

rearrangement collisions, such as $d + \alpha \rightarrow d + \alpha$ or ${}^6\text{Li} + \gamma \rightarrow p + {}^5\text{He}$, and so on, where again the different combinations will be real or virtual depending on whether the total center-of-mass system energy is sufficient to reach the combined rest-mass energies of the final channel.

As even these few examples show, systems with many degrees of freedom arise in almost every field of modern physics. In fact in a quantum theory the uncertainty principle offers the intrinsic possibility of introducing many degrees of freedom in a problem that seemed only to involve a few particles (even two, or one, or for that matter none—since empty space may dissociate virtually into antiparticle pairs such as e^+e^- or $\pi^+\pi^-$ or $p\bar{p}$, say). It is our purpose here to study the numerous common aspects of the description of systems with many degrees of freedom. In the case of systems with a fixed but large number of particles we must be able to deal correctly with the boson or fermion statistics of the particles. For situations where particles are produced or annihilated, we must have a way of keeping track of these changes in the number of particles. In both cases we wish to develop special techniques for handling the complex dynamics of the system by a calculational device that keeps track of the number of particles of each variety that are present at each moment in time.

1.1 SINGLE-PARTICLE CREATION AND ANNIHILATION

We consider a rewriting of the usual description of a single particle by means of a wave function in terms of an operator that will depict the state of the particle at the moment of time in question. In fact before we can do that usefully we must first define the vacuum state $|0\rangle$, a state with no physical particles present; in our notation here, the zero inside the ket indicates the number of physical particles in the vacuum state. Suppose we are interested in a single particle occupying a state characterized by a complete set of quantum numbers that we shall designate by ρ . This set might include, for example, the momentum of the particle k , its spin and spin projection, its isospin and isospin projection, and other internal quantum numbers for the particle. We characterize this single-particle state by the action of a creation operator $a_\rho^\dagger$ on the vacuum to produce a ket with one particle in the state ρ , namely

$$|1_\rho\rangle = a_\rho^\dagger |0\rangle. \quad (1)$$

To spell out a little more explicitly what our notation means in terms of a basis of single-particle states designated by the (sets of) quantum numbers $\xi, \rho, \sigma, \tau, \dots$, the vacuum really refers to no occupation of any of these states,

$$|0\rangle = |\dots, 0_\xi, 0_\rho, 0_\sigma, 0_\tau, \dots\rangle, \quad (2)$$

and the single-particle ket to the occupation of only one of them (and that by one particle),

$$|1_\rho\rangle = |\dots, 0_\xi, 1_\rho, 0_\sigma, 0_\tau, \dots\rangle. \quad (3)$$

The projection of this single-particle ket onto configuration space is then what we mean by a single-particle wave function,

$$u_\rho(\mathbf{r}) = \langle \mathbf{r} | 1_\rho \rangle = \langle \mathbf{r} | a_\rho^\dagger | 0 \rangle. \quad (4)$$

For the annihilation or destruction of a particle we use the Hermitian conjugate of the creation operator; thus

$$a_\rho |1_\rho\rangle = |0\rangle. \quad (5)$$

If there are no particles present to be annihilated in the single-particle state in question, then the operation leads to a null result, e.g.,

$$a_\rho |1_\sigma\rangle = 0, \quad \rho \neq \sigma, \quad (6)$$

or, taking these together,

$$a_\rho |1_\sigma\rangle = a_\rho a_\sigma^\dagger |0\rangle = \delta_{\rho\sigma} |0\rangle. \quad (7)$$

Since the vacuum state is unoccupied for any single-particle label,

$$a_\rho |0\rangle = 0. \quad (8)$$

For our present purpose we assume that the vacuum state is unique, and thus the scheme for building up occupied states should also be unique.

1.2 MORE THAN ONE PARTICLE: COMMUTATION AND ANTICOMMUTATION, STATISTICS

Suppose we have two particles present in the system. These may be in different single-particle states,

$$|1_\rho 1_\sigma\rangle \sim a_\rho^\dagger a_\sigma^\dagger |0\rangle, \quad (9)$$

or in the same single-particle modes,

$$|2_\rho\rangle \sim a_\rho^\dagger a_\rho^\dagger |0\rangle. \quad (10)$$

In these expressions we have assumed that acting twice with creation

operators on the vacuum will produce two-particles states, though these need not necessarily be normalized even if the vacuum and single-particle states are. Generalizations for states with more particles are obvious: we merely list the number of particles in each single-particle mode; for instance, for three particles, two in the single-particle state ρ and one in σ ,

$$|2_\rho 1_\sigma\rangle \sim a_\rho^\dagger a_\rho^\dagger a_\sigma^\dagger |0\rangle, \quad (11)$$

and so forth. From the left-hand side of this equation, it is clear why this is called the *number representation*; for most of the manipulations we consider the right-hand form will be more useful. The space in which these kets exist is called *Fock space*, after the name of the physicist who introduced its use. And the whole procedure is often referred to as *second quantization*, since one views the first quantization as that which gives discrete levels as embodied in the single-particle Schrödinger equation, and this one as yielding a description in terms of discrete particles.

Now in what order should we write the creation operators when more than one particle is present? For two identical particles, say, it is clear that is equivalent to (i.e., refers to the same state as)

$$|1_\rho 1_\sigma\rangle \sim a_\rho^\dagger a_\sigma^\dagger |0\rangle \quad (12a)$$

$$|1_\sigma 1_\rho\rangle \sim a_\sigma^\dagger a_\rho^\dagger |0\rangle, \quad (12b)$$

and so these should be related by a phase. We are free to choose this phase as we wish at a given moment in time, and we take it here as real. In fact we are easily guided in our procedure at this point because we know that two identical bosons are to be described by symmetrical states, and two identical fermions by antisymmetrical ones. Within the selection of the real phase this motivates, for *bosons*,

$$|1_\rho 1_\sigma\rangle = |1_\sigma 1_\rho\rangle \quad (13a)$$

and the *commutation relations*

$$a_\rho^\dagger a_\sigma^\dagger = a_\sigma^\dagger a_\rho^\dagger, \quad (13b)$$

while for *fermions* we have

$$|1_\rho 1_\sigma\rangle = -|1_\sigma 1_\rho\rangle \quad (14a)$$

and *anticommutation relations*

$$a_\rho^\dagger a_\sigma^\dagger = -a_\sigma^\dagger a_\rho^\dagger. \quad (14b)$$

For the fermion case we immediately see

$$a_\rho^\dagger a_\rho^\dagger = -a_\rho^\dagger a_\rho^\dagger = 0, \quad (14c)$$

so that two fermions cannot occupy the same single-particle state and the Pauli exclusion principle is immediately satisfied. For bosons, of course, one may have an arbitrary number, 0, 1, 2, 3, ... of particles in a given single-particle state. If this state ρ has energy ω_ρ , each additional particle adds energy ω_ρ to the system, just as if we had a harmonic oscillator of energy ω_ρ that we excited to successively higher levels of excitation; each such excitation adds energy ω_ρ . In fact we can exploit this analogy quite completely by associating a corresponding oscillator with each single-particle mode and using its degree of excitation to "count" the number of particles in the system and their contribution to the total system energy. As is developed in Exercise 1.1 at the end of this chapter, the creation and annihilation operators then have the formal analogy of the ladder operators for the harmonic oscillator. These have the explicit representation

$$a^\dagger = \frac{1}{\sqrt{2m\omega}} (p + im\omega x), \quad a = \frac{1}{\sqrt{2m\omega}} (p - im\omega x), \quad (15a, b)$$

for each mode ρ , σ , ... , where ω is the mode frequency or energy* and m is the oscillator mass, the Hamiltonian being given by

$$H = \frac{1}{2m} p^2 + \frac{1}{2} m\omega^2 x^2 = \omega(a^\dagger a + \frac{1}{2}). \quad (15c)$$

Let us explore further the description of boson systems, returning later to fermions. The Hermitian conjugate of the commutation relation (13b) immediately yields also

$$a_\sigma a_\rho = a_\rho a_\sigma. \quad (16)$$

From Eqs. 7 and 8 we are led to consider

$$(a_\rho a_\sigma^\dagger - a_\sigma^\dagger a_\rho)|0\rangle = \delta_{\rho\sigma}|0\rangle, \quad (17)$$

which suggests the further extension of the commutation relations to**

$$a_\rho a_\sigma^\dagger - a_\sigma^\dagger a_\rho = \delta_{\rho\sigma}. \quad (18)$$

*Here and throughout this book we use units such that $\hbar = 1$. We also take the velocity of light to be unity, $c = 1$. To transcribe units, it is useful to remember that $\hbar c = 197.33 \text{ MeV}\cdot\text{fm} = 1973.3 \text{ eV}\cdot\text{\AA}$.

**This equation may be taken as a definition for a system of elementary bosons.

Thus altogether we expect to get a description of boson properties that has the symmetry properties expected by taking for our creation and annihilation operators the commutation relations

$$[a_\rho, a_\rho] = 0, \quad [a_\rho, a_\rho^\dagger] = 0, \quad [a_\rho, a_\sigma^\dagger] = \delta_{\rho\sigma}. \quad (19a-c)$$

We now define the *number operator* for a given mode ρ ,

$$N_\rho = a_\rho^\dagger a_\rho, \quad (20)$$

or for the total system,

$$N_{\text{tot}} \equiv \sum_\rho N_\rho = \sum_\rho a_\rho^\dagger a_\rho. \quad (21)$$

This operator simply counts the number of particles in each mode. From the commutation relations 19 and the relationships

$$[A, BC] = B[A, C] + [A, B]C \quad (22a)$$

and

$$[AB, C] = A[B, C] + [A, C]B, \quad (22b)$$

we have

$$\begin{aligned} [N_\rho, a_\rho] &= [a_\rho^\dagger a_\rho, a_\rho] \\ &= a_\rho^\dagger [a_\rho, a_\rho] + [a_\rho^\dagger, a_\rho] a_\rho = -\delta_{\rho\rho} a_\rho, \end{aligned} \quad (23a)$$

and similarly

$$[N_\rho, a_\rho^\dagger] = \delta_{\rho\rho} a_\rho^\dagger, \quad (23b)$$

while

$$\begin{aligned} [N_\rho, N_\sigma] &= [N_\rho, a_\rho^\dagger a_\rho] = a_\rho^\dagger [N_\rho, a_\rho] + [N_\rho, a_\rho^\dagger] a_\rho \\ &= \delta_{\rho\sigma} (-a_\rho^\dagger a_\rho + a_\rho^\dagger a_\rho) = 0. \end{aligned} \quad (23c)$$

Thus the numbers of particles in the different modes are diagonal or “sharp” in this representation, as one might expect if the counting of the occupations of the different single-particle states is to be independent and well defined.

The counting of the number of particles in a given mode now proceeds as follows (we suppress the mode index ρ for a while): We populate the mode by constructing

$$(a^\dagger)^n |0\rangle = \underbrace{a^\dagger a^\dagger \cdots a^\dagger}_{n \text{ operators}} |0\rangle \quad (24a)$$

and to verify the number of particles in this state we act on it with the number operator $N = a^\dagger a$ for that mode

$$\begin{aligned} N(a^\dagger)^n |0\rangle &= N \underbrace{a^\dagger a^\dagger \cdots a^\dagger}_n |0\rangle = a^\dagger (1 + N) \underbrace{a^\dagger a^\dagger \cdots a^\dagger}_{n-1} |0\rangle \\ &= a^\dagger a^\dagger (2 + N) \underbrace{a^\dagger a^\dagger \cdots a^\dagger}_{n-2} |0\rangle \\ &= \cdots = \underbrace{a^\dagger a^\dagger \cdots a^\dagger}_{n} (n + N) |0\rangle \\ &= (a^\dagger)^n (n + a^\dagger a) |0\rangle = n(a^\dagger)^n |0\rangle, \end{aligned} \quad (24b)$$

where we have used Eq. 23b and $a|0\rangle = 0$. Thus the state constructed in 24a is an eigenstate of the number operator N_ρ for the mode in question, with eigenvalue equal to the number of particles $n = n_\rho$ placed in that mode. We label the states by the occupation number, $|n_\rho\rangle \sim (a_\rho^\dagger)^{n_\rho} |0\rangle$.

These states have not yet been normalized. For that purpose we consider

$$a_\rho^\dagger |n_\rho\rangle = c_+(n_\rho) |n_\rho + 1\rangle, \quad a_\rho |n_\rho\rangle = c_-(n_\rho) |n_\rho - 1\rangle, \quad (25a, b)$$

where $c_\pm(n_\rho)$ are the normalization coefficients which we must determine; we anticipate that they may depend on the present occupation number. Then for the normalization condition $\langle n_\rho \pm 1 | n_\rho \pm 1 \rangle = 1$ we have (as in the harmonic-oscillator problem)

$$|c_-(n_\rho)|^2 = \langle n_\rho | a_\rho^\dagger a_\rho | n_\rho \rangle = n_\rho \quad (26a)$$

and

$$|c_+(n_\rho)|^2 = \langle n_\rho | a_\rho a_\rho^\dagger | n_\rho \rangle = n_\rho + 1. \quad (26b)$$

Again choosing a real phase, we have

$$a_\rho^\dagger |n_\rho\rangle = \sqrt{n_\rho + 1} |n_\rho + 1\rangle, \quad a_\rho |n_\rho\rangle = \sqrt{n_\rho} |n_\rho - 1\rangle. \quad (27a, b)$$

Since we shall encounter these relationships time and again in what follows, it is useful to note the mnemonic suggested by Feynman. The argument in the radical is always the larger of the two occupation numbers involved in the relation. Of course a simple test case is Eq. 8, which is immediately embodied in 27b here.

As we have generated the eigenstates of the number operator here it is clear by construction that they must involve an integral number of particles. We now also check that these are the only admissible form of number eigenstates. First consider

$$n_\rho = \langle n_\rho | N_\rho | n_\rho \rangle = \langle n_\rho | a_\rho^\dagger a_\rho | n_\rho \rangle \\ = (a_\rho | n_\rho \rangle)^\dagger (a_\rho | n_\rho \rangle) \geq 0, \quad (28)$$

showing that the number-operator eigenvalues must be positive. Next we note that n_ρ must be an integer, since otherwise the repeated action of a_ρ on $|n_\rho\rangle$, as in $(a_\rho)^{n_\rho+1}|n_\rho\rangle$, would eventually yield a negative number label, which is impossible by virtue of Eq. 28. If n_ρ is an integer we are spared this by Eq. 8 or 27b, since we eventually reach $a_\rho|0_\rho\rangle = 0$. (We assume implicitly here that the vacuum state $|0_\rho\rangle$ is unique.) Thus all the eigenstates of N_ρ are those reached by the successive action of $a_\rho^\dagger$ operators on the vacuum, namely

$$a_\rho^\dagger|0\rangle = |1_\rho\rangle, \quad a_\rho^\dagger|1_\rho\rangle = \sqrt{2}|2_\rho\rangle, \dots \quad (29)$$

An explicit representation for the creation and annihilation operators, and hence for the number operator and its eigenstates, is immediately provided by the harmonic-oscillator analogy of Eqs. 15 and Exercise 1.1, or by direct verification of the commutation relations 19 and definition 20. We have, for the mode ρ ,

$$a_\rho = \begin{bmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{2} & 0 & 0 & \cdots \\ 0 & 0 & 0 & \sqrt{3} & 0 & \cdots \\ 0 & 0 & 0 & 0 & \sqrt{4} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}_\rho,$$

$$a_\rho^\dagger = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \cdots \\ \sqrt{1} & 0 & 0 & 0 & 0 & \cdots \\ 0 & \sqrt{2} & 0 & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{3} & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}_\rho,$$

$$N_\rho = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 1 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 2 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 3 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}_\rho,$$

and

$$|0_\rho\rangle = \begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{bmatrix}_\rho, \quad |1_\rho\rangle = \begin{bmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{bmatrix}_\rho, \quad |2_\rho\rangle = \begin{bmatrix} 0 \\ 0 \\ 1 \\ \vdots \end{bmatrix}_\rho, \dots \quad (30)$$

The analogous results for fermions are rather simpler because the exclusion principle guarantees that single-particle occupation is binary in character: a given mode is either occupied or unoccupied. As we saw in Eqs. 14, the antisymmetry of fermion states implies anticommutators, and, instead of Eqs. 19, we expect*

$$\{a_\rho, a_\sigma\} \equiv a_\rho a_\sigma + a_\sigma a_\rho = 0, \quad \{a_\rho^\dagger, a_\sigma^\dagger\} = 0, \quad (31a, b)$$

$$\{a_\rho, a_\sigma^\dagger\} = \delta_{\rho\sigma}, \quad (31c)$$

with the immediate corollaries

$$a_\rho^\dagger a_\rho^\dagger = 0, \quad a_\rho a_\rho = 0. \quad (32a, b)$$

The number operator is defined as before,

$$N_\rho = a_\rho^\dagger a_\rho, \quad (33)$$

and we immediately see that

$$N_\rho^2 = a_\rho^\dagger a_\rho a_\rho^\dagger a_\rho = a_\rho^\dagger (1 - a_\rho^\dagger a_\rho) a_\rho = a_\rho^\dagger a_\rho = N_\rho. \quad (34)$$

Thus the number eigenvalues must satisfy $n_\rho^2 = n_\rho$, or $n_\rho = 0$ or 1, exactly as we would expect on the basis of the exclusion principle. Thus all we need consider for a given mode ρ are the states $|0_\rho\rangle$ and $|1_\rho\rangle$ with

$$|1_\rho\rangle = a_\rho^\dagger |0_\rho\rangle, \quad a_\rho |1_\rho\rangle = |0_\rho\rangle. \quad (35)$$

An explicit representation for the operators and states in the case of fermions is

$$a_\rho = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}_\rho, \quad a_\rho^\dagger = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}_\rho, \\ N_\rho = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}_\rho, \quad (36)$$

and

$$|0_\rho\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}_\rho, \quad |1_\rho\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}_\rho.$$

*Equation 31c may be taken as a definition for a system of elementary fermions; see Eq. 18 and footnote.

As we shall see in the many applications of the coming chapters, the use of fermion creation and annihilation operators greatly simplifies the treatment of antisymmetrization as opposed to the construction of explicitly antisymmetric wave functions or Slater determinants. Of course it is quite crucial to keep careful track of the minus signs introduced by the anticommutation relations of Eqs. 31a–c.

In order to complete the picture of the method based on creation and annihilation operators, we show the explicit mapping of two-particle states for in Fock space into conventional symmetrized or antisymmetrized states for bosons or fermions, respectively. For particles in two different single-particle states these are

$$|1, 1_\sigma\rangle = \frac{1}{\sqrt{1!1!}} a_\rho^\dagger a_\sigma^\dagger |0\rangle$$

$$\rightarrow \frac{1}{\sqrt{2}} [u_\rho(\mathbf{r})u_\sigma(\mathbf{r}') \pm u_\sigma(\mathbf{r})u_\rho(\mathbf{r}')], \quad \rho \neq \sigma, \quad (37a)$$

while for particles in the same mode

$$|2_\rho\rangle = \frac{1}{\sqrt{2!}} a_\rho^\dagger a_\rho^\dagger |0\rangle$$

$$\rightarrow \frac{1}{2} [u_\rho(\mathbf{r})u_\rho(\mathbf{r}') \pm u_\rho(\mathbf{r})u_\rho(\mathbf{r}')] \\ = \begin{cases} u_\rho(\mathbf{r})u_\rho(\mathbf{r}'), & \text{bosons,} \\ 0, & \text{fermions;} \end{cases} \quad (37b)$$

the upper signs apply, obviously, to bosons and the lower signs to fermions. For two particles in the same single-particle states, the product wave function is immediately symmetrical for the boson case, while it vanishes for fermions. We have shown the mapping of Fock states to configuration-space wave functions explicitly for the situation of two particles because that is the most transparent case in which particle statistics are nontrivial. Naturally the scheme generalizes immediately to the construction of completely symmetrized or antisymmetrized states for bosons or fermions, respectively, when more than two particles of a given species are present.

1.3 CONSTRUCTION OF ONE- AND TWO-PARTICLE OPERATORS

In treating systems with many degrees of freedom we shall constantly encounter situations in which we must count the contribution of the particles present to various quantities that characterize the system. These quantities may be of one-particle nature, that is, each particle present makes its separate contribution to the total system value, without reference to other particles. Examples of one-particle quantities are the number operator of

Eqs. 20 and 21 itself, the kinetic energy in the system, the angular momentum, and so on. It is also very common to encounter two-particle quantities, that is, features of the system whose characterization requires knowledge concerning two particles together, as for example the interaction energy arising from a potential that acts between two particles. One may also require a description of three-, four-, or many-particle aspects of the system, which arise, for instance, in nuclear systems where two-particle interactions may not exhaust the nature of the potentials. We shall not, however, deal much with these many-particle situations. This is mainly because their thorough treatment generally requires a prior detailed knowledge of the nature and consequences of the two-particle forces, which often have not yet been adequately mastered. It is also partly because at least the early stages of the generalization to three-particle forces, or still more complex situations, follow as a straightforward generalization of the two-particle case.

To make clear the nature of one-particle operators, consider, as an example, a collection of noninteracting bosons; these could be, for instance, the photons in a blackbody cavity, which to an excellent approximation are noninteracting. The energy operator or Hamiltonian for this system is, in Fock space,

$$H = \sum_{\mathbf{k}s} \omega_{\mathbf{k}s} a_{\mathbf{k}s}^\dagger a_{\mathbf{k}s}, \quad (38)$$

where $\mathbf{k}$ is the particle momentum and s is the particle spin. We have assumed that the energy $\omega_{\mathbf{k}}$ is independent of the spin (and of the direction of $\mathbf{k}$), though that is not at all a necessary assumption; for the photon example, $\omega_{\mathbf{k}} = |\mathbf{k}| = k$ in our units. The operator in Eq. 38 is so constructed that the number operator $a_{\mathbf{k}s}^\dagger a_{\mathbf{k}s}$ for each single-particle mode $\mathbf{k}, s$ counts how many particles are in the mode and weights that number with the energy $\omega_{\mathbf{k}}$ of the mode, summing over the modes. If we take the expectation value of this one-particle operator for a state having definite occupation numbers for the single-particle modes, we get

$$\langle n_{\mathbf{k}_1 s_1}, n_{\mathbf{k}_2 s_2}, n_{\mathbf{k}_3 s_3}, \dots | H | n_{\mathbf{k}_1 s_1}, n_{\mathbf{k}_2 s_2}, n_{\mathbf{k}_3 s_3}, \dots \rangle \\ = n_{\mathbf{k}_1 s_1} \omega_{\mathbf{k}_1} + n_{\mathbf{k}_2 s_2} \omega_{\mathbf{k}_2} + n_{\mathbf{k}_3 s_3} \omega_{\mathbf{k}_3} + \dots, \quad (39)$$

For more general situations, where we may not always be interested in diagonal matrix elements, we must extend the construction of the one-particle operator slightly. The kinetic energy for a system—also a one-particle operator—can thus be written in Fock space as

$$T = \sum_{\alpha\beta} \langle \alpha | t | \beta \rangle a_\alpha^\dagger a_\beta, \quad (40)$$

where t is the kinetic-energy operator for an individual particle, and α, β refer to the single-particle basis to which the number representation is being applied. For example, if this basis referred to configuration space, the matrix element might be evaluated as

$$\langle \alpha | t | \beta \rangle = \int u_{\alpha}^{\dagger}(\mathbf{r}) \left[-\frac{1}{2m} \nabla^2 \right] u_{\beta}(\mathbf{r}) d\mathbf{r}, \quad (41)$$

for particle mass m and wave functions $u_{\alpha, \beta}$, while in a momentum-space basis one would have

$$\langle \alpha | t | \beta \rangle = \int \tilde{u}_{\alpha}^{\dagger}(\mathbf{p}) \frac{p^2}{2m} \tilde{u}_{\beta}(\mathbf{p}) \frac{d\mathbf{p}}{(2\pi)^3}, \quad (42)$$

where $\mathbf{p}_{\alpha}$ is the momentum eigenvalue of the state $|\alpha\rangle$. We have here taken nonrelativistic forms in the explicit examples.

The Fock-space matrix elements of the one-particle kinetic-energy operator are, for one particle present,

$$\begin{aligned} \langle 1_{\rho} | T | 1_{\sigma} \rangle &= \langle 0 | a_{\rho} T a_{\sigma}^{\dagger} | 0 \rangle \\ &= \sum_{\alpha\beta} \langle \alpha | t | \beta \rangle \langle 0 | a_{\rho} a_{\alpha}^{\dagger} a_{\beta} a_{\sigma}^{\dagger} | 0 \rangle \\ &= \sum_{\alpha\beta} \langle \alpha | t | \beta \rangle \delta_{\alpha\rho} \delta_{\beta\sigma} = \langle \rho | t | \sigma \rangle, \end{aligned} \quad (43)$$

for bosons or for fermions. If the single-particle basis refers to plane-wave states, this last result is diagonal,

$$\langle 1_{\rho} | T | 1_{\sigma} \rangle = \langle \rho | t | \sigma \rangle = \frac{p_{\sigma}^2}{2m} \delta_{\rho\sigma}, \quad (44)$$

where $\mathbf{p}_{\sigma}$ is the momentum of the plane-wave state $|\sigma\rangle$. But this need not be the case, of course; one may expand in any complete set of single-particle states. For the structure of Eq. 40 it was, however, crucial that T be of one-particle character, which would evidence itself in configuration space, say, through the appearance of a sum of operators each referring to only one particle variable,

$$T = -\frac{1}{2m} (\nabla_1^2 + \nabla_2^2 + \nabla_3^2 + \cdots), \quad (45)$$

where we have also used the fact that the identical particles in the system will obviously all have the same mass m .

For a two-particle operator, such as a two-particle potential (again acting between identical particles),

$$V = \sum_{i < j} v(i, j) = \frac{1}{2} \sum_{i \neq j} v(i, j), \quad (46)$$

the corresponding Fock-space two-particle operator will be

$$V = \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | v | \gamma\delta \rangle a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} a_{\gamma}, \quad (47a)$$

where we again have in mind expansion on *any* complete, single-particle basis. The matrix element here is

$$\langle \alpha\beta | v | \gamma\delta \rangle = \int u_{\alpha}^{\dagger}(\mathbf{r}) u_{\beta}^{\dagger}(\mathbf{r}') v(\mathbf{r}, \mathbf{r}') u_{\gamma}(\mathbf{r}) u_{\delta}(\mathbf{r}') d\mathbf{r} d\mathbf{r}'. \quad (47b)$$

The change from alphabetical order in the factor $a_{\delta} a_{\gamma}$ of Eq. 47a is immaterial for bosons, where a_{δ} and a_{γ} commute, but flips a sign of matrix elements for fermions, where they anticommute. We can verify the validity of Eq. 47, and in particular of this sign reversal, by evaluating matrix elements of V when two identical particles are present,

$$\begin{aligned} \langle 1_{\rho} 1_{\sigma} | V | 1_{\tau} 1_{\nu} \rangle &= \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | v | \gamma\delta \rangle \langle 0 | a_{\rho} a_{\sigma} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} a_{\gamma} a_{\tau}^{\dagger} a_{\nu}^{\dagger} | 0 \rangle \\ &= \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | v | \gamma\delta \rangle [(\delta_{\alpha\rho} \delta_{\beta\sigma} \pm \delta_{\alpha\sigma} \delta_{\beta\rho})(\delta_{\gamma\tau} \delta_{\delta\nu} \pm \delta_{\gamma\nu} \delta_{\delta\tau})] \\ &= \frac{1}{2} [\langle \rho\sigma | v | \tau\nu \rangle + \langle \sigma\rho | v | \nu\tau \rangle \pm (\langle \sigma\rho | v | \tau\nu \rangle + \langle \rho\sigma | v | \nu\tau \rangle)] \\ &= \langle \rho\sigma | v | \tau\nu \rangle \pm \langle \rho\sigma | v | \nu\tau \rangle, \end{aligned} \quad (48)$$

where, again, the upper sign refers to bosons and the lower sign to fermions. In deriving Eq. 48 it is convenient to note that just as $a_{\xi}^{\dagger} | 0 \rangle = 0$, one also has $\langle 0 | a_{\xi}^{\dagger} = 0$. In addition we have made use of the natural symmetry of the matrix element for the mutual interaction between two identical particles,

$$\begin{aligned} \langle \beta\alpha | v | \delta\gamma \rangle &= \int u_{\beta}^{\dagger}(\mathbf{r}) u_{\alpha}^{\dagger}(\mathbf{r}') v(\mathbf{r}, \mathbf{r}') u_{\delta}(\mathbf{r}) u_{\gamma}(\mathbf{r}') d\mathbf{r} d\mathbf{r}' \\ &= \langle \alpha\beta | v | \gamma\delta \rangle, \end{aligned} \quad (49)$$

here written explicitly in configuration space, as an example.

The final result of Eq. 48 gives clear expression to the symmetry or antisymmetry that we expect for bosons or fermions. Indeed, it is convenient to incorporate this into the notation by introducing a subscript to indicate the status of the matrix element, symmetric or antisymmetric as the case may be:

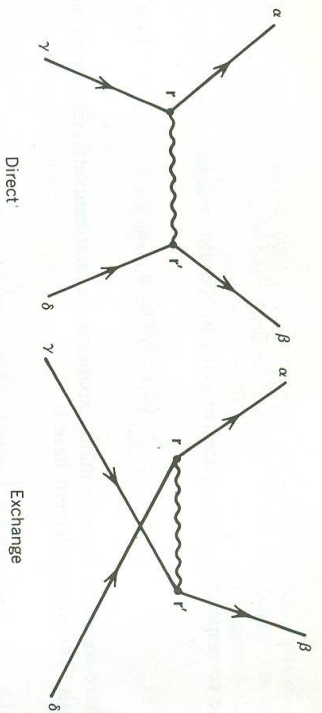


FIGURE 1.1 Direct and exchange graphs for two-particle interaction matrix elements.

$$\begin{aligned} \langle 1_\rho 1_\sigma | V | 1_\tau 1_\nu \rangle &= \langle \rho\sigma | v | \tau\nu \rangle \pm \langle \rho\sigma | v | \nu\tau \rangle \\ &= \begin{cases} \langle \rho\sigma | v | \tau\nu \rangle_s, & \text{bosons (+)} \\ \langle \rho\sigma | v | \tau\nu \rangle_A, & \text{fermions (-)} \end{cases} \end{aligned} \quad (50)$$

In view of this inevitable symmetry feature it is also useful on occasion to rewrite Eq. 47 in a completely equivalent way as

$$V = \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | v | \gamma\delta \rangle_A \text{ or } s \, a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma. \quad (51)$$

Last, we note that it is frequently convenient to draw diagrams that represent the interaction matrix elements of Eqs. 48 and 50. The case for two particles is shown in Figure 1.1.

1.4 THE FERMI GAS IN FOCK SPACE

Partly as an exercise in the techniques of second quantization for the fermion case, and partly because of its enormous usefulness as a zero-order approximation in the treatments of the many-fermion system that follow, we develop here the basic features of a noninteracting gas of N nonrelativistic fermions with mass m . The N fermions in question are viewed as existing in a cubic box of volume Ω , eventually taken very large, with periodic boundary conditions applied. The single-particle basis then refers to definite momentum $\mathbf{k}$ and spin projection s , taken here for spin $\frac{1}{2}$ to have values $s = \pm \frac{1}{2}$; one could also consider other internal degrees of freedom, such as isospin for nuclear applications. The wave functions in question are

$$u_\alpha(\mathbf{r}) = \frac{1}{\sqrt{\Omega}} e^{i\mathbf{k}\cdot\mathbf{r}} \chi_s, \quad \alpha = \{\mathbf{k}, s\}, \quad (52)$$

with energy $\epsilon_k = k^2/2m$, degenerate in spin $s = \pm \frac{1}{2}$.

To construct the ground state of the Fermi gas we populate the lowest available single-particle levels with one fermion each, in accordance with Pauli's exclusion principle. This population is by pairs in the sense that, since the single-particle energies do not depend on spin, for each ϵ_k we have one fermion with spin up and one with spin down. The filled levels are referred to as the Fermi sea, and the last level filled is called the Fermi surface (in momentum or energy space) and designated by ϵ_F or k_F ; the Fermi energy or momentum (see Figure 1.2). The ground state then has the structure

$$|\Phi_0\rangle = \prod_s \prod_{k \leq k_F} a_{ks}^\dagger |0\rangle. \quad (53)$$

The number of particles in this state (which by construction is to be N) is easily determined using the number operator $\sum_{\mathbf{k}s} a_{\mathbf{k}s}^\dagger a_{\mathbf{k}s}$; the particle density ρ_0 is then that number divided by the volume Ω . Thus

$$\begin{aligned} \rho_0 &= \frac{1}{\Omega} \langle \Phi_0 | \sum_{\mathbf{k}s} a_{\mathbf{k}s}^\dagger a_{\mathbf{k}s} | \Phi_0 \rangle \\ &= \frac{1}{\Omega} \sum_{\substack{s=\pm 1/2 \\ \mathbf{k}, k \leq k_F}} 1 = \frac{1}{\Omega} \sum_{\mathbf{k}s} \theta(k_F - k) \\ &\xrightarrow{\Omega \rightarrow \infty} \frac{1}{\Omega} \sum_{s=\pm 1/2} 1 \cdot \int \frac{\Omega d\mathbf{k}}{(2\pi)^3} \theta(k_F - k) \\ &= 2 \int_0^{k_F} \frac{k^2 dk}{(2\pi)^3} \int d\hat{\mathbf{k}} = 2 \times 4\pi \times \frac{k_F^3}{3(2\pi)^3} = \frac{2k_F^3}{6\pi^2}. \end{aligned} \quad (54)$$

The factor 2 in the numerator is simply the spin degeneracy factor $\sum_{s=\pm 1/2} 1$ and in general would be replaced by the degeneracy factor $\sum_s 1$ dictated by the number of (degenerate) substates for the internal quantum numbers in question, e.g., 4 for nuclei with spin up and down and isospin up and down (protons and neutrons). Thus the more general version of Eq. 54 is

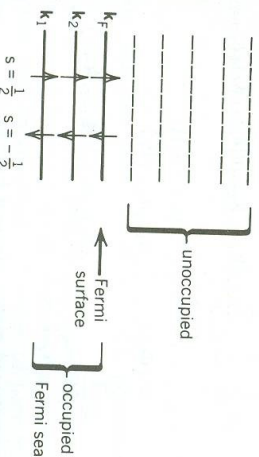


FIGURE 1.2 A pictorial representation of the ground state of a Fermi gas.