4.3: Second Quantization

In the usual tensor product notation, symmetric and antisymmetric states become quite cumbersome to deal with when the number of particles is large. We will now introduce a formalism called **second quantization**, which greatly simplifies manipulations of such multi-particle states. (The reason for the name "second quantization" will not be apparent until later; it is a bad name, but one we are stuck with for historical reasons.)

We start by defining a convenient way to specify states of multiple identical particles, called the **occupation number representation**. Let us enumerate a set of single-particle states, $\{|1\rangle, |2\rangle, |3\rangle, \cdots\}$, that form a complete orthonormal basis for the single-particle Hilbert space $\mathscr{H}^{(1)}$. Then, we build multi-particle states by specifying how many particles are in state $|1\rangle$, denoted n_1; how many are in state $|2\rangle$, denoted n_2; and so on. Thus,

$$|n_1, n_2, n_3, \ldots\rangle \tag{4.3.1}$$

is *defined* as the appropriate symmetric or antisymmetric multi-particle state, constructed using Equation (4.2.6) if we're dealing with bosons (Section 4.2), or using Equation (4.2.14) if we're dealing with fermions (Section 4.2).

Let us run through a couple of examples:

Example 4.3.1

The two-particle state $|0, 2, 0, 0, \ldots\rangle$ has both particles in the single-particle state $|2\rangle$. This is only possible if the particles are bosons, since fermions cannot share the same state. Written out in tensor product form, the symmetric state is

$$|0, 2, 0, 0, \ldots\rangle \equiv |2\rangle|2\rangle. \tag{4.3.2}$$

Example 4.3.2

The three-particle state $|1, 1, 1, 0, 0, \ldots\rangle$ has one particle each occupying $|1\rangle$, $|2\rangle$, and $|3\rangle$. If the particles are bosons, this corresponds to the symmetric state

$$\begin{aligned}|1,1,1,0,0,\ldots\rangle \equiv \frac{1}{\sqrt{6}}\Big(&|1\rangle|2\rangle|3\rangle + |3\rangle|1\rangle|2\rangle + |2\rangle|3\rangle|1\rangle \\ &+ |1\rangle|3\rangle|2\rangle + |2\rangle|1\rangle|3\rangle + |3\rangle|2\rangle|1\rangle\Big).\end{aligned} \tag{4.3.3}$$

And if the particles are fermions, the appropriate antisymmetric state is

$$\begin{aligned}|1,1,1,0,0,\ldots\rangle \equiv \frac{1}{\sqrt{6}}\Big(&|1\rangle|2\rangle|3\rangle + |3\rangle|1\rangle|2\rangle + |2\rangle|3\rangle|1\rangle \\ &- |1\rangle|3\rangle|2\rangle - |2\rangle|1\rangle|3\rangle - |3\rangle|2\rangle|1\rangle\Big).\end{aligned} \tag{4.3.4}$$

Fock space

There is a subtle point that we have glossed over: what Hilbert space do these state vectors reside in? The state $|0, 2, 0, 0, \ldots\rangle$ is a bosonic two-particle state, which is a vector in the two-particle Hilbert space $\mathscr{H}^{(2)} = \mathscr{H}^{(1)} \otimes \mathscr{H}^{(1)}$. However, $\mathscr{H}^{(2)}$ also contains two-particle states that are not symmetric under exchange, which is not allowed for bosons. Thus, it would be more rigorous for us to narrow the Hilbert space to the space of state vectors that are symmetric under exchange. We denote this reduced space by $\mathscr{H}_S^{(2)}$.

Likewise, $|1,1,1,0,\dots\rangle$ is a three-particle state lying in $\mathscr{H}^{(3)}$. If the particles are bosons, we can narrow the space to $\mathscr{H}_S^{(3)}$. If the particles are fermions, we can narrow it to the space of three-particle states that are antisymmetric under exchange, denoted by $\mathscr{H}_A^{(3)}$. Thus, $|1,1,1,0,\dots\rangle \in \mathscr{H}_{S/A}^{(3)}$, where the subscript S/A depends on whether we are dealing with symmetric states (S) or antisymmetric states (A).

We can make the occupation number representation more convenient to work with by defining an "extended" Hilbert space, called the **Fock space**, that is the space of bosonic/fermionic states *for arbitrary numbers of particles*. In the formal language of linear algebra, the Fock space can be written as

$$\mathscr{H}_{S/A}^{F} = \mathscr{H}^{(0)} \oplus \mathscr{H}^{(1)} \oplus \mathscr{H}_{S/A}^{(2)} \oplus \mathscr{H}_{S/A}^{(3)} \oplus \mathscr{H}_{S/A}^{(4)} \oplus \cdots \tag{4.3.5}$$

Here, $\oplus$ represents the **direct sum** operation, which combines vector spaces by directly grouping their basis vectors into a larger basis set; if $\mathscr{H}_1$ has dimension d_1 and $\mathscr{H}_2$ has dimension d_2, then $\mathscr{H}_1 \oplus \mathscr{H}_2$ has dimension $d_1 + d_2$. (By contrast, the space $\mathscr{H}_1 \otimes \mathscr{H}_2$, defined via the tensor product, has dimension $d_1 d_2$.) Once again, the subscript S/A depends on whether we are dealing with bosons (S) or fermions (A).

The upshot is that any multi-particle state that we can write down in the occupation number representation, $|n_1, n_2, n_3, \dots\rangle$, is guaranteed to lie in the Fock space $\mathscr{H}_{S/A}^{F}$. Moreover, these states form a complete basis for $\mathscr{H}_{S/A}^{F}$.

In Equation (4.3.5), the first term of the direct sum is $\mathscr{H}^{(0)}$, the "Hilbert space of 0 particles". This Hilbert space contains only one distinct state vector, denoted by

$$|\varnothing\rangle \equiv |0,0,0,0,\dots\rangle. \tag{4.3.6}$$

This refers to the **vacuum state**, a quantum state in which there are literally no particles. Note that $|\varnothing\rangle$ is *not* the same thing as a zero vector; it has the standard normalization $\langle\varnothing|\varnothing\rangle = 1$. The concept of a "state of no particles" may seem silly, but we will see that there are very good reasons to include it in the formalism.

Another subtle consequence of introducing the Fock space concept is that it is now legitimate to write down quantum states that lack definite particle numbers. For example,

$$\frac{1}{\sqrt{2}}\Big(|1,0,0,0,0,\dots\rangle + |1,1,1,0,0,\dots\rangle\Big) \tag{4.3.7}$$

is a valid state vector describing the superposition of a one-particle state and a three-particle state. We will revisit the phenomenon of quantum states with indeterminate particle numbers in Section 4.3, and in the next chapter.

Second quantization for bosons

After this lengthy prelude, we are ready to introduce the formalism of second quantization. Let us concentrate on bosons first.

We define an operator called the **boson creation operator**, denoted by $\hat{a}_\mu^\dagger$ and acting in the following way:

$$\hat{a}_\mu^\dagger \Big|n_1, n_2, \dots, n_\mu, \dots\Big\rangle = \sqrt{n_\mu + 1}\, \Big|n_1, n_2, \dots, n_\mu + 1, \dots\Big\rangle. \tag{4.3.8}$$

In this definition, there is one particle creation operator for each state in the single-particle basis $\{|\varphi_1\rangle, |\varphi_2\rangle, \dots\}$. Each creation operator is defined as an operator acting on state vectors in the Fock space $\mathscr{H}_S^F$, and has the effect of incrementing the occupation number of its single-particle state by one. The prefactor of $\sqrt{n_\mu + 1}$ is defined for later convenience.

Applying a creation operator to the vacuum state yields a single-particle state:

$$\hat{a}^\dagger_\mu|\varnothing\rangle \;=\; |0,\ldots,0,\underset{\leftarrow\,\mu}{1},0,0,\ldots\rangle. \tag{4.3.9}$$

The creation operator's Hermitian conjugate, $\hat{a}_\mu$, is the **boson annihilation operator**. To characterize it, first take the Hermitian conjugate of Equation (4.3.8):

$$\Big\langle n_1, n_2, \ldots \Big|\hat{a}_\mu = \sqrt{n_\mu + 1}\;\Big\langle n_1, n_2, \ldots, n_\mu + 1, \ldots \Big|. \tag{4.3.10}$$

Right-multiplying by another occupation number state $|n_1', n_2', \ldots\rangle$ results in

$$\begin{aligned}\Big\langle n_1, n_2, \ldots \Big|\hat{a}_\mu\Big|n_1', n_2', \ldots\Big\rangle &= \sqrt{n_\mu + 1}\;\Big\langle \ldots, n_\mu + 1, \ldots \Big| \ldots, n_\mu', \ldots \Big\rangle \\ &= \sqrt{n_\mu + 1}\;\delta^{n_1}_{n_1'}\,\delta^{n_2}_{n_2'}\cdots\delta^{n_\mu+1}_{n_\mu'}\;\cdots \\ &= \sqrt{n_\mu'}\;\delta^{n_1}_{n_1'}\,\delta^{n_2}_{n_2'}\cdots\delta^{n_\mu+1}_{n_\mu'}\;\cdots\end{aligned} \tag{4.3.11}$$

From this, we can deduce that

$$\hat{a}_\mu\Big|n_1', n_2', \ldots, n_\mu', \ldots\Big\rangle = \begin{cases}\sqrt{n_\mu'}\;\Big|n_1', n_2', \ldots, n_\mu' - 1, \ldots\Big\rangle, & \text{if } n_\mu' > 0\\ 0, & \text{if } n_\mu' = 0.\end{cases} \tag{4.3.12}$$

In other words, the annihilation operator decrements the occupation number of a specific single-particle state by one (hence its name). As a special exception, if the given single-particle state is unoccupied ($n_\mu = 0$), applying $\hat{a}_\mu$ results in a zero vector (note that this is *not* the same thing as the vacuum state $|\varnothing\rangle$).

The boson creation/annihilation operators obey the following commutation relations:

$$[\hat{a}_\mu, \hat{a}_\nu] = [\hat{a}^\dagger_\mu, \hat{a}^\dagger_\nu] = 0, \qquad [\hat{a}_\mu, \hat{a}^\dagger_\nu] = \delta_{\mu\nu}. \tag{4.3.13}$$

These can be derived by taking the matrix elements with respect to the occupation number basis. We will go through the derivation of the last commutation relation; the others are left as an exercise (Exercise 4.5.5).

To prove that $[\hat{a}_\mu, \hat{a}^\dagger_\nu] = \delta_{\mu\nu}$, first consider the case where the creation/annihilation operators act on the same single-particle state:

$$\begin{aligned}\left\langle n_1, n_2, \ldots \left|\hat{a_\mu}\hat{a}_\mu^\dagger\right| n_1', n_2' \ldots\right\rangle &= \sqrt{(n_\mu+1)(n_\mu'+1)}\,\left\langle \ldots, n_\mu+1, \ldots \middle| \ldots, n_\mu'+1, \ldots\right\rangle \\ &= \sqrt{(n_\mu+1)(n_\mu'+1)}\,\delta_{n_1'}^{n_1}\,\delta_{n_2'}^{n_2}\,\cdots\delta_{n_\mu'+1}^{n_\mu+1}\cdots \\ &= (n_\mu+1)\delta_{n_1'}^{n_1}\,\delta_{n_2'}^{n_2}\,\cdots\delta_{n_\mu'}^{n_\mu}\cdots \\ \left\langle n_1, n_2, \ldots \left|\hat{a}_\mu^\dagger\hat{a_\mu}\right| n_1', n_2' \ldots\right\rangle &= \sqrt{n_\mu n_\mu'}\,\left\langle \ldots, n_\mu-1, \ldots \middle| \ldots, n_\mu'-1, \ldots\right\rangle \\ &= \sqrt{n_\mu n_\mu'}\delta_{n_1'}^{n_1}\,\delta_{n_2'}^{n_2}\,\cdots\delta_{n_\mu'-1}^{n_\mu-1}\cdots \\ &= n_\mu\delta_{n_1'}^{n_1}\,\delta_{n_2'}^{n_2}\,\cdots\delta_{n_\mu'}^{n_\mu}\cdots\end{aligned} \tag{4.3.14}$$

In the second equation, we were a bit sloppy in handling the $n_\mu = 0$ and $n_\mu' = 0$ cases, but you can check for yourself that the result on the last line remains correct. Upon taking the difference of the two equations, we get

$$\left\langle n_1, n_2, \ldots \middle| \left(\hat{a_\mu}\hat{a}_\mu^\dagger - \hat{a}_\mu^\dagger\hat{a_\mu}\right) \middle| n_1', n_2' \ldots\right\rangle = \delta_{n_1'}^{n_1}\,\delta_{n_2'}^{n_2}\,\cdots\delta_{n_\mu'}^{n_\mu}\cdots = \left\langle n_1, n_2, \ldots \middle| n_1', n_2' \ldots\right\rangle. \tag{4.3.15}$$

Since the occupation number states form a basis for $\mathscr{H}_S^F$, we conclude that

$$\hat{a_\mu}\hat{a}_\mu^\dagger - \hat{a}_\mu^\dagger\hat{a_\mu} = \hat{I}. \tag{4.3.16}$$

Next, consider the case where $\mu \neq \nu$:

$$\begin{aligned}\left\langle n_1, \ldots \left|\hat{a_\mu}\hat{a}_\nu^\dagger\right| n_1', \ldots\right\rangle &= \sqrt{(n_\mu+1)(n_\nu'+1)}\,\langle \ldots, n_\mu+1, \ldots, n_\nu, \ldots \mid \ldots, n_\mu', \ldots, n_\nu'+1, \ldots\rangle \\ &= \sqrt{n_\mu' n_\nu}\;\delta_{n_1'}^{n_1}\,\cdots\delta_{n_\mu'}^{n_\mu+1}\cdots\delta_{n_\nu'+1}^{n_\nu}\cdots \\ \left\langle n_1, \ldots \left|\hat{a}_\nu^\dagger\hat{a_\mu}\right| n_1', \ldots\right\rangle &= \sqrt{n_\mu' n_\nu}\,\langle \ldots, n_\mu, \ldots, n_\nu-1, \ldots \mid \ldots, n_\mu'-1, \ldots, n_\nu' \ldots\rangle \\ &= \sqrt{n_\mu' n_\nu}\;\delta_{n_1'}^{n_1}\,\cdots\delta_{n_\mu'-1}^{n_\mu}\cdots\delta_{n_\nu'}^{n_\nu-1}\cdots \\ &= \sqrt{n_\mu' n_\nu}\;\delta_{n_1'}^{n_1}\,\cdots\delta_{n_\mu'}^{n_\mu+1}\cdots\delta_{n_\nu'+1}^{n_\nu}\cdots\end{aligned} \tag{4.3.17}$$

Hence,

$$\hat{a_\mu}\hat{a}_\nu^\dagger - \hat{a}_\nu^\dagger\hat{a_\mu} = 0 \quad \text{for} \quad \mu \neq \nu. \tag{4.3.18}$$

Combining these two results gives the desired commutation relation, $[\hat{a_\mu}, \hat{a}_\nu^\dagger] = \delta_{\mu\nu}$.

Another useful result which emerges from the first part of this proof is that

$$\left\langle n_1, n_2, \ldots \left|\hat{a}_\mu^\dagger\hat{a_\mu}\right| n_1', n_2' \ldots\right\rangle = n_\mu\left\langle n_1, n_2, \ldots \middle| n_1', n_2' \ldots\right\rangle. \tag{4.3.19}$$

Hence, we can define the Hermitian operator

$$\hat{n_\mu} \equiv \hat{a}_\mu^\dagger\hat{a_\mu}, \tag{4.3.20}$$

whose eigenvalue is the occupation number of single-particle state μ.

If you are familiar with the method of creation/annihilation operators for solving the quantum harmonic oscillator, you will have noticed the striking similarity with the particle creation/annihilation operators for bosons. This is no mere coincidence. We will examine the relationship between harmonic oscillators and bosons in the next chapter.

Second quantization for fermions

For fermions, the multi-particle states are antisymmetric. The fermion creation operator can be defined as follows:

$$\begin{aligned}\hat{c}_\mu^\dagger |n_1, n_2, \dots, n_\mu, \dots\rangle &= \begin{cases} (-1)^{n_1+n_2+\cdots+n_{\mu-1}}\, |n_1, n_2, \dots, n_{\mu-1}, 1, \dots\rangle & \text{if } n_\mu = 0 \\ 0 & \text{if } n_\mu = 1. \end{cases} \\ &= (-1)^{n_1+n_2+\cdots+n_{\mu-1}}\ \delta_0^{n_\mu}\, \Big|n_1, n_2, \dots, n_{\mu-1}, 1, \dots \Big\rangle. \end{aligned} \tag{4.3.21}$$

In other words, if state μ is unoccupied, then $\hat{c}_\mu^\dagger$ increments the occupation number to 1, and multiplies the state by an overall factor of $(-1)^{n_1+n_2+\cdots+n_{\mu-1}}$ (i.e, $+1$ if there is an even number of occupied states preceding μ, and -1 if there is an odd number). The role of this factor will be apparent later. Note that this definition requires the single-particle states to be ordered in some way; otherwise, it would not make sense to speak of the states "preceding" μ. It does not matter which ordering we choose, so long as we make *some* choice, and stick to it consistently.

If μ is occupied, applying $\hat{c}_\mu^\dagger$ gives the zero vector. The occupation numbers are therefore forbidden from being larger than 1, consistent with the Pauli exclusion principle.

The conjugate operator, $\hat{c}_\mu$, is the fermion annihilation operator. To see what it does, take the Hermitian conjugate of the definition of the creation operator:

$$\langle n_1, n_2, \dots, n_\mu, \dots|\hat{c}_\mu = (-1)^{n_1+n_2+\cdots+n_{\mu-1}}\ \delta_0^{n_\mu} \Big\langle n_1, n_2, \dots, n_{\mu-1}, 1, \dots\Big|. \tag{4.3.22}$$

Right-multiplying this by $|n_1', n_2', \dots\rangle$ gives

$$\langle n_1, n_2, \dots, n_\mu, \dots|\hat{c}_\mu|n_1', n_2', \dots\rangle = (-1)^{n_1+\cdots+n_{\mu-1}}\ \delta_{n_1'}^{n_1} \cdots \delta_{n_{\mu-1}'}^{n_{\mu-1}} \left(\delta_0^{n_\mu}\delta_{n_\mu'}^1\right) \delta_{n_{\mu+1}'}^{n_{\mu+1}} \cdots \tag{4.3.23}$$

Hence, we deduce that

$$\begin{aligned}\hat{c}_\mu |n_1', \dots, n_\mu', \dots\rangle &= \begin{cases} 0 & \text{if } n_\mu' = 0 \\ (-1)^{n_1'+\cdots+n_{\mu-1}'}\, |n_1', \dots, n_{\mu-1}', 0, \dots\rangle & \text{if } n_\mu' = 1. \end{cases} \\ &= (-1)^{n_1'+\cdots+n_{\mu-1}'}\ \delta_{n_\mu'}^1\, \Big|n_1', \dots, n_{\mu-1}', 0, \dots \Big\rangle. \end{aligned} \tag{4.3.24}$$

In other words, if state μ is unoccupied, then applying $\hat{c}_\mu$ gives the zero vector; if state μ is occupied, applying $\hat{c}_\mu$ decrements the occupation number to 0, and multiplies the state by the aforementioned factor of ± 1.

With these definitions, the fermion creation/annihilation operators can be shown to obey the following *anticommutation* relations:

Definition: Anticommutation Relations

$$\left\{\hat{c}_\mu, \hat{c}_\nu\right\} = \left\{\hat{c}_\mu^\dagger, \hat{c}_\nu^\dagger\right\} = 0, \qquad \left\{\hat{c}_\mu, \hat{c}_\nu^\dagger\right\} = \delta_{\mu\nu}. \tag{4.3.25}$$

Here, $\{\cdot,\cdot\}$ denotes an anticommutator, which is defined by

$$\left\{\hat{A}, \hat{B}\right\} \equiv \hat{A}\hat{B} + \hat{B}\hat{A}. \tag{4.3.26}$$

Similar to the bosonic commutation relations (4.3.13), the anticommutation relations (4.3.25) can be derived by taking matrix elements with occupation number states. We will only go over the last one, $\left\{\hat{c_\mu}, \hat{c_\nu^\dagger}\right\} = \delta_{\mu\nu}$; the others are left for the reader to verify.

First, consider creation/annihilation operators acting on the same single-particle state μ:

$$\begin{aligned}\Big\langle \ldots, n_\mu, \ldots \Big|\hat{c_\mu}\hat{c_\mu^\dagger}\Big| \ldots, n'_\mu, \ldots \Big\rangle &= (-1)^{n_1+\cdots+n_{\mu-1}}\,(-1)^{n'_1+\cdots+n'_{\mu-1}}\;\delta_0^{n_\mu}\delta_{n'_\mu}^0 \\ &\quad\times \Big\langle n_1, \ldots, n_{\mu-1}, 1, \ldots \Big| n'_1, \ldots, n'_{\mu-1}, 1, \ldots \Big\rangle \\ &= \delta_{n'_\mu}^0 \;\cdot\; \delta_{n'_1}^{n_1}\,\delta_{n'_2}^{n_2}\cdots\delta_{n'_\mu}^{n_\mu}\cdots\end{aligned} \tag{4.3.27}$$

By a similar calculation,

$$\Big\langle \ldots, n_\mu, \ldots \Big|\hat{c_\mu^\dagger}\hat{c_\mu}\Big| \ldots, n'_\mu, \ldots \Big\rangle = \delta_{n'_\mu}^1 \;\cdot\; \delta_{n'_1}^{n_1}\,\delta_{n'_2}^{n_2}\cdots\delta_{n'_\mu}^{n_\mu}\cdots \tag{4.3.28}$$

By adding these two equations, and using the fact that $\delta_{n'_\mu}^0 + \delta_{n'_\mu}^1 = 1$, we get

$$\Big\langle \ldots, n_\mu, \ldots \Big|\left\{\hat{c_\mu}, \hat{c_\mu^\dagger}\right\}\Big| \ldots, n'_\mu, \ldots \Big\rangle = \Big\langle \ldots, n_\mu, \ldots \Big| \ldots, n'_\mu, \ldots \Big\rangle \tag{4.3.29}$$

And hence,

$$\left\{\hat{c_\mu}, \hat{c_\mu^\dagger}\right\} = \hat{I}. \tag{4.3.30}$$

Next, we must prove that $\left\{\hat{c_\mu}, \hat{c_\nu^\dagger}\right\} = 0$ for $\mu \neq \nu$. We will show this for $\mu < \nu$ (the $\mu > \nu$ case follows by Hermitian conjugation). This is, once again, by taking matrix elements:

$$\begin{aligned}\Big\langle \ldots, n_\mu, \ldots, n_\nu, \ldots \Big|\hat{c_\mu}\hat{c_\nu^\dagger}\Big| \ldots, n'_\mu, \ldots, n'_\nu, \ldots \Big\rangle &= (-1)^{n_1+\cdots+n_{\mu-1}}\,(-1)^{n'_1+\cdots+n'_{\nu-1}}\;\delta_0^{n_\mu}\delta_{n'_\nu}^0 \\ &\quad\times \Big\langle \ldots, 1, \ldots, n_\nu, \ldots \Big| \ldots, n'_\mu, \ldots, 1, \ldots \Big\rangle \\ &= (-1)^{n'_\mu+\cdots+n'_{\nu-1}}\;\delta_{n'_1}^{n_1}\,\delta_{n'_2}^{n_2}\cdots\left(\delta_0^{n_\mu}\delta_{n'_\mu}^1\right)\cdots\left(\delta_1^{n_\nu}\delta_{n'_\nu}^0\right)\cdots \\ &= (-1)^{1+n_{\mu+1}+\cdots+n_{\nu-1}}\;\delta_{n'_1}^{n_1}\,\delta_{n'_2}^{n_2}\cdots\left(\delta_{n_\mu}^0\delta_{n'_\mu}^1\right)\cdots\left(\delta_{n'_\nu}^0\delta_{n_\nu}^1\right)\cdots \\ \Big\langle \ldots, n_\mu, \ldots, n_\nu, \ldots \Big|\hat{c_\nu^\dagger}\hat{c_\mu}\Big| \ldots, n'_\mu, \ldots, n'_\nu, \ldots \Big\rangle &= (-1)^{n_1+\cdots+n_{\nu-1}}\,(-1)^{n'_1+\cdots+n'_{\mu-1}}\;\delta_1^{n_\nu}\delta_{n'_\mu}^1 \\ &\quad\times \Big\langle \ldots, n_\mu, \ldots, 0, \ldots \Big| \ldots, 0, \ldots, n'_\nu, \ldots \Big\rangle \\ &= (-1)^{n_\mu+\cdots+n_{\nu-1}}\;\delta_{n'_1}^{n_1}\,\delta_{n'_2}^{n_2}\cdots\left(\delta_0^{n_\mu}\delta_{n'_\mu}^1\right)\cdots\left(\delta_1^{n_\nu}\delta_{n'_\nu}^0\right)\cdots \\ &= (-1)^{0+n_{\mu+1}+\cdots+n_{\nu-1}}\;\delta_{n'_1}^{n_1}\,\delta_{n'_2}^{n_2}\cdots\left(\delta_0^{n_\mu}\delta_{n'_\mu}^1\right)\cdots\left(\delta_1^{n_\nu}\delta_{n'_\nu}^0\right)\cdots\end{aligned} \tag{4.3.31}$$

The two equations differ by a factor of -1, so adding them gives zero. Putting everything together, we conclude that $\left\{c_\mu, c_\nu^\dagger\right\} = \delta_{\mu\nu}$, as stated in (4.3.25).

As you can see, the derivation of the fermionic anticommutation relations is quite hairy, in large part due to the $(-1)^{(\cdots)}$ factors in the definitions of the creation and annihilation operators. But once these relations have been derived, we can deal entirely with the creation and annihilation operators, without worrying about the underlying occupation number representation and its $(-1)^{(\cdots)}$ factors. By the way, if we had chosen to omit the $(-1)^{(\cdots)}$ factors in the definitions, the creation and annihilation operators would still satisfy the *anticommutation* relation $\{\hat{c_\mu}, \hat{c_\nu^\dagger}\} = \delta_{\mu\nu}$, but two creation operators or two annihilation operators would *commute* rather than *anticommute*.

During subsequent calculations, the “algebra” of creation and annihilation operators ends up being much harder to deal with.

Second-quantized operators

One of the key benefits of second quantization is that it allows us to express multi-particle quantum operators clearly and succinctly, using the creation and annihilation operators defined in Section 4.3 as “building blocks”.

Non-interacting particles

Consider a system of *non-interacting* particles. When there is just one particle ($N = 1$), let the single-particle Hamiltonian be $\hat{H}^{(1)}$, which is a Hermitian operator acting on the single-particle Hilbert space $\mathscr{H}^{(1)}$. For general N, the multi-particle Hamiltonian $\hat{H}$ is a Hermitian operator acting on the Fock space $\mathscr{H}^F$. How is $\hat{H}$ related to $\hat{H}^{(1)}$?

Let us take the bosonic case. Then the multi-particle Hamiltonian should be

$$\hat{H} = \sum_{\mu\nu} \hat{a}_\mu^\dagger H_{\mu\nu} \hat{a}_\nu, \quad \text{where} \quad H_{\mu\nu} = \langle \mu | \hat{H}^{(1)} | \nu \rangle, \tag{4.3.32}$$

where $\hat{a}_\mu$ and $\hat{a}_\mu^\dagger$ are the boson creation and annihilation operators, and $|\mu\rangle$, $|\nu\rangle$ refer to single-particle state vectors drawn from some orthonormal basis for $\mathscr{H}^{(1)}$.

To understand why Equation (4.3.32) is right, consider its matrix elements with respect to various states. First, for the vacuum state $|\varnothing\rangle$,

$$\langle \varnothing | \hat{H} | \varnothing \rangle = 0. \tag{4.3.33}$$

This makes sense. Second, consider the matrix elements between single-particle states:

$$\begin{aligned} \langle n_\mu = 1 | \hat{H} | n_\nu = 1 \rangle &= \langle \varnothing | a_\mu \Big(\sum_{\mu'\nu'} \hat{a}_{\mu'}^\dagger H_{\mu'\nu'} \hat{a}_{\nu'} \Big) a_\nu^\dagger | \varnothing \rangle \\ &= \sum_{\mu'\nu'} H_{\mu'\nu'} \, \langle \varnothing | a_\mu \hat{a}_{\mu'}^\dagger \hat{a}_{\nu'} \, a_\nu^\dagger | \varnothing \rangle \\ &= \sum_{\mu'\nu'} H_{\mu'\nu'} \, \delta_{\mu'}^{\mu} \delta_{\nu'}^{\nu} \\ &= H_{\mu\nu}. \end{aligned} \tag{4.3.34}$$

This exactly matches the matrix element defined in Equation (4.3.32).

Finally, consider the case where $\{|\mu\rangle\}$ forms an eigenbasis of $\hat{H}_1$. Then

$$\hat{H}^{(1)} |\mu\rangle = E_\mu |\mu\rangle \quad \Rightarrow \quad H_{\mu\nu} = E_\mu \, \delta_{\mu\nu} \quad \Rightarrow \quad \hat{H} = \sum_\mu E_\mu \, \hat{n}_\mu. \tag{4.3.35}$$

As previously noted, $\hat{n}_\mu = \hat{a}_\mu^\dagger \hat{a}_\mu$ is the number operator, an observable corresponding to the occupation number of single-particle state μ. Thus, the total energy is the sum of the single-particle energies, as expected for a system of non-interacting particles.

We can also think of the Hamiltonian $\hat{H}$ as the generator of time evolution. Equation (4.3.32) describes an infinitesimal time step that consists of a superposition of alternative evolution processes. Each term in the superposition, $\hat{a}_\mu^\dagger H_{\mu\nu} \hat{a}_\nu$, describes a particle being annihilated in state ν, and immediately re-created in state μ, which is equivalent to "transferring" a particle from ν to μ. The quantum amplitude for this process is described by the matrix element $H_{\mu\nu}$. This description of time evolution is applicable not just to single-particle states, but also to multi-particle states containing any number of particles.

Note also that the number of particles does not change during time evolution. Whenever a particle is annihilated in a state ν, it is immediately re-created in some state μ. This implies that the Hamiltonian commutes with the total particle number operator:

$$[\hat{H}, \hat{N}] = 0, \quad \text{where} \;\; \hat{N} \equiv \sum_\mu \hat{a}_\mu^\dagger \hat{a}_\mu. \tag{4.3.36}$$

The formal proof for this is left as an exercise (see Exercise 4.5.6). It follows directly from the creation and annihilation operators' commutation relations (for bosons) or anticommuattion relations (for fermions).

Apart from the total energy, other kinds of observables—the total momentum, total angular momentum, etc.—can be expressed in a similar way. Let $\hat{A}^{(1)}$ be a single-particle observable. For a multi-particle system, the operator corresponding to the "total A" is

$$\hat{A} = \sum_{\mu\nu} \hat{a}_\mu^\dagger A_{\mu\nu} \hat{a}_\nu, \quad \text{where} \;\; A_{\mu\nu} = \langle\mu|\hat{A}^{(1)}|\nu\rangle. \tag{4.3.37}$$

For fermions, everything from Equation (4.3.32)–(4.3.37) also holds, but with the a operators replaced by fermionic c operators.

Change of basis

A given set of creation and annihilation operators is defined using a basis of single-particle states $\{|\mu\rangle\}$, but such a choice is obviously not unique. Suppose we have a different single-particle basis $\{|\alpha\rangle\}$, such that

$$|\alpha\rangle = \sum_\mu U_{\alpha\mu}|\mu\rangle, \tag{4.3.38}$$

where $U_{\alpha\mu}$ are the elements of a unitary matrix. Let $\hat{a}_\alpha^\dagger$ and $\hat{a}_\mu^\dagger$ denote the creation operators defined using the two different basis (once again, we will use the notation for bosons, but the equations in this section are valid for fermions too). Writing Equation (4.3.38) in terms of the creation operators,

$$\hat{a}_\alpha^\dagger|\varnothing\rangle = \sum_\mu U_{\alpha\mu}\hat{a}_\mu^\dagger|\varnothing\rangle,$$

We therefore deduce that

$$\hat{a}_\alpha^\dagger = \sum_\mu U_{\alpha\mu}\hat{a}_\mu^\dagger, \quad \hat{a}_\alpha = \sum_\mu U_{\alpha\mu}^*\hat{a}_\mu. \tag{4.3.39}$$

Using the unitarity of $U_{\alpha\mu}$, we can verify that $\hat{a}_\alpha$ and $\hat{a}_\alpha^\dagger$ satisfy bosonic commutation relations if and only if $\hat{a}_\mu$ and $\hat{a}_\mu^\dagger$ do so. For fermions, we put c operators in place of a operators in Equation (4.3.39), and use anticommutation rather than commutation relations.

To illustrate how a basis change affects a second quantized Hamiltonian, consider a system of non-interacting particles whose single-particle Hamiltonian is diagonal in the α basis. The multi-particle Hamiltonian is

$$\hat{H} = \sum_{\alpha} E_{\alpha} \hat{a}_{\alpha}^{\dagger} \hat{a}_{\alpha}, \tag{4.3.40}$$

consistent with Equation (4.3.36). Applying Equation (4.3.39),

$$\hat{H} = \sum_{\mu\nu} \hat{a}_{\mu}^{\dagger} \left(\sum_{\alpha} E_{\alpha} U_{\alpha\mu} U_{\alpha\nu}^{*} \right) \hat{a}_{\nu} \tag{4.3.41}$$

Compare this to single-particle bracket

$$\begin{aligned} H_{\mu\nu} \equiv \langle \mu | \hat{H}^{(1)} | \nu \rangle &= \sum_{\alpha\beta} \langle \alpha | U_{\alpha\mu} \hat{H}^{(1)} U_{\beta\nu}^{*} | \beta \rangle \\ &= \sum_{\alpha\beta} U_{\alpha\mu} U_{\beta\nu}^{*} E_{\beta} \, \delta_{\alpha\beta} \\ &= \sum_{\alpha} E_{\alpha} \, U_{\alpha\mu} U_{\alpha\nu}^{*}. \end{aligned} \tag{4.3.42}$$

This precisely matches the term in parentheses in Equation (4.3.41). This is consistent with the general form of $\hat{H}$ for non-interacting particles, Equation (4.3.32).

Particle interactions

Hermitian operators can also be constructed out of other kinds of groupings of creation and annihilation operators. For example, a pairwise (two-particle) potential can be described with a superposition of creation and annihilation operator pairs, of the form

$$\hat{V} = \frac{1}{2} \sum_{\mu\nu\lambda\sigma} \hat{a}_{\mu}^{\dagger} \hat{a}_{\nu}^{\dagger} \, V_{\mu\nu\lambda\sigma} \, \hat{a}_{\sigma} \hat{a}_{\lambda}. \tag{4.3.43}$$

The prefactor of 1/2 is conventional. In terms of time evolution, $\hat{V}$ "transfers" (annihilates and then re-creates) a *pair* of particles during each infinitesimal time step. Since the number of annihilated particles is always equal to the number of created particles, the interaction conserves the total particle number. We can ensure that $\hat{V}$ is Hermitian by imposing a constraint on the coefficents:

$$\hat{V}^{\dagger} = \frac{1}{2} \sum_{\mu\nu\lambda\sigma} \hat{a}_{\lambda}^{\dagger} \hat{a}_{\sigma}^{\dagger} \, V_{\mu\nu\lambda\sigma}^{*} \, \hat{a}_{\nu} \hat{a}_{\mu} = \hat{V} \quad \Leftarrow \quad V_{\lambda\sigma\mu\nu}^{*} = V_{\mu\nu\lambda\sigma}. \tag{4.3.44}$$

Suppose we are given the two-particle potential as an operator $\hat{V}^{(2)}$ acting on the two-particle Hilbert space $\mathscr{H}^{(2)}$. We should be able to express the second-quantized operator $\hat{V}$ in terms of $\hat{V}^{(2)}$, by comparing their matrix elements. For example, consider the two-boson states

$$\begin{aligned} |n_{\mu} = 1, n_{\nu} = 1\rangle &= \frac{1}{\sqrt{2}} \Big(|\mu\rangle|\nu\rangle + |\nu\rangle|\mu\rangle \Big), \\ |n_{\lambda} = 1, n_{\sigma} = 1\rangle &= \frac{1}{\sqrt{2}} \Big(|\lambda\rangle|\sigma\rangle + |\sigma\rangle|\lambda\rangle \Big), \end{aligned} \tag{4.3.45}$$

where $\mu \neq \nu$ and $\lambda \neq \sigma$. The matrix elements of $V^{(2)}$ are

$$\begin{aligned} &\langle n_\mu = 1, n_\nu = 1 | V^{(2)} | n_\lambda = 1, n_\sigma = 1 \rangle \\ = \frac{1}{2}\Big(&\langle \mu | \langle \nu | V^{(2)} | \lambda \rangle \sigma \rangle + \langle \nu | \langle \mu | V^{(2)} | \lambda \rangle \sigma \rangle + \langle \mu | \langle \nu | V^{(2)} | \sigma \rangle \lambda \rangle + \langle \nu | \langle \mu | V^{(2)} | \sigma \rangle \lambda \rangle \Big). \end{aligned} \tag{4.3.46}$$

On the other hand, the matrix elements of the second-quantized operator $\hat{V}$ are

$$\langle n_\mu = 1, n_\nu = 1 | \hat{V} | n_\lambda = 1, n_\sigma = 1 \rangle = \sum_{\mu'\nu'\lambda'\sigma'} V_{\mu'\nu'\lambda'\sigma'} \langle \varnothing | \hat{a}_\nu \hat{a}_\mu \hat{a}^\dagger_{\mu'} \hat{a}^\dagger_{\nu'} \hat{a}_{\sigma'} \hat{a}_{\lambda'} \hat{a}^\dagger_\lambda \hat{a}^\dagger_\sigma | \varnothing \rangle \tag{4.3.47}$$

$$= \frac{1}{2} \big(V_{\mu\nu\lambda\sigma} + V_{\mu\nu\sigma\lambda} + V_{\nu\mu\lambda\sigma} + V_{\nu\mu\sigma\lambda} \big) \,. \tag{4.3.48}$$

In going from Equation (4.3.47) to (4.3.48), we use the bosonic commutation relations repeatedly to “pushing” the annihilation operators to the right (so that they can act upon $|\varnothing\rangle$) and the creation operators to the left (so that they can act upon $\langle\varnothing|$). Comparing Equation (4.3.46) to Equation (4.3.48), we see that the matrix elements match if we take

$$V_{\mu\nu\lambda\sigma} = \langle \mu | \langle \nu | V^{(2)} | \lambda \rangle | \sigma \rangle. \tag{4.3.49}$$

For instance, if the bosons have a position representation, we would have something like

$$V_{\mu\nu\lambda\sigma} = \int d^d r_1 \int d^d r_2 \; \varphi^*_\mu(r_1)\, \varphi^*_\nu(r_2)\, V(r_1, r_2)\, \varphi_\lambda(r_1)\, \varphi_\sigma(r_2). \tag{4.3.50}$$

The appropriate coefficients for $\mu = \nu$ and/or $\lambda = \sigma$, as well as for the fermionic case, are left for the reader to work out.

Other observables?

Another way to build a Hermitian operator from creation and annihilation operators is

$$\hat{A} = \sum_\mu \left(\alpha_\mu \hat{a}^\dagger_\mu + \alpha^*_\mu \hat{a}_\mu \right) \,. \tag{4.3.51}$$

If such a term is added to a Hamiltonian, it breaks the conservation of total particle number. Each infinitesimal time step will include processes that decrement the particle number (due to $\hat{a}_\mu$), as well as processes that increment the particle number (due to $\hat{a}^\dagger_\mu$). Even if the system starts out with a fixed number of particles, such as the vacuum state $|\varnothing\rangle$, it subsequently evolves into a superposition of states with different particle numbers. In the theory of quantum electrodynamics, this type of operator is used to describe the emission and absorption of photons caused by moving charges.

Incidentally, the name “second quantization” comes from this process of using creation and annihilation operators to define Hamiltonians. The idea is that single-particle quantum mechanics is derived by “quantizing” classical Hamiltonians via the imposition of commutation relations like $[x, p] = i\hbar$. Then, we extend the theory to multi-particle systems by using the single-particle states to define creation/annihilation operators obeying commutation or anticommutation relations. This can be viewed as a “second” quantization step.
