Many-body systems; Bosons and Fermions

The topic of many-body systems and particle statistics properly belongs to quantum field theory, but it is traditional to attempt to treat these subjects within the paradigm of standard quantum mechanics. This leads to a fair amount of mysticism, which one should view simply as ‘rules of thumb’ intended to help us perform calculations within standard QM that are consistent with what would be calculated rigorously using QFT. I have to say that I really don’t like the discussion in Cohen-Tannoudji et al, so Merzbacher Chapter 21 is my preferred reading this week, but you may want to have a look at C-T Ch. XIV anyway to get a feeling for the more standard presentation.

Identical particles

So far in this course we have built up a fairly complete and consistent picture of the mechanics of individual quantum systems, and we have looked at a few examples of interacting systems as well. To what we have learned so far we must now add some new physics, which becomes relevant when considering systems of identical particles. As a remarkable reflection of the underlying quantum field nature of the real world, identical particles whose wave-functions are not orthogonal can behave in a concerted and coordinated manner, even when there is no ‘real’ physical interaction between them in the sense of an interaction Hamiltonian! This type of intrinsic coordination in the behavior of systems of many identical particles has particularly strong consequences for statistical mechanics in ‘quantum’ regimes, such as very low temperature (liquid Helium) or very high density (neutron stars).

In terms of many-body behavior, the known particles break up fairly cleanly into two families. Particles with integer total intrinsic spin obey Bose-Einstein statistics and are known as Bosons, whereas particles with half-integer total intrinsic spin obey Fermi-Dirac statistics and are known as Fermions. Here the term ‘particle’ must be understood to include elementary particles such as quarks and electrons, and under certain conditions also composite particles such as nucleons, atoms, or molecules. Roughly speaking, such composite objects must be treated as identical particles when a collection of them are prepared in exactly the same internal state and can somehow be constrained to stay that way. This can be arranged, for example, for a collection of atoms prepared in a non-degenerate ground state by ensuring that the energy scale of all physical processes involved is much less than that required to reach the lowest-lying excited state. A now famous example of this is the Bose-Einstein condensation of alkali atoms such as Rubidium and Sodium. Certain types of ‘quasi-particle’ excitations in condensed-matter systems can actually obey a more general type of statistics, and are known as anyons. These play an important role in the quantum Hall effect, and it is hoped that a particularly exotic (and so-far completely hypothetical) class of quasi-particles known as non-Abelian anyons could
be used for intrinsically fault-tolerant quantum computation.

The general idea, in my picture of things, is that the quantum mechanics we know and love with particles and wave functions is really just an approximation to quantum field theory. The things we like to think of as individual elementary particles are really just excitations of some corresponding field, but we can think of these particles as independent ‘entities’ living in their own Hilbert spaces so long as we don’t consider situations in which more than one identical particle ends up in precisely the same ‘mode.’ In the latter type of situation, the particles can behave in a coordinated manner even in the absence of Hamiltonian interaction because they are really excitations of the same field, e.g., the electromagnetic field (photons) or the electron field (electrons and positrons). Where composite particles are concerned, I suppose we must believe that the field-field interactions that support the relevant bound states, e.g. of the electron and positron in a hydrogen atom, can somehow be wrapped up into a single ‘effective’ field of which the composite particles may be considered elementary excitations.

**Fock spaces and particle creation/annihilation operators**

Say we have a system of many identical particles. If our description of any single one of them would have involved a Hilbert space $H^p$, then in principle we can think of the joint state as living in the multiple-tensor product space

$$H^{tot} \sim H^p \otimes H^p \otimes H^p \otimes \cdots.$$ 

Suppose the set of kets $\{|X_k\rangle\}$ represents a basis for $H^p$, perhaps the energy basis but not necessarily. Then the spirit of quantum many-body theory is to describe the overall state of the multiparticle system solely in terms of the occupation numbers $n_k$, where $n_0$ represents the number of particles in state $|X_0\rangle$, $n_1$ represents the number of particles in state $|X_1\rangle$, etc. A state vector representing the overall multiparticle state may therefore be written

$$|n_0 n_1 n_2 n_3 \cdots\rangle,$$

where if the total number of particles is fixed at $N$ we should require

$$\sum_k n_k = N.$$

Note however that quantum many-body theory is perfectly capable of describing situations in which the total number of particles is not fixed (e.g. photon absorption/emission, electron-positron annihilation), in which case we would allow basis vectors with arbitrary $\sum n_k$. When we view $H^{tot}$ as being the space spanned by occupation-number states of the above form (Fock states), we refer to it as Fock space.

What we need for dynamics is to define operators that change the occupation number of a given state. Then for example the transition of one particle from state $j$ to state $k$ can be thought of as a process in which $n_j \mapsto n_j - 1$ and $n_k \mapsto n_k + 1$. These operators are commonly called creation and annihilation operators, and for Bosons they bear formal resemblance to the ladder operators for a harmonic oscillator. In general (for any particle statistics), we define

$$a_j |n_0 n_1 n_2 n_3 \cdots n_{j-1} n_j n_{j+1} \cdots\rangle \propto |n_0 n_1 n_2 n_3 \cdots n_{j-1} (n_j - 1) n_{j+1} \cdots\rangle,$$

$$a_k^\dagger |n_0 n_1 n_2 n_3 \cdots n_{k-1} n_k n_{k+1} \cdots\rangle \propto |n_0 n_1 n_2 n_3 \cdots n_{k-1} (n_k + 1) n_{k+1} \cdots\rangle.$$
where the constants of proportionality must be derived, and the action of operators such as \( a_j \) and \( a_k \) are the obvious
\[
\begin{align*}
    a_j^\dagger | n_0 n_1 n_2 n_3 \cdots n_{j-1} n_j n_{j+1} \cdots \rangle & \propto | n_0 n_1 n_2 n_3 \cdots n_{j-1} (n_j + 1) n_{j+1} \cdots \rangle, \\
    a_k^\dagger | n_0 n_1 n_2 n_3 \cdots n_{k-1} n_k n_{k+1} \cdots \rangle & \propto | n_0 n_1 n_2 n_3 \cdots n_{k-1} (n_k - 1) n_{k+1} \cdots \rangle.
\end{align*}
\]
Note that an annihilation operator \( a_j \) is related to the corresponding creation operator \( a_j^\dagger \) by Hermitian conjugate, so these operators are certainly not Hermitian.

The Fock state with no particles at all, which we shall write \( |0\rangle \), is by convention known as the vacuum state. An elementary requirement for the creation and annihilation operators is that
\[
a_j |0\rangle = 0
\]
for all \( j \). We can also make a start at fixing the constants of proportionality in the above expressions (matrix elements of the operators) by requiring
\[
\begin{align*}
a_j^\dagger |0\rangle &= |0000 \cdots n_j = 1 \cdots \rangle, \\
a_k^\dagger |0000 \cdots n_j = 1 \cdots \rangle &= a_k a_j^\dagger |0\rangle \\
&= \delta_{jk} |0\rangle.
\end{align*}
\]
In order to proceed any further, however, we must establish the commutation relations among these operators.

In order to do that, we must first introduce a simple but crucial assumption about our theory, known as the principle of unitary symmetry. This principle states that our Fock-space description of a many-body system should be equivalent for any choice of single-particle basis \( \{|X_k\}\). Suppose for example that we want to transform to a basis spanned by the kets \( \{|Y_q\}\), specified by
\[
|X_k\rangle = \sum_q |Y_q\rangle \langle Y_q |X_k\rangle,
\]
where the complex coefficients \( \langle Y_q |X_k\rangle \) form a unitary matrix. Relative to this new choice of basis, we will have new occupation numbers \( \tilde{n}_q \) and a modified set of annihilation and creation operators \( \{b_q, b_q^\dagger\} \) for the Fock space. Thinking about just the one-particle states, and noting that one particle in \( H_{tot} \) is one particle in \( H_{tot} \) regardless of our choice of basis in \( H_P \), we must have
\[
\begin{align*}
a_k^\dagger |0\rangle &= |n_k = 1\rangle \\
&= \sum_q |\tilde{n}_q = 1\rangle \langle \tilde{n}_q = 1 |n_k = 1\rangle \\
&= \sum_q |\tilde{n}_q = 1\rangle \langle Y_q |X_k\rangle \\
&= \sum_q b_q^\dagger |0\rangle \langle Y_q |X_k\rangle
\end{align*}
\]
where \( \langle Y_q |X_k\rangle \) are elements of the same unitary matrix that defines the transformation of basis \( \{|X_k\}\) \( \rightarrow \) \( \{|Y_q\}\). At the operator level, then, at least as far as their action on the vacuum state is concerned, we may write
\[ a_k^\dagger = \sum_q b_q^\dagger \langle Y_q | X_k \rangle. \]

It turns out that this general relation, as well as the Hermitian conjugate expression
\[ a_k = \sum_q \langle X_k | Y_q \rangle b_q, \]
may be consistently enforced on the entire Fock space. The resulting picture is that, in general, the creation (or destruction) of a particle of type \( |X_k\rangle \) is strictly equivalent to the creation (or destruction) of a ‘superposition of particles’ \( |Y_q\rangle \) so long as the coefficients of the terms in this superposition are consistent with \( \langle Y_q | X_k \rangle \). For example, we might have
\[ |n_k = 1\rangle = \sum_q c_q |\bar{n}_q = 1\rangle, \]
\[ = \sum_q c_q b_q^\dagger |\bar{0}\rangle, \]
where it should be emphasized that the expression on the RHS is strictly a one-particle state as long as
\[ \sum_q |c_q|^2 = 1. \]

This can be seen by defining number operators in analogy to the harmonic oscillator case. For any given mode,
\[ n_i = a_i^\dagger a_i, \]
\[ \bar{n}_q = b_q^\dagger b_q \]
and the total number of particles in any mode is given by
\[ N = \sum_i n_i \]
\[ = \sum_q \bar{n}_q. \]

Then
\[ \langle n_k = 1 | N | n_k = 1 \rangle = \left[ \sum_q c_q^* \langle \bar{n}_q = 1 \rangle \right] \left[ N \sum_q c_q |\bar{n}_q = 1\rangle \right] \]
\[ \langle n_k = 1 | \sum_i a_i^\dagger a_i | n_k = 1 \rangle = \left[ \sum_q c_q^* \langle \bar{n}_q = 1 \rangle \right] \left[ \sum_j b_j^\dagger b_j \left[ \sum_q c_q |\bar{n}_q = 1\rangle \right] \right] \]
\[ 1 = \left[ \sum_q c_q^* \langle \bar{n}_q = 1 \rangle \right] \left[ \sum_q c_q |\bar{n}_q = 1\rangle \right] \]
\[ = \sum_q |c_q|^2. \]

**Operator algebra**
Let's now consider the simultaneous action of two creation operators,
\[ |\Psi\rangle \rightarrow a_i^+ a_j^+ |\Psi\rangle, \]
where \(|\Psi\rangle\) is an arbitrary state in the Fock space. Now it stands to reason that if we were to apply the creation operators in the opposite order, the final state should be the same (we are still just adding the same two particles) but perhaps the constant of proportionality would be different. Hence,
\[ a_i^+ a_j^+ |\Psi\rangle = \lambda a_j^+ a_i^+ |\Psi\rangle. \]

Our task now is to determine \(\lambda\), which equivalently fixes the commutator of \(a_i^+\) and \(a_j^+\) since
\[ a_i^+ a_j^+ - \lambda a_j^+ a_i^+ = 0 \]

\[ = a_i^+ a_j^+ - a_j^+ a_i^+ - (\lambda - 1) a_j^+ a_i^+, \]

\[ \left[ a_i^+, a_j^+ \right] = (\lambda - 1) a_j^+ a_i^+. \]

To do this we need to apply our principle of unitary symmetry. Written in the transformed basis,
\[
a_i^+ a_j^+ = \left[ \sum_k b_k^+ \langle Y_k | X_i \rangle \right] \left[ \sum_l b_l^+ \langle Y_l | X_j \rangle \right] = \sum_{k,l} \langle Y_k | X_i \rangle \langle Y_l | X_j \rangle b_k^+ b_l^+, \]

\[ \lambda a_j^+ a_i^+ = \lambda \left[ \sum_l b_l^+ \langle Y_l | X_j \rangle \right] \left[ \sum_k b_k^+ \langle Y_k | X_i \rangle \right] = \lambda \sum_{k,l} \langle Y_k | X_i \rangle \langle Y_l | X_j \rangle b_l^+ b_k^+, \]

\[ (a_i^+ a_j^+ - \lambda a_j^+ a_i^+) |\Psi\rangle = \sum_{k,l} \langle Y_k | X_i \rangle \langle Y_l | X_j \rangle \left( b_k^+ b_l^+ - \lambda b_l^+ b_k^+ \right) |\Psi\rangle = 0. \]

Since the transformation coefficients \(\langle Y_k | X_i \rangle \langle Y_l | X_j \rangle\) are arbitrary up to unitarity, the above equation can be satisfied for all possible \(|\Psi\rangle\) only if, for every possible value of \(k\) and \(l\),
\[ b_k^+ b_l^+ - \lambda b_l^+ b_k^+ = 0. \]

Since \(k\) and \(l\) are arbitrary in this expression, and for example can therefore be swapped, then with the same \(\lambda\) we also require
\[ b_k^+ b_l^+ - \lambda b_l^+ b_k^+ = 0. \]

We can now substitute the second expression into the first to obtain
\[ b_k^+ b_l^+ - \lambda^2 b_l^+ b_k^+ = 0, \]
meaning
\[ \lambda = \pm 1. \]

Since our choices of initial and transformed representations are completely arbitrary, it thus follows that the set of creation operators for any given representation of the Fock space must satisfy one of two possible commutation relations:
\[ a_i^+ a_j^+ - a_j^+ a_i^+ = 0, \]
or
\[ a_i^\dagger a_j^\dagger + a_j^\dagger a_i^\dagger = 0. \]
In the former case we say that the operators commute, in the latter case we say that the operators \textit{anticommute}. Likewise, by Hermitian conjugate, we have
\[ a_i a_j - a_j a_i = 0, \quad \text{OR} \]
\[ a_i a_j + a_j a_i = 0. \]
It turns out that a given species of particle has consistent \( \lambda \) for the annihilation and creation operators.

Now considering
\[ a_i a_j |\Psi\rangle = \mu a_j^\dagger a_i |\Psi\rangle, \]
we have the condition
\[ (a_i a_j^\dagger - \mu a_j a_i^\dagger) |\Psi\rangle = \sum_{k,l} \langle X_i | Y_k \rangle \langle Y_j | X_l \rangle \left( b_k b_l^\dagger - \mu b_l b_k^\dagger \right) |\Psi\rangle = 0 \]
for any state \( |\Psi\rangle \). Since we now have one creation and one annihilation operator in each term, we must take care of the unitarity condition
\[ \sum_k \langle X_i | Y_k \rangle \langle Y_k | X_j \rangle = \delta_{ij}, \]
since we may get special cancellations in the summation for \( l = k \). For the case \( k \neq l \), we can still argue that we must have
\[ b_i b_j^\dagger - \mu b_j b_i^\dagger = 0 \quad \text{for } k \neq l \]
\[ a_i a_j^\dagger - \mu a_j a_i^\dagger = 0 \quad \text{for } i \neq j. \]
Substituting the former result back into the general expression, we get
\[ (a_i a_j^\dagger - \mu a_j a_i^\dagger) |\Psi\rangle = \sum_{k,l} \langle X_i | Y_k \rangle \langle Y_j | X_l \rangle \left( b_k b_l^\dagger - \mu b_l b_k^\dagger \right) |\Psi\rangle \]
\[ = \sum_k \langle X_i | Y_k \rangle \langle Y_k | X_j \rangle \left( b_k b_k^\dagger - \mu b_k b_k^\dagger \right) |\Psi\rangle. \]
Next we note that as long as
\[ b_k b_k^\dagger - \mu b_k b_k^\dagger = A, \]
where \( A \) is some operator independent of the index \( k \), we’ll get
\[ (a_i a_j^\dagger - \mu a_j a_i^\dagger) |\Psi\rangle = \sum_k \langle X_i | Y_k \rangle \langle Y_k | X_j \rangle \left( b_k b_k^\dagger - \mu b_k b_k^\dagger \right) |\Psi\rangle \]
\[ = A \sum_k \langle X_i | Y_k \rangle \langle Y_k | X_j \rangle |\Psi\rangle \]
\[ = A \delta_{ij} |\Psi\rangle. \]
Looking at the case \( j = i \), we note that this implies
\[ a_i a_i^\dagger - \mu a_i a_i^\dagger = A \]
as well, meaning that the operator \( A \) appearing in the commutation relation is \textit{basis-independent} and the same for every quantum number \( i \). If we let this expression act on the vacuum, we find
\[ A \left| \vec{0} \right> = (a_i a_i^\dagger - \mu a_i^\dagger a_i) \left| \vec{0} \right> \]
\[ = a_i a_i^\dagger \left| \vec{0} \right> \]
\[ = \left| \vec{0} \right>. \]

meaning that we may choose \( A = 1 \) (the identity operator). Hence, \( a_i a_i^\dagger - \mu a_i^\dagger a_i = 1. \)

In order to finally pin down \( \mu \), we must consider commutators with the number operator \( n_k \). Clearly we require, for \( j \neq k \),

\[ n_j a_j = a_j n_k, \]
\[ n_k a_j^\dagger = a_j^\dagger n_k, \]

since we don’t want the particle count in mode \( k \) to depend on the addition or subtraction of particles in a different mode. Within a given mode, we require

\[ n_i a_k = a_k (n_k - 1), \]
\[ n_i a_k - a_k^\dagger n_k = -a_k, \]
\[ n_i a_k^\dagger = a_k^\dagger (n_k + 1), \]
\[ n_i a_k^\dagger - a_k n_i = a_k, \]

in order to have proper counting. For these to be consistent with the commutation relations derived above, we finally require

\[ (1 \pm \mu) n_i a_k = 0 \]

for all \( i \neq k \). This expression is derived with a plus sign for the case \( \lambda = +1 \), and with a minus sign for the case \( \lambda = -1 \).

Collecting everything together, we finally have

**Bose-Einstein case** :
\[ a_k a_i - a_i a_k = 0, \]
\[ a_k a_i^\dagger - a_i^\dagger a_k^\dagger = 0, \]
\[ a_i a_i^\dagger - a_i^\dagger a_i = \delta_{ii} 1. \]

**Fermi-Dirac case** :
\[ a_k a_i + a_i a_k = 0, \]
\[ a_k a_i^\dagger + a_i^\dagger a_k^\dagger = 0, \]
\[ a_i a_i^\dagger + a_i^\dagger a_i = \delta_{ii} 1. \]

As it turns out, a deep connection between particle statistics and the transformation of states under spatial rotations can be understood from quantum field theory, resulting in the fact that particles with zero or integer spin are Bosons, whereas particles with half-integer spin are Fermions.

A final detail to clean up are those constants of proportionality in the definitions of the annihilation and creation operators. In general there are phase ambiguities, but the following definitions are conventional and consistent with the commutation relations:
Bose-Einstein case:
\[
\begin{align*}
    a_k |n_k\rangle &= \sqrt{n_k} |n_k - 1\rangle, \\
    a_k^\dagger |n_k\rangle &= \sqrt{n_k + 1} |n_k + 1\rangle,
\end{align*}
\]

Fermi-Dirac case:
\[
\begin{align*}
    a_k |n_k = 0\rangle &= 0, \\
    a_k |n_k = 1\rangle &= \exp(i\alpha) |n_k = 0\rangle, \\
    a_k^\dagger |n_k = 0\rangle &= \exp(-i\alpha) |n_k = 1\rangle, \\
    a_k^\dagger |n_k = 1\rangle &= 0.
\end{align*}
\]

Here \(\exp(i\alpha)\) may be chosen to equal 1 if the number of occupied one-particle states with index less than \(k\) is even, or \(-1\) if this number is odd. Other conventions are possible but one must take care to stay consistent with the Fermionic commutation relations.

A remarkable immediate consequence of all this is that for Fermions,
\[
a_k^\dagger a_k + a_k a_k^\dagger = 0,
\]

implying \(a_k^\dagger a_k = 0\). In other words, \textit{no two Fermions can occupy exactly the same quantum state}, a principle which you may know otherwise as the Pauli exclusion principle!

A corresponding result for Bosons is that matrix elements of transition operators such as
\[
a_l^\dagger a_k, \quad l \neq k,
\]

which ‘scatter’ one particle from mode \(k\) to mode \(l\), have matrix elements that scale as \(\sqrt{n_l + 1}\), and therefore induce transition rates (where Fermi’s Golden Rule applies) that scale as \(n_l + 1\). Note that the corresponding scaling with \(n_k\) may not be so surprising (more candidates to perform the transition) but the scaling with \(n_l\) is actually rather strange – as if Bosons like to ‘sympathetically’ go to final states that already have lots of Bosons! This phenomenon is sometimes referred to as Bose enhancement.