# Chapter 2

# Second quantization

The present chapter introduces a method which greatly facilitates working with many-fermion or many-boson states. For this purpose the fermion addition operator is defined in Sec. 2.1 and the notion of the Fock space is introduced. After determining the action of the adjoint of the particle addition operator one may proceed to derive the important anticommutation relations among these operators. Many-particle states with the correct symmetry properties can then be constructed quite easily by acting with these operators on the state without particles, the socalled vacuum state. Similar results for bosons are presented in Sec. 2.2. The form of one- and two-body operators in terms of particle addition and removal operators are discussed in Secs. 2.3 and 2.4, respectively. Some simple applications are discussed in Sec. 2.5.

## 2.1 Fermion addition and removal operators

Dealing with symmetric or antisymmetric many-particle states is simplified considerably by using the occupation number representation (second quantization). In this section the relevant concepts for fermions are presented. Instead of working in the space of a fixed number of particles, one employs the vector space which is the direct sum of the vacuum state $|0\rangle$, which contains no particles, the complete set of sp states $\{|\alpha\rangle\}$, the complete set of antisymmetric two-particle states $\{|\alpha_1\alpha_2\rangle\}$, and so on until infinite particle number. This space is referred to as Fock space. Completeness of the states in this space, using ordered sp quantum numbers, is expressed by

$$\sum_{N=0}^{\infty} \sum_{\alpha_1\alpha_2..\alpha_N}^{ordered} |\alpha_1\alpha_2...\alpha_N\rangle \langle\alpha_1\alpha_2...\alpha_N| \;=\; 1. \tag{2.1}$$

States with different particle number are automatically orthogonal.

An important operator is the fermion addition operator, often called creation operator, defined by

$$a_\alpha^\dagger \left|\alpha_1\alpha_2...\alpha_N\right\rangle \equiv \left|\alpha\alpha_1\alpha_2...\alpha_N\right\rangle \tag{2.2}$$

which adds to an antisymmetric state in which $N$ particles occupy sp levels $\{\alpha_1, \alpha_2, ..., \alpha_N\}$ a particle with quantum numbers $\alpha$, resulting in an antisymmetric $N+1$-particle state. Note that if the level characterized by $\alpha$ is already occupied, the result is zero. Observe also that the $N+1$-particle state containing $\alpha$ may not yet be ordered and the ordering of $\alpha$ among the $\alpha_i$ could therefore result in an extra minus sign.

The adjoint of $a_\alpha^\dagger$ is called a particle removal (destruction) operator based on the following result

$$\begin{aligned}
a_\alpha \left|\alpha_1\alpha_2...\alpha_N\right\rangle &= \sum_{M=0}^{\infty} \sum_{\alpha_1'\alpha_2'..\alpha_M'}^{ordered} \left|\alpha_1'\alpha_2'..\alpha_M'\right\rangle \left\langle\alpha_1'\alpha_2'..\alpha_M'\right| a_\alpha \left|\alpha_1\alpha_2..\alpha_N\right\rangle \\
&= \sum_{M=0}^{\infty} \sum_{\alpha_1'\alpha_2'..\alpha_M'}^{ordered} \left|\alpha_1'\alpha_2'..\alpha_M'\right\rangle \left\langle\alpha_1\alpha_2..\alpha_N\right| a_\alpha^\dagger \left|\alpha_1'\alpha_2'..\alpha_M'\right\rangle^* \\
&= \sum_{M=0}^{\infty} \sum_{\alpha_1'\alpha_2'..\alpha_M'}^{ordered} \left|\alpha_1'\alpha_2'..\alpha_M'\right\rangle \left\langle\alpha_1\alpha_2..\alpha_N|\alpha\alpha_1'\alpha_2'..\alpha_M'\right\rangle^*.
\end{aligned} \tag{2.3}$$

The last line is obtained by using the definition of the particle addition operator. In addition, $M = N-1$ since states containing different particle number are orthogonal. As discussed in Sec. 1.5, the normalization of antisymmetric states can be chosen to be real and therefore one can omit the complex conjugation sign in Eq. (2.3). It is also clear that once $\alpha$ has been ordered among the $\alpha'$ states, one can simply apply Eq. (1.52). Suppose $\alpha$ must be placed before $\alpha_i'$. If $i=1$, no sign change will result, therefore ordering leads to the phase $(-1)^{i-1}$. Eq. (1.52) then gives

$$\left\langle\alpha_1\alpha_2...\alpha_N|\alpha_1'\alpha_2'...\alpha\alpha_i'...\alpha_M'\right\rangle = \delta_{\alpha_1,\alpha_1'}\delta_{\alpha_2,\alpha_2'}...\delta_{\alpha_i,\alpha}\delta_{\alpha_{i+1},\alpha_i'}...\delta_{\alpha_N,\alpha_{N-1}'}. \tag{2.4}$$

As a result one obtains

$$a_\alpha \left|\alpha_1\alpha_2...\alpha_N\right\rangle = (-1)^{i-1} \left|\alpha_1\alpha_2...\alpha_{i-1}\alpha_{i+1}...\alpha_N\right\rangle \qquad \text{if } \alpha = \alpha_i, \tag{2.5}$$

and

$$a_\alpha \left|\alpha_1\alpha_2...\alpha_N\right\rangle = 0 \qquad \text{if } \alpha \neq \alpha_i. \tag{2.6}$$

As a consequence, one also has

$$a_\alpha \left|0\right\rangle = 0. \tag{2.7}$$

These results show that the operator $a_\alpha$ has the property that upon acting on an antisymmetric $N$-particle state, it produces an antisymmetric $N-1$-particle state provided the sp state $\alpha$ is occupied (otherwise the result is zero).

The fermion addition and removal operators obey the following, extremely important, operator relations (sometimes called fundamental anti-commutation relations) :

$$\{a_\alpha, a_\beta^\dagger\} = a_\alpha a_\beta^\dagger + a_\beta^\dagger a_\alpha = \delta_{\alpha,\beta}, \tag{2.8}$$

$$\{a_\alpha, a_\beta\} = \{a_\alpha^\dagger, a_\beta^\dagger\} = 0. \tag{2.9}$$

A typical analysis to obtain these results will be given in the following. Consider an $N$-particle ket in which $\alpha$ is not occupied:

$$a_\alpha a_\alpha^\dagger \left|\alpha_1\alpha_2...\alpha_N\right\rangle = a_\alpha \left|\alpha\alpha_1\alpha_2...\alpha_N\right\rangle = \left|\alpha_1\alpha_2...\alpha_N\right\rangle. \tag{2.10}$$

In addition

$$a_\alpha^\dagger a_\alpha \left|\alpha_1\alpha_2...\alpha_N\right\rangle = 0 \tag{2.11}$$

in that case. These two results combined show that

$$\{a_\alpha, a_\alpha^\dagger\} \left|\alpha_1\alpha_2...\alpha_N\right\rangle = \left|\alpha_1\alpha_2...\alpha_N\right\rangle \tag{2.12}$$

When the $N$-particle ket does contain the sp state $\alpha$ one can assume without loss of generality that $\alpha_1 = \alpha$. One then obtains

$$a_\alpha a_\alpha^\dagger \left|\alpha\alpha_2...\alpha_N\right\rangle = 0 \tag{2.13}$$

and

$$a_\alpha^\dagger a_\alpha \left|\alpha\alpha_2...\alpha_N\right\rangle = a_\alpha^\dagger \left|\alpha_2...\alpha_N\right\rangle = \left|\alpha\alpha_2...\alpha_N\right\rangle \tag{2.14}$$

which shows that

$$\{a_\alpha, a_\alpha^\dagger\} \left|\alpha\alpha_2...\alpha_N\right\rangle = \left|\alpha\alpha_2...\alpha_N\right\rangle. \tag{2.15}$$

Since this procedure can be applied for any $N$ and, as shown above, for fixed $N$ for any state, one concludes that

$$\{a_\alpha, a_\alpha^\dagger\} = 1 \tag{2.16}$$

holds as an operator identity. A similar strategy can be used for the proof of the other identities.

Antisymmetric $N$-particle states can now be obtained by repeated application of particle addition operators to the vacuum state

$$\begin{aligned} |\alpha_1\alpha_2\alpha_3...\alpha_N\rangle &= a_{\alpha_1}^\dagger |\alpha_2\alpha_3...\alpha_N\rangle = a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger |\alpha_3...\alpha_N\rangle = ... \\ &= a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger ... a_{\alpha_N}^\dagger |0\rangle = \prod_i a_{\alpha_i}^\dagger |0\rangle . \end{aligned} \tag{2.17}$$

Note that anticommutation relation 2.9 automatically ensures that the Pauli principle is incorporated in the above construction. Indeed, one can write for example

$$\begin{aligned} |\alpha_1\alpha_2...\alpha_N\rangle &= a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger ... a_{\alpha_N}^\dagger |0\rangle = -a_{\alpha_2}^\dagger a_{\alpha_1}^\dagger ... a_{\alpha_N}^\dagger |0\rangle \\ &= - |\alpha_2\alpha_1...\alpha_N\rangle , \end{aligned} \tag{2.18}$$

which shows that the state with $\alpha_1 = \alpha_2$ does not exist.

## 2.2 Boson addition and removal operators

In dealing with boson addition and removal operators it is convenient to use the notation that characterizes the occupation of each sp state

$$|\alpha_1\alpha_2...\alpha_N\rangle = \left[\frac{N!}{n_\alpha! n_{\alpha'}!...}\right]^{1/2} S\, |\alpha_1\alpha_2...\alpha_N) = |n_\alpha n_{\alpha'}...\rangle , \tag{2.19}$$

where in the last ket the $n_\alpha$ correspond to the number of particles that occupy the sp level $\alpha$ etc. It is customary to only include those $n_\alpha$ in Eq. (2.19) that are different from zero. Addition and removal operators may be introduced as in the case of fermions. For sp states one has

$$|\alpha\rangle = a_\alpha^\dagger |0\rangle . \tag{2.20}$$

For two-particle states one has

$$|\alpha\beta\rangle = a_\alpha^\dagger a_\beta^\dagger |0\rangle \tag{2.21}$$

when $\alpha \neq \beta$. In the case $\alpha = \beta$ one must include an extra normalization factor

$$|\alpha\alpha\rangle = |n_\alpha = 2\rangle = \frac{1}{\sqrt{2}} a^\dagger_\alpha a^\dagger_\alpha |0\rangle . \tag{2.22}$$

In the general case one obtains

$$|n_\alpha n_\beta ... n_\omega\rangle = \frac{1}{[n_\alpha! n_\beta! ... n_\omega!]^{1/2}} \left(a^\dagger_\alpha\right)^{n_\alpha} \left(a^\dagger_\beta\right)^{n_\beta} ... \left(a^\dagger_\omega\right)^{n_\omega} |0\rangle . \tag{2.23}$$

The boson addition and removal operators obey the following fundamental commutation relations :

$$[a_\alpha, a^\dagger_\beta] = a_\alpha a^\dagger_\beta - a^\dagger_\beta a_\alpha = \delta_{\alpha,\beta}, \tag{2.24}$$

$$[a_\alpha, a_\beta] = [a^\dagger_\alpha, a^\dagger_\beta] = 0. \tag{2.25}$$

These results can be obtained in a similar way as for the fermion operators and are related to the requirement that symmetric states are obtained after the action of an addition or removal operator of a boson sp state. It should be noted that the commutation relations for a given sp state are identical to those for harmonic oscillator quanta. It is therefore not surprising that the following relations hold

$$a^\dagger_\alpha |n_\alpha n_\beta ... n_\omega\rangle = \sqrt{n_\alpha + 1} |n_\alpha + 1 \ n_\beta ... n_\omega\rangle , \tag{2.26}$$

$$a_\alpha |n_\alpha n_\beta ... n_\omega\rangle = \sqrt{n_\alpha} |n_\alpha - 1 \ n_\beta ... n_\omega\rangle , \tag{2.27}$$

and similarly for operators involving other sp quantum numbers. The results of Eqs. (2.26) and (2.27) can be verified by using Eq. (2.23) and the commutation relations.

## 2.3 One-body operators in Fock space

Relevant operators to consider in many-particle systems involve only the coordinates of one or two (and in unusual cases three) particles. It is therefore important to translate the action of such operators into the language of particle addition and removal operators. To determine the corresponding operator in Fock space, consider first an operator which acts only on one particle. Such a one-body operator, $F$, acting in a sp space can be written as

$$F = \sum_{\alpha} \sum_{\beta} |\alpha\rangle \langle\alpha| F |\beta\rangle \langle\beta| \tag{2.28}$$

and is completely determined by all its matrix elements $\langle\alpha| F |\beta\rangle$ in a chosen sp basis. In an $N$-particle space the corresponding extension of this operator is simply

$$F_N = F(1) + F(2) + ... + F(N) = \sum_{i=1}^{N} F(i), \tag{2.29}$$

where each operator $F(i)$ acts only on particle $i$. Using Eq. (2.28) the action of $F(i)$ on a product state (note the round bracket) is given by

$$\begin{aligned} F(i)|\alpha_1\alpha_2\alpha_3...\alpha_N) &= |\alpha_1\rangle |\alpha_2\rangle ... |\alpha_{i-1}\rangle \Big\{ \sum_{\beta_i} |\beta_i\rangle \langle\beta_i| F |\alpha_i\rangle \Big\} |\alpha_{i+1}\rangle ... |\alpha_N\rangle \\ &= \sum_{\beta_i} \langle\beta_i| F |\alpha_i\rangle |\alpha_1...\alpha_{i-1}\beta_i\alpha_{i+1}...\alpha_N). \end{aligned} \tag{2.30}$$

Note that the matrix elements of $F$ do not depend on which particle is considered. The matrix element $\langle\beta_i| F |\alpha_i\rangle$ in the above expression will therefore be the same for any particle. Calculation of this matrix element for another particle will in fact only involve a change in dummy variables. For the operator $F_N$ one then obtains

$$\begin{aligned} F_N|\alpha_1\alpha_2\alpha_3...\alpha_N) &= F(1)\,|\alpha_1\rangle |\alpha_2\rangle ... |\alpha_N\rangle + |\alpha_1\rangle F(2)\,|\alpha_2\rangle ... |\alpha_N\rangle + ... \\ &\quad + |\alpha_1\rangle |\alpha_2\rangle ... F(N)\,|\alpha_N\rangle \\ &= \sum_{\beta_1} \langle\beta_1| F |\alpha_1\rangle |\beta_1\alpha_2...\alpha_N) \\ &\quad + \sum_{\beta_2} \langle\beta_2| F |\alpha_2\rangle |\alpha_1\beta_2...\alpha_N) + ... \\ &\quad + \sum_{\beta_N} \langle\beta_N| F |\alpha_N\rangle |\alpha_1\alpha_2...\beta_N) \\ &= \sum_{i=1}^{N} \sum_{\beta_i} \langle\beta_i| F |\alpha_i\rangle |\alpha_1\alpha_2...\alpha_{i-1}\beta_i\alpha_{i+1}...\alpha_N). \end{aligned} \tag{2.31}$$

To obtain the action of $F_N$ on an antisymmetric or symmetric $N$-particle state, one notes that $F_N$ is symmetric and therefore commutes with the antisymmetrizer $A$ or the symmetrizer $S$ (remember the example of two particles in which $H$ commutes with $P_{12}$ discussed in Sec. 1.3). As a result

$$F_N \left|\alpha_1\alpha_2\alpha_3...\alpha_N\right\rangle = \sum_{i=1}^{N}\sum_{\beta_i} \left\langle\beta_i\right| F \left|\alpha_i\right\rangle \left|\alpha_1\alpha_2...\alpha_{i-1}\beta_i\alpha_{i+1}...\alpha_N\right\rangle . \quad (2.32)$$

One can now show that the Fock-space operator (note the "^" notation for a Fock-space operator)

$$\hat{F} = \sum_{\alpha\beta} \left\langle\alpha\right| F \left|\beta\right\rangle a_\alpha^\dagger a_\beta \quad (2.33)$$

gives the same result for any $N$ when acting on Eq. (2.17) for fermions and Eq. (2.23) for bosons. In order to show this, consider the following commutator in the case of fermions

$$\begin{aligned}[\hat{F}, a_{\alpha_i}^\dagger] &= \sum_{\alpha\beta} \left\langle\alpha\right| F \left|\beta\right\rangle [a_\alpha^\dagger a_\beta, a_{\alpha_i}^\dagger] = \sum_{\alpha\beta} \left\langle\alpha\right| F \left|\beta\right\rangle (a_\alpha^\dagger a_\beta a_{\alpha_i}^\dagger - a_{\alpha_i}^\dagger a_\alpha^\dagger a_\beta) \\ &= \sum_{\alpha\beta} \left\langle\alpha\right| F \left|\beta\right\rangle a_\alpha^\dagger (a_\beta a_{\alpha_i}^\dagger + a_{\alpha_i}^\dagger a_\beta) = \sum_{\alpha\beta} \left\langle\alpha\right| F \left|\beta\right\rangle a_\alpha^\dagger \delta_{\beta,\alpha_i} \\ &= \sum_{\alpha} \left\langle\alpha\right| F \left|\alpha_i\right\rangle a_\alpha^\dagger = \sum_{\beta_i} \left\langle\beta_i\right| F \left|\alpha_i\right\rangle a_{\beta_i}^\dagger , \end{aligned} \quad (2.34)$$

where the fundamental anticommutation relation (2.8) has been used. One can use this result in the following manipulation

$$\begin{aligned}\hat{F}\left|\alpha_1\alpha_2\alpha_3...\alpha_N\right\rangle &= \hat{F} a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger ... a_{\alpha_N}^\dagger \left|0\right\rangle \\ &= [\hat{F}, a_{\alpha_1}^\dagger] a_{\alpha_2}^\dagger ... a_{\alpha_N}^\dagger \left|0\right\rangle + a_{\alpha_1}^\dagger \hat{F} a_{\alpha_2}^\dagger ... a_{\alpha_N}^\dagger \left|0\right\rangle \\ &= [\hat{F}, a_{\alpha_1}^\dagger] a_{\alpha_2}^\dagger ... a_{\alpha_N}^\dagger \left|0\right\rangle + a_{\alpha_1}^\dagger [\hat{F}, a_{\alpha_2}^\dagger] ... a_{\alpha_N}^\dagger \left|0\right\rangle \\ &+ ... + a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger ... [\hat{F}, a_{\alpha_N}^\dagger] \left|0\right\rangle \\ &= \sum_{i=1}^{N}\sum_{\beta_i} \left\langle\beta_i\right| F \left|\alpha_i\right\rangle a_{\alpha_1}^\dagger ... a_{\alpha_{i-1}}^\dagger a_{\beta_i}^\dagger a_{\alpha_{i+1}}^\dagger ... a_{\alpha_N}^\dagger \left|0\right\rangle \\ &= \sum_{i=1}^{N}\sum_{\beta_i} \left\langle\beta_i\right| F \left|\alpha_i\right\rangle \left|\alpha_1 ... \alpha_{i-1}\beta_i\alpha_{i+1}...\alpha_N\right\rangle \end{aligned} \quad (2.35)$$

which proves the equivalence for fermions of Eqs .(2.32) and (2.35) for a given $N$. Since this result can be obtained for any $N$, one may conclude that Eq. (2.33) has the required form of a one-body operator in Fock space. For bosons one may proceed in a similar way to obtain Eq. (2.33).

## 2.4 Two-body operators in Fock space

An example of an operator involving the coordinates of two particles, is the two-body interaction $V$. In order to establish the corresponding Fock-space operator, consider first the two-body operator $V$ acting on states in the two-particle space of product states

$$V = \sum_{\alpha\beta} \sum_{\gamma\delta} |\alpha\beta)(\alpha\beta|V|\gamma\delta)(\gamma\delta|. \tag{2.36}$$

In an $N$-particle space the corresponding extension of this operator is given by

$$V_N = \begin{cases} V(1,2) + V(1,3) + V(1,4) + \ldots + & V(1,N) + \\ \quad\quad V(2,3) + V(2,4) + \ldots + & V(2,N) + \\ \quad\quad\quad\quad V(3,4) + \ldots + & V(3,N) + \\ \quad\quad\quad\quad\quad\quad \ddots & \vdots \\ & V(N-1,N) \end{cases}$$
$$= \sum_{i<j=1}^{N} V(i,j) = \frac{1}{2} \sum_{i \neq j}^{N} V(i,j), \tag{2.37}$$

where each operator $V(i,j)$ acts only on particles $i$ and $j$. The action of $V(i,j)$ on a product state of $N$ particles is given by

$$V(i,j)|\alpha_1..\alpha_i..\alpha_j..\alpha_N) = \sum_{\beta_i\beta_j} (\beta_i\beta_j|V|\alpha_i\alpha_j) \times |\alpha_1..\alpha_{i-1}\beta_i\alpha_{i+1}..\alpha_{j-1}\beta_j\alpha_{j+1}..\alpha_N). \tag{2.38}$$

Note that the matrix elements of $V$ do not depend on which pair of particles is considered. The matrix elements $(\beta_i\beta_j|V|\alpha_i\alpha_j)$ in the above expression will therefore be the same for any pair of particles as long as the same quantum numbers are involved. For the operator $V_N$ one then obtains

$$V_N|\alpha_1\alpha_2\alpha_3...\alpha_N) = \sum_{i<j=1}^{N} \sum_{\beta_i\beta_j} (\beta_i\beta_j|V|\alpha_i\alpha_j)|\alpha_1...\beta_i...\beta_j...\alpha_N). \tag{2.39}$$

To obtain the action of $V_N$ on an antisymmetric or symmetric $N$-particle state, one notes that $V_N$ is symmetric and therefore commutes with the antisymmetrizer $A$ or symmetrizer $S$. As a result

$$V_N \left|\alpha_1\alpha_2\alpha_3...\alpha_N\right\rangle = \sum_{i<j=1}^{N} \sum_{\beta_i\beta_j} (\beta_i\beta_j|V|\alpha_i\alpha_j) \left|\alpha_1...\beta_i...\beta_j...\alpha_N\right\rangle . \quad (2.40)$$

One can now show that the Fock space operator (note again the "ˆ" notation for a Fock-space operator)

$$\hat{V} = \frac{1}{2} \sum_{\alpha\beta\gamma\delta} (\alpha\beta|V|\gamma\delta) a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma \quad (2.41)$$

gives the same result for any $N$ when acting on Eq. (2.17) for fermions and Eq. (2.23) for bosons. In order to show this in the case of fermions, consider the following commutator

$$[\hat{V}, a_{\alpha_i}^\dagger] = \sum_{\beta_i\beta_{i'}\alpha_{i'}} (\beta_i\beta_{i'}|V|\alpha_i\alpha_{i'}) a_{\beta_i}^\dagger a_{\beta_{i'}}^\dagger a_{\alpha_{i'}} , \quad (2.42)$$

which is obtained in a similar way as Eq. (2.34). To obtain this result one has to make use of the symmetry $V(i,j) = V(j,i)$ which implies

$$(\alpha\beta|V|\gamma\delta) = (\beta\alpha|V|\delta\gamma). \quad (2.43)$$

One can use this result to demonstrate that

$$\hat{V} \left|\alpha_1\alpha_2\alpha_3...\alpha_N\right\rangle = \sum_{i=1}^{N} \sum_{j>i}^{N} \sum_{\beta_i\beta_j} (\beta_i\beta_j|V|\alpha_i\alpha_j) a_{\alpha_1}^\dagger ... a_{\beta_i}^\dagger ... a_{\beta_j}^\dagger ... a_{\alpha_N}^\dagger \left|0\right\rangle \quad (2.44)$$

which proves the equivalence. Note that in obtaining this result one makes use of

$$\sum_{\beta_{i'}\alpha_{i'}} f(\beta_{i'}, \alpha_{i'}) [a_{\beta_{i'}}^\dagger a_{\alpha_{i'}}, a_{\alpha_j}^\dagger] = \sum_{\beta_{i'}} f(\beta_{i'}, \alpha_j) a_{\beta_{i'}}^\dagger \quad (2.45)$$

for each $j > i$. Eq. (2.44) is equivalent to Eq. (2.39) and this result holds for any $N$. Eq. (2.41) therefore represents the extension of the two-particle operator $V_N$ in Fock space. For bosons one can proceed in a similar fashion yielding the same result for the two-body interaction in Fock space (Eq. (2.41)). An alternative form for $\hat{V}$ in the case of fermions is given by

$$\hat{V} = \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \left\langle\alpha\beta\right| V \left|\gamma\delta\right\rangle a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma \quad (2.46)$$

where

$$\langle\alpha\beta|\, V\,|\gamma\delta\rangle \equiv (\alpha\beta|V|\gamma\delta) - (\alpha\beta|V|\delta\gamma) = \langle\alpha\beta|\,\hat{V}\,|\gamma\delta\rangle\,. \tag{2.47}$$

It should be noted that the last expression in Eq. (2.47) contains the second quantized two-body operator $\hat{V}$. One should also note that in the expressions for $\hat{V}$ in (2.41) and (2.46) the order of the quantum numbers $\gamma$ and $\delta$ in the matrix element is different from the ordering of the corresponding particle removal operators. Depending on the nature of the interaction $V$ it can be useful to choose the unsymmetrized version of $\hat{V}$ (Eq. (2.41)) or the symmetrized version (Eq. (2.46)). Using thes Fock space formulation of one- and two-body operators it is now possible to write the hamiltonian of a many-particle system in second quantized form

$$\begin{aligned}\hat{H} &= \hat{T} + \hat{V} \\ &= \sum_{\alpha\beta} \langle\alpha|\, T\,|\beta\rangle\, a^\dagger_\alpha a_\beta + \frac{1}{2}\sum_{\alpha\beta\gamma\delta} (\alpha\beta|V|\gamma\delta) a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma\end{aligned} \tag{2.48}$$

for both fermions and bosons. For fermions it also useful to consider the alternative result for the two-body interaction given in Eq. (2.46). For a given choice of sp basis and two-body interaction $V$, it is possible to calculate the relevant one- and two-body matrix elements which appear in $\hat{H}$ (although this can be very tedious and computer time consuming sometimes). The calculation of matrix elements of $\hat{H}$ between many-particle states is therefore reduced to manipulating particle addition and removal operators using their (anti)commutation relations. This represents a considerable practical advantage over other methods that deal with the calculation of matrix elements of operators between symmetric or antisymmetric many-particle states.

In the case an explicit three-body interaction (symmetric in the coordinates of the particles) needs to be considered one can use the first quantized version in the $N$-particle space

$$W_N = \sum_{i<j<k=1}^{N} W(i,j,k) \tag{2.49}$$

and the Fock space operator

$$\hat{W} = \frac{1}{6}\sum_{\alpha\beta\gamma}\sum_{\alpha'\beta'\gamma'} (\alpha\beta\gamma|W|\alpha'\beta'\gamma')\, a^\dagger_\alpha a^\dagger_\beta a^\dagger_\gamma a_{\gamma'} a_{\beta'} a_{\alpha'}\,. \tag{2.50}$$

## 2.5 Examples

As an example of a second quantized one-body operator consider

$$\hat{N} = \sum_{\alpha} a^{\dagger}_{\alpha} a_{\alpha}. \tag{2.51}$$

Using the results of Eqs. (2.34) and (2.35) one easily obtains

$$\hat{N} \left|\alpha_1 ... \alpha_N\right\rangle = N \left|\alpha_1 ... \alpha_N\right\rangle \tag{2.52}$$

for any $N$ and any set $\alpha_i$. This operator is therefore called the number operator since it simply counts the number of particles in the state on which it acts. When the state has a fixed number of particles it is an eigenstate of $\hat{N}$.

To explain the name second quantization it is useful to mention the confusing convention to denote the addition operators for particles with quantum numbers $\boldsymbol{r}, m_s$ by

$$\psi^{\dagger}_{m_s}(\boldsymbol{r}) \equiv a^{\dagger}_{\boldsymbol{r} m_s} \tag{2.53}$$

and similarly for the removal operators. Using this basis the kinetic energy matrix element becomes

$$\langle \boldsymbol{r} m_s | \, T \, | \boldsymbol{r}' m'_s \rangle = \frac{-\hbar^2}{2m} \nabla^2 \delta(\boldsymbol{r} - \boldsymbol{r}') \delta_{m_s, m'_s}. \tag{2.54}$$

For a conventional spin-independent local two-particle interaction one has in addition

$$\begin{aligned}(\boldsymbol{r}_1 m_{s_1} \; \boldsymbol{r}_2 m_{s_2} | V(\boldsymbol{r}, \boldsymbol{r}') | \boldsymbol{r}_3 m_{s_3} \; \boldsymbol{r}_4 m_{s_4}) = \delta(\boldsymbol{r}_1 - \boldsymbol{r}_3) \delta(\boldsymbol{r}_2 - \boldsymbol{r}_4) \\ \times \, \delta_{m_{s_1}, m_{s_3}} \delta_{m_{s_2}, m_{s_4}} V(|\boldsymbol{r}_3 - \boldsymbol{r}_4|).\end{aligned} \tag{2.55}$$

Using these results the hamiltonian can be rewritten as

$$\begin{aligned}\hat{H} &= \sum_{m_s} \int d^3 r \; \psi^{\dagger}_{m_s}(\boldsymbol{r}) \{ \frac{-\hbar^2}{2m} \nabla^2 \} \psi_{m_s}(\boldsymbol{r}) \\ &+ \frac{1}{2} \sum_{m_s m'_s} \int d^3 r \int d^3 r' \; \psi^{\dagger}_{m_s}(\boldsymbol{r}) \psi^{\dagger}_{m'_s}(\boldsymbol{r}') V(|\boldsymbol{r} - \boldsymbol{r}'|) \psi_{m'_s}(\boldsymbol{r}') \psi_{m_s}(\boldsymbol{r}).\end{aligned} \tag{2.56}$$

This expression can of course easily lead to the wrong interpretation when one mistakenly thinks of $\psi$ as a wave function. In order to avoid this pitfall the notation $a^{\dagger}_{\boldsymbol{r} m_s}$ will be used to denote an operator which adds a particle with sp quantum numbers $\{\boldsymbol{r}m_s\}$ to a many-particle state (and similarly for $a_{\boldsymbol{r}m_s}$, the removal operator).

A change of sp basis in sp space can be rewritten in the following way

$$a_\alpha^\dagger \left|0\right\rangle = \left|\alpha\right\rangle = \sum_\lambda \left|\lambda\right\rangle \left\langle\lambda|\alpha\right\rangle = \sum_\lambda a_\lambda^\dagger \left|0\right\rangle \left\langle\lambda|\alpha\right\rangle. \tag{2.57}$$

This procedure can be repeated for $a_\alpha^\dagger$ acting on any state in Fock space and one therefore obtains the operator equation

$$a_\alpha^\dagger = \sum_\lambda \langle\lambda|\alpha\rangle a_\lambda^\dagger \tag{2.58}$$

and similarly

$$a_\alpha = \sum_\lambda \langle\alpha|\lambda\rangle a_\lambda. \tag{2.59}$$

Note that this transformation is unitary as any basis transformation.

## 2.6 Exercises

(1) Perform the analysis to obtain the remaining anticommution relations in Eqs. (2.8) and (2.9).
(2) Obtain the commutation relations for boson addition and removal operators Eqs. (2.24) and (2.25).
(3) Check Eqs. (2.26) and (2.27).
(4) Calculate the commutator in Eq. (2.42) for both the fermion and the boson case and check the relation (2.44).
(5) Determine the second-quantized form of

- the density operator

$$\rho_N(\boldsymbol{r}) = \sum_{i=1}^N \delta(\boldsymbol{r} - \boldsymbol{r}_i) \tag{2.60}$$

- the electrical current density operator

$$\boldsymbol{j}_N(\boldsymbol{r}) = \frac{1}{2}\sum_{i=1}^N \{\boldsymbol{v}_i \delta(\boldsymbol{r} - \boldsymbol{r}_i) + \delta(\boldsymbol{r} - \boldsymbol{r}_i)\boldsymbol{v}_i\} \tag{2.61}$$

- the three components of the spin density operator

$$\boldsymbol{s}_N(\boldsymbol{r}) = \sum_{i=1}^{N} \boldsymbol{s}_i \delta(\boldsymbol{r} - \boldsymbol{r}_i) \tag{2.62}$$

in the case of fermions and using the $\{\boldsymbol{r}, m_s\}$ basis.

(6) Determine the second-quantized form of the two-body Coulomb interaction for fermions in the $\{\boldsymbol{r}, m_s\}$ basis.

(7) Show that for any $n$-body operator $\hat{F}^{(n)}$ the relation

$$\sum_{\alpha} c_{\alpha}^{\dagger} [c_{\alpha}, \hat{F}^{(n)}] = n\hat{F}^{(n)} \tag{2.63}$$

holds, for both fermions and bosons.

(8) Use the result from the previous problem to show that, in case of a hamiltonian $\hat{H} = \hat{T} + \hat{V}$ consisting of a one-body operator $\hat{T}$ and a two-body operator $\hat{V}$, the energy expectation value $E_0^N = \langle \Psi_0^N | \hat{H} | \Psi_0^N \rangle$ in an arbitrary $N$-body state $|\Psi_0^N\rangle$ can be written as

$$E_0^N = \frac{1}{2} \Bigg\{ \langle \Psi_0^N | \hat{T} | \Psi_0^N \rangle + \sum_{\alpha} \sum_{\nu(N-1)} \left[ E_0^N - E_\nu^{N-1} \right] | \langle \Psi_\nu^{N-1} | a_\alpha | \Psi_0^N \rangle |^2 \Bigg\},$$

where the $|\Psi_\nu^{N-1}\rangle$ form the complete set of eigenstates of $\hat{H}$ in the $(N-1)$-particle Fock space.