intractable (i.e., nonseparable). This analytical intractability includes the important physical case in which the potential energy of the system arises from pairwise interactions of the form

$$V = \frac{1}{2}\sum_{\substack{\alpha,\beta \\ \alpha\neq\beta}} V(\vec{r}_\alpha - \vec{r}_\beta). \tag{4.35}$$

Solutions of problems of this sort are fundamental to the study of atomic and molecular physics when N is relatively small ($N \leq 200$, typically) and to the study of more general forms of matter (i.e., condensed phases, liquids, solids, etc.) when N is very large ($N \sim 10^{24}$). Under these circumstances one is often led to consider the development of approximate solutions developed, e.g., using the techniques of perturbation theory.

An important, and in principle soluble special case is that of noninteracting particles, for which the potential can be written in the form

$$V = \sum_{\alpha=1}^{N} V_\alpha(\vec{r}_\alpha) \tag{4.36}$$

corresponding to a situation in which each particle separately responds to its own external potential. In fact, using potentials of this type it is often possible, in an approximate sense, to treat more complicated real interactions such as those described by (4.35). In fact, if all but one of the particles in the system were fixed in some well-defined state, then this remaining particle could be treated as moving in the potential field generated by all the others. If suitable potentials $V_\alpha(\vec{r}_\alpha)$ could thus be generated that, in some average sense, took into account the states that the particles actually end up in, then the actual Hamiltonian

$$H = \sum_\alpha \frac{P_\alpha^2}{2m_\alpha} + V$$

could be rewritten in the form

$$\begin{aligned} H &= \sum_\alpha \left[\frac{P_\alpha^2}{2m_\alpha} + V_\alpha(\vec{r}_\alpha)\right] + \Delta V \\ &= H_0 + \Delta V \end{aligned}$$

where

$$\Delta V = V - \sum_\alpha V_\alpha(\vec{r}_\alpha)$$

would, it is to be hoped, represent a small perturbation. The exact solution could then be expanded about the solutions to the noninteracting problem associated with the Hamiltonian

$$H_0 = \sum_\alpha \left[\frac{P_\alpha^2}{2m_\alpha} + V_\alpha(\vec{r}_\alpha)\right].$$

In this limit, it turns out, the eigenvalue equation can, in principle, be solved by the method of separation of variables. To obtain the same result, we observe that in this limit the Hamiltonian can be written as a sum

$$H_0 = \sum_{\alpha=1}^{N} \left[\frac{P_\alpha^2}{2m_\alpha} + V_\alpha(\vec{R}_\alpha)\right] = \sum_{\alpha=1}^{N} H_\alpha, \tag{4.37}$$

of single particle operators, where the operator H_α acts only on that part of the state associated with the single particle space $S(\alpha)$. In each single particle space the eigenstates $|E_{n_\alpha}\rangle$ of H_α form an ONB for the associated single particle space. Thus the many particle space has as an ONB the simultaneous eigenstates $|E_{n_1}, E_{n_2}, \ldots, E_{n_N}\rangle$ of the commuting set of operators $\{H_1, H_2, \ldots, H_N\}$. These are automatically eigenstates of the total

Hamiltonian H_0, i.e.,

$$\begin{aligned} H_0|E_{n_1}, E_{n_2}, \ldots, E_{n_\alpha}, \ldots, E_{n_N}\rangle &= \sum_\alpha H_\alpha |E_{n_1}, E_{n_2}, \ldots, E_{n_\alpha}, \ldots, E_{n_N}\rangle \\ &= \sum_\alpha E_{n_\alpha} |E_{n_1}, E_{n_2}, \ldots, E_{n_\alpha}, \ldots, E_{n_N}\rangle \\ &= E\,|E_{n_1}, E_{n_2}, \ldots, E_{n_\alpha}, \ldots, E_{n_N}\rangle, \end{aligned} \tag{4.38}$$

where the total energy $E = \sum_\alpha E_{n_\alpha}$ is just the sum of the single particle energies (as it is classically). The corresponding wave function associated with such a state is

$$\langle \vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N | E_{n_1}, E_{n_2}, \ldots, E_{n_N}\rangle = \phi_{n_1}(\vec{r}_1)\phi_{n_2}(\vec{r}_2)\ldots\phi_{n_N}(\vec{r}_N) \tag{4.39}$$

which is just the product of the associated single particle eigenfunctions of the operators H_α, the same result that one would find by using the process of separation of variables. Indeed, the standard process of solving a partial differential equation by the method of separation of variables can be interpreted as the decomposition of an original functional space of several variables into the direct product of the functional spaces associated with each.

4.4 Systems of Identical Particles

The developments in this chapter derive their importance from the fact that there exist experimental systems of considerable interest which contain more than one particle. It is useful at this point to consider the implications of another important empirical fact: in many of these systems the particles of interest belong to distinct classes of (apparently) **indistinguishable or identical particles**. We use names (protons, electrons, neutrons, silver ions, etc.) to distinguish the different classes of indistinguishable particles from one another. Operationaly, this means that two members of a given class (e.g., two electrons) are not just similar, but are in fact *identical* to one another, i.e., that there exists no experiment which could possibly distinguish one from the other. This leads us to ask the following question: What constraint, if any, does indistinguishability impose upon the state vector of a system of identical particles?

To explore this question, consider first a system of N distinguishable, but physically similar, particles each of which is associated with a state space $S(\alpha)$ which is isomorphic to all the others. If the set of vectors $\{|\phi_\nu\rangle^{(\alpha)} \mid \nu = 1, 2, \cdots\}$ forms an ONB for the space of the αth particle then the many particle space $S^{(N)}$ is spanned by basis vectors of the form

$$|\phi_{\nu_1}, \phi_{\nu_2}, \ldots, \phi_{\nu_N}\rangle = |\phi_{\nu_1}\rangle^{(1)}|\phi_{\nu_2}\rangle^{(2)}\ldots|\phi_{\nu_N}\rangle^{(N)} \tag{4.40}$$

which corresponds to a state in which particle 1 is in state ϕ_{ν_1}, particle 2 in state ϕ_{ν_2}, and so on.

Consider, now, the operation of "interchanging" two of the particles in the system. Formally, we can define a set of $N(N-1)/2$ unitary **exchange operators** $U_{\alpha\beta}$ through their action on any direct product basis as follows:

$$U_{\alpha\beta}|\phi_{\nu_1}, \ldots, \phi_{\nu_\alpha}, \ldots, \phi_{\nu_\beta}, \ldots, \phi_{\nu_N}\rangle = |\phi_{\nu_1}, \ldots, \phi_{\nu_\beta}, \ldots, \phi_{\nu_\alpha}, \ldots, \phi_{\nu_N}\rangle \tag{4.41}$$

which puts particle α in the state formerly occupied by particle β, puts particle β in the state formerly occupied by particle α, and leaves all other particles alone (we assume

$\alpha \neq \beta$). We note in passing that each exchange operator is unitary since it maps any direct product basis onto itself, but in a different order. We note also that the product of any exchange operator with itself gives the identity operator, as is easily verified by multiplying the equation above by $U_{\alpha\beta}$,.and which is consistent with the intuitive idea that two consecutive exchanges is equivalent to none. Thus, we deduce that $U_{\alpha\beta}^2 = \mathbf{1}$.

These properties of the exchange operators aside, the important physical point is that for distinguishable particles an exchange of this sort leaves the system in a physically different state (assuming $\nu_\alpha \neq \nu_\beta$). The two states $|\phi_{\nu_1}, \ldots, \phi_{\nu_\beta}, \ldots, \phi_{\nu_\alpha}, \ldots, \phi_{\nu_N}\rangle$ and $U_{\alpha\beta}|\phi_{\nu_1}, \ldots, \phi_{\nu_\beta}, \ldots, \phi_{\nu_\alpha}, \ldots, \phi_{\nu_N}\rangle$, are linearly independent.

When we mentally repeat this exercise of exchanging particles with a system of indistinguishable particles, however, we must confront the fact that there can be no experiment which can tell which particle is in which state, since there is no way of distinguishing the different particles in the system from one another. That is to say, we cannot know that particle α is in the state $|\phi_{\nu_\alpha}\rangle$, but only that the state $|\phi_{\nu_\alpha}\rangle$ is occupied by one of the particles. Thus, an ordered list enumerating which particles are in which states, such as that labeling the direct product states above, *contains more information than is actually knowable*. For the moment, let $|\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle^{(I)}$ denote the *physical state* of a system of N indistinguishable particles in which the states $\phi_{\nu_1}, \ldots, \phi_{\nu_N}$ are occupied. We then invoke the principle of indistinguishability and assert that this state and the one

$$U_{\alpha\beta}|\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle^{(I)} \tag{4.42}$$

obtained from it by switching two of the particles must represent the *same* physical state of the system. This means that they can differ from one another by at most a phase factor, i.e., a unimodular complex number of the form $\lambda = e^{i\theta}$. Thus, we assert that there exists some λ for which

$$U_{\alpha\beta}|\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle^{(I)} = \lambda|\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle^{(I)}. \tag{4.43}$$

Note, however, that exchanging two particles twice in succession must return the system to its original state, i.e.,

$$U_{\alpha\beta}[U_{\alpha\beta}|\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle^{(I)}] = |\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle^{(I)}. \tag{4.44}$$

This last statement is true whether applied to distinguishable or indistinguishable particles. The implication for the undetermined phase factor, however, is that

$$U_{\alpha\beta}^2|\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle^{(I)}] = \lambda^2|\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle^{(I)} = |\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle^{(I)} \tag{4.45}$$

from which we deduce that $\lambda^2 = 1$. This implies that $\lambda = \pm 1$, so that

$$U_{\alpha\beta}|\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle^{(I)} = \pm|\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle^{(I)}. \tag{4.46}$$

Thus, we have essentially proved the following theorem: The physical state of a system of N identical particles is a simultaneous eigenstate of the set of exchange operators $\{U_{\alpha\beta}\}$ with eigenvalue equal either to $+1$ or -1. A state is said to be **symmetric** under exchange of the particles α and β if it is an eigenvector of $U_{\alpha\beta}$ with eigenvalue $+1$, and is **antisymmetric** if it is an eigenvector of $U_{\alpha\beta}$ with eigenvalue -1. It is **totally symmetric** if it is symmetric under all exchanges and **totally antisymmetric** if it is antisymmetric under all exchanges.

Now it is not hard to see that the set of *all* totally symmetric states of N particles forms a *subspace* $S_S^{(N)}$of the original product space $S^{(N)}$, (since any linear combination

of such states is still totally symmetric). We shall call $S_S^{(N)}$ the **symmetric subspace** of $S^{(N)}$. Similarly the set of all totally antisymmetric states forms the **antisymmetric subspace** $S_A^{(N)}$ of $S^{(N)}$. Our theorem shows that all physical states of a system of N indistinguishable particles must lie either in $S_S^{(N)}$ or $S_A^{(N)}$. (We can't have a physical state symmetric under some exchanges and antisymmetric under others, since this would imply a physical difference between some of the particles.) Moreover, if a given class of identical particles had some states that were symmetric and some that were antisymmetric, it would be possible to form linear combinations of each, forming physical states that were neither, and thus violating our theorem. We deduce, therefore, that each class of identical particles can have physical states that lie *only* in $S_S^{(N)}$ or *only* in $S_A^{(N)}$; it cannot have some states that are symmetric and some that are antisymmetric.

Experimentally, it is indeed found that the identifiable classes of indistinguishable particles divide up naturally into those whose physical states are *all* antisymmetric and those whose physical states are *all* symmetric under the exchange of any two particles in the system. Particles which are antisymmetric under exchange, such as electrons, protons, and neutrons, are referred to as **fermions**. Particles which are symmetric under exchange, such as photons, are referred to as **bosons**.

4.4.1 Construction of the Symmetric and Antisymmetric Subspaces

We find ourselves in an interesting formal position. We have found that it is a straightforward exercise to construct the Hilbert space $S^{(N)}$ of N distinguishable particles as a direct product of N single particle spaces. We see now that the *physical* states associated with N *indistinguishable* particles are necessarily restricted to one or the other of two *subspaces* of the originally constructed direct product space. We still have not said how to actually construct these subspaces or indeed how to actually produce a physical state of such a system. This would be straightforward, of course, if we had at our disposal the *projectors* P_S and P_A onto the corresponding symmetric and antisymmetric subspaces, for then we could start with *any* state in $S^{(N)}$ and simply project away those parts of it which were not symmetric or antisymmetric, respectively. These projectors, if we can construct them, must satisfy the condition obeyed by any projectors, namely,

$$P_S^2 = P_S \qquad P_A^2 = P_A. \tag{4.47}$$

In addition, if $|\psi_S\rangle$ and $|\psi_A\rangle$ represent, respectively, any completely symmetric or antisymmetric states in $S^{(N)}$, then we must have

$$P_S|\psi_S\rangle = |\psi_S\rangle \qquad P_A|\psi_S\rangle = 0 \tag{4.48}$$

$$P_A|\psi_A\rangle = |\psi_A\rangle \qquad P_S|\psi_A\rangle = 0 \tag{4.49}$$

the right-hand relations follow because an antisymmetric state must be orthogonal to all symmetric states and *vice versa*. It turns out that the projectors P_S and P_A are straightforward to construct once one has assembled a rather formidable arsenal of unitary operators referred to as **permutation operators**, which are very closely related to, and in a sense constructed from, the exchange operators. To this end it is useful to enumerate some of the basic properties of the exchange operators $U_{\alpha\beta}$:

1. All exchange operators are *Hermitian*, since, as we have seen, they have real eigenvalues $\lambda = \pm 1$.

2. All exchange operators are *nonsingular*, since they are equal to their own inverses, a fact that we have already used by observing, effectively, that $U_{\alpha\beta}^2 = 1$, hence $U_{\alpha\beta}^{-1} = U_{\alpha\beta}$.

3. All exchange operators are *unitary* since they are Hermitian and equal to their own inverses; it follows that $U_{\alpha\beta} = U^{+}_{\alpha\beta} = U^{-1}_{\alpha\beta}$. Thus each one transforms any complete direct product basis for $S^{(N)}$ onto another, equivalent, direct product basis.

4. Different exchange operators do not generally commute. This makes sense on a physical basis; if we first exchange particles α and β and *then* exchange particles β (which is the original particle α) and γ we get different results then if we make these exchanges in the reverse order.

The product of two or more exchange operators is not, in general, simply another exchange operator, but is a unitary operator that has the effect of inducing a more complicated *permutation* of the particles among themselves. Thus, a product of two or more exchange operators is one of the $N!$ possible *permutation operators* the members of which set we will denote by the symbol U_ξ, where

$$\xi \equiv \begin{pmatrix} 1,\ 2\ ,\ldots,\ N \\ \xi_1, \xi_2, \ldots, \xi_N \end{pmatrix} \tag{4.50}$$

denotes an arbitrary permutation, or reordering of the integers $(1,\ 2\ ,\ldots,\ N)$ into a new order, denoted by $(\xi_1, \xi_2, \ldots, \xi_N)$. Thus the operator U_ξ has the effect of replacing particle 1 with particle ξ_1, particle 2 with particle ξ_2 and so on, i.e.

$$U_\xi |\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle = |\phi_{\nu_{\xi_1}}, \ldots, \phi_{\nu_{\xi_N}}\rangle$$

There are $N!$ such permutations of N particles. The set of $N!$ permutation operators share the following properties, some of which are given without proof:

1. The product of any two permutation operators is another permutation operator. In fact, they form a *group,* the identity element of which is the identity permutation that maps each particle label onto itself. Symbolically, we can write $U_\xi U_{\xi'} = U_{\xi''}$. The group property also insures that this relation applies to the whole set of permutation operators, i.e., for any fixed permutation operator U_ξ the set of products $\{U_\xi U_{\xi'}\}$ is equivalent to the set $\{U_\xi\}$ of permutation operators itself. This important property will be used below.

2. Each permutation ξ, or permutation operator U_ξ can be classified as being either "even" or "odd". An even permutation operator can be written as a product

   $$U_\xi = U_{\alpha\beta} U_{\gamma\delta} \cdots U_{\mu\nu}$$

   of an even number of *exchange* operators, and odd permutation as a product of an odd number of exchange operators. This factorization of each U_ξ is not unique, since we can obviously insert an even number of factors of $U_{\alpha\beta}$ in the product without changing the permutation (or the even-odd classification). This is equivalent to the observation that an arbitrary permutation of N particles can be built up through a series of simple exchanges in many different ways.

3. The *exchange parity* ε_ξ of a given permutation operator is defined to be $+1$ if U_ξ is even and -1 if it is odd. Equivalently, if U_ξ can be written as a product of n exchange operators then $\varepsilon_\xi = (-1)^n$.

It turns out that for a given number N of particles, there are an equal number of even and odd permutation operators (indeed multiplying any even permutation operator by one exchange operator makes it an odd permutation operator and vice versa.). It is also fairly easy to see that if a state $|\psi_S\rangle$ is symmetric (i.e., invariant) under all exchanges, it is also symmetric under any product thereof, and thus is symmetric under the entire set of permutation operators, i.e.,

$$U_\xi|\psi_S\rangle = |\psi_S\rangle. \tag{4.51}$$

Physically, this means that it is invariant under an arbitrary permutation of the particles in the system. Alternatively, it means that $|\psi_S\rangle$ is an eigenstate of U_ξ with eigenvalue 1.

On the other hand, a state $|\psi_A\rangle$ which is antisymmetric under all exchanges will be left unchanged after an even number of exchanges (i.e., after being operated on by an even number of exchange operators), but will be transformed into its negative under an odd number of exchanges. Thus is succinctly expressed by the relation

$$U_\xi|\psi_A\rangle = \varepsilon_\xi|\psi_A\rangle. \tag{4.52}$$

Thus, an antisymmetric state is an eigenstate of U_ξ with eigenvalue ε_ξ.

With these properties in hand, we are now ready to display the form of the projectors onto the symmetric and antisymmetric subspaces of $S^{(N)}$. These are expressible as relatively simple sums of the permutation operators as follows; the symmetric projector is essentially the symmetric sum

$$P_S = \frac{1}{N!}\sum_\xi U_\xi \tag{4.53}$$

of all the permutation operators, while the antisymmetric projector has a form

$$P_A = \frac{1}{N!}\sum_\xi U_\xi\varepsilon_\xi. \tag{4.54}$$

that weights each of the permutation operators by its exchange parity of ± 1. Thus, half the terms in the antisymmetric projector have a -1 and half have a $+1$.

The proof that these operators do indeed satisfy the basic properties of the projectors as we described earlier is straightforward. First we note that if $|\psi_S\rangle$ is a symmetric state, then

$$P_S|\psi_S\rangle = \frac{1}{N!}\sum_\xi U_\xi|\psi_S\rangle = \frac{1}{N!}\sum_\xi |\psi_S\rangle = |\psi_S\rangle \tag{4.55}$$

where the sum over the $N!$ permutations ξ eliminates the normalization factor. Similarly, we have

$$P_A|\psi_S\rangle = \frac{1}{N!}\sum_\xi \varepsilon_\xi U_\xi|\psi_S\rangle = \frac{1}{N!}\sum_\xi \varepsilon_\xi|\psi_S\rangle = 0, \tag{4.56}$$

where we have used the fact that there are equal numbers of even and odd permutations to evaluate the alternating sum in the last expression. Similarly, if $|\psi_A\rangle$ is an antisymmetric state,

$$P_A|\psi_A\rangle = \frac{1}{N!}\sum_\xi \varepsilon_\xi U_\xi|\psi_A\rangle = \frac{1}{N!}\sum_\xi \varepsilon_\xi^2|\psi_A\rangle = |\psi_A\rangle \tag{4.57}$$

while

$$P_S|\psi_A\rangle = \frac{1}{N!}\sum_\xi U_\xi|\psi_A\rangle = \frac{1}{N!}\sum_\xi \varepsilon_\xi|\psi_A\rangle = 0. \tag{4.58}$$

Finally, we must show that $P_S^2 = P_S$, and $P_A^2 = P_A$. To show this we note first that

$$U_\xi P_S = \frac{1}{N!}\sum_{\xi'} U_\xi U_{\xi'} = \frac{1}{N!}\sum_{\xi''} U_{\xi''} = P_S, \tag{4.59}$$

where we have used the group property which ensures that the set of permutation operators simply reproduces itself when multiplied by any single permutation operator. Thus for the symmetric projector we have

$$P_S P_S = \frac{1}{N!}\sum_{\xi} U_\xi P_S = \frac{1}{N!}\sum_{\xi''} P_S = P_S, \tag{4.60}$$

showing that it is indeed a projection operator.

To prove a similar result for the antisymmetric projector, we note first that the exchange parity of the product of any two permutation operators is the product of their individual parities. Thus if $U_\xi U_{\xi'} = U_{\xi''}$, then

$$\varepsilon_{\xi''} = \varepsilon_\xi \varepsilon_{\xi'}. \tag{4.61}$$

This can be seen by factorizing both permutation operators in the product into exchange operators. If U_ξ and $U_{\xi'}$ contain n and m factors, respectively, then $U_{\xi''}$ contains $n+m$ factors, so $\varepsilon_{\xi''} = (-1)^{n+m} = (-1)^n(-1)^m = \varepsilon_\xi\varepsilon_{\xi'}$. Using this, along with the obvious relation $\varepsilon_\xi^2 = 1$, it follows that

$$\begin{aligned} U_\xi P_A &= \frac{1}{N!}\sum_{\xi'} U_\xi U_{\xi'}\varepsilon_{\xi'} = \frac{1}{N!}\sum_{\xi'} \varepsilon_\xi U_\xi U_{\xi'}\varepsilon_\xi\varepsilon_{\xi'} = \varepsilon_\xi \frac{1}{N!}\sum_{\xi''}\varepsilon_{\xi''}U_{\xi''} \\ &= \varepsilon_\xi P_A, \end{aligned} \tag{4.62}$$

Thus for the antisymmetric projector we have

$$P_A P_A = \frac{1}{N!}\sum_{\xi} \varepsilon_\xi U_\xi P_A = \frac{1}{N!}\sum_{\xi} \varepsilon_\xi^2 P_A = \frac{1}{N!}\sum_{\xi} P_A = P_A, \tag{4.63}$$

which is the desired idempotency relation for the antisymmetic projector.

Using these projectors, the *physical state* of a system of N identical particles is constructed by projection. To each state $|\psi\rangle \in S^{(N)}$ there corresponds at most one state $|\psi_S\rangle \in S_S^{(N)}$ and one state $|\psi_A\rangle \in S_A^{(N)}$. For bosons, the normalized symmetrical state is given by the projection

$$|\psi_S\rangle = \frac{P_S|\psi\rangle}{\sqrt{\langle\psi|P_S|\psi\rangle}} \tag{4.64}$$

onto $S_S^{(N)}$, while for fermions we have

$$|\psi_A\rangle = \frac{P_A|\psi\rangle}{\sqrt{\langle\psi|P_A|\psi\rangle}}. \tag{4.65}$$

It is important to point out that the projection may give the null vector if, for example, the original state is entirely symmetric or antisymmetric to begin with.

Example: Two Identical Bosons - Let $|\phi\rangle$ and $|\chi\rangle$ be two orthonormal single particle states. The state $|\phi^{(1)}, \chi^{(2)}\rangle = |\phi, \chi\rangle = |\psi\rangle$ is in the two-particle direct product space $S^{(2)}$. The projection of $|\psi\rangle$ onto the symmetric subspace of $S^{(2)}$ is

$$P_S|\psi\rangle = \frac{1}{2}\left[U_{12} + U_{21}\right]|\phi, \chi\rangle = \frac{1}{2}\left[|\phi, \chi\rangle + |\chi, \phi\rangle\right]. \tag{4.66}$$

To normalize we evaluate

$$\frac{1}{2}\left[\langle\phi,\chi| + \langle\chi,\phi|\right]\frac{1}{2}\left[|\phi,\chi\rangle + |\chi,\phi\rangle\right] = \frac{1}{4}\left[1+0+0+1\right] = \frac{1}{2}, \tag{4.67}$$

so

$$|\psi_S\rangle = \frac{1}{\sqrt{2}}\left[|\phi,\chi\rangle + |\chi,\phi\rangle\right]. \tag{4.68}$$

Notice that if $\phi = \chi$, then the original state is already symmetric, i.e., $P_S|\phi,\phi\rangle = |\phi,\phi\rangle$. Thus, it is possible for two (or more) bosons to be in the same single particle state. Also notice that if $\phi \neq \chi$, then the states $|\phi,\chi\rangle$ and $|\chi,\phi\rangle$ are both projected onto the same physical state, i.e., $P_S|\phi,\chi\rangle = P_S|\chi,\phi\rangle$. This fact, namely that there are generally many states in $S^{(N)}$ that correspond to the same physical state in $S_S^{(N)}$ is referred to as a lifting of the exchange degeneracy of $S^{(N)}$.

Example: Two Identical Fermions - Again let $|\phi\rangle$ and $|\chi\rangle$ be two orthonormal single particle states, and $|\phi^{(1)},\chi^{(2)}\rangle = |\phi,\chi\rangle = |\psi\rangle$ be the associated two-particle state in $S^{(2)}$. The projection of $|\psi\rangle$ onto the antisymmetric part of $S^{(2)}$ is

$$P_A|\psi\rangle = \frac{1}{2}\left[\varepsilon_{12}U_{12} + \varepsilon_{21}U_{21}\right]|\phi,\chi\rangle = \frac{1}{2}\left[|\phi,\chi\rangle - |\chi,\phi\rangle\right]. \tag{4.69}$$

To normalize we evaluate

$$\frac{1}{2}\left[\langle\phi,\chi| - \langle\chi,\phi|\right]\frac{1}{2}\left[|\phi,\chi\rangle - |\chi,\phi\rangle\right] = \frac{1}{4}\left[1-0-0+1\right] = \frac{1}{2}, \tag{4.70}$$

so

$$|\psi_A\rangle = \frac{1}{\sqrt{2}}\left[|\phi,\chi\rangle - |\chi,\phi\rangle\right]. \tag{4.71}$$

Again, the projection of the states $|\phi,\chi\rangle$ and $|\chi,\phi\rangle$ onto $S_A^{(2)}$correspond to the same physical state, (a lifting of the exchange degeneracy) although they differ from one another by a phase factor, i.e., $P_S|\phi,\chi\rangle = -P_A|\chi,\phi\rangle = e^{i\pi}P_S|\phi,\chi\rangle$. Notice, however, that if $\phi = \chi$, then the projection of the original state vanishes. Thus, two identical fermions cannot occupy the same physical state. This fact, which follows from the symmetrization requirement is referred to as the **Pauli exclusion principle**.

It is possible to write the fermion state derived above in a convenient mathematical form involving a determinant, i.e., if we write

$$|\psi_A\rangle = \frac{1}{\sqrt{2}}\begin{vmatrix} |\phi^{(1)}\rangle & |\phi^{(2)}\rangle \\ |\chi^{(1)}\rangle & |\chi^{(2)}\rangle \end{vmatrix} \tag{4.72}$$

and formally evaluate the determinant of this odd matrix we obtain

$$\begin{aligned} |\psi_A\rangle &= \frac{1}{\sqrt{2}}\left[|\phi^{(1)}\rangle|\chi^{(2)}\rangle - |\chi^{(1)}\rangle|\phi^{(2)}\rangle\right] \\ &= \frac{1}{\sqrt{2}}\left[|\phi,\chi\rangle - |\chi,\phi\rangle\right] \end{aligned} \tag{4.73}$$

This determinantal way of expressing the state vector (or the wave function) is referred to as a **Slater determinant**, and generalizes to a system of N particles. Thus, if $|\phi_{\nu_1}\rangle, |\phi_{\nu_2}\rangle, \cdots, |\phi_{\nu_N}\rangle$ represent a set of N orthonormal single particle states, then the Slater determinant

$$|\psi_A\rangle = \frac{1}{\sqrt{N!}}\begin{vmatrix} |\phi_{\nu_1}^{(1)}\rangle & |\phi_{\nu_1}^{(2)}\rangle & \cdots & |\phi_{\nu_1}^{(N)}\rangle \\ |\phi_{\nu_2}^{(1)}\rangle & |\phi_{\nu_2}^{(2)}\rangle & \cdots & |\phi_{\nu_2}^{(N)}\rangle \\ \cdots & \cdots & \cdots & \cdots \\ |\phi_{\nu_N}^{(1)}\rangle & |\phi_{\nu_N}^{(2)}\rangle & \cdots & |\phi_{\nu_N}^{(N)}\rangle \end{vmatrix} \tag{4.74}$$

is a properly normalized state of N fermions. Note that if any two states $|\phi_{\nu_\alpha}\rangle$ and $|\phi_{\nu_\beta}\rangle$ are the same, then the corresponding rows will be identical and the resulting state will vanish, automatically satisfying the Pauli exclusion principle.

4.4.2 Number Operators and Occupation Number States

We now turn to the task of identifying and constructing ONB's for the symmetric (or bosonic) subspace describing a collection of N identical bosons and the antisymmetric (or fermionic) subspace describing a collection of N identical fermions. As we have seen, from a given set of single particle states $\{|\phi_\nu\rangle \; |\nu = 1, 2, \cdots\}$ we can form for the direct product space $S^{(N)}$ of N distinguishable particles an ONB of direct product states $|\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle$, in which particle 1 is in state $|\phi_{\nu_1}\rangle$, particle 2 in state $|\phi_{\nu_2}\rangle$, and so on. It is useful at this point to introduce a set of operators $\{N_\nu \; |\nu = 1, 2, \cdots\}$ associated with this representation which "count" the number of particles that are in each single-particle state, i.e., by definition,

$$\begin{aligned} N_1|\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle &= n_1|\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle \\ N_2|\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle &= n_2|\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle \\ &\vdots \\ N_\nu|\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle &= n_\nu|\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle \\ &\vdots \end{aligned} \tag{4.75}$$

where, e.g., n_1 represents the number of times the symbol ϕ_1 appears in the list $(\phi_{\nu_1}, \ldots, \phi_{\nu_N})$, i.e., it describes the number of particles in the collection occupying the single-particle state $|\phi_1\rangle$. Similarly, the eigenvalue

$$n_\nu = \sum_{\alpha=1}^{N} \delta_{\nu,\nu_\alpha} \tag{4.76}$$

is, for this state, the number of particles in the single-particle state $|\phi_\nu\rangle$. Thus the direct product states of this representation are simultaneous eigenstates of this set of **number operators** $\{N_\nu\}$, and each such state is characterized by a specific set of eigenvalues $\{n_\nu\}$. The eigenvalues n_ν are referred to as the **occupation numbers** associated with this representation of single particle states. Now, typically, the number of single-particle states $\{|\phi_\nu\rangle\}$ is infinite, and so most of the occupation numbers $\{n_\nu\}$ characterizing any given basis state $|\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle$ are equal to zero. In fact, it is clear that at most N of them are not zero, and this maximum can be obtained only if all the particles are in different single-particle states. On the other hand, at least one of the occupation numbers is not zero, since the sum of the occupation numbers is equal to the total number of particles in the system, i.e.,

$$N = \sum_\nu n_\nu. \tag{4.77}$$

Now for distinguishable particles, the occupation numbers $\{n_\nu\} = \{n_1, n_2, \cdots\}$ generally do not determine uniquely the corresponding basis states. This is because the occupation numbers, by construction, contain information about which single-particle states are filled, but contain no information about which particles are in which states. Thus, e.g., if $|\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle$ is a direct product state characterized by a certain set of occupation numbers $\{n_\nu\}$, any permutation of the particles in the system among the same specified set of single-particle states will leave the system in a state $U_\xi|\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle$ having exactly the *same* set of single-particle states filled (albeit by different particles than in the original). The set of occupation numbers for any such state will, therefore, be identical with that of the unpermuted state. If all of the occupied single-particle states

$\phi_{\nu_1}, \ldots, \phi_{\nu_N}$ are distinct (i.e., if all the associated occupation numbers are either zero or one) , then there will be $N!$ linearly independent states $U_\xi|\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle$ associated with the same set of occupation numbers $\{n_\nu\}$. If, however, some of the single-particle states are multiply occupied, then any permutation that simply rearranges those particles in the *same* occupied state will leave the system in exactly the same state as before. If, e.g., there are n_1 particles in the state $|\phi_1\rangle$ then there will be $n_1!$ permutations that simply permute these n_1 particles among themselves, and so on. Arguing in this way for each multiply-occupied state, we deduce that the number of linearly-independent states $\left\{U_\xi|\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle\right\}$ of N distinguishable particles associated with a given set $\{n_\nu\}$ of occupation numbers is given by the expression

$$g\left(\{n_\nu\}\right) = \frac{N!}{n_1! n_2! \cdots} \,. \tag{4.78}$$

Recall that $0! = 1! = 1$, so that this expression reduces to $N!$ when there are N distinct single-particle states filled. This number $g\left(\{n_\nu\}\right)$ defines more closely the term **exchange degeneracy** introduced earlier, since it is, in fact, the degeneracy in $S^{(N)}$ associated with the set of simultaneous eigenvalues $\{n_\nu\}$ of the number operators $\{N_\nu\}$, a degeneracy that arises entirely due to the distinguishability of the particles described.

Now when the basis vectors $\left\{|\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle\right\}$ of this representation of $S^{(N)}$ are projected onto the symmetric or anti-symmetric subspaces, they generate an ONB for each of these two smaller subspaces. As we might expect, however, there is a reduction in the number of linearly-independent basis vectors that survive the projection. In particular, projection onto either the symmetric or anti-symmetric spaces eliminates any information regarding which particle is in which single-particle state. As a consequence, all the basis vectors $\left\{U_\xi|\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle\right\}$ associated with a given set $\{n_\nu\}$ of occupation numbers project onto *at most one linearly independent basis vector* of each subspace. This dramatic reduction (which is the essence of the removal of the exchange degeneracy that we observed in the two-particle case) allows us to label each such basis vector by the associated set of occupation numbers, and provides us with what is referred to as the **occupation number representation** associated with a given set of single-particle states. In what follows we describe the projection process independently for the bosonic and fermionic subspaces.

The projection of the basis vector $|\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle$ onto the symmetric subspace $S_S^{(N)}$ of N-identical bosons is, by definition, the vector $P_S|\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle$. On the other hand the projection of the state $U_\xi|\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle$, which is associated with the same set of occupation numbers, is given by the vector $P_S U_\xi|\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle$. But, we note that

$$P_S U_\xi = \frac{1}{N!}\sum_{\xi'} U_{\xi'} U_\xi = \frac{1}{N!}\sum_{\xi''} U_{\xi''} = P_S, \tag{4.79}$$

where we have used the group properties of the permutation operators. Thus we find that

$$P_S U_\xi|\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle = P_S|\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle, \tag{4.80}$$

and hence deduce that all $g\left(\{n_\nu\}\right)$ basis vectors of $S^{(N)}$ associated with the same set $\{n_\nu\}$ of occupation numbers project onto precisely the same vector in $S_S^{(N)}$. As a consequence, the basis vectors obtained in this way by projection onto $S_S^{(N)}$ can be uniquely labeled by the occupation numbers $\{n_\nu\}$ that characterize them. We thus denote by

$$|n_1, n_2, \ldots\rangle = \frac{P_S|\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle}{||P_S|\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle||} \tag{4.81}$$

the symmetric state of N identical bosons containing n_1 particles in state ϕ_1, n_2 particles in state ϕ_2, and so on. The set of such states with $\sum_\nu n_\nu = N$ span the symmetric subspace $S_S^{(N)}$ of N identical bosons, and form what is referred to as the occupation number representation associated with this set of single particle states. (Note that any such ONB of single particle states generates a similar representation.) For any such representation for the symmetric subspace, therefore, we can write an orthonormality relation

$$\langle n_1, n_2, \ldots | n_1', n_2', \ldots \rangle = \delta_{n_1,n_1'} \delta_{n_2,n_2'} \cdots \tag{4.82}$$

showing that two occupation number states are orthogonal unless they have exactly the same set of occupation numbers, and a completeness relation

$$\sum_{\{n_\nu\}} |n_1, n_2, \ldots\rangle\langle n_1, n_2, \ldots| = 1 \tag{4.83}$$

for the symmetric space, where the sum is over all sets of occupation numbers consistent with the constraint $\sum_\nu n_\nu = N$. We note in passing that the number operators $\{N_\nu\}$ form a complete set of commuting observables (CSCO) for this symmetric subspace, since each basis vector in this occupation number representation is uniquely labeled by the associated set of eigenvalues.

Construction of the occupation number representation for the antisymmetric space of N identical fermions is similar, but some important differences arise. In particular, we note first that the projection onto $S_A^{(N)}$ of any basis vector $|\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle$ of $S_S^{(N)}$ having more than one particle in any given single particle state vanishes, since the corresponding Slater determinant (4.74) will have repeated rows. Thus most of the basis states of $S^{(N)}$ have no physical counterpart in the antisymmetric subspace. (In this sense, threfore, fermionic spaces are always smaller than bosonic spaces.) In general, only those direct product states $|\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle$ with each particle in a distinct single-particle state $\phi_{\nu_1}, \ldots, \phi_{\nu_N}$ will have a non-vanishing projection $P_A|\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle$ onto $S_A^{(N)}$. In that case, the projection of the $N!$ linearly independent states $U_\xi|\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle$ characterized by the same set $\{n_\nu\}$ of occupation numbers (which will now all be 0's or 1's) will take the form $P_A P_\xi|\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle$. But this product of operators can also be simplified, i.e.,

$$\begin{aligned} P_A U_\xi &= \frac{1}{N!}\sum_{\xi'} \varepsilon_{\xi'} U_{\xi'} U_\xi = \frac{\varepsilon_\xi}{N!}\sum_{\xi'} \varepsilon_{\xi'}\varepsilon_\xi U_{\xi'} U_\xi \\ &= \varepsilon_\xi \left[\frac{1}{N!}\sum_{\xi''} \varepsilon_{\xi''} U_{\xi''}\right] = \varepsilon_\xi P_A \end{aligned} \tag{4.84}$$

where we have used the group properties of the permutation operators and the identity $\varepsilon_\xi^2 = 1$. Thus, we find that

$$P_A U_\xi |\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle = \varepsilon_\xi P_A |\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle = \pm P_A |\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle. \tag{4.85}$$

Thus, the even permutations project onto the vector $P_A|\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle$ and the odd permutations onto its negative $-P_A|\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle$. Of course, although these two states differ by a phase factor of unit modulus ($-1 = e^{i\pi}$), they represent precisely the same *physical state* in Hilbert space. Thus, with a suitable phase convention, we find that all of the basis vectors associated with a given acceptable set $\{n_\nu\}$of occupation numbers project onto the same basis vector of $S_A^{(N)}$, and so are uniquely labeled by the occupation numbers that

characterize them. Thus, the number operators $\{N_\nu\}$ form a complete set of commuting observables (CSCO) for the antisymmetric subspace, as well. We thus denote by

$$|n_1, n_2, \ldots\rangle = \frac{P_A|\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle}{||P_A|\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle||} \tag{4.86}$$

the antisymmetric state of N identical fermions containing n_1 particles in state ϕ_1, n_2 particles in state ϕ_2, and so on, where all $n_\nu \in \{0, 1\}$, and where $\sum_\nu n_\nu = N$. To unambiguously fix the phase of the associated occupation number basis state $|n_1, n_2, \ldots\rangle$, we note that of all the $N!$ states $\left\{U_\xi|\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle\right\}$ associated with the same set of occupation numbers $\{n_\nu\}$, only one of them has the occupied states ordered so that the first particle is in the lowest occupied state, the second is in the next-to-lowest occupied state, and so on. It is this state (or any even permutation thereof) that we project onto $S_A^{(N)}$ to produce the basis state. Thus $|n_1, n_2, \ldots\rangle$ is identified with the normalized antisymmetric projection of that state $|\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle$ that has the correct set of occupation numbers and for which

$$\nu_1 < \nu_2 < \cdots < \nu_N. \tag{4.87}$$

Another way of putting it is that we identify the basis state $|n_1, n_2, \ldots\rangle$ with that Slater determinant (4.74) in which the indices ν_α of the single particle states are strictly increasing in going from the top row to the bottom row.

For this set of states, we can write completeness and orthonormality relations essentially identical to those that we wrote for the occupation number representation of the bosonic subspace, except for the restriction on the allowed set of occupation numbers to those for which $n_\nu \in \{0, 1\}$.

4.4.3 Evolution and Observables of a System of Identical Particles

The state vector $|\psi(t)\rangle$ describing a collection of identical bosons or fermions, if it is to continue to describe such a system for all times, must remain within the bosonic or fermionic space in which it starts. What does this imply about the structure of the corresponding Hamiltonian and of the observables for such a system? To address this question we note that, as for any quantum system, evolution of the state vector is governed by Schrödinger's equation

$$i\hbar\frac{d}{dt}|\psi(t)\rangle = H|\psi(t)\rangle \tag{4.88}$$

where H is the Hamiltonian governing the many-particle system. Now the state vector of a collection of bosons must remain symmetric under the exchange of any two particles in the system, and the state vector of a collection of identical fermions must remain antisymmetric under any such exchange. Thus, we can write that, for all times t,

$$U_{\alpha\beta}|\psi(t)\rangle = \lambda|\psi(t)\rangle \tag{4.89}$$

where $\lambda = +1$ for bosons and -1 for fermions. Applying $U_{\alpha\beta}$ to the evolution equation we determine that

$$\begin{aligned} i\hbar\lambda\frac{d}{dt}|\psi(t)\rangle &= U_{\alpha\beta}H|\psi(t)\rangle \\ &= \lambda U_{\alpha\beta}HU_{\alpha\beta}^+|\psi(t)\rangle \end{aligned} \tag{4.90}$$

where we have inserted a factor of $1 = U_{\alpha\beta}^+U_{\alpha\beta}$ between H and the state vector. Canceling the common factor of λ, and comparing the result to the original evolution equation we find that

$$i\hbar\frac{d}{dt}|\psi(t)\rangle = U_{\alpha\beta}HU_{\alpha\beta}^+|\psi(t)\rangle = H|\psi(t)\rangle \tag{4.91}$$

which is satisfied provided that

$$H = U_{\alpha\beta} H U_{\alpha\beta}^{+}. \tag{4.92}$$

This shows that H, if it is to preserve the exchange symmetry of the state vector, must be invariant under the unitary transformations that exchange particles in the system. An *operator* A is said to be symmetric under the exchange of particles α and β if $U_{\alpha\beta} A U_{\alpha\beta}^{+} = A$ and is said to be antisymmetric under exchange if $U_{\alpha\beta} A U_{\alpha\beta}^{+} = -A$. Using this terminology, we see that the Hamiltonian of a collection of identical bosons or fermions must be symmetric under all particle exchanges in the system. Another way of expressing the same thing is obtained by multiplying (4.92) through on the right by $U_{\alpha\beta}$ to obtain the result $HU_{\alpha\beta} = U_{\alpha\beta} H$, or,

$$[U_{\alpha\beta}, H] = 0 \tag{4.93}$$

Thus, any operator that is symmetric under particle exchange commutes with the exchange operators. If H commutes with all of the exchange operators, then it commutes with any product of exchange operators, i.e., with any permutation operator U_ξ, thus

$$[U_\xi, H] = 0. \tag{4.94}$$

Since the projectors P_S and P_A onto the bosonic and fermionic subspaces are linear combinations of permutation operators, they must also commute with H, i.e.,

$$[P_S, H] = 0 = [P_A, H]\,. \tag{4.95}$$

From the basic theorems that we derived for commuting observables, it follows that the eigenspaces of P_S and P_A, in particular, the subspaces $S_S^{(N)}$ and $S_A^{(N)}$, must be *globally-invariant* under the action of the Hamiltonian H. In other words, H connects no state inside either subspace to any state lying outside the subspace in which it is contained. Indeed, this is the way that H keeps the state vector inside the relevant subspace. It follows, for example, that if the symmetric and antisymmetric projectors commute with the Hamiltonian at each instant, then they also commute with the evolution operator $U(t, t_0)$ which can be expressed as a function of the Hamiltonian. This means, e.g., that if $|\psi(t_0)\rangle$ is some arbitrary initial state vector lying in $S^{(N)}$ which evolves into the state $|\psi(t)\rangle = U(t, t_0)|\psi(t_0)\rangle$, then the projection of $|\psi(t)\rangle$ onto the symmetric subspace can be written

$$|\psi_S(t)\rangle = P_S|\psi(t)\rangle = P_S U(t, t_0)|\psi(t_0)\rangle = U(t, t_0) P_S|\psi(t_0)\rangle = U(t, t_0)|\psi_S(t_0)\rangle \tag{4.96}$$

and the projection onto the antisymmetric space can be written

$$|\psi_A(t)\rangle = P_A|\psi(t)\rangle = P_A U(t, t_0)|\psi(t_0)\rangle = U(t, t_0) P_A|\psi(t_0)\rangle = U(t, t_0)|\psi_A(t_0)\rangle \tag{4.97}$$

which shows that we can project an arbitrary initial state first to get an initial state vector with the right symmetry, and then evolve within the subspace, or simply evolve the arbitrary initial state and project at the end of the evolution process to get the state that evolves out of the appropriate projection of the initial state.

The fact that the Hamiltonian commutes with P_S and P_A also means that there exists an orthonormal basis of energy eigenstates spanning each of the two subspaces of interest. This also makes sense from the point of view of the measurement process. If this were not the case, then an arbitrary state in either subspace would have to be represented as a linear combination of energy eigenstates some of which lie outside (or have components that lie outside) the subspace of interest. An energy measurement would then have a nonzero probability of collapsing the system onto one of these inadmissible

energy eigenstates, i.e., onto a state that is not physically capable of describing a collection of identical particles, since it lies outside the relevant subspace.

Clearly, arguments of this sort based upon what can happen during a measurement process must apply as well to *any observable* of a system of identical particles. That is, in order for a measurement of an observable A not leave the system in an inadmissible state, it must have a complete set of eigenstates spanning the relevant subspace, and must, therefore, be symmetric under all particle exchanges.

So what kind of operators are, in fact, symmetric under all particle exchanges? As we have seen, the number operators $\{N_\nu\}$ associated with a given direct product representation of $S^{(N)}$ have the property that they count the number of particles in any given single particle state, but are completely insensitive to which particles are in which state. Indeed, if the state $|\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle$ is characterized by a given set of occupation numbers $\{n_\nu\}$ (i.e., is an eigenstate of the number operators $\{N_\nu\}$ with a particular set of eigenvalues) then so is any state $U_\xi|\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle$ obtained from this one by a permutation of the particles. In other words, it follows that if

$$N_\nu|\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle = n_\nu|\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle \tag{4.98}$$

then

$$\begin{aligned} N_\nu\left[U_\xi|\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle\right] &= n_\nu\left[U_\xi|\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle\right] \\ &= U_\xi N_\nu|\phi_{\nu_1}, \ldots, \phi_{\nu_N}\rangle. \end{aligned} \tag{4.99}$$

Since this holds for each vector of the basis set, it follows that $N_\nu U_\xi = U_\xi N_\nu$, hence

$$[U_\xi, N_\nu] = 0, \tag{4.100}$$

which implies that

$$[P_S, N_\nu] = 0 = [P_A, N_\nu]\,. \tag{4.101}$$

Indeed, the number operators form a CSCO for the two subspaces of interest, and clearly have a complete ONB of eigenvectors (i.e., the occupation number states) spanning each subspace. It follows that any observable that can be expressed as a function of the number operators will also be symmetric under all particle exchanges.

It is also possible to form suitable observables as appropriate linear combinations of single-particle operators. To see how this comes about, consider as a specific example, a system of two particles, each of which we can associate with a position operator $\vec{R}_1$ and $\vec{R}_2$ whose eigenstates in the two particle space S^2 are the direct product position states $\{|\vec{r}_1, \vec{r}_2\rangle\}$ and have the property that

$$\vec{R}_1|\vec{r}_1, \vec{r}_2\rangle = \vec{r}_1|\vec{r}_1, \vec{r}_2\rangle \qquad \vec{R}_2|\vec{r}_1, \vec{r}_2\rangle = \vec{r}_2|\vec{r}_1, \vec{r}_2\rangle \tag{4.102}$$

To see what happens under particle exchange, consider the operator

$$U_{21}\vec{R}_1U_{21} = U_{21}\vec{R}_1U_{21}^+, \tag{4.103}$$

where $U_{21} = U_{21}^+$ exchanges particles 1 and 2. Thus, we find that

$$\begin{aligned} U_{21}\vec{R}_1U_{21}|\vec{r}_1, \vec{r}_2\rangle &= U_{21}\vec{R}_1|\vec{r}_2, \vec{r}_1\rangle = U_{21}\vec{r}_2|\vec{r}_2, \vec{r}_1\rangle \\ &= \vec{r}_2|\vec{r}_1, \vec{r}_2\rangle = \vec{R}_2|\vec{r}_1, \vec{r}_2\rangle \end{aligned} \tag{4.104}$$

Thus, as we might have anticipated,

$$U_{21}\vec{R}_1U_{21}^+ = \vec{R}_2. \tag{4.105}$$

More generally, in a system of N particles if B_α is a single-particle operator associated with particle α, then its transform under $U_{\alpha\beta}$

$$U_{\alpha\beta} B_\alpha U_{\alpha\beta}^+ = B_\beta \tag{4.106}$$

is the corresponding operator for particle β. In this light, any symmetric combination of operators such as $\vec{R}_\alpha + \vec{R}_\beta$ is readily verified to be symmetric under the associated particle exchange, i.e.,

$$U_{\alpha\beta} \left(\vec{R}_\alpha + \vec{R}_\beta \right) U_{\alpha\beta}^+ = \vec{R}_\beta + \vec{R}_\alpha \tag{4.107}$$

whereas any antisymmetric combination, such as that related to the relative displacement of two particles is antisymmetric, since

$$U_{\alpha\beta} \left(\vec{R}_\alpha - \vec{R}_\beta \right) U_{\alpha\beta}^+ = \vec{R}_\beta - \vec{R}_\alpha = - \left(\vec{R}_\alpha - \vec{R}_\beta \right). \tag{4.108}$$

On the other hand, the relative distance between the particles $\left| \vec{R}_\beta - \vec{R}_\alpha \right|$, being an even function of the $\vec{R}_\beta - \vec{R}_\alpha$ is symmetric. Thus any function of a symmetric operator is symmetric, while an even function of antisymmetric operators is also symmetric.

Extending this to a system of N particles, any observable of a system of identical particles must be symmetric under all particle exchanges and permutations. This would include, e.g., any complete sum

$$B = \sum_{\alpha=1}^{N} B_\alpha \tag{4.109}$$

of the corresponding single particle operators for each particle in the system. Examples of operators of this type include the location of the center of mass

$$\vec{R} = \frac{1}{N} \sum_{\alpha=1}^{N} \vec{R}_\alpha \tag{4.110}$$

(recall that all the particles are assumed identical, so the masses are all the same), and the total linear and angular momentum

$$\vec{P} = \sum_{\alpha=1}^{N} \vec{P}_\alpha \qquad\qquad \vec{L} = \sum_{\alpha=1}^{N} \vec{L}_\alpha. \tag{4.111}$$

As we have seen, a system of noninteracting particles has a Hamiltonian that is of precisely this type, i.e.,

$$H = \sum_{\alpha=1}^{N} H_\alpha \tag{4.112}$$

where, e.g.,

$$H_\alpha = \frac{P_\alpha^2}{2m} + V(R_\alpha). \tag{4.113}$$

Actually, although we have constructed these operators as symmetric linear combinations of single-particle operators, it is easy to show that any operator of this type can also represented in terms of the number operators associated with a particular occupation number representation. Suppose, e.g., that the single-particle states $|\phi_\nu\rangle^{(\alpha)}$ are eigenstates of the single-particle operator B_α with eigenvalues b_ν. Thus, e.g., $B_\alpha |\phi_\nu\rangle^{(\alpha)} = b_\nu |\phi_\nu\rangle^{(\alpha)}$.

Then the direct product states formed from this set will be simultaneous eigenstates of the all the related operators B_α,

$$B_\alpha|\phi_{\nu_1},\ldots,\phi_{\nu_\alpha},\ldots,\phi_{\nu_N}\rangle = b_{\nu_\alpha}|\phi_{\nu_1},\ldots,\phi_{\nu_\alpha},\ldots,\phi_{\nu_N}\rangle \tag{4.114}$$

and so will be an eigenstate of the symmetric operator $B = \sum_\alpha B_\alpha$, i.e.,

$$\begin{aligned} B|\phi_{\nu_1},\ldots,\phi_{\nu_N}\rangle &= \sum_\alpha B_\alpha|\phi_{\nu_1},\ldots,\phi_{\nu_N}\rangle = \sum_\alpha b_{\nu_\alpha}|\phi_{\nu_1},\ldots,\phi_{\nu_\alpha},\ldots,\phi_{\nu_N}\rangle \\ &= b|\phi_{\nu_1},\ldots,\phi_{\nu_\alpha},\ldots,\phi_{\nu_N}\rangle \end{aligned} \tag{4.115}$$

where the collective eigenvalue b is the sum of the individual single-particle eigenvalues

$$b = \sum_{\alpha=1}^{N} b_{\nu_\alpha} = \sum_{\alpha=1}^{N}\sum_\nu b_\nu \delta_{\nu,\nu_\alpha} = \sum_\nu b_\nu n_\nu \tag{4.116}$$

where we have reexpressed the sum over the particle index α by a sum over the state index ν, and collected all the eigenvalues associated with the n_ν particles in the same single-particle state ϕ_ν together. Thus we can reexpress the eigenvalue equation above as

$$\begin{aligned} B|\phi_{\nu_1},\ldots,\phi_{\nu_N}\rangle &= \sum_\nu b_\nu n_\nu|\phi_{\nu_1},\ldots,\phi_{\nu_N}\rangle \\ &= \sum_\nu b_\nu N_\nu|\phi_{\nu_1},\ldots,\phi_{\nu_N}\rangle \end{aligned} \tag{4.117}$$

and, through a simple process of identification, reexpress the operator B in the form

$$B = \sum_\nu b_\nu N_\nu. \tag{4.118}$$

Thus, e.g., the noninteracting particle Hamiltonian above can be expressed in terms of the single particle energy eigenstates $|\phi_\nu\rangle$ obeying the equation $H_\alpha|\phi_\nu\rangle = \varepsilon_\nu|\phi_\nu\rangle$ in the form

$$H = \sum_\nu \varepsilon_\nu N_\nu. \tag{4.119}$$

There is a real sense in which this way of expressing the Hamiltonian is to be preferred over the earlier form, particularly when we are dealing with identical particles. The operators N_ν are not labeled by particle numbers, but by the single-particle states that can be occupied or not. Thus in expressing the Hamiltonian in this fashion, we are not using a notation that suggests (erroneously!) that we can actually label the individual particles in the system, unlike, e.g., (4.112), which explicitly includes particle labels as well as the number of particles in the system. The operator (4.119), on the other hand , makes no explicit reference either to particle labels or to the number of particles in the system, and therefore has exactly the same form in any of the spaces $S^{(N)}$ associated with any number $N = 1, 2, \cdots$ of identical particles.

Operators of this type, which can be expressed as a sum of single-particle operators, or equivalently, as a simple linear function of the number operators associated with a particular occupation number representation, we will refer to as one-body operators, since they really depend only on single-particle properties. In addition to these, there are also operators that depend upon multiple-particle properties. For example, interactions between particles are often represented by "two-body" operators of the form

$$V_{\rm int} = \frac{1}{2}\sum_{\substack{\alpha,\beta \\ \alpha\neq\beta}} V(\vec{R}_\alpha - \vec{R}_\beta) \tag{4.120}$$

which is a symmetrized sum of operators that each depend upon the properties of just two particles. It turns out that operators of this type can usually be expressed as a simple bilinear function of the number operators associated with *some* set of single-particle states. Typically, however, the Hamiltonian contains both one-body and two-body parts, and the representation in which the one-body part is expressible in the form (4.119) is not one in which the two-body part is expressible as a simple function of the number operators. Conversely, a representation in which the interactions are expressible in terms of number operators is not one in which the one-body part is, also. The reason for this is that, typically, the interactions induce *transitions* between single-particle eigenstates, i.e., they take particles out of the single-particle states that they occupy and place them back into other single particle states. In the process, they *change* the occupation numbers characterizing the state of the system. It is useful, therefore, to define operators that are capable of inducing transitions of this type.

We have, in a sense, already encountered operators that do this sort of thing in our study of the harmonic oscillator. The energy eigenstates $\{|n\rangle\}$of the 1D harmonic oscillator are each characterized by an integer $n \in \{0, 1, 2, \cdots\}$ that can be viewed as an "occupation number" characterizing the number of vibrational quanta (now considered as a kind of "particle") in the system. The annihilation, creation, and number operators a, a^+, and $N = a^+a$ decrease, increase, and count the number of these quanta.

In the 3D harmonic isotropic oscillator, which is separable in Cartesian coordinates, the energy eigenstates $\{|n_x, n_y, n_z\rangle\}$ are characterized by a set of three occupation numbers $\{n_\nu \,|\nu = 1, 2, 3\}$ characterizing the number of vibrational quanta associated with each Cartesian degree of freedom, and there are a set of annihilation, creation, and number operators a_ν, a_ν^+, and N_ν for each axis. The different annihilation and creation operators obey characteristic commutation relations

$$[a_\nu, a_{\nu'}] = 0 = \left[a_\nu^+, a_{\nu'}^+\right] \tag{4.121}$$

$$\left[a_\nu, a_{\nu'}^+\right] = \delta_{\nu,\nu'} \tag{4.122}$$

that, as we have seen, completely determine the associated integer spectrum of the number operators $N_\nu = a_\nu^+ a_\nu$.

Within this context, we now note that product operators of the form $a_x^+ a_y$ have the effect

$$a_x^+ a_y \{|n_x, n_y, n_z\rangle\} = \sqrt{n_x + 1}\sqrt{n_y}\,\{|n_x + 1, n_y - 1, n_z\rangle\} \tag{4.123}$$

of transferring a quantum of vibrational excitation from one axis to another, i.e., of inducing transitions in the states of the quanta. It is precisely operators of this type, that are capable of creating, destroying, and counting material particles in different single particle states that we wish to define for a collection of identical particles.

In order to carry this plan out, however, we need to realize that these creation and annhilation operators have the effect of taking the system out of the space of N-particles, and into a space containing $N+1$, or $N-1$ particles. Thus, we need to expand our space in a way that allows us to put together, in the same space, states of the system containing *different* particle numbers. The mathematical procedure for doing this is to combine the different N-particle spaces together in what is referred to as a *direct sum* of vector spaces which is, in a way, similar to that associated with the direct product of vector spaces that we have already encountered.. The definition and details associated with this procedure are explored in the next section.

4.4.4 Fock Space as a Direct Sum of Vector Spaces

The idea of expressing a vector space as a sum of smaller vector spaces is actually implicitly contained in some of the concepts that we have already encountered. Consider, e.g., an

arbitrary observable A of a linear vector space S. By definition, the observable A possesses a complete orthonormal basis $\{|a,\tau\rangle\}$ of eigenstates spanning the space. The eigenstates associated with a particular eigenvalue a form a subspace S_a of S, the vectors of which are orthogonal to the vectors in any of the other eigenspaces of A. Also, any vector $|\psi\rangle$ in S can be written as a linear combination of vectors taken from each of the orthogonal subspaces S_a, i.e.,

$$|\psi\rangle = \sum_a |\psi_a\rangle \tag{4.124}$$

where

$$|\psi_a\rangle = \sum_\tau \psi_{a,\tau}|a,\tau\rangle = P_a|\psi\rangle. \tag{4.125}$$

Under these circumstances, we say that the space S can be decomposed into a **direct sum** of the eigenspaces associated with the observable A, and symbolically represent this decomposition in the form

$$S = S_a \oplus S_{a'} \oplus S_{a''} \oplus \cdots \tag{4.126}$$

The vector space S has a dimension equal to the sum of the dimensions of all the eigenspaces S_a, as can be seen by counting up the basis vectors needed to span each orthogonal subspace.

This idea of decomposing larger spaces into direct sums of smaller spaces can be reversed. Thus, given two separate vector spaces S_1 and S_2 of dimension N_1 and N_2, respectively, defined on the same field of scalars, we produce a larger vector space S of dimension $N = N_1 + N_2$ as the direct sum

$$S = S_1 \oplus S_2. \tag{4.127}$$

The space S then contains, by definition, all vectors in S_1, all vectors in S_2, and all possible linear combinations of the vectors in S_1 and S_2 (the latter two spaces now being relegated to the role of orthogonal subspaces of S), with each vector in S_1 orthogonal, by construction, to each vector in S_2.

It is this procedure that we carry out with the different N-particle spaces associated with a collection of identical particles. In particular, we define the **Fock Space** of a collection of identical bosons or fermions, respectively, as the space obtained by forming the direct sum of the corresponding spaces describing $N = 0, 1, 2, \cdots$ particles. In particular, the Fock space of a set of identical bosons is written as the direct sum

$$S_S = S_S^0 \oplus S_S^1 \oplus S_S^2 \oplus S_S^3 \oplus \cdots \tag{4.128}$$

of the symmetric spaces $S_S^{(N)}$ for each possible value of N. The space S_S^0 of zero particles is assumed to contain exactly one linearly-independent basis vector, referred to as **the vacuum** and denoted by $|0\rangle$, and vectors from different N-particle spaces are assumed to be automatically orthogonal to each other.

Similarly, the Fock space associated with a collection of identical fermions is written as the direct sum

$$S_A = S_A^0 \oplus S_A^1 \oplus S_A^2 \oplus S_A^3 \oplus \cdots \tag{4.129}$$

of the antisymmetric spaces $S_S^{(N)}$ for each value of N, where, again, the space of zero particles contains one basis vector, the vacuum, denoted by $|0\rangle$, and the different N-particle subspaces are assumed orthogonal. In what follows we explore separately the different structure of the bosonic and fermionic Fock spaces.

4.4.5 The Fock Space of Identical Bosons

As we have seen, the symmetric occupation number states

$$|n_1, n_2, \ldots\rangle \qquad \sum_\nu n_\nu = N \tag{4.130}$$

associated with a given set of single-particle states $|\phi_\nu\rangle$ forms an ONB for the space $S_S^{(N)}$ of N identical bosons. The collection of such states, therefore, with no restriction on the sum of the occupation numbers, forms a basis for the Fock space S_S of a set of identical bosons. In particular, the vacuum state is associated, in this (and any) occupation number representation with the vector

$$|0\rangle = |0, 0, \ldots\rangle \tag{4.131}$$

in which $n_\nu = 0$ for all single particle states ϕ_ν. The single-particle states $|\phi_\nu\rangle$ themselves can be expressed in this representation in the form

$$\begin{aligned} |\phi_1\rangle &= |1, 0, 0, \ldots\rangle \\ |\phi_2\rangle &= |0, 1, 0, \ldots\rangle \\ &\vdots \end{aligned} \tag{4.132}$$

and so on. These basis states of Fock space are all simultaneous eigenvectors of the number operators N_ν associated with this set of single particle states, and are uniquely labeled by the associated set of occupation number $\{n_\nu\}$. Thus, the operators $\{N_\nu\}$ form a CSCO for Fock space, just as they do for each of the symmetric N-particle subspaces $S_S^{(N)}$. Thus, we can write a completeness relation for this representation of the form

$$\sum_{n_1=0}^{\infty} \sum_{n_2=0}^{\infty} \cdots \; |n_1, n_2, \ldots\rangle\langle n_1, n_2, \ldots| = 1. \tag{4.133}$$

We now wish to introduce operators that change the occupation numbers in a way similar to that associated with the harmonic oscillator. Because we are interested at present in describing bosons we want the spectrum of each number operator N_ν to be exactly the same as for the harmonic oscillator, i.e., $n_\nu \in \{0, 1, 2, \cdots\}$. Thus, we can actually model the bosonic creation and annihilation operators *directly* on those of the oscillator system, i.e., we introduce for each single particle state $|\phi_\nu\rangle$ an annihilation and creation operator, whose action is defined on the occupation number states of this representation such that

$$a_\nu^+ |n_1, \ldots, n_\nu, \ldots\rangle = \sqrt{n_\nu + 1}|n_1, \ldots, n_\nu + 1, \ldots\rangle \tag{4.134}$$

and

$$a_\nu |n_1, \ldots, n_\nu, \ldots\rangle = \sqrt{n_\nu}|n_1, \ldots, n_\nu - 1, \ldots\rangle. \tag{4.135}$$

It follows from this definition, as special cases, that the single-particle state $|\phi_\nu\rangle$ (which lies in the subspace containing just one boson) can be written in a form

$$|\phi_\nu\rangle = a_\nu^+ |0\rangle = a_\nu^+ |0, 0, \ldots\rangle \tag{4.136}$$

in which it is created "from nothing" by the operator a_ν^+. It also follows that any annihilation operator acting on the vacuum

$$a_\nu |0\rangle = 0 \tag{4.137}$$

destroys it, i.e., maps it onto the null vector (not the vacuum!). Thus, the operator a_ν^+ creates a boson in the state ϕ_ν and the operator a_ν removes a boson from that state.

Expressing the same idea in a somewhat more pedestrian fashion, the operators a_ν and a_ν^+ simply connect states in adjacent subspaces $S_S^{(N)}$ of the bosonic Fock space S_S. Consistent with the definitions above, annihilation and creation operators associated with different single particle states commute with one another, allowing us to write the commutation relations for the complete set of such operators in the form

$$[a_\nu, a_{\nu'}] = 0 = \left[a_\nu^+, a_{\nu'}^+\right] \tag{4.138}$$

$$\left[a_\nu, a_{\nu'}^+\right] = \delta_{\nu,\nu'}, \tag{4.139}$$

which are usually referred to as "boson commutation relations". It also follows from the definition given above that

$$a_\nu^+ a_\nu |n_1, \ldots, n_\nu, \ldots\rangle = n_\nu |n_1, \ldots, n_\nu, \ldots\rangle \tag{4.140}$$

which allows us to identify this product of operators with the associated number operator, i.e., $N_\nu = a_\nu^+ a_\nu$, which obey the commutation relations

$$[N_\nu, N_{\nu'}] = 0 \tag{4.141}$$

$$[N_\nu, a_{\nu'}] = -a_\nu \delta_{\nu,\nu'} \qquad \left[N_\nu, a_{\nu'}^+\right] = a_\nu^+ \delta_{\nu,\nu'} \tag{4.142}$$

Finally, just as it is possible to create the single particle state $|\phi_\nu\rangle$ from the vacuum, so it is possible to express any of the occupation number states of this representation in a form in which they are created out of the vacuum by an appropriate product of creation operators, i.e., it is readily verified that

$$|n_1, \ldots, n_\nu, \ldots\rangle = \frac{(a_1^+)^{n_1}(a_2^+)^{n_2}(a_3^+)^{n_3}\cdots}{\sqrt{n_1!}\sqrt{n_2!}\sqrt{n_3!}\cdots}|0\rangle, \tag{4.143}$$

the normalization factors taking the same form, for each single particle state, as in the simple harmonic oscillator.

4.4.6 The Fock Space of Identical Fermions

The construction of the Fock space of a set of identical fermions proceeds in a similar fashion, but some interesting differences arise as a result of the antisymmetric structure of the states associated with this space. For the fermionic space, we know that the antisymmetric occupation number states

$$|n_1, n_2, \ldots\rangle \qquad \sum_\nu n_\nu = N \tag{4.144}$$

generated from a given set of single-particle states $|\phi_\nu\rangle$ forms an ONB for the space $S_S^{(N)}$ of N identical fermions, provided that, as required by the exclusion principle, all occupation numbers only take the values $n_\nu = 0$ or $n_\nu = 1$. Lifting the restriction on the *sum* of the occupation numbers, we obtain a basis for the Fock space S_A of this set of fermions. As in the bosonic case, the vacuum state is associated with the vector

$$|0\rangle = |0, 0, \ldots\rangle \tag{4.145}$$

in which all $n_\nu = 0$, and the single-particle states $|\phi_\nu\rangle$ can be written as

$$\begin{aligned} |\phi_1\rangle &= |1, 0, 0, \ldots\rangle \\ |\phi_2\rangle &= |0, 1, 0, \ldots\rangle \\ &\vdots \end{aligned} \tag{4.146}$$

and so on. These basis states $|n_1, n_2, \ldots\rangle$ of the fermionic Fock space are also simultaneous eigenvectors of the operators N_ν, and are uniquely labeled by their occupation numbers $\{n_\nu\}$. Thus, the operators $\{N_\nu\}$ form a CSCO for the fermionic Fock space as well. The completeness relation differs from that of the bosonic space only by the limits on the summations involved, i.e.,

$$\sum_{n_1=0}^{1}\sum_{n_2=0}^{1}\cdots\ |n_1, n_2, \ldots\rangle\langle n_1, n_2, \ldots| = 1. \tag{4.147}$$

As in the bosonic case, we now wish to introduce operators that change the occupation numbers. Clearly, however, we cannot model the fermion annihilation and creation operators directly on those of the harmonic oscillator, since to do so would result in a fermion number spectrum inappropriately identical to that of the bosons. In the fermion case we require that the number operator have eigenvalues restricted to the set $\{0, 1\}$.

It is a remarkable fact that a very slight modification to the commutation relations associated with the annihilation and creation operators of the harmonic oscillator yield a set of operators that have precisely the properties that we need. To partially motivate this modification we note that the commutator $[A, B]$ of two operators simply gives, if it is known, a rule or prescription for reversing the order of a product of these two operators whenever it is convenient to do so. Thus if we know the operator $[A, B]$ then we can replace the operator AB wherever it appears with the operator $BA + [A, B]$. Any rule that allows us to perform a similar reversal would serve the same purpose. For example, it sometimes occurs that the **anticommutator** $\{A, B\}$ of two operators, defined as the *sum*

$$\{A, B\} = AB + BA \tag{4.148}$$

rather than the difference of the operator product taken in each order, is actually a simpler operator than the commutator. Under these circumstances, we can use the anticommutator to replace AB whenever it occurs with the operator $-BA + \{A, B\}$.

With this in mind, we now consider an operator a and its adjoint a^+ which obey *anticommutation* relations that have the same structure as the *commutation* relations of those associated with the harmonic oscillator, i.e., suppose that

$$\{a, a\} = 0 = \left\{a^+, a^+\right\} \tag{4.149}$$

$$\left\{a, a^+\right\} = 1. \tag{4.150}$$

Let us also define, as in the oscillator case, the positive operator $N = a^+a$ and let us assume that N has at least one nonzero eigenvector $|\nu\rangle$, square normalized to unity, with eigenvalue ν, i.e., $N|\nu\rangle = \nu|\nu\rangle$. The following statements are then easily shown:

1. $a^2 = 0 = (a^+)^2$
2. $aa^+ = 1 - N$
3. Spectrum$(N) = \{0, 1\}$
4. If $\nu = 0$, then $a|0\rangle = 0$ and $a^+|0\rangle = |1\rangle$, i.e., $a^+|0\rangle$ is a square normalized eigenvector of N with eigenvalue 1.
5. If $\nu = 1$, then $a^+|1\rangle = 0$ and $a|1\rangle = |0\rangle$, i.e., $a|1\rangle$ is a square normalized eigenvector of N with eigenvalue 0.

The first item follows directly upon expanding the anticommutation relations $\{a, a\} = 0 = \{a^+, a^+\}$. The second item follows from the last anticommutation relation $\{a, a^+\} = aa^+ + a^+a = 1$, which implies that $aa^+ = 1 - a^+a = 1 - N$. To show that the spectrum can only contain the values 0 an 1, we multiply the relation $aa^+ + a^+a = 1$ by $N = a^+a$ and use the fact that $aa = 0$ to obtain $N^2 = N$, which implies that N is a projection operator and so can only have the eigenvalues specified . To show that both of these actually occur, we prove the last two items, which together show that if one of the eigenvalues occurs in the spectrum of N then so does the other. These statements follow from the following observations

$$||a|0\rangle||^2 = \langle 0|a^+a|0\rangle = \langle 0|N|0\rangle = 0 \tag{4.151}$$

$$||a^+|0\rangle||^2 = \langle 0|aa^+|0\rangle = \langle 0|\,(1-N)\,|0\rangle = \langle 0|0\rangle = 1 \tag{4.152}$$

$$\begin{aligned} Na^+|0\rangle &= a^+aa^+|0\rangle = a^+\,(1-N)\,|0\rangle \\ &= a^+|0\rangle \end{aligned} \tag{4.153}$$

which prove the fourth item, and

$$||a^+|1\rangle||^2 = \langle 1|aa^+|1\rangle = \langle 1|\,(1-N)\,|1\rangle = 0 \tag{4.154}$$

$$||a|1\rangle||^2 = \langle 1|a^+a|1\rangle = \langle 1|N|1\rangle = \langle 1|1\rangle = 1 \tag{4.155}$$

$$Na|1\rangle = a^+aa|1\rangle = 0 \tag{4.156}$$

which proves the final item.

It should be clear that operators of this type have precisely the properties we require for creating and destroying fermions, since they only allow for occupation numbers of 0 and 1. We thus define, for the fermion Fock space, a complete set of annihilation, creation, and number operators a_ν, a_ν^+, and $N_\nu = a_\nu^+ a_\nu$ that remove, create, and count fermions in the single particle states $|\phi_\nu\rangle$. To define these operators completely, we need to specify the commutation properties obeyed by annihilation and creation operators associated with different single particle states. It turns out the antisymmetry of the states in this space under particle exchange require that operators associated with different states *anticommute*, so that, collectively, the operators associated with this occupation number representation obey the following **fermion commutation relations**

$$\begin{aligned} \{a_\nu, a_{\nu'}\} = 0 = \left\{a_\nu^+, a_{\nu'}^+\right\} \\ \left\{a_\nu, a_{\nu'}^+\right\} = \delta_{\nu,\nu'}, \end{aligned} \tag{4.157}$$

which are just like those for bosons, except for replacement of the commutator bracket with the anticommutator bracket. It is importnat to emphasize that, according to these defintions, operators associated with different single-particle states do not commute, they anticommute, which means for example that

$$a_\nu^+ a_{\nu'}^+ = -a_{\nu'}^+ a_\nu^+. \tag{4.158}$$

Thus, the order in which particles are created in or removed from various states makes a difference. This reversal of sign is reminiscent of, and stems from the same source, as the sign change that occurs when different direct product states in $S^{(N)}$ are projected into the anti-symmetric subspace, i..e., it arises from the antisymmetry exhibited by the states under particle exchange.

The action of these fermion annihilation and creation operators on the vacuum is essentially the same as for the boson operators, i.e.,

$$a_\nu^+|0\rangle = |\phi_\nu\rangle \qquad\qquad a_\nu|0\rangle = 0, \tag{4.159}$$

and in a similar fashion we can represent an arbitrary occupation number state of this representation in terms of the vacuum state through the expression

$$|n_1, \ldots, n_\nu, \ldots\rangle = (a_1^+)^{n_1}(a_2^+)^{n_2}(a_3^+)^{n_3}\cdots|0\rangle. \tag{4.160}$$

Note that normalization factors are not necessary in this expression, since all the occupation numbers are equal to either 0 or 1. Also, the order of the creation operators in the expression is important, with higher occupied states (states with large values of ν) filled first, since the creation operators for such states are closer to the vacuum state being acted upon than those with lower indices. This way of representing the occupation number state $|n_1, \ldots, n_\nu, \ldots\rangle$ as an ordered array of creation operators acting on the vacuum is often referred to as **standard form**.

When an annihilation or creation operator acts upon an arbitrary occupation number state the result depends upon the whether the corresponding single particle states is already occupied, as well as on the number and kind of single particle states already occupied. Specifically, it follows from the anticommutation relations above that

$$a_\nu|n_1, \ldots, n_\nu, \ldots\rangle = \begin{cases} 0 & \text{if } n_\nu = 0 \\ (-1)^m\,|n_1, \ldots, n_\nu - 1, \ldots\rangle & \text{if } n_\nu = 1 \end{cases} \tag{4.161}$$

and

$$a_\nu^+|n_1, \ldots, n_\nu, \ldots\rangle = \begin{cases} (-1)^m\,|n_1, \ldots, n_\nu + 1, \ldots\rangle & \text{if } n_\nu = 0 \\ 0 & \text{if } n_\nu = 1 \end{cases} \tag{4.162}$$

where

$$m = \sum_{\nu'<\nu} n_{\nu'} \tag{4.163}$$

are the number of states with $\nu' < \nu$ already occupied. The phase factors $(-1)^m$ are easily proven using the anticommutation relations. For example, the action of a_ν^+ on the state $|n_1, \ldots, n_\nu, \ldots\rangle$ can be determined by expressing the latter in standard form, and then anticommuting the creation operator through those with indices less than ν until it is sitting in its standard position. Each anticommutation past another creation operator generates a factor of -1, since $a_\nu^+ a_{\nu'}^+ = -a_{\nu'}^+ a_\nu^+$. The product of all these factors gives -1 raised to the power $m = \sum_{\nu'<\nu} n_{\nu'}$.

It is worth noting that, although the fermion creation and annihilation operators anticommute, the corresponding number operators $N_\nu = a_\nu^+ a_\nu$, actually *commute* with one another. This follows from the basic definition of these operators in terms of their action on the occupation number states, but is also readily obtained using the anticommutation relations. To see this, consider

$$N_\nu N_{\nu'} = a_\nu^+ a_\nu a_{\nu'}^+ a_{\nu'} \qquad\qquad \text{with } \nu \neq \nu', \tag{4.164}$$

and note that each time $a_{\nu'}^+$ is moved to the left one position it incurs a minus sign. When it moves two positions, all the way to the left, we have a product of two minus signs, so $N_\nu N_{\nu'} = a_{\nu'}^+ a_\nu^+ a_\nu a_{\nu'}$. But now we do the same thing with a_ν, moving it two positions to the left and so find that

$$N_\nu N_{\nu'} = a_{\nu'}^+ a_{\nu'} a_\nu^+ a_\nu = N_{\nu'} N_\nu. \tag{4.165}$$

In a similar fashion, e.g., we deduce, using the anticommutator $a_{\nu'}a_\nu^+ + a_\nu^+ a_{\nu'} = \delta_{\nu,\nu'}$, that

$$\begin{aligned} N_\nu a_{\nu'} &= a_\nu^+ a_\nu a_{\nu'} = -a_\nu^+ a_{\nu'} a_\nu \\ &= a_{\nu'}^+ a_\nu^+ a_{\nu'} - a_\nu \delta_{\nu,\nu'} = a_{\nu'}(N_\nu - \delta_{\nu,\nu'}) \end{aligned} \tag{4.166}$$

which shows that

$$[N_\nu, a_{\nu'}] = -a_{\nu'}\delta_{\nu,\nu'} \tag{4.167}$$

which is the same *commutation* relation as for bosons. In a similar fashion it is readily established that $a_\nu a_{\nu'}^+ = \delta_{\nu\nu'} - a_{\nu'}^+ a_\nu$

$$\begin{aligned} N_\nu a_{\nu'}^+ &= a_\nu^+ a_\nu a_{\nu'}^+ = a_\nu^+(\delta_{\nu\nu'} - a_{\nu'}^+ a_\nu) \\ &= a_{\nu'}^+ \delta_{\nu\nu'} + a_{\nu'}^+ a_\nu^+ a_\nu = a_{\nu'}^+ \delta_{\nu\nu'} + a_{\nu'}^+ N_\nu \end{aligned} \tag{4.168}$$

which shows that

$$\left[N_\nu, a_{\nu'}^+\right] = +a_{\nu'}^+ \delta_{\nu,\nu'} \tag{4.169}$$

also as for bosons.

4.4.7 Observables of a System of Identical Particles Revisited

Having compiled an appropriate set of operators capable of describing transitions between different occupation number states we now reconsider the form that general observables of a system of identical particles take when expressed as operators of Fock space. Recall that the problem that led to our introduction of Fock space was basically that different parts of the same operator (e.g. the Hamiltonian) are expressible as simple functions of number operators in different occupation number representations. The problem is similar to that encountered in simpler quantum mechanical problems where the question often arises as to whether to work in the position representation, the momentum representation, or some other representation altogether. We are thus led to consider how the occupation number representations associated with different sets of single particle states are related to one another.

Recall that any orthonormal basis of single-particle states generates its own occupation number representation. Thus, e.g. an ONB of states $\{|\phi_\nu\rangle \mid \nu = 1, 2, \cdots\}$ generates a representation of states $|n_1, \ldots, n_\nu, \ldots\rangle$ that are expressible in terms of a set of creation, annihilation, and number operators a_ν^+, a_ν, and $N_\nu = a_\nu^+ a_\nu$, while a different ONB of states $\{|\chi_\mu\rangle \mid \mu = 1, 2, \cdots\}$ generates a different representation of states $|\tilde{n}_1, \ldots, \tilde{n}_\mu, \ldots\rangle$, say, expressible in terms of a different set of creation, annihilation, and number operators b_μ^+, b_μ, and $N_\nu = b_\mu^+ b_\mu$. We know, on the other hand, that the two sets of single-particle states are related to one another through a unitary transformation U such that, e.g.,

$$|\phi_\nu\rangle = U|\chi_\nu\rangle \qquad\qquad \nu = 1, 2, \cdots \tag{4.170}$$

with matrix elements

$$U_{\mu\nu} = \langle\chi_\mu|U|\chi_\nu\rangle = \langle\chi_\mu|\phi_\nu\rangle \tag{4.171}$$

that are the inner products of one basis set in terms of the other. This allows us to write, e.g., that

$$|\chi_\mu\rangle = \sum_\nu |\phi_\nu\rangle\langle\phi_\nu|\chi_\mu\rangle = \sum_\nu U_{\mu\nu}^* |\phi_\nu\rangle \tag{4.172}$$

where $U_{\mu\nu}^* = \langle\chi_\mu|\phi_\nu\rangle^* = \langle\phi_\nu|\chi_\mu\rangle$. But we also know that the single-particle states $|\phi_\nu\rangle$ can be expressed in terms of the vacuum state through the relation

$$|\phi_\nu\rangle = a_\nu^+|0\rangle. \tag{4.173}$$

Using this in the expression for $|\chi_\mu\rangle$, we find that

$$\begin{aligned} |\chi_\mu\rangle &= \sum_\nu U^*_{\mu\nu}|\phi_\nu\rangle = \sum_\nu U^*_{\mu\nu} a^+_\nu \, |0\rangle \\ &= b^+_\mu|0\rangle \end{aligned} \tag{4.174}$$

where we have identified the operator

$$b^+_\mu = \sum_\nu U^*_{\mu\nu} a^+_\nu \tag{4.175}$$

that creates $|\chi_\mu\rangle$ out of the vacuum. The adjoint of this relation gives the corresponding annihilation operator

$$b_\mu = \sum_\nu U_{\mu\nu} a_\nu. \tag{4.176}$$

Thus the annihilation/creation operators of one occupation number representation are linear combinations of the annihilation/creation operators associated with any other occupation number representation, with the coefficients being the matrix elements of the unitary transformation connecting the two sets of single particle states involved. It is straightforward to show that this unitary transformation of annihilation and creation operators preserves the boson or fermion commuation relation that must be obeyed for each type of particle. To treat both types of particles simultaneously, we introduce the notation $[A, B]_\pm = AB \pm BA$, where the minus sign stands for the commutator (and applies to boson operators) and the plus sign stands for the anticommutator (which applies to fermion operators). Thus, if the operators a_ν and a^+_ν obey the relations

$$\begin{aligned} [a_\nu, a_{\nu'}]_\pm = 0 = \left[a^+_\nu, a^+_{\nu'}\right] \\ \left[a_\nu, a^+_{\nu'}\right]_\pm = \delta_{\nu,\nu'} \end{aligned} \tag{4.177}$$

Then, using the transformation law we can calculate the corresponding relation for the operators b_μ and b^+_μ. Thus, e.g.,

$$\begin{aligned} [b_\mu, b_{\mu'}]_\pm &= b_\mu b_{\mu'} \pm b_{\mu'} b_\mu \\ &= \sum_{\nu,\nu'} U_{\mu\nu} U_{\mu'\nu'} (a_\nu a_{\nu'} \pm a_{\nu'} a_\nu) \\ &= \sum_{\nu,\nu'} U_{\mu\nu} U_{\mu'\nu'} \, [a_\nu, a_{\nu'}]_\pm = 0 \end{aligned} \tag{4.178}$$

where in the last line we have used the appropriate relations for each type of particle. The adjoint of this relation shows that $\left[b^+_\mu, b^+_{\mu'}\right]_\pm = 0$, as well. In a similar fashion we see that

$$\begin{aligned} \left[b_\mu, b^+_{\mu'}\right]_\pm &= \sum_{\nu,\nu'} U_{\mu\nu} U^*_{\mu'\nu'} \left[a_\nu, a^+_{\nu'}\right]_\pm = \sum_{\nu,\nu'} U_{\mu\nu} U^*_{\mu'\nu'} \delta_{\nu,\nu'} = \sum_\nu U_{\mu\nu} U^*_{\mu'\nu} \\ &= \sum_\nu \langle\chi_\mu|\phi_\nu\rangle\langle\phi_\nu|\chi_{\mu'}\rangle = \langle\chi_\mu|\chi_{\mu'}\rangle = \delta_{\mu,\mu'} \end{aligned} \tag{4.179}$$

where we have used the completeness of the states $|\phi_\nu\rangle$ and the orthonormality of the states $|\chi_\mu\rangle$. Thus, the b's and b^+'s obey the same kind of commutation/anticommutation relations as the a's and a^+'s.

We are now in a position to see what different one-body and two-body operators look like in various representations. Suppose, e.g., that H_1 is a one-body operator that is represented in the occupation number states generated by the single-particle states $|\chi_\mu\rangle$ in the form

$$H_1 = \sum_\mu \varepsilon_\mu N_\mu = \sum_\mu \varepsilon_\mu b_\mu^+ b_\mu. \tag{4.180}$$

This implies, e.g., that in the space of single-particle, the states $|\chi_\mu\rangle$ are the associated eigenstates of H_1, i.e., $H_1|\chi_\mu\rangle = \varepsilon_\mu|\chi_\mu\rangle$. To find the form that this takes in any other occupation number representation we simply have to express the annihilation and creation operators in (4.180) as the appropriate linear combinations of the new annihilation and creation operators, i.e.,

$$\begin{aligned} H_1 &= \sum_{\nu,\nu'\mu} \varepsilon_\mu U^*_{\mu\nu} U_{\mu'\nu'} a_\nu^+ a_{\nu'} \\ &= \sum_{\nu,\nu'} a_\nu^+ H_{\nu\nu'} a_{\nu'} \end{aligned} \tag{4.181}$$

where

$$\begin{aligned} H_{\nu\nu'} &= \sum_\mu U^*_{\mu\nu} \varepsilon_\mu U_{\mu'\nu'} = \sum_\mu \langle\phi_\nu|\chi_\mu\rangle \varepsilon_\mu \langle\chi_\mu|\phi_{\nu'}\rangle \\ &= \langle\phi_\nu|H_1^{(1)}|\phi_{\nu'}\rangle \end{aligned} \tag{4.182}$$

in which we have identified the expansion

$$H_1^{(1)} = \sum_\mu |\chi_\mu\rangle \varepsilon_\mu \langle\chi_\mu| \tag{4.183}$$

of the operator H_1, as it is defined in the one-particle subspace. Although we have expressed this in a notation suggestive of Hamiltonians and energy eigenstates, the same considerations apply to any one-body operator. Thus, a general one body operator can be represented in Fock space in an arbitrary occupation number representation in the form

$$B_1 = \sum_{\nu,\nu'} a_\nu^+ B_{\nu\nu'} a_{\nu'} \qquad\qquad B_{\nu\nu'} = \langle\phi_\nu|B_1^{(1)}|\phi_{\nu'}\rangle. \tag{4.184}$$

In the special case when B is diagonal in the specified single particle representation, the double sum collapses into a single sum, and the resulting operator is reduced to a simple function of the number operators of that representation. Thus, a one-body operator B induces single particle transitions, taking a particle out of state $\phi_{\nu'}$ and putting it into state ϕ_ν with amplitude $B_{\nu\nu'}$.

As we noted earlier, two body operators are often associated with interactions between particles. Often, a representation can be found in which such an operator can be expressed in the following form

$$H_2 = \frac{1}{2} \sum_{\substack{\mu,\mu' \\ \mu\neq\mu'}} N_\mu N_{\mu'} V_{\mu\mu'} + \frac{1}{2} \sum_\mu N_\mu (N_\mu - 1) V_{\mu\mu} \tag{4.185}$$

where in the first term $V_{\mu\mu'}$ is the interaction energy between a particle in the state $|\chi_\mu\rangle$ and another particle in a different state $|\chi_{\mu'}\rangle$. The second term includes the interactions between particles in the same states, and takes this form because a particle in a given

state does not interact with itself (Note that $\frac{1}{2}N_\mu(N_\mu-1)$ is the number of distinct pairs of N_μ particles). Both terms can be combined by inserting an appropriate Kronecker delta, i.e.,

$$H_2 = \frac{1}{2}\sum_{\mu,\mu'} N_\mu(N_{\mu'} - \delta_{\mu\mu'})V_{\mu\mu'}. \tag{4.186}$$

This can be simplified further. Using the commutation laws $[N_{\mu'}, b_\mu] = -b_\mu\delta_{\mu\mu'}$ obeyed by both fermion and boson operators (see the discussion in the last section) it follows that

$$N_{\mu'}b_\mu = b_\mu(N_{\mu'} - \delta_{\mu\mu'}). \tag{4.187}$$

Multiplying this on the left by b_μ^+, we deduce that

$$b_\mu^+ N_{\mu'}b_\mu = b_\mu^+ b_{\mu'}^+ b_{\mu'}b_\mu = N_\mu(N_{\mu'} - \delta_{\mu\mu'}), \tag{4.188}$$

which allows us to write

$$H_2 = \frac{1}{2}\sum_{\mu,\mu'} b_\mu^+ b_{\mu'}^+ V_{\mu\mu'}b_{\mu'}b_\mu. \tag{4.189}$$

Thus, in this form the two-body interaction is a sum of products involving two annihilation and two creation operators, but it only involves two summation indices, since each annihilation operator is paired off with a creation operator of each type.

To see what this looks like in any other occupation number representation we just have to transform each of the annihilation and creation operators in the sum. Thus we find that in a representation associated with a set of states $|\phi_\nu\rangle = U|\chi_\nu\rangle$,

$$\begin{aligned} H_2 &= \frac{1}{2}\sum_{\mu,\mu'} b_\mu^+ b_{\mu'}^+ V_{\mu\mu'}b_{\mu'}b_\mu \\ &= \frac{1}{2}\sum_{q,r,s,t}\sum_{\mu,\mu'} U^*_{\mu q}U^*_{\mu' r}U_{\mu' s}U_{\mu t}V_{\mu\mu'}a_q^+ a_{r'}^+ a_s a_t. \end{aligned} \tag{4.190}$$

where we have used the roman indices q, r, s, and t to avoid the proliferation of multiply-primed ν's. To simplify this we now re-express the matrix elements of the unitary transformation in terms of the inner products between basis vectors

$$\sum_{\mu,\mu'} U^*_{\mu q}U^*_{\mu' r}U_{\mu' s}U_{\mu t}V_{\mu\mu'} = \sum_{\mu,\mu'}\langle\phi_q|\chi_\mu\rangle\langle\phi_r|\chi_{\mu'}\rangle V_{\mu\mu'}\langle\chi_{\mu'}|\phi_s\rangle\langle\chi_\mu|\phi_t\rangle \tag{4.191}$$

and notice that each pair of inner products on the right and left of $V_{\mu\mu'}$ can be expressed as a single inner product between direct product states in the space $S^{(2)}$ of just two particles, i.e.,

$$\begin{aligned} \sum_{\mu,\mu'}\langle\phi_q|\chi_\mu\rangle\langle\phi_r|\chi_{\mu'}\rangle V_{\mu\mu'}\langle\chi_{\mu'}|\phi_s\rangle\langle\chi_\mu|\phi_t\rangle &= \sum_{\mu,\mu'}\langle\phi_q,\phi_r|\chi_\mu,\chi_{\mu'}\rangle V_{\mu\mu'}\langle\chi_\mu,\chi_{\mu'}|\phi_t,\phi_s\rangle \\ &= \langle\phi_q,\phi_r|H_2^{(2)}|\phi_t,\phi_s\rangle \end{aligned} \tag{4.192}$$

where the order of the terms has been chosen to reproduce the original set of four inner products, and where we have identified

$$H_2^{(2)} = \sum_{\mu,\mu'}|\chi_\mu,\chi_{\mu'}\rangle V_{\mu\mu'}\langle\chi_\mu,\chi_{\mu'}| \tag{4.193}$$

as the form that this operator takes in the space $S^{(2)}$ of just two particles. Working our way back up, we find that in an arbitrary occupation number representation, a general two-body interaction can be written in the form

$$H_2 = \frac{1}{2}\sum_{q,r,s,t} a_q^+ a_r^+ V_{qrts} a_s a_t \tag{4.194}$$

where

$$V_{qrts} = \langle \phi_q, \phi_r | H_2^{(2)} | \phi_t, \phi_s \rangle \tag{4.195}$$

is the matrix element of the operator taken between states of just two (distinguishable) particles. Thus, to construct such an operator for an arbitrary occupation number representation we simply need to be able to takes its matrix elements with respect to the corresponding set of two-particle direct-product states.

As an example, we note that the Coulomb interaction

$$V(\vec{r}_1, \vec{r}_2) = \frac{e}{|\vec{r}_1 - \vec{r}_2|} \tag{4.196}$$

between particles can be written in the form

$$V = \frac{1}{2}\sum_{q,r,s,t} a_q^+ a_{r'}^+ V_{qrts} a_s a_t \tag{4.197}$$

where the matrix elements are evaluated, e.g., in the two-particle position representation as

$$\begin{aligned} V_{qrts} &= \langle \phi_q, \phi_r | V | \phi_t, \phi_s \rangle \\ &= \int d^3r \int d^3r' \; \phi_q^*(\vec{r}) \phi_r^*(\vec{r}\,') \frac{e}{|\vec{r} - \vec{r}\,'|} \phi_t(\vec{r}) \phi_s(\vec{r}\,') \end{aligned} \tag{4.198}$$

in terms of the wave functions associated with this set of single particle states.

4.4.8 Field Operators and Second Quantization

The use of creation and annihilation operators of the type we have just considered is often referred to as the method of **second quantization** . The "first quantization" implied by this phrase is that developed, e.g., by Schrödinger, in which the dynamical variables x_i and p_i of classical mechanics are now viewed as operators, and the state of the system is characterized by wave functions $\psi(x_i, t)$ or $\psi(p_i, t)$ of one or another of this set of variables. On the other hand, there are other systems studied by classical mechanics that cannot be described as particles, e.g., waves traveling on a string or through an elastic medium, or Maxwell's electric and magnetic field equations, where the classical dynamical variables are just the field amplitudes $\psi(x, t)$ at each point, which like the position and momentum of classical particles always have a well-defined value, and where x is now simply viewed as a continuous index labeling the different dynamical variables $\psi(x)$ that are collectively needed to fully describe the configuration of the system. In a certain sense, Schrödinger's wave function $\psi(x, t)$ for a single particle can also be viewed "as a sort of classical field" and Schrödinger's equation of motion can be viewed as simply the "classical" wave equation obeyed by this field. One can then ask what happens when this classical system is quantized, with the corresponding field amplitudes being associated with operators. It is actually possible to follow this path from classical fields to quantum ones through a detailed study of the objects of classical field theory, including Lagrangian densities, conjugate fields, and so on.

As it turns out, however, the end result of such a process is actually implicitly contained in the mathematical developments that we have already encountered. The key to seeing this comes from the realization that the procedure for transforming between different occupation number representations applies, in principle, to any two sets of single-particle states. Until now we have focused on transformations between discrete ONB's, e.g., $\{|\phi_\nu\rangle\}$ and $\{|\chi_\mu\rangle\}$, but it is possible to consider transformations that include continuously indexed basis sets as well.

A case of obvious interest would be the basis states $\{|\vec{r}\rangle\}$ of the position representation. The transformation law between these states and those of some other single-particle representation, e.g., $\{|\phi_\nu\rangle\}$ takes the form

$$|\phi_\nu\rangle = \int d^3r\ |\vec{r}\rangle\langle\vec{r}|\phi_\nu\rangle = \int d^3r\ \phi_\nu(\vec{r})\ |\vec{r}\rangle = \int d^3r\ U_\nu(\vec{r})\ |\vec{r}\rangle \tag{4.199}$$

and

$$|\vec{r}\rangle = \sum_\nu |\phi_\nu\rangle\langle\phi_\nu|\vec{r}\rangle = \sum_\nu \phi_\nu^*(\vec{r})|\phi_\nu\rangle = \sum_\nu U_\nu^*(\vec{r})|\phi_\nu\rangle \tag{4.200}$$

where $U_\nu(\vec{r}) = \langle\vec{r}|\phi_\nu\rangle$ and $U_\nu^*(\vec{r}) = \langle\phi_\nu|\vec{r}\rangle$ are simply the wave functions (and conjugates) for the single particle states $|\phi_\nu\rangle$ in the position representation. Expressing, the single-particle state $|\phi_\nu\rangle$ in terms of the vacuum state, and substituting into the expansion for the state $|\vec{r}\rangle$, we find that

$$|\vec{r}\rangle = \sum_\nu \phi_\nu^*(\vec{r})a_\nu^+\ |0\rangle. \tag{4.201}$$

This allows us to identify the operator that creates out of the vaccum a particle at the point $\vec{r}$, (i.e., in the single-particle state $|\vec{r}\rangle$) as a linear combination of creation operators associated with the states $|\phi_\nu\rangle$. We will denote this new creation operator with the symbol $\hat{\psi}^+(\vec{r})$, i.e.,

$$\hat{\psi}^+(\vec{r}) = \sum_\nu \phi_\nu^*(\vec{r})a_\nu^+. \tag{4.202}$$

The adjoint of the operator $\hat{\psi}^+(\vec{r})$ gives the corresponding annihilation operator

$$\hat{\psi}(\vec{r}) = \sum_\nu \phi_\nu(\vec{r})a_\nu \tag{4.203}$$

These two families of operators are referred to as **field operators**, since they define an operator-valued field of the real space position parameter $\vec{r}$. Thus $\hat{\psi}^+(\vec{r})$ creates a particle at $\vec{r}$, and $\hat{\psi}(\vec{r})$ destroys or removes a particle from that point. The fact that the basis states $|\vec{r}\rangle$ of this single-particle representation are not square-normalizable leads to some slight but fairly predictable differences between the field operators and the annihilation and creation operators associated with discrete representations. For example, the commutation/anticommutation relations obeyed by the field operators now take a form more appropriate to the continuous index associated with this set of operators. The transformation law is derived as in the discrete case, and we find that

$$\left[\hat{\psi}(\vec{r}), \hat{\psi}(\vec{r}\,')\right]_\pm = \sum_{\nu,\nu'} \phi_\nu(\vec{r})\phi_{\nu'}(\vec{r}\,')\,[a_\nu, a_{\nu'}]_\pm = 0 \tag{4.204}$$

$$\left[\hat{\psi}^+(\vec{r}), \hat{\psi}^+(\vec{r}\,')\right]_\pm = \sum_{\nu,\nu'} \phi_\nu^*(\vec{r})\phi_{\nu'}^*(\vec{r}\,')\,\left[a_\nu^+, a_{\nu'}^+\right]_\pm = 0 \tag{4.205}$$

and

$$\begin{aligned}\left[\hat{\psi}(\vec{r}),\hat{\psi}^{+}(\vec{r}\,')\right]_{\pm} &= \sum_{\nu,\nu'}\phi_{\nu}(\vec{r})\phi^{*}_{\nu'}(\vec{r}\,')\left[a^{+}_{\nu},a^{+}_{\nu'}\right]_{\pm}\\ &= \sum_{\nu,\nu'}\phi_{\nu}(\vec{r})\phi^{*}_{\nu'}(\vec{r}\,')\delta_{\nu\nu'} = \sum_{\nu,\nu}\phi_{\nu}(\vec{r})\phi^{*}_{\nu}(\vec{r}\,')\\ &= \sum_{\nu,\nu}\langle\vec{r}|\phi_{\nu}\rangle\langle\phi_{\nu}|\vec{r}\,'\rangle = \langle\vec{r}|\vec{r}\,'\rangle\\ &= \delta(\vec{r}-\vec{r}\,') \end{aligned} \tag{4.206}$$

Also, as a consequence of the normalization, the product of $\hat{\psi}^{+}(\vec{r})$ and $\hat{\psi}(\vec{r})$ does not give a number operator, but a number density operator, i.e.,

$$\hat{n}(\vec{r}) = \hat{\psi}^{+}(\vec{r})\hat{\psi}(\vec{r}) \tag{4.207}$$

counts the number of particles per unit volume at the point $\vec{r}$. That the product has the correct units to describe a number density follows directly from the commutation relations just derived. From this we can define number operators N_{Ω} that count the number of particles in any region of space Ω, as the integral

$$N_{\Omega} = \int_{\vec{r}\in\Omega} d^3r\ \hat{\psi}^{+}(\vec{r})\hat{\psi}(\vec{r}) \tag{4.208}$$

with the total number operator N obtained by extending the integral to all space.

Finally, we can express various one-body and two body operators using this representation, by sightly extending our results obtained with discrete representations. Thus, e.g., a general one-body operator can be expressed in terms of the field operators through the expression

$$H_1 = \int d^3r \int d^3r'\ \hat{\psi}^{+}(\vec{r})H_1(\vec{r},\vec{r}\,')\hat{\psi}(\vec{r}) \qquad\qquad H_1(\vec{r},\vec{r}\,') = \langle\vec{r}|H^{(1)}_1|\vec{r}\,'\rangle. \tag{4.209}$$

For a collection of noninteracting identical particles moving in a common potential, e.g.,

$$H(\vec{r},\vec{r}\,') = \langle\vec{r}|\frac{P^2}{2m}|\vec{r}\,'\rangle + \langle\vec{r}|V|\vec{r}\,'\rangle = -\frac{\hbar^2}{2m}\nabla^2\delta(\vec{r}-\vec{r}\,') + V(\vec{r})\delta(\vec{r}-\vec{r}\,') \tag{4.210}$$

which reduces the previous expression to the familiar looking form

$$H = \int d^3r\ \left[\psi^{+}(\vec{r})\left(-\frac{\hbar^2}{2m}\right)\nabla^2\psi(\vec{r}) + \psi^{+}(\vec{r})V(\vec{r})\psi(\vec{r})\right] \tag{4.211}$$

which, it is to be emphasized is an operator in Fock space, although it looks just like a simple expectation value. Similarly, a general two-body operator can be expressed in the somewhat more cumbersome form

$$H_2 = \int d^3r_1 \int d^3r_2 \int d^3r_3 \int d^3r_4\ \hat{\psi}^{+}(\vec{r}_1)\hat{\psi}^{+}(\vec{r}_2)\langle\vec{r}_1,\vec{r}_2|H_2|\vec{r}_3,\vec{r}_4\rangle\hat{\psi}(\vec{r}_4)\hat{\psi}(\vec{r}_3). \tag{4.212}$$

The form that this takes for the Coulomb interaction is left as an exercise for the reader.