Harmonic Oscillator, $a$, $a^\dagger$, Fock Space, Identicle Particles, Bose/Fermi

This set of lectures introduces the algebraic treatment of the Harmonic Oscillator and applies the result to a string, a prototypical system with a large number of degrees of freedom. That system is used to introduce Fock space, discuss systems of identicle particles and introduce Bose/Fermi annihilation and creation operators.

■ Harmonic Oscillator

■ Classic SHO

The classical Hamiltonian for the simple harmonic oscillator is

$$H = \frac{1}{2m} p^2 + \frac{k}{2} x^2 = \frac{1}{2m} p^2 + \frac{m\omega^2}{2} x^2$$

This leads to simple harmonic motion with frequency $\omega = \sqrt{k/m}$.

■ QM: wave mechanics

Make the replacement $p = -i \hbar \frac{\partial}{\partial x}$, and solve for the wave functions. For example, Merzbacher chapter 5.

■ QM: operator approach

Introduce raising and lowering operators ($a$ and $a^\dagger$) and solve simple algebraic eigenvalue problem. Note: in some contexts (field theory) $a$, $a^\dagger$ are also known as annihilation and creation operators.

■ Set up of problem, introduction of $a$, $a^\dagger$, and $N$

■ For convenience simplify $H$

Define: $p' = \frac{p}{\sqrt{m\omega}}$ and $x' = \sqrt{m\omega} x$, in which case $H$ can be rewritten as

$$H = \frac{\omega}{2} (p'^2 + x'^2)$$

■ Define $a$ and $a^\dagger$.

Further, define the operator

$$a = \frac{1}{\sqrt{2}} (x' + ip')$$

and since $x$ and $p$ are hermitian, the adjoint is

$$a^\dagger = \frac{1}{\sqrt{2}} (x' - ip').$$
Also note that $x'$ and $p'$ can be rewritten as

$$x' = \frac{1}{\sqrt{2}} (a^\dagger + a) \quad \text{and} \quad p' = \frac{i}{\sqrt{2}} (a^\dagger - a).$$

The commutator of $a$ and $a^\dagger$ is

$$[a, a^\dagger] = \frac{1}{2} [x' + ip', x' - ip'] = i[p', x'] = i[p, x] = 1$$

and

$$a^\dagger a = \frac{1}{2} (x' - ip')(x' + ip') = \frac{1}{2} (x'^2 + p'^2 + i[x', p']) = \frac{1}{2} (x'^2 + p'^2) - \frac{1}{2}$$

$$a a^\dagger = \frac{1}{2} (x' + ip')(x' - ip') = \frac{1}{2} (x'^2 + p'^2 - i[x', p']) = \frac{1}{2} (x'^2 + p'^2) + \frac{1}{2}$$

■ Define $N$ and rewrite $H$

It is convenient to recast $H$

$$H = \frac{\omega}{2} (p'^2 + x'^2)$$

$$= \omega (a^\dagger a + \frac{1}{2})$$

$$= \omega (N + \frac{1}{2})$$

where the "number" operator is $N = a^\dagger a$. It should be obvious that $[H, N] = 0$, and so $H$ and $N$ can be simultaneously diagonalized. Determining the spectrum of energy eigenstates can be reclassified as determining the spectrum of $N$.

■ The spectrum of states

Define $\{|n\rangle\}$ as the normalized eigenstates of $N$, and let it be understood that the states are labeled by the eigenvalue, i.e.

$$N |n\rangle = n |n\rangle$$

■ Show $n$ is positive definite

Consider the quantity $\langle n | N | n\rangle = n \langle n | n\rangle = n$.

It is convenient to define $|b\rangle = a |n\rangle$. Since $N = a^\dagger a$ we also have

$$\langle n | N | n\rangle = \langle n | a^\dagger a | n\rangle = \langle b | b\rangle \geq 0.$$

It follows that $n$ is real and positive-definite.

■ Show that $a$ is a lowering operator.

$$[a, N] = a (a^\dagger a) - (a^\dagger a) a$$

$$= (a a^\dagger) a - (a^\dagger a) a$$

$$= [a, a^\dagger] a$$

$$= a$$
Again, let $|b\rangle = a |n\rangle$, so that

\[
N |b\rangle = N a |n\rangle
\]
\[
= (\{N, a\} + a N) |n\rangle
\]
\[
= (-a + a n) |n\rangle
\]
\[
= (n - 1) a |n\rangle
\]
\[
= (n - 1) |b\rangle
\]

i.e. $|b\rangle$ is an eigenstate of $N$, with eigenvalue $(n - 1)$, or

$\alpha|n\rangle = c_n |n - 1\rangle$

where $c_n$ is some as yet undetermined coefficient.

We can evaluate $c_n$ by considering

\[
n = \langle n | N | n \rangle = \langle n | a^\dagger a | n \rangle = |c_n|^2.
\]

which gives $c_n = e^{i\phi} \sqrt{n}$. Conventionally $\phi = 0$, which gives

$\alpha|n\rangle = \sqrt{n} |n - 1\rangle$.

**and $\alpha^\dagger$ is a raising operator**

Similarly $[N, a^\dagger] = a^\dagger$ and $a^\dagger |n\rangle = b_{n+1} |n + 1\rangle$, where $b_n = \sqrt{n}$ as well. $a^\dagger$ acts as a raising operator -

$\alpha^\dagger |n\rangle = \sqrt{n + 1} |n + 1\rangle$.

It is often more convenient in this form. $\alpha^\dagger |n - 1\rangle = \sqrt{n} |n\rangle$, where we can easily see

\[
N |n\rangle = \alpha^\dagger a |n\rangle = \alpha^\dagger \sqrt{n} |n - 1\rangle = n |n\rangle.
\]

**spectrum**

So far we have showed how to construct a set of states $|n\rangle$ with $n$ values separated by integers. There are, however, many such sets, but only one is a viable set of states for the SHO. Recall that we have the constraint that $n \geq 0$.

Suppose $n$ is in the interval $(0, 1)$. Then operating with $a$ would give a state with $n < 0$, which is not allowed. The only possibility is that operating with $a$ gives 0, but that would violate the relation for $c_n$ - unless $n = 0$. It seems the only possibility is for $n$ to be integral. In this case we can satisfy the boundary condition by $a |0\rangle = 0 |0\rangle = 0$. The spectrum of states is then given by $\{ |n\rangle, n = \{0, 1, 2, \ldots\}\}$.

This seems very reasonable. As the Hamiltonian is positive definite, the expectation value is required to be positive. Even with the extra contribution of $\frac{1}{2}$ it is not unreasonable that $N$ is also positive.

One can build normalized states by iterative use of the raising operator.

\[
|n\rangle = \frac{(\alpha^\dagger)^n}{\sqrt{n!}} |0\rangle
\]
Matrix form for operators

$H$, $N$, $a$, $a^\dagger$. It is straightforward to express the operators in matrix form (see Merzbacher). $H$ and $N$ are diagonal. $a$ and $a^\dagger$ are off diagonal. e.g.

$$H = \omega \begin{pmatrix} \frac{1}{2} & 0 & \cdots \\ 0 & \frac{3}{2} & 0 \\ \vdots & 0 & \ddots \end{pmatrix}, \quad a = \begin{pmatrix} 0 & \sqrt{1} & 0 & \cdots \\ 0 & 0 & \sqrt{2} & 0 \\ 0 & 0 & 0 & \sqrt{3} \\ \vdots & 0 & 0 & \ddots \end{pmatrix}$$

or $a = \sum_n \sqrt{n} \ |n-1\rangle \langle n|$. 

Useful relation

A useful fact for doing some manipulations (for example problem 2.18) is

$$[a, f(a^\dagger)] = \frac{\partial}{\partial \omega} f(a^\dagger)$$

This is similar to $[k, x] = -i \frac{\partial}{\partial x}$

Fock Space - "2nd quantization"

The harmonic oscillator provides a starting point for discussing a number of more advanced topics, including multiparticle states, identical particles and field theory.

As an introduction, consider the problem of quantizing a classical string (e.g. a guitar string). This is done by treating the oscillating modes of the string as a set of harmonic oscillators. Each H.O. can be quantized, so that the quantum state of the string is given by specifying the quantum state of each oscillator. This is sometime referred to as "second quantization". Presumably the term is meant to suggest that the first quantization is determining the eigenmodes of the system, and the second quantization is determining the excitation level of each mode.

An alternative language for discussing the quantized string is to label the excitations of the individual modes as particles. This language naturally carries over to any number of classical systems that exhibit oscillatory behavior, including transverse phonons on a string, longitudinal phonons through a medium, and photons as quantized oscillations of the electromagnetic radiation. These particles are all examples of Bosons. Bose systems may exhibit a large degree of excitation. In the particle language this is equivalent to discussing a system with a large number of particles. the particles are identicle, although they may be found in different states. Accordingly, it is natural to discuss the quantum theory of identical particles at this time. The concept of annihilation and creation operators for Bosons, can be extended to describe Fermi systems as well.

Quantize simple string

The energy for a classical string is given by the sum of the kinetic and potential energies.

$$E = T + U$$
To be specific, consider boundary conditions where the string is stretched between two fixed end points at \( x = (0, L) \), the string has mass density \( \rho \), and tension \( \kappa \). Let the position of string be \( y(x, t) \). Then

\[
T = \frac{\mu}{2} \int_0^L y'^2 \\
U = \frac{\kappa}{2} \int_0^L y'^2
\]

**Expansion in eigenfunctions**

Next, expand \( y \) in terms of normalized eigenfunctions for the string.

\[
y(x, t) = \sum_n y_n(t) \sqrt{\frac{2}{L}} \sin\left(\frac{n \pi x}{L}\right)
\]

Then, the kinetic and potential energy terms can be reexpressed as a sum over modes.

\[
\int_0^L y'^2 = \int_0^L \left( \sum_n \dot{y}_n \sqrt{\frac{2}{L}} \sin\left(\frac{n \pi x}{L}\right) \right) \left( \sum_m \dot{y}_m \sqrt{\frac{2}{L}} \sin\left(\frac{m \pi x}{L}\right) \right) \\
= \sum_{n,m} \dot{y}_n \dot{y}_m \sqrt{\frac{2}{L}} \int_0^L \sin\left(\frac{n \pi x}{L}\right) \sin\left(\frac{m \pi x}{L}\right) \\
= \sum_{n,m} \dot{y}_n \dot{y}_m \delta_{nm} \\
= \sum_n |y_n|^2
\]

\[
\int_0^L y'^2 = \int_0^L \left( \sum_n y_n \sqrt{\frac{2}{L}} \cos\left(\frac{n \pi x}{L}\right) \right) \left( \sum_m y_m \sqrt{\frac{2}{L}} \cos\left(\frac{m \pi x}{L}\right) \right) \\
= \sum_{n,m} y_n y_m \sqrt{\frac{2}{L}} \left( \frac{n \pi}{L} \right) \left( \frac{m \pi}{L} \right) \int_0^L \cos\left(\frac{n \pi x}{L}\right) \cos\left(\frac{m \pi x}{L}\right) \\
= \sum_{n,m} y_n y_m \left( \frac{n \pi}{L} \right) \left( \frac{m \pi}{L} \right) \delta_{nm} \\
= \sum_n \left( \frac{n \pi}{L} \right)^2 |y_n|^2 \\
= \sum_n k_n^2 |y_n|^2
\]

**string = sum over harmonic oscillators**

These results can be used to reexpress the Hamiltonian as a sum over harmonic oscillators.

\[
H = \frac{1}{2} \sum_n \rho |\dot{y}_n|^2 + \kappa k_n^2 |y_n|^2 \\
= \sum_n \frac{\rho}{2} \left( p_n^2 + q_n^2 \right) = \sum_n \omega_n (a_n^+ a_n + \frac{1}{2})
\]

where
\[ p_n = \frac{\dot{y}_n}{\sqrt{\rho \omega_n}} \]
\[ q_n = y_n \frac{1}{\sqrt{\rho \omega_n}} \]
\[ a_n = \frac{1}{\sqrt{2}} (q_n + i p_n) \]
\[ a_n^\dagger = \frac{1}{\sqrt{2}} (q_n - i p_n) \]
\[ \omega_n = \sqrt{\rho / k} \ k_n = c \ k_n = \omega_0 \ n \]
\[ \omega_0 = \frac{2 \pi}{L} \]

**Fock space: basis states for the string**

From the above discussion, a continuous string can be described by a large (infinite) number of QM harmonic oscillators, one harmonic oscillator for each eigenfunction describing the string's motion. Denote the oscillators by the subscript \( i \). The basis states for each oscillator can be chosen to be the eigenstates of the number operator \( N_i \), and the basis states for the string may be taken to be a product of the individual oscillator basis states. A string basis state can therefore be described by an infinite dimensional vector specifying the state of each of the harmonic oscillators.

\[ |\vec{n}\rangle = |n_1\rangle \otimes |n_2\rangle \otimes |n_3\rangle \otimes ... = |n_1, n_2, n_3, ... \rangle \]

and each of the \( n_i \) may be a non-negative integer. An arbitrary state of the string \( |\alpha\rangle \) would be given by a superposition

\[ |\alpha\rangle = \sum_{n_1=0}^{\infty} \sum_{n_2=0}^{\infty} \sum_{n_3=0}^{\infty} \ldots c_n \ |\vec{n}\rangle \]

where the \( c_n \) are complex numbers.

The lowest energy state of the string is one where all the \( n_i \) are 0. Note that the lowest energy state has infinite energy, from summing up all the zero point energies for each of the individual oscillators, \( E_0 = \sum \frac{\omega_i}{2} = \infty \). It is conventional to ignore this infinity, noting that absolute energy scales are not observable, only relative energy scales. With this subtraction, the energy of a string state is

\[ E = \langle \vec{n} | H | \vec{n}\rangle = \langle \vec{n} | \sum_i \omega_i \ | \vec{n}\rangle = \sum_i n_i \omega_i \]

The basis states of the string can be built up from the ground state by operating with appropriate raising operators. For example,

\[ |1, 0, 0, ...\rangle = a_1^\dagger \ |0, 0, 0, ...\rangle \]

The operator \( a_1^\dagger \) raises the excitation level of the lowest mode by 1.

It is important to distinguish the effect of raising the excitation amplitude of a given mode, from the effect of shifting excitations to a higher mode. In the context of a guitar string, shifting to a higher mode corresponds to a higher frequency or a higher "note". Increasing the excitation of a given mode, corresponds to making that note "louder". For example, suppose the string is in the \( n_1 = 1 \) state, \( |1, 0, 0, ...\rangle \). The energy is \( \omega_0 \). We can increase the energy to \( 2 \omega_0 \) either by increasing the amplitude to the \( n_1 = 2 \) state, or by increasing the frequency by shifting the excitation to the 2\(^{nd} \) mode.

\[ |2, 0, 0, ...\rangle = a_1^\dagger |1, 0, 0, ...\rangle \quad \text{or} \quad |0, 1, 0, ...\rangle = a_1^\dagger a_1 |1, 0, 0, ...\rangle \]
For a highly excited string there is a large amount of degeneracy...all states where \( E = \omega_0 \sum_i n_i \) such that the \( i n_i \) add up to the same total are degenerate.

- **Particles as excitations**

At this point, each of the \( n_i \) specifies the degree of excitation of the \( i \)th mode of the string. There is, however, a natural interpretation where the excitations may be thought of as "particles", and the \( n_i \) represent the number of particles in a given mode. In the case of excitations on a string, the oscillations of the string correspond to sound waves, and we call the particles "phonons". The concept can be extended to any "field". In the present case, the field is the lateral or transverse displacement of the string. The restoring force which provides for the potential energy is the string tension.

In the case of sound waves in a liquid or gas, the field is the longitudinal displacement of the atoms in the material, and the restoring force is pressure in the fluid. When considering electromagnetic radiation, the field is the vector potential \( A \), and the potential energy is associated with gradients of \( A \) providing tension in the field (also known as \( E \) and \( B \)). Such particles are called photons. We will develop the concept of photons more thoroughly when discussing radiative transitions.

The analogy is a bit more difficult when discussing electrons. What, after all, is supposed to play the role of the field? A couple of comments are in order. First, phonons and photons are massless. As a result the spectrum of modes includes long wavelength, low frequency oscillations. We can observe the effects of such modes with macroscopic instruments. Electrons, on the other hand, have mass. Even low momentum modes have energies comparable to the mass, and thus oscillate at a high frequency, not easily measured by humans. More importantly, phonons and photons are bosons, and the spectrum of states includes occupation numbers with large values of individual \( n_i \). Such states are recognized as classical fields. Electrons, however, are fermions which admit to \( n_i = 0 \) or \( 1 \) (see below). Large occupation numbers are not permitted, and there is no analog of the classical field. That does not mean electrons cannot be described in terms of a field theory, only that we do not have direct experience with the field in a classical configuration. Thus, at this juncture, there is no reason not to consider electrons as excitations of an underlying field theory. Instead of discussing the state of an electron, we could discuss the number of excitations for a given mode of the electron field.

When using the particle language, it is common to refer to the raising and lowering operators as creation and annihilation operators. In the example above, The operator \( a_1^\dagger \) creates a phonon in lowest mode. Similarly, \( a_1 \) destroys or annihilates a phonon from the first mode. If there are no phonons in the mode, the result of operating with \( a_1 \) is 0.

The total number of particles in the state is given by the number operator, \( N = \Sigma_i N_i \), which has the expectation value

\[
\langle N \rangle = \left| \begin{array}{c} n_1, n_2, \ldots \\ \Sigma_i N_i \\ n_1, n_2, \ldots \end{array} \right|
= \sum_i n_i \langle n_1, n_2, \ldots \mid n_1, n_2, \ldots \rangle
= \sum_i n_i \langle n_1, n_2, \ldots \rangle
= n
\]

Each of the \( N_i \) acts only on its own mode. The energy of the state is the sum of the particle energies in the individual modes

\[
\langle E \rangle = \left| \begin{array}{c} n_1, n_2, \ldots \\ \Sigma_i N_i \omega_i \\ n_1, n_2, \ldots \end{array} \right|
= \sum_i N_i \omega_i
\]
For the string, the frequencies are evenly spaced. This result is a feature of a 1-dimensional system with a massless eigenmode spectrum, $E_i = c p_i$. For a 3-dimensional system, the lattice of momentum states leads to uneven spacing of energy levels. In addition, for a massive relativistic ($E_i^2 = m^2 c^4 + c^2 p_i^2$) or non-relativistic ($E_i = p_i^2 \frac{1}{2m}$) spectrum, the splitting is not proportional to $p_i$.

### Identical particles

Considering particles as excitations of an underlying field theory is one way to approach a discussion of identical particles. Consider the string system above. Viewed as excitations, there is no way to distinguish the phonons in the system, other than by which mode they are in. The same is true when considering two electrons. There is no way to distinguish which is which. A full description of the system is given by specifying the occupation numbers for the various electron modes. The individual electrons have no identity.

### Traditional discussion of exchange symmetry

Before continuing with the Fock space description, it may be useful to review the traditional discussion, given in terms of exchange symmetry.

Consider a system consisting of two identical particles. Let one (the first) be in state $|k'\rangle$ and the other be in state $|k''\rangle$. To distinguish the two particles, write the combined state in a specific order $|k', k''\rangle$. More generally, in this language, an $N$ particle state is written $|k_1, k_2, \ldots, k_N\rangle$, where the "slots" in the state vector identify the particle, and the value of the slot identifies the mode. (Note that this is different than the nomenclature for Fock states, where the slots identify the modes and the value of the slot indicates the excitation level of that mode, or how many particles are in each mode.) The particle nomenclature makes sense if the particles are distinguishable, in which case the two-particle states are product states of the one-particle states for the two particles. When the particles are identical, the situation is less clear. How, for example, does one distinguish between the state $|k', k''\rangle$ and the state where the particle identities are exchanged $|k'', k'\rangle$? It would seem that for any pair of quantum numbers $k', k''$, there is a degenerate two state system, i.e. $|k', k''\rangle$, $|k'', k'\rangle$, or any linear combination of basis kets $c_d |k', k''\rangle + c_x |k'', k'\rangle$ where $d$ or $x$ indicates "direct" or "exchange" should lead to the same observables.

To aid the discussion, introduce the exchange operator $P_{12}$ which acts to exchange the state of the two particles

$$P_{12} |k', k''\rangle = |k'', k'\rangle$$

Acting with $P_{12}$ twice gives one back the original state, $P_{12}^2 = 1$. Operating on a general linear combination

$$P_{12}(c_d |k', k''\rangle + c_x |k'', k'\rangle) = c_d |k'', k'\rangle + c_x |k', k''\rangle$$

The eigenstates of $P_{12}$ are the symmetric and antisymmetric linear combinations

$$|s_{12}\rangle = \frac{1}{\sqrt{2}} (|k'', k'\rangle + |k', k''\rangle)$$

$$|a_{12}\rangle = \frac{1}{\sqrt{2}} (|k'', k'\rangle - |k', k''\rangle)$$

with $P_{12} |s_{12}\rangle = +|s_{12}\rangle$ and $P_{12} |a_{12}\rangle = -|a_{12}\rangle$. 
Since the particles cannot be distinguished, it is reasonable that \[ P_{12}, H = 0 \], in which case the "exchange parity" of the system is conserved. The space of states can be divided into symmetric and antisymmetric subspaces.

Until this point in the discussion either state, or a linear combination, would be acceptable. In fact, however, Nature appears to choose either \( |\psi\rangle \) states or \( |\alpha\rangle \) states but not both for a particular particle species. Particles with integral spin (spin = 0, 1, 2, ... ) form symmetric states, and are known as bosons (after Bose). Similarly, particles with half-integral spin (spin = \( \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, ... \) ) form antisymmetric states, and are called fermions (after Fermi).

From the perspective of non-relativistic quantum mechanics, I think these rules are not derivable, and must be treated as additional assumptions.

### Discussion

There is something a bit odd about this discussion. It starts with the assumption that the two-particle vector space consists of states \( |k', k''\rangle \) which are different, but in the end it turns out these states are not valid. Rather the physical vector space is restricted to either \( |\psi_{12}\rangle \) or \( |\alpha_{12}\rangle \). An alternative approach is to assume from the beginning that there is no exchange degeneracy, but rather that specifying quantum numbers for a two particle state yields a unique description of the state. In this case, \( |k', k'', \lambda\rangle \) fully specifies the state, where \( \lambda = \pm 1 \) is the eigenvalue of the exchange operator. Bosons have \( \lambda = 1 \) and fermions have \( \lambda = -1 \).

\[
P_{12} |k', k'', \lambda\rangle = |k'', k', \lambda\rangle = \lambda |k', k'', \lambda\rangle
\]

In this picture, \( |k', k'', \lambda\rangle \) and \( |k'', k', \lambda\rangle \) represent states that differ only by a phase, which is constrained to be \( \pm 1 \) by the condition \( P_{12}^2 = 1 \). Either state may be used as the basis ket for the two particle system. For fermions, a two particle state cannot be formed with the same set of quantum numbers occupied twice, i.e.

\[
|k', k', -1\rangle = -|k', k', -1\rangle = 0
\]

### Permutation symmetry and totally symmetric/antisymmetric multiparticle states

The above approach can be generalized. Consider an \( N \) particle state. Where \( N \) modes \( (k_1, k_2, ... k_N) \) are occupied. Then one possible assignment of particles to states is to put the first particle in \( k_1 \), the second in \( k_2 \), etc. We could, however, equally well consider any other assignment, e.g. put the 1st particle in the mode \( k_5 \), the 2nd is assigned to \( k_{23} \), ... In general, all such permutations must be considered. If there are \( N \) particles there are \( N! \) permutations, and the full description of the state is a sum over all permutations with appropriate weights,

\[
|\Psi\rangle = \sum_{i=1}^{N!} c_i |i\rangle
\]

where the sum over \( i \) is over all permutations, and \( |i\rangle \) represents a particular assignment of particles to modes, e.g. \( |k_5, k_{23}, ...\rangle \). Then the generalization of the two particle states above is that for bosons all permutations have weight

\[
c_i = \frac{1}{\sqrt{N!}},
\]

while for fermions the coefficients have alternating signs

\[
c_i = \frac{(-1)^p}{\sqrt{N!}}, \text{ where } p = 0 \text{ if the permutation is even},
\]

and

\[
p = 1 \text{ if the permutation is odd.}
\]

The definition of an even/odd permutation is that the permutation can be generated from the identity permutation \( |k_1, k_2, ...\rangle \) by an even/odd number of two particle exchanges.
With these rules, boson states are "totally symmetric", and fermion states are "totally anti-symmetric". The fermion rule reproduces the Pauli exclusion principle since exchange of any two particles in the same mode reproduces the same state, but with a change in the even/odd nature of the permutation. Such an exchange produces two components of the state which are identical, but of opposite sign. The amplitude for the state as a whole is identically zero. Two identical fermions cannot occupy the same mode.

**Space and Spin**

Notice that it is the complete state of the system that is either symmetric or antisymmetric. It is typical to write the full state of a system as the product of its spin state and its space state. In this case, the full exchange symmetry of the state is the product of the spin exchange symmetry and the space exchange symmetry. For example, denote the full state by \( |\psi\rangle \), the spin state by \( |\chi\rangle \), and the spatial state by \( |\varphi\rangle \), and denote exchange symmetry by a subscript \( A \) or \( S \). Then, for fermions, either

\[
|\psi_A\rangle = |\chi_A\rangle |\varphi_S\rangle
\]

are valid states, while for bosons we have the possibilities

\[
|\psi_S\rangle = |\chi_S\rangle |\varphi_A\rangle
\]

**Discussion in terms of Fock space, creation and annihilation operators**

**creation operators and multiparticle states**

Now consider multiparticle states in terms of occupation numbers, beginning with two particle basis kets. Suppose the occupation numbers of the \( i^{th} \) and \( j^{th} \) modes are 1, and all other \( n_k = 0 \). This ket may be written as

\[
|0, 0, \ldots, n_i = 1, \ldots, n_j = 1, \ldots\rangle \equiv |n_i = 1, n_j = 1\rangle
\]

where in the second form modes with \( n_i = 0 \) are suppressed. A two particle state, with the quantum numbers for modes \( i \) and \( j \) will generally be described by a complex phase times the ket. Next, consider the production of a two particle state from the ground state by the application of creation operators.

\[
a_j^\dagger a_i^\dagger |0\rangle = c_{ij} |n_i = 1, n_j = 1\rangle
\]

where the phase of the ground state has been taken to be 1. Alternatively, one could create a two particle state by

\[
a_i^\dagger a_j^\dagger |0\rangle = c_{ji} |n_i = 1, n_j = 1\rangle
\]

where \( \lambda_{ij} = c_{ji}/c_{ij} \). One might ask if \( c_{ij} = c_{ji} \), or, what are the allowed values of \( \lambda_{ij} \)? Does the order of the creation operators matter? Does \( \lambda_{ij} \) depend on the modes \( i, j \)?

Merzbacher discusses this questions in chapter 21. Here is a simple version of his argument. Consider three modes 1,2,3. Then
\[
\begin{align*}
\hat{a}_1^\dagger \hat{a}_2^\dagger |0\rangle &= \lambda_{12} \hat{a}_2^\dagger \hat{a}_1^\dagger |0\rangle \\
\hat{a}_1^\dagger \hat{a}_3^\dagger |0\rangle &= \lambda_{13} \hat{a}_3^\dagger \hat{a}_1^\dagger |0\rangle
\end{align*}
\]

Now, for the purpose of forming a set of orthogonal eigenfunctions \(\langle x | i \rangle\) upon which to build the basis kets \(|\bar{n}\rangle\), there is nothing special about \(\langle x | 2 \rangle\) and \(\langle x | 3 \rangle\). One could just as well use another linear combination of these eigenfunctions, e.g. \(\langle x | \pm \rangle = \frac{1}{\sqrt{2}} (\langle x | 2 \rangle \pm \langle x | 3 \rangle)\), which would be created by \(\hat{a}_\pm^\dagger = \frac{1}{\sqrt{2}} (\hat{a}_2^\dagger \pm \hat{a}_3^\dagger)\). To resolve the question of operator order, one may now consider

\[
\hat{a}_1^\dagger \hat{a}_\pm^\dagger |0\rangle = \lambda_{1\pm} \hat{a}_\pm^\dagger \hat{a}_1^\dagger |0\rangle \\
= \frac{1}{\sqrt{2}} (\lambda_{1\pm} \hat{a}_2^\dagger \pm \hat{a}_3^\dagger) \hat{a}_1^\dagger |0\rangle \\
= \frac{1}{\sqrt{2}} (\lambda_{1\pm} \hat{a}_2^\dagger \hat{a}_1^\dagger \pm \lambda_{1\pm} \hat{a}_3^\dagger \hat{a}_1^\dagger) |0\rangle
\]

Alternatively, the left side is

\[
\hat{a}_1^\dagger \hat{a}_\pm^\dagger |0\rangle = \frac{1}{\sqrt{2}} \hat{a}_1^\dagger (\hat{a}_2^\dagger \pm \hat{a}_3^\dagger) |0\rangle \\
= \frac{1}{\sqrt{2}} (\hat{a}_1^\dagger \hat{a}_2^\dagger \pm \hat{a}_1^\dagger \hat{a}_3^\dagger) |0\rangle \\
= \frac{1}{\sqrt{2}} (\lambda_{12} \hat{a}_2^\dagger \hat{a}_1^\dagger \pm \lambda_{13} \hat{a}_3^\dagger \hat{a}_1^\dagger) |0\rangle
\]

Since \(\hat{a}_2^\dagger\) and \(\hat{a}_3^\dagger\) create different states, the expressions can be equal only if \(\lambda_{12} = \lambda_+ = \lambda_- = \lambda_3\). Generalizing, \(\lambda_{ij}\) must have a common value for any pair of modes, independent of \(i\) and \(j\). Carrying out the exchange operation twice,

\[
\hat{a}_i^\dagger \hat{a}_j^\dagger |0\rangle = \lambda_{ij} \hat{a}_j^\dagger \hat{a}_i^\dagger |0\rangle \\
= \lambda_{ij} \lambda_{ji} \hat{a}_i^\dagger \hat{a}_j^\dagger |0\rangle \\
= \lambda^2 \hat{a}_i^\dagger \hat{a}_j^\dagger |0\rangle
\]

one can see that \(\lambda^2 = 1\), or there are two possibilities \(\lambda = \pm 1\).

For \(\lambda = 1\), (bosons) the operators obey the commutator relation \([\hat{a}_i^\dagger, \hat{a}_j^\dagger] = 0\), and for \(\lambda = -1\), (fermions) the operators obey the anti-commutator relation \(\{\hat{a}_i^\dagger, \hat{a}_j^\dagger\} = 0\). Often to distinguish between the two types of operators, creation operators for the case \(\lambda = -1\) are denoted by \(c^\dagger\) or \(b^\dagger\). I’ll use \(c^\dagger\). The importance of the sign of \(\lambda\), arises dramatically when considering the case \(i = j\). For the fermi case, the spectrum of states cannot include \(n_i = 2\) for any \(i\).

\[
c_i^\dagger c_i^\dagger |0\rangle = -c_i^\dagger c_i^\dagger |0\rangle = 0
\]

In the language of annihilation and creation operators it is natural to consider either bosons or fermions, but not a mixture of the two, whereas in the traditional approach that assumption has to be introduced separately.

### Annihilation operators

Taking the adjoint of the commutation relation for the creation operators, one finds that annihilation operators must also obey either \([a_i, a_j] = 0\) or \(\{c_i, c_j\} = 0\), with the same sign for \(\lambda\) as for the creation operators.
\[ \{ c, c^\dagger \} = 1 \] or \( [a, a^\dagger] = 1 \)?

It remains to show which statistic is followed when the order of an annihilation and a creation operator is changed. Before considering the more general case of \( a_i \) and \( a_j^\dagger \), start by considering a single degree of freedom \( (i = j) \). The discussion began with the assumption that there was a number operator \( N \), the states were eigenstates of \( N \), labeled by \( |n\rangle \), and that \( a \) and \( a^\dagger \) act as annihilation and creation operators.

Let us make one more assumption, that a ground state with no particles exists, \( N |0\rangle = 0 \). When acting on the ground state \( aa^\dagger |0\rangle = |0\rangle \), assuming an appropriate normalization. When acting on the ground state, there are two possibilities

\[
\{a, a^\dagger\} |0\rangle = (aa^\dagger + a^\dagger a) |0\rangle = (1 + 0) |0\rangle = 1 |0\rangle \quad \text{or} \\
\{a, a^\dagger\} |0\rangle = (aa^\dagger - a^\dagger a) |0\rangle = (1 - 0) |0\rangle = 1 |0\rangle
\]

Evidently, we have two possibilities, \( \{a, a^\dagger\} = 1 \), or \( [a, a^\dagger] = 1 \).

Next, consider the operation of \( N \) on the state \( |1\rangle = a^\dagger |0\rangle \) and study the possibility that \( [a, a^\dagger] = 1 \). By definition \( N |1\rangle = |1\rangle \), while at the same time

\[
N |1\rangle = a^\dagger a |1\rangle = a^\dagger aa^\dagger |0\rangle \\
= (aa^\dagger - [a, a^\dagger]) a^\dagger |0\rangle \\
= (aa^\dagger - 1) a^\dagger |0\rangle
\]

Again there are two possibilities. If the annihilation and creation operators commute \( [a, a] = 0 \) and \( [a^\dagger, a^\dagger] = 0 \) then one has the case of bose or harmonic oscillator statistics. In this case \( aa^\dagger |1\rangle = 2 |1\rangle \) and everything is fine. The relation \( [a, a^\dagger] = 1 \) is consistent with \( [a, a] = 0 \) and \( [a^\dagger, a^\dagger] = 0 \). On the other hand, if one has fermi statistics \( [a^\dagger, a^\dagger] = 0 \) or \( a^\dagger a^\dagger = 0 \), then \( aa^\dagger |1\rangle = aa^\dagger a^\dagger |0\rangle = 0 \) and \( (aa^\dagger - 1) a^\dagger |0\rangle = -|1\rangle \). Evidently, choosing \( [a, a^\dagger] = 1 \) and \( [a^\dagger, a^\dagger] = 0 \), leads to \( N |1\rangle = -|1\rangle \), which is inconsistent.

Similarly, consider \( \{a, a^\dagger\} = 1 \), in which case

\[
N |1\rangle = a^\dagger a |1\rangle = a^\dagger aa^\dagger |0\rangle \\
= ([a, a^\dagger] - aa^\dagger) a^\dagger |0\rangle \\
= (1 - aa^\dagger) a^\dagger |0\rangle
\]

In this case, fermi statistics gives \( (1 - aa^\dagger) a^\dagger |0\rangle = a^\dagger |0\rangle = |1\rangle \), which is fine. Now it is bose statistics which leads to the inconsistency.

One may conclude that for a consistent definition of \( N \) and raising and lowering operators, the choice of statistics obeyed by annihilation operators, by creation operators, and between annihilation and creation operators must be the same.

\( N, c, c^\dagger \)

Although \( c \) and \( c^\dagger \) act to change \( |n\rangle \) it remains to evaluate the constants \( \lambda_- , \lambda_+ \) in the relations

\[
c |n\rangle = \lambda_- |n - 1\rangle \\
c^\dagger |n\rangle = \lambda_+ |n + 1\rangle
\]

For \( c \), proceed as in the Bose case and compare to \( \langle n | N | n\rangle = n \)
\[ |\lambda_-|^2 = \langle n | c^\dagger c | n \rangle \]
\[ = \langle n | N | n \rangle \]
\[ = n \]

For \( c^\dagger \),
\[ |\lambda_+|^2 = \langle n | cc^\dagger | n \rangle \]
\[ = \langle n | 1 - c^\dagger c | n \rangle \]
\[ = \langle n | 1 - N | n \rangle \]
\[ = 1 - n \]

Together, these relations give
\[ c |n\rangle = \sqrt{n} |n\rangle \]
\[ c^\dagger |n\rangle = \sqrt{1 - n} |n + 1\rangle \]

which apart from a change of sign from \( \sqrt{1 + n} \rightarrow \sqrt{1 - n} \) is similar to that for bose operators.

All this may seem a bit fancy. The full set of possibilities for \( c \) and \( c^\dagger \) to operate is given by the short list
\[
\begin{align*}
c |0\rangle &= 0 \\
c |1\rangle &= |0\rangle \\
c^\dagger |0\rangle &= |1\rangle \\
c^\dagger |1\rangle &= 0
\end{align*}
\]

\[ \{c_i, c_j^\dagger\} \]

By an argument similar to that given for creation operators above, for different modes \( i \neq j \) one has either \([a_i, a_j^\dagger] = 0\) or \(\{c_i, c_j^\dagger\} = 0\). Taking into account the possibility that \( i = j \), the two cases are bosons: \([a_i, a_j^\dagger] = \delta_{ij}\) and fermions: \(\{c_i, c_j^\dagger\} = \delta_{ij}\).

\[ \text{Field operators} \]

Having established the commutation relations for the annihilation and creation operators of the modes, one can define field operators and commutation relations for them. For example, the Bose field operator defined as an expansion in orthogonal eigenfunctions is
\[ a(x) = \sum_n a_n \phi_n(x) \]

and the commutator
\[
\begin{align*}
[a(x), a^\dagger(x')] &= \left[ \sum_n a_n \phi_n(x), \sum_n a_n^\dagger \phi_n^*(x') \right] \\
&= \sum_n \sum_{n'} \phi_n(x) \phi_{n'}^*(x') [a_n, a_{n'}^\dagger] \\
&= \sum_n \sum_{n'} \phi_n(x) \phi_{n'}^*(x') \delta_{nn'} \\
&= \sum_n \phi_n(x) \phi_n^*(x') \\
&= \delta(x - x')
\end{align*}
\]
Similarly \([a(x), a(x')] = [a^\dagger(x), a^\dagger(x')] = 0\). For fermionic operators \([c(x), c^\dagger(x)] = 1\), etc.

### One particle operators

In a multiparticle system one distinguishes between single and multiparticle operators. Single particle operators depend only the state of a single particle. If the particles are distinct, this is a straightforward sum. For example, neglecting interactions between particles, the energy is a straightforward sum over the individual kinetic energies and an external potential

\[
H = \sum_i H_i = \sum_i \frac{p_i^2}{2m_i} + V_i(x_i)
\]

Single particle operators should extend to a multiparticle state of identical particles as well. Consider a two particle system, without a consideration of statistics

\[
(H_1 + H_2) |k'k''\rangle = E' + E'' = (H_1 + H_2) |k''k'\rangle
\]

As discussed earlier, the energies of these two states are degenerate. Accordingly, the symmetric and anti-symmetric states have the same single particle energies.

In Fock space, the single particle Hamiltonian takes the form

\[
H = \sum_i H_i = \sum_i a_i^\dagger a_i E_i
\]

where the sum is over modes, not particles. Each mode is weighted by \(N_i = a_i^\dagger a_i\). For the example at hand, the mode energies are calculated by \(E_i = \frac{p_i^2}{2m_i} + V_i(x_i)\).

Other single particle operators are given similarly by \(O = \sum_i N_i O_i\) where \(O_i = \langle i | O | i \rangle\) where \(i\) denotes the \(i^{th}\) eigenmode.

### Interactions and two particle operators

The interaction potential between two particles is the next level of complexity. In the particle picture, the interaction energy would be written as

\[
V_{12} = \langle \Psi_{12} | V(x_1, x_2) | \Psi_{12} \rangle = \int d x_1 d x_2 \Psi^{\dagger}(x_1, x_2) V(x_1, x_2) \Psi(x_1, x_2)
\]

For non-identical particles one would use single particle wave-functions, e.g. \(\Psi_{i}(x_1, x_2) = \Psi_i(x_1) \Psi_j(x_2)\) if particle 1 is in the state \(i\) and particle 2 is in state \(j\). For identical particles, one needs symmetric or antisymmetric wave-functions. For example, for fermions \(\Psi_{i}(x_1, x_2) = \frac{1}{\sqrt{2}} (\Psi_i(x_1) \Psi_j(x_2) - \Psi_j(x_1) \Psi_i(x_2))\). This leads to two contributions to the energy, a direct term \(V_d\) and an exchange term \(V_x\).

\[
V_d = \int d x_1 d x_2 \Psi_i^\dagger(x_1) \Psi_j^\dagger(x_2) V(x_1, x_2) \Psi_i(x_1) \Psi_j(x_2)
\]

\[
V_x = \int d x_1 d x_2 \Psi_i^\dagger(x_1) \Psi_j^\dagger(x_2) V(x_1, x_2) \Psi_i(x_1) \Psi_j(x_2)
\]

\(V = V_d - V_x\)

Using Fock space, the two body potential is written as
\[ V_{12} = \frac{1}{2} \sum_{ijkl} a_{k}^{\dagger} a_{l}^{\dagger} a_{i} a_{j} \langle kl | V | ij \rangle \]

where the matrix element \( \langle kl | V | ij \rangle = \int dx_{1} dx_{2} \Psi_{k}^{\dagger}(x_{1}) \Psi_{l}(x_{2}) V(x_{1}, x_{2}) \Psi_{i}(x_{1}) \Psi_{j}(x_{2}) \) is an integral over the mode functions, and the algebra of annihilation and creation operators automatically takes care of the direct and exchange terms. For example, if one wanted the expectation of the interaction potential for a particular two particle state \( | n_{r} = 1, n_{s} = 1 \rangle \), then

\[
V_{rs} = \langle n_{r} = 1, n_{s} = 1 | \left( \frac{1}{2} \sum_{ijkl} a_{k}^{\dagger} a_{l}^{\dagger} a_{i} a_{j} \langle kl | V | ij \rangle \right) | n_{r} = 1, n_{s} = 1 \rangle
\]

\[
= \frac{1}{2} \sum_{ijkl} \langle kl | V | ij \rangle \langle n_{r} = 1, n_{s} = 1 | a_{k}^{\dagger} a_{l}^{\dagger} a_{i} a_{j} | n_{r} = 1, n_{s} = 1 \rangle
\]

\[
= \frac{1}{2} \sum_{ijkl} \langle kl | V | ij \rangle \langle n_{r} = 1, n_{s} = 1 | a_{k}^{\dagger} a_{l}^{\dagger} (\delta_{ir} \delta_{js} \pm \delta_{is} \delta_{jr}) | 0 \rangle
\]

\[
= \frac{1}{2} \sum_{kl} \sum_{ijkl} \langle kl | V | rs \rangle \pm \langle kl | V | sr \rangle \langle n_{r} = 1, n_{s} = 1 | a_{k}^{\dagger} a_{l}^{\dagger} | 0 \rangle
\]

\[
= \frac{1}{2} \sum_{kl} (\langle kl | V | rs \rangle \pm \langle kl | V | sr \rangle) (\delta_{kr} \delta_{ls} - \delta_{ks} \delta_{jr})
\]

\[
= \langle rs | V | rs \rangle \pm \langle rs | V | sr \rangle
\]

which has the form of \( V_{d} \pm V_{x} \), where \( \pm \) applies for Bose/Fermion statistics.