Chapter 1

Identical Particles

Two particles are said to be identical if they are exact replicas of each other in every respect - there should be no experiment that detects any intrinsic difference between them. By intrinsic we mean properties inherent to the particle, such as its charge or mass and not its location or momentum. Although the definition of identical particles is the same classically and quantum mechanically, the implications are different in the two cases.

1.1 The Classical Case

Imagine a billiard table with four holes, numbered 1 through 4. Near holes 1 and 2 rest two identical billiard balls. Let us call these balls 1 and 2. The difference between the labels reflects not any intrinsic difference in the balls (for they are identical) but rather a difference in their environments, namely, the holes near which they find themselves. Now, it follows from the definition of identity, that if these two balls are exchanged, the resulting configuration would appear exactly the same. Nonetheless these two configurations are treated as distinct in classical physics. Let us discuss an experiments which could distinguish the two balls.

Imagine that at time \( t = 0 \), two players propel the balls toward the center of the table. At once two physicists \( P_1 \) and \( P_2 \) take the initial-value data and make the following predictions:

- \( P_1 \): ball 1 goes to hole 3 and ball 2 goes to hole 4 at \( t = T \)
- \( P_2 \): ball 1 goes to hole 4 and ball 2 goes to hole 3 at \( t = T \)

Say at time \( T \) we find that ball 1 ends up in hole 3 and ball 2 in hole 4. We declare that \( P_1 \) is correct and \( P_2 \) is wrong. Now, the configurations predicted by them for \( t = T \) differ only by the exchange of two identical particles. If seen in isolation they would appear identical: an observer who walks in just at \( t = T \) and is given the predictions of \( P_1 \) and \( P_2 \) will conclude that both are right. But the persons who have been around the table from the beginning of the experiment know the history of the balls and can say who is right. Although both balls appear identical to the newcomer, we are able to trace the ball in hole 3 back to the vicinity of hole 1 and the one in hole 4 back to hole 2. Similarly at \( t = 0 \), the two balls which seemed identical to us would be distinguishable to someone who had been following them from an earlier period. Now of course it is not really necessary that either we or any other observer be actually present in order for
this distinction to exist. One imagines in classical physics the fictitious observer who sees everything and disturbs nothing; if he can make the distinction, the distinction exists.

To summarize, it is possible in classical mechanics to distinguish between identical particles by following their nonidentical trajectories (without disturbing them in any way). Consequently two configurations related by exchanging the identical particles are physically nonequivalent.

An immediate consequence of the above reasoning, and one that will play a dominant role in what follows, is that in quantum theory, which completely outlaws the notion of continuous trajectories for the particles, there exists no physical basis for distinguishing between identical particles. Consequently two configurations related by the exchange of identical particles must be treated as one and the same configuration and described by the same state vector. We now proceed to deduce the consequences of this restriction.

1.2 Two-particle Systems - Symmetric and Antisymmetric States

Suppose we have a system of two distinguishable particles 1 and 2 and a position measurement on the system shows particle 1 to be at \( x = a \) and particle 2 to be at \( x = b \). We write the state just after measurement as

\[
|\psi\rangle = |x_1 = a, x_2 = b\rangle = |ab\rangle
\]

(1.1)

where we are adopting the convention that the state of particle 1 is described by the first label (\( a \)) and that of particle 2 by the second label (\( b \)). Since the particles are distinguishable, the state obtained by exchanging them is distinguishable from the above. It is given by

\[
|\psi\rangle = |ba\rangle
\]

and corresponds to having found particle 1 at \( b \) and particle 2 at \( a \).

Suppose we repeat the experiment with two identical particles and catch one at \( x = a \) and the other at \( x = b \). Is the state vector just after measurement \( |ab\rangle \) or \( |ba\rangle \)? The answer is, neither. We have seen that in quantum theory two configurations related by the exchange of identical particles must be viewed as one and the same and be described by the same state. Since \( |\psi\rangle \) and \( \alpha|\psi\rangle \) are physically equivalent, we require that \( |\psi(a, b)\rangle \), the state vector just after the measurement, satisfy the constraint

\[
|\psi(a, b)\rangle = \alpha|\psi(b, a)\rangle
\]

(1.2)

where \( \alpha \) is any complex number. Since under the exchange \( |ab\rangle \rightarrow |ba\rangle \) and the two vectors are not multiples of each other (i.e., physically distinct) neither is acceptable. The problem is that our position measurement yields not an ordered pair of numbers (as in the distinguishable particle case) but just a pair of numbers: to assign them to the particles in a definite way is to go beyond what is physically meaningful in quantum theory. What our measurement does permit
us to conclude is that the state vector is an eigenstate of \(X_1 + X_2\) with eigenvalue \(a + b\), the sum of the eigenvalue being insensitive to how the values \(a\) and \(b\) are assigned to the particles. In other words, given an unordered pair of numbers \(a\) and \(b\) we can still define a unique sum (but not difference). Now, there are just two product vectors, \(|ab\rangle\) and \(|ba\rangle\) with this eigenvalue, and the state vector lies somewhere in the two-dimensional degenerate (with respect to \(X_1 + X_2\)) eigenspace spanned by them. Let \(|\psi(a, b)\rangle = \beta|ab\rangle + \gamma|ba\rangle\) be the allowed vector. If we impose the constraint Eq. (1.2)

\[
\beta|ab\rangle + \gamma|ba\rangle = \alpha[\beta|ba\rangle + \gamma|ab\rangle]
\]

we find, upon equating the coefficients of \(|ab\rangle\) and \(|ba\rangle\) that

\[
\beta = \alpha \gamma, \quad \gamma = \alpha \beta
\]

so that

\[
\alpha = \pm 1
\]

(1.3)

It is now easy to construct the allowed state vectors. They are

\[
|ab, S\rangle = |ab\rangle + |ba\rangle
\]

(1.4)

called the symmetric state vector (\(\alpha = 1\)) and

\[
|ab, A\rangle = |ab\rangle - |ba\rangle
\]

(1.5)

called the antisymmetric state vector (\(\alpha = -1\)). (Notice that these vectors are still unnormalized).

### 1.3 Bosons and Fermions

Although both \(S\) and \(A\) states seem physically acceptable (in that they respect the indistinguishability of the particles) we can go a step further and make the following assertion:

A given species of particles must choose once and for all between \(S\) and \(A\) states.

Suppose the contrary were true, and the Hilbert space of two identical particles contained both \(S\) and \(A\) vectors. Then the space also contains linear combinations such as

\[
|\psi\rangle = \alpha|\omega_1 \omega_2, S\rangle + \beta|\omega'_1 \omega'_2, A\rangle
\]

which are neither symmetric nor antisymmetric. So we rule out this possibility.

Nature seems to respect the constraints we have deduced. Particles such as the pion, photon, and graviton are always found in symmetric states and are called bosons, and particles such as the electron, proton, and neutron are always found in antisymmetric states and are called fermions.

Thus, if we catch two identical bosons, one at \(x = a\) and the other at \(x = b\), the state vector immediately following the measurement is

\[
|\psi\rangle = |x_1 = a, x_2 = b\rangle + |x_1 = b, x_2 = a\rangle = |ab\rangle + |ba\rangle = |ab, S\rangle.
\]
Had the particles been fermions, the state vector after the measurement would have been

$$|\psi\rangle = |x_1 = a, x_2 = b\rangle - |x_1 = b, x_2 = a\rangle = |ab\rangle - |ba\rangle = |ab, A\rangle.$$}

Note that although we still use the labels $x_1$ and $x_2$, we do not attach them to the particles in any particular way. Thus having caught the bosons at $x = a$ and $x = b$, we need not agonize over whether $x_1 = a$ and $x_2 = b$ or vice-versa. Either choice leads to the same $|\psi\rangle$ for bosons, and to state vectors differing only by an overall sign for fermions.

We are now in a position to deduce a fundamental property of fermions, which results from the antisymmetry of their state vectors. Consider a two-fermion state

$$|\omega_1\omega_2, A\rangle = |\omega_1\omega_2\rangle - |\omega_2\omega_1\rangle.$$}

Let us now set $\omega_1 = \omega_2 = \omega$. We find

$$|\omega\omega, A\rangle = |\omega\omega\rangle - |\omega\omega\rangle = 0.$$}

This is the celebrated Pauli exclusion principle: Two identical fermions cannot be in the same quantum state. This principle has profound consequences - in statistical mechanics, in understanding chemical properties of atoms, in nuclear theory, astrophysics, etc.

Let us come back to an essential point: our analysis has only told us that a given type of particle, say a pion, has to be either a boson or a fermion, but does not say which one. There are two ways to the answer. The first is within the framework of quantum field theory, which relates the spin of the particle to its “statistics” - which is the term physicists use to refer to its bosonic or fermionic nature. Since the relevant arguments are beyond the scope of this course, we merely quote the results here. Recall that the spin of the particle is its internal angular momentum. The magnitude of spin happens to be an invariant for a particle (and thus serves as a label, like its mass or charge) and can have only one of the following values: 0, $\hbar/2$, $3\hbar/2$, $2\hbar$, ... The spin statistics theorem, provable in quantum field theory, asserts that particles with (magnitude of) spin equal to an even multiple of $\hbar/2$ are bosons, and those with spin equal to an odd multiple of $\hbar/2$ are fermions. However, this connection, proven in three dimensions, does not apply to one dimension, where it is not possible to define spin or any form of angular momentum (this should be clear classically). Thus the only way to find if a particle in one dimension is a boson or fermion is to determine the symmetry of the wave function experimentally. This is the second method, to be discussed in the following.

Before going on to this second method, let us note that the requirement that the state vector of two identical particles be symmetric or antisymmetric (under the exchange of the quantum numbers labeling them) applies in three dimensions as well, as will be clear by going through the arguments in one dimension. The only difference will be the increase in the number of labels. For example, the position eigenket of a spin-zero boson will be labeled by three numbers $x$, $y$, and $z$. For fermions, which have spin at least equal to $\hbar/2$, the states will be labeled by the orientation of the spin as well as the orbital labels that describe spinless
bosons. We shall consider just spin-1/2 particles, for which this label can take only two values, call them + and − or spin up and down (the meaning of these terms will be clear later). If we denote by ω all the orbital labels and s the spin label, the state vector of the fermion that is antisymmetric under the exchange of the particles, i.e., under the exchange of all the labels, will be of the form
\[
|ω_1s_1, ω_2s_2, A⟩ = |ω_1s_1, ω_2s_2⟩ - |ω_2s_2, ω_1s_1⟩.
\]

We see that the state vector vanishes if
\[
ω_1 = ω_2 \quad \text{and} \quad s_1 = s_2.
\]

Thus we find once again that two fermions cannot be in the same quantum state, but we mean by a quantum state a state of definite ω and s. Thus two electrons can be in the same orbital state if their spin orientations are different.

1.4 Determination of particle statistics

Let us now show how does one determine empirically the statistics of a given species without turning to the spin statistics theorem. For concreteness, let us say we have two identical noninteracting pions and wish to find out if they are bosons or fermions. Let us put them in a one-dimensional box and make an energy measurement. Say we find one in the state \( n = 3 \) and the other in the state \( n = 4 \). The probability distribution in \( x \) space would be, depending on their statistics

\[
P_{S/A}(x_1, x_2) = 2|ψ_{S/A}(x_1, x_2)|^2
\]

\[
= 2|2^{-1/2}[ψ_3(x_1)ψ_4(x_2) ± ψ_4(x_1)ψ_3(x_2)]|^2
\]

\[
= |ψ_3(x_1)|^2|ψ_4(x_2)|^2 + |ψ_4(x_1)|^2|ψ_3(x_2)|^2
\]

\[
±[ψ_3^*(x_1)ψ_4(x_1)ψ_4^*(x_2)ψ_3(x_2) + ψ_4^*(x_1)ψ_3(x_1)ψ_3^*(x_2)ψ_4(x_2)].
\]

Compare this situation with two particles carrying labels 1 and 2, but otherwise identical, with particle 1 in state 3 and described by a probability distribution \( |ψ_3(x)|^2 \), and particle 2 in state 4 and described by the probability distribution \( |ψ_4(x)|^2 \). In this case, the first term represents the probability that particle 1 is at \( x_1 \) and particle 2 is at \( x_2 \), while the second gives the probability for the exchanged event. The sum of these two terms then gives \( P_D(x_1, x_2) \), the probability for finding one at \( x_1 \) and the other at \( x_2 \), with no regard paid to their labels. (The subscript \( D \) denotes distinguishable). The next two terms, called interference terms, remind us that there is more to identical particles in quantum theory than just their identical characteristics: they have no separate identities. There is a parallel between this situation and the double slit experiment, where the probabilities for finding a particle at a given point \( x \) on the screen with both slits open was not the sum of probabilities with either slit open. In both cases, the interference terms arise, because in quantum theory, when an event can take place in two (or more) indistinguishable ways, we add the corresponding amplitudes and not the corresponding probabilities.
The interference terms tell us if the pions are bosons or fermions. The difference between the two cases is more dramatic as \( x_1 \to x_2 \to x \):

\[
P_A(x_1 \to x, x_2 \to x) \to 0 \quad \text{Pauli principle applied to state } |x\rangle
\]

whereas

\[
P_S(x_1 \to x, x_2 \to x) = 2|\psi_3(x)|^2|\psi_4(x)|^2 + |\psi_4(x)|^2|\psi_3(x)|^2
\]

is twice as big as \( P_D(x_1 \to x, x_2 \to x) \), the probability density for two distinct label carrying (but otherwise identical) particles, whose labels are disregarded in the position measurement.

One refers to the tendency of fermions to avoid each other (i.e., avoid the state \( x_1 = x_2 = x \)) as obeying “Fermi-Dirac statistics” and the tendency of bosons to conglomerate as obeying “Bose-Einstein statistics,” after the physicists who first explored the consequences of the antisymmetrization and symmetrization requirements on the statistical mechanics of an ensemble of fermions and bosons, respectively. This is the reason for referring to the bosonic/fermionic nature of a particle as its statistics.

Given the striking difference in the two distributions, we can readily imagine deciding (once and for all) whether pions are bosons or fermions by preparing an ensemble of systems (with particles in \( n = 3 \) and \( 4 \)) and measuring \( P(x_1, x_2) \).

Note that \( P(x_1, x_2) \) helps us decide not only whether the particles are bosons or fermions, but also whether they are identical in the first place. In other words, if particles that we think are identical differ with respect to some label that we are not aware of, the nature of the interference term will betray this fact. Imagine, for example, two bosons, call them \( K \) and \( \bar{K} \), which are identical with respect to mass and charge, but different with respect to a quantum number called “hypercharge.” Let us assume we are ignorant of hypercharge. In preparing an ensemble that we think contains \( N \) identical pairs, we will actually be including some \((K, K)\) pairs, some \((\bar{K}, \bar{K})\) pairs. If we now make measurements on the ensemble and extract the distribution \( P(x_1, x_2) \) (once again ignoring the hypercharge), we will find the interference term has the + sign but is not as big as it should be. If the ensemble contained only identical bosons, \( P(x, x) \) should be twice as big as \( P_D(x, x) \), which describes label-carrying particles; if we get a ratio less than 2, we know the ensemble is contaminated by label-carrying particles which produce no interference terms.

From the above discussions, it is also clear that one cannot hastily conclude, upon catching two electrons in the same orbital state in three dimensions that they are not fermions. In this case, the label we are ignoring is the spin orientation \( s \). As mentioned earlier on, \( s \) can have only two values, call them + and –. If we assume that \( s \) never changes (during the course of the experiment) it can serve as a particle label that survives with time. If \( s = + \) for one electron and \( – \) for the other, they are like two distinct particles and \emph{can} be in the same orbital state. The safe thing to do here is once again to work with an ensemble rather than an isolated measurement. Since we are ignorant of spin, our ensemble will contain \((+,+)\) pairs, \((-,-)\) pairs, and \((+,–)\) pairs. The \((+,+)\) and \((-,-)\) pairs are
identical fermions and will produce a negative interference term, while the (+, −) pairs will not. Thus we will find $P(r, r)$ is smaller than $P_D(r, r)$ describing labeled particles, but not zero. This will tell us that our ensemble has identical fermion pairs contaminated by pairs of distinguishable particles. It will then be up to us to find the nature of the hidden degree of freedom which provides the distinction.

**Literature**

Chapter 2

Second quantization, electrons and phonons

The formalism of second quantization permits to treat in a unified way systems with a large number of particles, this number being conserved or not. Here we give an introduction to this formalism and illustrate it with the example of the electron-phonon systems.

We consider an assembly of $N$ identical bosons or fermions without internal structure in a large box of volume $V = L^3$. We set $x_i = (r_i, \sigma_i)$ where $r_i$ is the position in the box and $\sigma_i = -s, -s + 1, \ldots, s - 1, +s$ the spin state. The Hilbert space for $N$ particles, $\mathcal{H}_\pm^N$, consists of wave functions $\psi(x_1, \ldots, x_N)$ that are symmetric under permutations of $x_1, \ldots, x_N$ for bosons

$$\psi(x_1, \ldots, x_N) = \psi(x_{\pi(1)}, \ldots, x_{\pi(N)}) \quad (2.1)$$

and antisymmetric for fermions

$$\psi(x_1, \ldots, x_N) = (-1)^{sgn(\pi)}\psi(x_{\pi(1)}, \ldots, x_{\pi(N)}). \quad (2.2)$$

In (2.2) $sgn(\pi)$ is the signature of the permutation $\pi$ of $N$ particles. The wave functions of $\mathcal{H}_\pm^N$ are square summable

$$\int dx_1 \cdots \int dx_N |\psi(x_1, \ldots, x_N)|^2 < \infty \quad (2.3)$$

where we use the notation

$$\int d\xi = \sum_{\sigma = -s}^{+s} \int_V dr.$$

2.1 Occupation number representation

Often there exists a natural basis for one-particle states, i.e. states belonging to the Hilbert space $\mathcal{H}$ with $N = 1$. For example this basis may be related to the energy levels of an atom, or to the plane waves of a free particle in a cubic
box with periodic boundary conditions. The $N$-particle states can be constructed from those of the single-particle basis.

Let \( \{ \phi_i(x), i = 1, 2, \ldots \} \) be an orthonormal basis of \( \mathcal{H} \),

\[
\int dx \overline{\phi_i(x)} \phi_j(x) = \langle \phi_i | \phi_j \rangle = \delta_{ij}.
\] (2.4)

We consider the special class of $N$-particle states obtained by symmetrising or antisymmetrising the tensor product of single-particle states of the basis

\[
S_{\pm} \{ \phi_{i_1}(x_1) \phi_{i_2}(x_2) \cdots \phi_{i_N}(x_N) \}
\]

\[
= \frac{1}{N!} \sum \sigma \left( \prod \phi_{i_1}(x_{\pi(1)}) \phi_{i_2}(x_{\pi(2)}) \cdots \phi_{i_N}(x_{\pi(N)}) \right)
\] (2.5)

where the sum carries over all $N!$ permutations of $N$ particles. In the notation of Dirac equation (2.5) becomes

\[
|\phi_{i_1} \cdots \phi_{i_N}\rangle_{\pm} = S_{\pm} \{ |\phi_{i_1}\rangle \otimes |\phi_{i_2}\rangle \otimes \cdots \otimes |\phi_{i_N}\rangle \}.
\] (2.6)

Instead of specifying the states (2.5) by the set of quantum numbers $i_1, i_2, \ldots, i_N$ one could indicate the number of times that a single-particle state appears in the product $\phi_{i_1} \phi_{i_2} \cdots \phi_{i_N}$. Let us call $n_i$ the number of times that the state $\phi_i$ appears in the product $\phi_{i_1} \phi_{i_2} \cdots \phi_{i_N}$. This number $n_i$ is the occupation number of the state $\phi_i$. Then the state (2.6) can be specified by the ket

\[
|n_1, n_2, \ldots, n_N\rangle_{\pm}, \quad \sum_{i=1}^{+\infty} n_i = N
\] (2.7)

where \pm refers to the statistics (fermions or bosons) and where there are $n_1$ particles in state $\phi_1$, $n_2$ particles in the state $\phi_2$ and so forth. By definition the wave function is

\[
\langle x_1, x_2, \ldots, x_N | n_1, n_2, \ldots \rangle_{\pm} = \frac{\sqrt{N!}}{\sqrt{n_1! n_2! \cdots}} S_{\pm} \{ \phi_{i_1}(x_1) \phi_{i_2}(x_2) \cdots \phi_{i_N}(x_N) \}.
\] (2.8)

For fermions $n_i = 0, 1$ according to the Pauli principle, and for bosons $n_i = 0, 1, 2, 3, \ldots$. For an $N$-particle state we have the restriction $\sum_{i=1}^{+\infty} n_i = N$.

It is important to realize that the occupation number representation (2.7) depends on the choice of the single particle basis of $\mathcal{H}$. In general one tries to make a judicious choice dictated by the physical problem at hand.

To keep the notation simpler we drop the subscript \pm in (2.7). But one has to remember that the states in the occupation number representation are symmetric (bosons) or antisymmetric (fermions).

One may show that the states (2.5) are orthogonal and thanks to the prefactor in (2.8) they form an orthonormal basis of $\mathcal{H}^N_{\pm}$. Their scalar product is

\[
\langle m_1, m_2, m_3, \ldots | n_1, n_2, n_3, \ldots \rangle = \delta_{m_1,n_1} \delta_{m_2,n_2} \delta_{m_3,n_3} \cdots
\] (2.9)
and all states of $\mathcal{H}_N^\pm$ can be obtained from linear combinations

$$|\psi\rangle = \sum_{\sum n_i = N} c(n_1, n_2, \ldots)|n_1, n_2, \ldots\rangle. \quad (2.10)$$

In (2.10) if we remove the restriction $\sum n_i = N$ we obtain a linear combination of states where the number of particles is not specified

$$|\psi\rangle = \sum_{n_1, n_2, \ldots} c(n_1, n_2, \ldots)|n_1, n_2, \ldots\rangle. \quad (2.11)$$

Clearly states with different total number of particles are orthogonal. Thus states of the form (2.11) belong to the Hilbert space formed by the direct sum

$$\bigoplus_{N=0}^{+\infty} \mathcal{H}_N^\pm = \mathcal{F}_\pm.$$

In this expression $\mathcal{H}_N^0 \cong \mathbb{C} \cong \{\lambda|0, 0, 0, \ldots\}, \lambda \in \mathbb{C}\} \text{ where } |0, 0, 0, \ldots\rangle \text{ is called the vacuum state. The space } \mathcal{F}_\pm \text{ is called the Fock space: it consists of symmetric (bosons) resp. antisymmetric (fermions) wave functions, the number of particles being unspecified. The Fock space is the appropriate Hilbert space for the formalism of second quantization.}

### 2.2 Creation and annihilation operators

**Bosons**

The creation operator $a^\dagger_i$ and annihilation operator $a_i$ of a boson in the state $\phi_i$ are defined by

$$a^\dagger_i|n_1, n_2, \ldots, n_i, \ldots\rangle = \sqrt{n_i + 1}|n_1, n_2, \ldots, n_i + 1, \ldots\rangle$$

$$a_i|n_1, n_2, \ldots, n_i, \ldots\rangle = \sqrt{n_i}|n_1, n_2, \ldots, n_i - 1, \ldots\rangle. \quad (2.12)$$

In (2.12) if $n_i = 0$, $a_i|n_1, n_2, \ldots, 0, \ldots\rangle = 0$. In addition to the two relations above we postulate that these operators are linear. In this way the creation and annihilation operators are completely defined. Relation (2.9) implies that the only non zero matrix elements of $a_i$ are

$$\langle n_1, n_2, \ldots, n_i - 1, \ldots|a_i|n_1, n_2, \ldots, n_i, \ldots\rangle = \sqrt{n_i}. \quad (2.13)$$

The only non zero matrix elements of $a^\dagger_i$ are

$$\langle n_1, n_2, \ldots, n_i, \ldots|a^\dagger_i|n_1, n_2, \ldots, n_i - 1, \ldots\rangle = (n_i - 1 + 1)\frac{i}{2} = (n_i)\frac{i}{2}. \quad (2.14)$$

Formulas (2.13) and (2.14) show that $a^\dagger_i$ is the adjoint of $a_i$: indeed the matrix elements of the adjoint of $a_i$ are obtained from (2.13) by taking the transpose and the complex conjugate.
From (2.12) one may also determine the algebra satisfied by these operators.

\[
[a_i, a_j^\dagger] = a_i a_j^\dagger - a_j^\dagger a_i = \delta_{ij} \\
[a_i, a_j] = [a_i^\dagger, a_j^\dagger] = 0
\]

(2.15)

For \( i = j \) the algebra is the same than that of the harmonic oscillator. Operators associated to different states \( |\phi_i\rangle \) and \( |\phi_j\rangle \) commute. Let us prove the first relation for \( i = j \):

\[
a_i a_i^\dagger |\ldots, n_i, \ldots\rangle = \sqrt{n_i + 1} a_i |\ldots, n_i + 1, \ldots\rangle \\
= \sqrt{n_i + 1} \sqrt{n_i + 1} |\ldots, n_i, \ldots\rangle \\
a_i^\dagger a_i |\ldots, n_i, \ldots\rangle = \sqrt{n_i} a_i^\dagger |\ldots, n_i - 1, \ldots\rangle \\
= \sqrt{n_i} \sqrt{n_i} |\ldots, n_i, \ldots\rangle
\]

Subtracting the two relations

\[
[a_i, a_i^\dagger] |\ldots, n_i, \ldots\rangle = |\ldots, n_i, \ldots\rangle.
\]

Using the linearity of the operators, we see that \( |\ldots, n_i, \ldots\rangle \) can be replaced by any linear combination, i.e. by any state of Fock space (in the last formula). Thus

\[
[a_i, a_i^\dagger] = 1.
\]

### Fermions

The creation and annihilation operators are linear and are defined by

\[
a_i^\dagger |n_1, n_2, \ldots, n_i, \ldots\rangle = (1 - n_i)(-1)^{\epsilon_i} |n_1, n_2, \ldots, n_i + 1, \ldots\rangle \\
a_i |n_1, n_2, \ldots, n_i, \ldots\rangle = n_i(-1)^{\epsilon_i} |n_1, n_2, \ldots, n_i - 1, \ldots\rangle.
\]

(2.16)

Here \( \epsilon_i = \sum_{s=1}^{i-1} n_s \) takes into account the Fermi statistics. Note that if state \( |\phi_i\rangle \) is already occupied (\( n_i = 1 \)) we have \( a_i^\dagger |n_1, n_2, \ldots, 1, \ldots\rangle = 0 \), which is an expression of the Pauli principle. As in the bosonic case \( a_i |n_1, n_2, \ldots, 0, \ldots\rangle = 0 \) if \( n_i = 0 \).

In a way analogous to (2.13)-(2.14) one shows that \( a_i^\dagger \) is the adjoint of \( a_i \). Moreover the algebra of these operators is

\[
\{a_i, a_j^\dagger\} = a_i a_j^\dagger + a_j^\dagger a_i = \delta_{ij} \\
\{a_i, a_j\} = \{a_i^\dagger, a_j^\dagger\} = 0.
\]

(2.17)

In particular \( a_i^2 = (a_i^\dagger)^2 = 0 \) which is again an expression of the Pauli principle. The proof of (2.17) is similar to the case of bosons (follows from (2.16) and linearity).
Particle number operator

From (2.12) or (2.16) we have (for both statistics)

\[ a_i^\dagger a_i | \ldots, n_i, \ldots \rangle = n_i | \ldots, n_i, \ldots \rangle. \] (2.18)

In other words the operator \( a_i^\dagger a_i \) can be implemented as the operator which counts the number of particles in the state \( |\phi_i\rangle \). The particle number operator or observable is

\[ N = \sum_{i=1}^{+\infty} a_i^\dagger a_i. \] (2.19)

We have

\[ N | n_1, n_2, n_3, \ldots \rangle = \sum_{i=1}^{+\infty} n_i | n_1, n_2, n_3, \ldots \rangle. \] (2.20)

Construction of states from the vacuum

The state corresponding to \( n_1 = 0, n_2 = 0, \ldots \) is denoted by \( |0\rangle \) and is commonly called the vacuum state. If one acts on \( |0\rangle \) with products (or polynomials) of \( a_i^\dagger \) and \( a_j \), one gets states in the Fock space. From the definitions of \( a_i^\dagger \) and \( a_j \) one shows that

\[ | n_1, n_2, \ldots, n_i, \ldots \rangle = \frac{(a_i^\dagger)^{n_1}(a_j^\dagger)^{n_2}}{\sqrt{n_1!}} \cdots \frac{(a_i^\dagger)^{n_i}}{\sqrt{n_i!}} \cdots |0\rangle. \] (2.21)

Intuitively this operation corresponds to fill specified energy levels, for example

\[ a_i^\dagger a_j^\dagger |0\rangle = |1, 0, 0, 1, 0, 0, \ldots \rangle. \]

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empty levels  levels 1 and 4 occupied

Since the Fock space is given by all linear combinations of the states in occupation number \( | n_1, n_2, \ldots, n_i, \ldots \rangle \) we see that all states can be obtained by acting on \( |0\rangle \) by polynomials \( P(a^\dagger, a) \).
2.3 Quantum fields or creation/annihilation operators in $x = (r, \sigma)$ representation

The creation and annihilation operators of a particle at position $r$ and spin state $\sigma$ (that is the state $|r, \sigma\rangle$) are

$$
\Psi^\dagger(x) = \sum_i \overline{\phi_i(x)} a_i^\dagger = \sum_i \langle x | \phi_i \rangle a_i^\dagger \\
\Psi(x) = \sum_i \phi_i(x) a_i = \sum_i \langle x | \phi_i \rangle a_i.
$$

(2.22)

These operators are also called quantum fields. From the orthonormality (2.4) of the simple particle basis $\{\phi_i, i = 1, 2, \ldots\}$ it follows that

$$a_i^\dagger = \int dx \, \overline{\phi_i(x)} \Psi^\dagger(x)$$
$$a_i = \int dx \, \phi_i(x) \Psi(x).$$

(2.23)

The particle number operator (2.19) becomes

$$N = \int dx \, \Psi^\dagger(x) \Psi(x)$$

(2.24)

which shows that $\Psi^\dagger(x) \Psi(x)$ can be interpreted as the density of particles of spin $\sigma$ at $r$. The proof of (2.24) is easy:

$$N = \sum_i a_i^\dagger a_i = \int dx \int dx' \sum_i \overline{\phi_i(x)} \phi_i(x') \Psi^\dagger(x) \Psi(x')$$
$$= \int dx \int dx' \, \delta(x - x') \Psi^\dagger(x) \Psi(x')$$
$$= \int dx \Psi^\dagger(x) \Psi(x)$$

We have used the closure relation in the second equality

$$\sum_i \langle x | \phi_i \rangle \langle \phi_i | x' \rangle = \delta(x - x') \quad (= \delta(r - r') \delta_{\sigma\sigma'}).$$

Remark

It is possible to define the creation and annihilation operators of any single particle state $|\chi\rangle$ by

$$a_i^\dagger(\chi) = \sum_i \overline{\langle \chi | \phi_i \rangle} a_i^\dagger, \quad a(\chi) = \sum_i \langle \chi | \phi_i \rangle a_i.$$

In principle one must show that $a_i^\dagger(\chi)$ and $a(\chi)$ are intrinsic, meaning that they do not depend on the choice of the basis $\{\phi_i\}$. This is also the case for $\Psi^\dagger(x)$,
\[ a^\dagger(\chi) = \sum_i \langle \chi | \phi_i \rangle a_i^\dagger \]
\[ = \sum_i \int dx \, \overline{\langle \chi | \phi_i \rangle} \phi_i(x) \Psi^\dagger(x) \]
\[ = \int dx \, \overline{\chi(x)} \Psi^\dagger(x) \]
and
\[ a(\chi) = \int dx \, \chi(x) \Psi(x). \]

Example

We consider electrons in a cubic box of size \( V = L^3 \) and take periodic boundary conditions. A simple basis is given by the plane waves

\[ \phi_{k\tau}(r, \sigma) = \langle k, \tau | r, \sigma \rangle = \frac{e^{ikr}}{V^{1/2}} \delta_{\tau \sigma} \]  
(2.25)

where \( k = \frac{2\pi}{L} n, n = (n_x, n_y, n_z) \in \mathbb{Z}^3 \). The creation and annihilation operators of an electron with wave vector \( k \) and spin \( \sigma \in \{\uparrow, \downarrow\} \) are \( a_{k\sigma}^\dagger \) and \( a_{k\sigma} \). The field operators of the electrons are given by the Fourier transforms

\[ \Psi_{\sigma}^\dagger(r) = \frac{1}{V^{1/2}} \sum_k e^{-ikr} a_{k\sigma}^\dagger \]

\[ \Psi_{\sigma}(r) = \frac{1}{V^{1/2}} \sum_k e^{ikr} a_{k\sigma}. \]  
(2.26)

The density operator at point \( r \) is

\[ n(r) = \Psi_\uparrow^\dagger(r) \Psi_\uparrow(r) + \Psi_\downarrow^\dagger(r) \Psi_\downarrow(r) \]  
(2.27)

and the total electron number operator is

\[ N = \sum_{\sigma - \uparrow, \downarrow} \int_V dr \, \Psi_{\sigma}^\dagger(r) \Psi_{\sigma}(r) = \sum_{k, \sigma} a_{k\sigma}^\dagger a_{k\sigma}. \]  
(2.28)

Commutation relations

From (2.22) one deduces the commutation relations for bosons

\[ [\Psi(x), \Psi^\dagger(x')] = \delta(x - x') = \delta(r - r') \delta_{\sigma \sigma'} \]

\[ [\Psi(x), \Psi(x')] = [\Psi^\dagger(x), \Psi^\dagger(x')] = 0 \]

and for fermions

\[ \{\Psi(x), \Psi^\dagger(x')\} = \delta(x - x') = \delta(r - r') \delta_{\sigma \sigma'} \]

\[ \{\Psi(x), \Psi(x')\} = \{\Psi^\dagger(x), \Psi^\dagger(x')\} = 0. \]  
(2.29)
2.4 A few examples of states in Fock space

a) The following identity

\[
\frac{1}{\sqrt{N!}}\Psi^\dagger(x_1)\Psi^\dagger(x_2)\cdots\Psi^\dagger(x_N)|0\rangle = \{|x_1, x_2, \ldots, x_N\rangle\}_{\pm}
\]

\[
= S_{\pm}\{x_1 \otimes x_2 \otimes \cdots \otimes x_N\}
\]

is intuitively clear since the product \(\Psi^\dagger(x_1)\Psi^\dagger(x_2)\cdots\Psi^\dagger(x_N)\) creates particles at \(x_1, x_2, \ldots, x_N\). Moreover the commutation relations assure that the state is properly symmetrised or antisymmetrised.

b) More generally

\[
\frac{1}{\sqrt{N!}}a^\dagger(\chi_1)a^\dagger(\chi_2)\cdots a^\dagger(\chi_N)|0\rangle = S_{\pm}\{\chi_1 \otimes \chi_2 \otimes \cdots \otimes \chi_N\}.
\]

This is nothing else but a Slater determinant \(\text{Det}\{\chi_i(x_j)\}\).

c) The Fermi sea for free electrons

\[
|F\rangle = \prod_{|k| < k_F} a^\dagger_{k\sigma}|0\rangle.
\]

d) The Bardeen-Cooper-Schrieffer state

\[
|BCS\rangle = \prod_k (u_k + v_k a^\dagger_{k\uparrow} a^\dagger_{-k\downarrow})|0\rangle, \quad |u_k|^2 + |v_k|^2 = 1
\]

where \(a^\dagger_{k\uparrow} a^\dagger_{-k\downarrow}|0\rangle\) is a Cooper pair.

e) A Bose condensate for \(N\) free bosons:

\[
\frac{(a^\dagger_{k=0})^N}{\sqrt{N!}}|0\rangle
\]

2.5 Representation of observables in second quantization

We have already encountered the number operator which may be expressed in terms of creation and annihilation operators (in the basis \(|\phi_i\rangle\)), \(\hat{N} = \sum_i a^\dagger_i a_i\). Here we shall explain how to express general observables in terms of \(a^\dagger\) and \(a\). In order to keep the discussion concrete we concentrate on three special, but important, observables. The kinetic energy of \(N\) particles

\[
T = \sum_{i=1}^N \frac{\hat{p}_i^2}{2m}
\]
The external potential
\[ V_{\text{ext}} = \sum_{i=1}^{N} U(\mathbf{r}_i) \]
and the two body interaction
\[ V_2 = \frac{1}{2} \sum_{i \neq j} V(x_i, x_j). \]

The first and the second observables are one-body observables while the third one is a two-body observable. For \( V_2 \) we take an interaction which is not necessarily translation invariant and may be spin dependent in order to sort out the general structure of formulas. However in most applications the two-body interaction is translation invariant and spin independent. Once the formulas for those three observables are established we will give the general representation.

**One-body observables**

**Kinetic energy** \( T \)

We start with the kinetic energy \( T \). Since it is diagonal in the basis of plane waves \( |k, \sigma\rangle \) we use the operators \( a^\dagger_{k\sigma}, a_{k\sigma} \). The number of particles in the state \( |k, \sigma\rangle \) is \( a^\dagger_{k\sigma}a_{k\sigma} \) so we expect
\[
T = \sum_{k, \sigma} \frac{|k|^2}{2m} a^\dagger_{k\sigma}a_{k\sigma}. \tag{2.30}
\]

We introduce the notation \( |k, \sigma\rangle = |k\rangle, a^\dagger_{k\sigma} = a^\dagger_k, a_{k\sigma} = a_k \). On a \( N \)-particle state
\[
|k_1, k_2, \ldots, k_N\rangle_{\pm} = a^\dagger_{k_1}a^\dagger_{k_2}\cdots a^\dagger_{k_N}|0\rangle
\]
\( T \) acts as
\[
T|k_1, k_2, \ldots, k_N\rangle_{\pm} = \left( \sum_{i=1}^{N} \frac{|k_i|^2}{2m} \right) |k_1, k_2, \ldots, k_N\rangle_{\pm}. \tag{2.31}
\]

In order to prove (2.30) it suffices to check that the second quantized expression acts in the same way. From the commutation relations (\( \epsilon = +1 \) for bosons, \(-1\) for fermions),
\[
(a^\dagger_{k_1}a_k)a^\dagger_{k_2}\cdots a^\dagger_{k_N}|0\rangle
\]
\[= a^\dagger_k(\delta_{kk_1} + \epsilon a^\dagger_{k_1}a_k)a^\dagger_{k_2}\cdots a^\dagger_{k_N}|0\rangle
\]
\[= \delta_{kk_1}a^\dagger_{k_1}a^\dagger_{k_2}\cdots a^\dagger_{k_N}|0\rangle + \epsilon a^\dagger_{k_1}a_{k_1}a^\dagger_{k_2}a^\dagger_{k_3}\cdots a^\dagger_{k_N}|0\rangle
\]
\[= \delta_{kk_1}a^\dagger_{k_1}a^\dagger_{k_2}\cdots a^\dagger_{k_N}|0\rangle + \epsilon\delta_{kk_2}a^\dagger_{k_2}a^\dagger_{k_1}a^\dagger_{k_3}\cdots a^\dagger_{k_N}|0\rangle
\]
\[+ \epsilon^2 a^\dagger_{k_1}a^\dagger_{k_2}a^\dagger_{k_3}\cdots a^\dagger_{k_N}|0\rangle
\]

The basic idea in this calculation is to use the commutation relations to bring the operator \( a_k \) on \( |0\rangle \) and use \( a_k|0\rangle = 0 \). We note that in the second term of the
last equality \(\epsilon a_k^{\dagger} a_k = a_k^{\dagger} a_k\). Finally one finds

\[
(a_k^{\dagger} a_k) a_{k_1}^{\dagger} a_{k_2}^{\dagger} \cdots a_{k_N}^{\dagger} |0\rangle = \left( \sum_{i=1}^{N} \delta_{kk_i} \right) a_{k_1}^{\dagger} a_{k_2}^{\dagger} \cdots a_{k_N}^{\dagger} |0\rangle \tag{2.32}
\]

In fact this identity could have been guessed by remarking that \(a_k^{\dagger} a_k\) counts the number of particles in the state \(|k, \sigma\rangle = |k\rangle\). From (2.32)

\[
\left( \sum_k |k|^2 \frac{a_k^{\dagger} a_k}{2m} \right) a_{k_1}^{\dagger} a_{k_2}^{\dagger} \cdots a_{k_N}^{\dagger} |0\rangle = \left( \sum_{i=1}^{N} \sum_k \frac{|k|^2}{2m} \delta_{kk_i} \right) a_{k_1}^{\dagger} a_{k_2}^{\dagger} \cdots a_{k_N}^{\dagger} |0\rangle = \left( \sum_{i=1}^{N} \frac{|k|^2}{2m} \right) a_{k_1}^{\dagger} a_{k_2}^{\dagger} \cdots a_{k_N}^{\dagger} |0\rangle
\]

which is identical to (2.31).

Expression (2.30) is simple and intuitive because the underlying basis diagonalises the kinetic energy. It is useful to have the representation of \(T\) in the \(|x\rangle = |r, \sigma\rangle\) basis. Inverting (2.26)

\[
a_{k\sigma}^{\dagger} = \frac{1}{V^2} \int_V dr e^{i k \cdot r} \Psi_{\sigma}^{\dagger}(r)
\]

\[
a_{k\sigma} = \frac{1}{V^2} \int_V dr e^{-i k \cdot r} \Psi_{\sigma}(r)
\]

we obtain

\[
T = \sum_\sigma \int_V \frac{1}{V} \int_V dr \int_V dr' \left( \sum_k e^{i k (r-r')} \frac{|k|^2}{2m} \right) \Psi_{\sigma}^{\dagger}(r) \Psi_{\sigma}(r').
\]

Since

\[
\frac{1}{V} \sum_k e^{i k (r-r')} \frac{|k|^2}{2m} = \left< r \left| \frac{\mathbf{p}^2}{2m} \right| r' \right>,
\]

we get

\[
T = \sum_\sigma \int_V dr \int_V dr' \Psi_{\sigma}^{\dagger}(r) \left< r \left| \frac{\mathbf{p}^2}{2m} \right| r' \right> \Psi_{\sigma}(r').
\]

Furthermore we note that \(\left< r \left| \frac{\mathbf{p}^2}{2m} \right| r' \right> = \delta(r - r') \left(-\frac{\hbar^2}{2m} \Delta r \right)\) so

\[
T = \sum_\sigma \int_V dr \Psi_{\sigma}^{\dagger}(r) \delta(r - r') \left(-\frac{\hbar^2}{2m} \Delta r \right) \Psi_{\sigma}(r').
\]

**External potential \(V_{ext}\)**

This one-body observable is diagonal in direct space:

\[
V_{ext} |x_1, x_2, \ldots, x_N\rangle = \left( \sum_{i=1}^{N} U(r_i) \right) |x_1, x_2, \ldots, x_N\rangle \tag{2.37}
\]
The representation in second quantization is

\[ V_{\text{ext}} = \sum_{\sigma} \int d\mathbf{r} U(\mathbf{r}) \Psi_{\sigma}^\dagger(\mathbf{r}) \Psi_{\sigma}(\mathbf{r}) \]

\[ = \int d\mathbf{r} U(\mathbf{r}) n(\mathbf{r}). \] (2.38)

This expression is similar to a classical formula except that here \( n(\mathbf{r}) \) is the density operator (see 2.27). To check formula (2.38) we compute the action of the right hand side on basis states

\[ |x_1, x_2, \ldots, x_N\rangle = \frac{1}{\sqrt{N!}} \Psi^\dagger(x_1) \Psi^\dagger(x_2) \cdots \Psi^\dagger(x_N)|0\rangle \] (2.39)

Here we use the notation \( \Psi^\dagger_{\sigma}(\mathbf{r}) = \Psi^\dagger(\mathbf{r}, \sigma) = \Psi^\dagger(\mathbf{r}) \). By communting \( \Psi(x) \), the annihilation operator, with all creators and using \( \Psi(x)|0\rangle = 0 \), we find (this is similar to (2.32))

\[ (\Psi^\dagger(x) \Psi(x)) \Psi^\dagger(x_1) \Psi^\dagger(x_2) \cdots \Psi^\dagger(x_N)|0\rangle \]

\[ = \left( \sum_{i=1}^{N} \delta(\mathbf{r} - \mathbf{r}_i) \delta_{\sigma_{\sigma_i}} \right) \Psi^\dagger(x_1) \Psi^\dagger(x_2) \cdots \Psi^\dagger(x_N)|0\rangle. \] (2.40)

This relation can be guessed by realizing that \( \sum_{i=1}^{N} \delta(\mathbf{r} - \mathbf{r}_i) \delta_{\sigma_{\sigma_i}} \) counts the number of particles in the state \( |\mathbf{r}, \sigma\rangle = |\mathbf{x}\rangle \). From (2.40) we obtain

\[ \left( \int d\mathbf{r} U(\mathbf{r}) n(\mathbf{r}) \right) \Psi^\dagger(x_1) \Psi^\dagger(x_2) \cdots \Psi^\dagger(x_N)|0\rangle \]

\[ = \left( \sum_{i=1}^{N} U(\mathbf{r}_i) \right) \Psi^\dagger(x_1) \Psi^\dagger(x_2) \cdots \Psi^\dagger(x_N)|0\rangle. \] (2.41)

which proves formula (2.37).

To obtain the expression of \( V_{\text{ext}} \) in the Fourier basis one replaces (2.25) in (2.38)

\[ V_{\text{ext}} = \sum_{\mathbf{k}, \mathbf{k}'} \left( \frac{1}{L^3} \int_V d\mathbf{r} U(\mathbf{r}) e^{-i(\mathbf{k}' - \mathbf{k}) \cdot \mathbf{r}} \right) \sum_{\sigma} a_{\mathbf{k}' \sigma}^\dagger a_{\mathbf{k} \sigma} \]

\[ = \frac{1}{L^3} \sum_{\mathbf{k}, \mathbf{k}', \sigma} \hat{U}(\mathbf{k}' - \mathbf{k}) a_{\mathbf{k}' \sigma}^\dagger a_{\mathbf{k} \sigma} \] (2.42)

where

\[ \hat{U}(\mathbf{k}) = \int_V d\mathbf{r} e^{-i\mathbf{k} \cdot \mathbf{r}} U(\mathbf{r}). \]

The result can be written in two equivalent forms

\[ V_{\text{ext}} = \sum_{\mathbf{k}, \mathbf{k}', \sigma} \langle \mathbf{k}', \sigma | U(\mathbf{k}, \sigma) a_{\mathbf{k}' \sigma}^\dagger a_{\mathbf{k} \sigma} \]

\[ = \frac{1}{L^3} \sum_{\mathbf{k}, \mathbf{q}, \sigma} \hat{U}(\mathbf{q}) a_{\mathbf{k} + \mathbf{q} \sigma}^\dagger a_{\mathbf{k} \sigma}. \] (2.43)

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Diagrammatic interpretation:

General expression of one-body observables

Thanks to the formulas (2.35) and (2.43) we can infer the general expression of any single-particle operator. Let \( A \) be a one-body observable: that is a selfadjoint operator from \( \mathcal{H} \rightarrow \mathcal{H} \), with matrix elements

\[
A_{ij} = \langle \phi_i | A | \phi_j \rangle
\]

(2.44)

and let \( a_i^\dagger, a_j \) the creation and annihilation operators of the basis states \( \{ | \phi_i \rangle \} \). The second quantized form of \( A \) is

\[
A = \sum_{i,j} \langle \phi_i | A | \phi_j \rangle a_i^\dagger a_j.
\]

(2.45)

The operator \( A \) is selfadjoint from \( \mathcal{F}_\pm \rightarrow \mathcal{F}_\pm \). Note that if \( A \) is diagonal for the basis \( \{ | \phi_i \rangle \} \) we have the simpler expression

\[
A = \sum_i \alpha_i a_i^\dagger a_i.
\]

(2.46)

Here \( A | \phi_i \rangle = \alpha_i | \phi_i \rangle \).

Two-body observables

We will concentrate on a two-body interaction, which is spin independent, and proceed in a way analogous to \( V_{\text{ext}} \). The observable is diagonal in direct space:

\[
V_2 | x_1, x_2, \ldots, x_N \rangle_\pm = \frac{1}{2} \sum_{i \neq j} V_2(r_i, r_j) | x_1, x_2, \ldots, x_N \rangle_\pm
\]

(2.47)

The second quantized expression is

\[
V_2 = \frac{1}{2} \int dx \int dx' V_2(x, x') \Psi^\dagger(x) \Psi^\dagger(x') \Psi(x') \Psi(x)
\]

(2.48)

Often this expression is rewritten in a form involving the density operators (2.27):

\[
V_2 = \frac{1}{2} \int_V dx \int_V dx' V_2(x, x') : n(x)n(x') :
\]

(2.49)
This formula has a familiar aspect except for the fact that the product of density operators at points \( x \) and \( x' \) is normal ordered. This means that all the creation operators are put on the left of the annihilation operators and that for fermions one hast to take into account \((-1)^{\text{sgn}(\pi)}\) \( \pi \) the permutation involved in the rearrangement of the operators.

\[
: n(r)n(r') : = : n(r, \sigma)n(r', \sigma') : \\
= : \Psi_\sigma^\dagger(r)\Psi_\sigma(r)\Psi_{\sigma'}^\dagger(r')\Psi_{\sigma'}(r') : \\
= \epsilon\Psi_\sigma^\dagger(r)\Psi_\sigma^\dagger(r')\Psi_\sigma(r)\Psi_{\sigma'}(r') \\
= \epsilon^2\Psi_\sigma^\dagger(r)\Psi_{\sigma'}^\dagger(r')\Psi_\sigma(r)\Psi_{\sigma'}(r) \\
= \Psi_\sigma^\dagger(r)\Psi_{\sigma'}^\dagger(r')\Psi_{\sigma'}(r)\Psi_\sigma(r) \\
(2.50)
\]

**Proof of (2.48)**

We have to check that (2.48) satisfies (2.47). The basic idea is to use the commutation relations to bring \( \Psi(x')\Psi(x) \) on \( |0\rangle \) and use \( \Psi(x')\Psi(x)|0\rangle = 0 \). To illustrate the method we concentrate on the simpler case of a two particle state in (2.47) : 
\[
|x_1, x_2\rangle = \Psi^\dagger(x_1)\Psi^\dagger(x_2)|0\rangle. \]

We have

\[
\Psi(x)\Psi^\dagger(x_1)\Psi^\dagger(x_2) \\
= \delta(x - x_1)\Psi^\dagger(x_2) + \epsilon\Psi^\dagger(x_1)\Psi(x)\Psi^\dagger(x_2) \\
= \delta(x - x_1)\Psi^\dagger(x_2) + \epsilon\delta(x - x_2)\Psi^\dagger(x_1) + \epsilon^2\Psi^\dagger(x_1)\Psi^\dagger(x_2)\Psi(x)
\]

and

\[
\Psi(x')\Psi(x)\Psi^\dagger(x_1)\Psi^\dagger(x_2) \\
= \delta(x - x_1)\delta(x' - x_2) + \epsilon\delta(x - x_1)\Psi^\dagger(x_2)\Psi(x') + \epsilon\delta(x - x_2)\Psi^\dagger(x_1)\Psi(x) \\
+ \epsilon^2\delta(x - x_1)\Psi^\dagger(x_1)\Psi(x) + \delta(x' - x_1)\Psi^\dagger(x_2)\Psi(x) \\
+ \epsilon\delta(x' - x_2)\Psi^\dagger(x_1)\Psi(x) + \Psi^\dagger(x_1)\Psi^\dagger(x_2)\Psi(x')\Psi(x). \\
\]

Multiplying on the right by \( |0\rangle \) we see that only two terms survive

\[
\Psi(x')\Psi(x)\Psi^\dagger(x_1)\Psi^\dagger(x_2)|0\rangle \\
= [\delta(x - x_1)\delta(x' - x_2) + \epsilon\delta(x - x_2)\delta(x' - x_1)]|0\rangle.
\]

Thus :

\[
[\Psi^\dagger(x)\Psi^\dagger(x')\Psi(x')\Psi(x)]\Psi^\dagger(x_1)\Psi^\dagger(x_2)|0\rangle \\
= \delta(x - x_1)\delta(x' - x_2)\Psi^\dagger(x)\Psi^\dagger(x')|0\rangle + \epsilon\delta(x - x_2)\delta(x' - x_1)\Psi^\dagger(x)\Psi^\dagger(x')|0\rangle \\
= \delta(x - x_1)\delta(x' - x_2)\Psi^\dagger(x_1)\Psi^\dagger(x_2)|0\rangle + \epsilon\delta(x - x_2)\delta(x' - x_1)\Psi^\dagger(x_1)\Psi^\dagger(x_2)|0\rangle \\
= \delta(x - x_1)\delta(x' - x_2)\Psi^\dagger(x_1)\Psi^\dagger(x_2)|0\rangle + \delta(x - x_2)\delta(x' - x_1)\Psi^\dagger(x_1)\Psi^\dagger(x_2)|0\rangle \\
= \delta(x - x_1)\delta(x' - x_2) + \delta(x - x_2)\delta(x' - x_1)\Psi^\dagger(x_1)\Psi^\dagger(x_2)|0\rangle \\
= \Psi^\dagger(x_1)\Psi^\dagger(x_2)|0\rangle \\
(2.51)
\]
Now we multiply the equality by \( V_2(x, x') \) and integrate over \( x \) and \( x' \). The contribution of the first term in (2.51) is

\[
\int dx \int dx' \delta(x - x_1)\delta(x' - x_2) V_2(x, x') \Psi^\dagger(x_1) \Psi^\dagger(x_2)|0\rangle = V_2(x_1, x_2)|x_1, x_2\rangle_\pm.
\]

The contribution of the second term in (2.51) is

\[
V_2(x_2, x_1)|x_1, x_2\rangle_\pm.
\]

For a symmetric potential \( V_2(x_1, x_2) = V_2(x_2, x_1) \) the two contributions are equal and add up. Because there is a \( \frac{1}{2} \) in (2.48) we obtain

\[
\left( \frac{1}{2} \int dx \int dx' V_2(x, x') \Psi^\dagger(x) \Psi^\dagger(x') \Psi(x) \right)|x_1, x_2\rangle_\pm = V_2(x_1, x_2)|x_1, x_2\rangle_\pm
\]

as required by (2.47).

Let us derive the expression for \( V_2 \) in momentum space. Replacing (2.25) in (2.49) we get

\[
V_2 = \frac{1}{2} \sum_{k_1, k_2, k_3, k_4} \sum_{\sigma_1, \sigma_2, \sigma_3, \sigma_4} \langle k_1, \sigma_1; k_2, \sigma_2| V_2| k_4, \sigma_4; k_3, \sigma_3 \rangle (2.52)
\]

where the matrix element of the two body interaction is explicitly

\[
\langle k_1, \sigma_1; k_2, \sigma_2| V_2| k_4, \sigma_4; k_3, \sigma_3 \rangle = \frac{1}{L^6} \sum_{\sigma} \int_V d\mathbf{r} \sum_{\sigma'} \int_V d\mathbf{r}' e^{-ik_1 \cdot \mathbf{r}} \delta_{\sigma_1 \sigma} e^{-ik_2 \cdot \mathbf{r}'} \delta_{\sigma_2 \sigma'} V_2(\mathbf{r}, \sigma; \mathbf{r}', \sigma') e^{-ik_4 \cdot \mathbf{r}} \delta_{\sigma_4 \sigma} e^{-ik_3 \cdot \mathbf{r}'} \delta_{\sigma_3 \sigma'}
\]

In most situations of interest the potential is spin independent and translation invariant : \( V_2(x, x') = V_2(\mathbf{r} - \mathbf{r}') \). Thus the summation over \( \sigma \) and \( \sigma' \) can be performed explicitly

\[
\langle k_1, \sigma_1; k_2, \sigma_2| V_2| k_4, \sigma_4; k_3, \sigma_3 \rangle = \delta_{\sigma_1 \sigma_4} \delta_{\sigma_2 \sigma_3} \langle k_1, k_2| V_2| k_4, k_3 \rangle (2.53)
\]

and

\[
\langle k_1, k_2| V_2| k_4, k_3 \rangle = \frac{1}{L^6} \int_V d\mathbf{r}' e^{i(k_3 - k_2) \cdot \mathbf{r}'} \int_V d\mathbf{r} V_2(\mathbf{r} - \mathbf{r}') e^{i(k_4 - k_1) \cdot \mathbf{r}}
\]

\[
= \frac{1}{L^6} \int_V d\mathbf{r}' e^{i(k_3 + k_4 - k_1 - k_2) \cdot \mathbf{r}'} \int_V d\mathbf{r} V_2(\mathbf{r}) e^{i(k_4 - k_1) \cdot \mathbf{r}}
\]

\[
= \frac{1}{L^3} \delta_{k_3 + k_4, k_1 + k_2} \hat{V}_2(\mathbf{k}_1 - \mathbf{k}_4). (2.54)
\]
It is important to remark that in the second equality we omit a "surface term" which comes from the fact that the spatial integrals are carried out for a finite volume. The result becomes exact in the thermodynamic limit \( L \to +\infty \). Finally the Kronecker symbol expresses the fact that the system is translation invariant and thus the momentum is conserved \( k_3 + k_4 = k_1 + k_2 \) in collision processes. Setting \( k_1 - k_4 = q \) and then \( k_4 = k \), \( k_3 = k' \), from (2.52), (2.53) and (2.54) we get the important result

\[
V_2 = \frac{1}{2L^3} \sum_{k,k',q \sigma,\sigma'} \hat{V}_2(q) a_{k+q,\sigma}^\dagger a_{k',-q,\sigma'}^\dagger a_{k',\sigma'}^\dagger a_{k,\sigma}. \tag{2.55}
\]

Graphical interpretation:

\[
\begin{array}{c}
\text{k,}\sigma \\
\bullet \\
\text{k+q,}\sigma \\
\text{q} \\
\text{k',}\sigma' \\
\bullet \\
\text{k'-q,}\sigma' \\
\end{array}
\]

Momentum is conserved at each vertex.

**General expression for a two-body observable**

Let \( V \) be a general two-body observable acting from \( \mathcal{H} \otimes \mathcal{H} \to \mathcal{H} \otimes \mathcal{H} \) with matrix elements

\[
V_{ij;kl} = \langle \phi_i \otimes \phi_j | V | \phi_k \otimes \phi_l \rangle \tag{2.56}
\]

in the basis \( |\phi_i \otimes \phi_j \rangle \) of \( \mathcal{H} \otimes \mathcal{H} \). From (2.52) one may infer the general structure of the second quantized operator

\[
V_2 = \frac{1}{2} \sum_{i,j,k,l} V_{ij;kl} a_i^\dagger a_j^\dagger a_l a_k. \tag{2.57}
\]

Observe the order of the indices.

### 2.6 Electrons and phonons

The description of electron-phonon interactions is a vast subject and plays an important role in a number of phenomena. Here we give a brief overview of the derivation of the basic electron-phonon Hamiltonian in second quantization.

We consider a simplified model for a metal in which the conduction electrons interact with ions of a crystal. For simplicity we suppose that there is one ion
per unit cell and label its position by $\mathbf{R}_i$. The total Hamiltonian is in first quantization

$$H = \sum_i \frac{p_i^2}{2m} + \frac{1}{2} \sum_{i \neq j} V_{ee}(\mathbf{r}_i - \mathbf{r}_j) + \sum_i \frac{p_i^2}{2M} + \frac{1}{2} \sum_{i \neq j} V_{ii}(\mathbf{R}_i - \mathbf{R}_j) + \sum_{i,j} V_{ei}(\mathbf{r}_i - \mathbf{R}_j) \quad (2.58)$$

The ion coordinates are supposed to have small fluctuations around equilibrium lattice sites $\{\mathbf{R}_i^0\}, i = 1, \ldots, N$.

$$\mathbf{R}_i = \mathbf{R}_i^0 + \delta \mathbf{R}_i \quad (2.59)$$

As a result we use the harmonic approximation in which the ion interaction is replaced by

$$V_{ii}(\mathbf{R}_i^0 - \mathbf{R}_j^0) + \frac{1}{2} \sum_{\mu,\nu=1}^3 (\delta \mathbf{R}_i - \delta \mathbf{R}_j)_\mu (\delta \mathbf{R}_i - \delta \mathbf{R}_j)_\nu \frac{\partial^2}{\partial \mathbf{R}_\mu \partial \mathbf{R}_\nu} V_{ii}(\mathbf{R}_i^0 - \mathbf{R}_j^0) \quad (2.60)$$

The first term is constant and is omitted by redefining the energy. The harmonic energy of the ions may be diagonalized by introducing the normal modes:

$$\delta \mathbf{R}_i = \frac{1}{\sqrt{NM}} \sum_{q,\lambda} Q_{q,\lambda} \epsilon_\lambda(q) e^{iq\mathbf{R}_i^0} \quad (2.61)$$

$$\mathbf{P}_i = \sqrt{\frac{M}{N}} \sum_{q,\lambda} \Pi_{q,\lambda} \epsilon_\lambda(q) e^{-iq\mathbf{R}_i^0} \quad (2.62)$$

In these formulas $\epsilon_\lambda(q), \lambda = 1, 2, 3$ are polarization vectors, i.e. eigenvectors of the normal mode equation

$$\sum_{\nu=1}^3 D_{\mu\nu}(q) \epsilon_\lambda'(q) = M \omega^2_{q,\lambda} \epsilon_\lambda(q)$$

where $D_{\mu\nu}(q)$ is the Fourier transform of $\frac{\partial^2 V_{ii}}{\partial \mathbf{R}_\mu \partial \mathbf{R}_\nu}(\mathbf{R})$. The sums over $q$ are restricted to the first Brillouin zone of the crystal.

In terms of normal modes (2.60) is diagonal

$$\frac{1}{2} \sum_{q,\lambda} \left( \Pi_{q,\lambda}^\dagger \Pi_{q,\lambda} + \omega^2_{q,\lambda} Q_{q,\lambda}^\dagger Q_{q,\lambda} \right) \quad (2.63)$$

The usual commutation relations $[\mathbf{R}_i^\mu, \mathbf{P}_j^{\nu}] = i\hbar \delta_{ij} \delta_{\mu\nu}$ imply

$$[Q_{q,\lambda}, \Pi_{q',\lambda'}] = i\hbar \delta_{qq'} \delta_{\lambda\lambda'}$$

$$[Q_{q,\lambda}, Q_{q',\lambda'}] = [\Pi_{q,\lambda}, \Pi_{q',\lambda'}] = 0$$

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and therefore (2.63) is just the Hamiltonian for a collection of independent harmonic oscillators for each mode \( q \) and polarization \( \lambda \). The creation and annihilation operators of phonons for the mode \( q \) and polarization \( \lambda \) can be defined by the usual relations

\[
Q_{q,\lambda} = \left( \frac{\hbar}{2\omega_q} \right)^{\frac{1}{2}} (b_{q\lambda} + b_{-q\lambda}^+) \\
\Pi_{q,\lambda} = i \left( \frac{\hbar\omega_q}{2} \right)^{\frac{1}{2}} (b_{q\lambda}^+ - b_{-q\lambda}).
\]

with boson commutation relations

\[
[b_{q\lambda}, b^*_{q',\lambda'}] = \delta_{qq'} \delta_{\lambda\lambda'} \\
[b_{q\lambda}, b_{q',\lambda'}] = [b^*_{q\lambda}, b^*_{q',\lambda'}] = 0.
\]

The Hamiltonian (2.63) takes the form

\[
\sum_{q,\lambda} \hbar\omega_{q\lambda} \left( b^*_{q\lambda} b_{q\lambda} + \frac{1}{2} \right) = \sum_{q\lambda} \hbar\omega_{q\lambda} \left( N_{q\lambda} + \frac{1}{2} \right) \tag{2.64}
\]

where \( N_{q\lambda} = b^*_{q\lambda} b_{q\lambda} \) is the number operator for phonons. This is the phonon Hamiltonian in the harmonic approximation. If one would take into account anharmonic terms, one would obtain interaction terms in (2.64), involving quartic monomials of operators \( b^* \) and \( b \).

The electron-ion interaction gives two contributions for small displacements of the ions around their equilibrium positions.

\[
\sum_{i,j} V_{ei}(r_i - R_j) = \sum_i \left( \sum_j V_{ei}(r_i - R^0_j) \right) + \sum_{i,j} \delta R_j \nabla V_{ei}(r_i - R^0_j) \tag{2.65}
\]

Let us first look at the first term. It represents an external potential for the electron, due to the periodic crystalline lattice, and it is natural to add it to the purely electronic part of (2.58). Thus the purely electronic part of the energy is

\[
\sum_i \left( \frac{p_i^2}{2m} + U(r_i) \right) + \frac{1}{2} \sum_{i,j} V_{ee}(r_i - r_j) \tag{2.66}
\]

with \( U(r) = \sum_j V_{ei}(r - R^0_j) \).

The one-body part of (2.66) can be diagonalized with the help of Bloch functions \( \chi_{kn}(r) \) satisfying

\[
\chi_{kn}(r + R) = e^{i k \cdot R} \chi_{kn}(r)
\]

where \( R \) is a lattice vector. The energy bands are described by dispersion relations \( \epsilon_n(k) \) where \( k \) is restricted to the first Brillouin zone and \( n \) indexes the energy band. To keep the notation a bit simple we work in an extended zone scheme : there is one function \( \epsilon(k) \) with discontinuities and \( n \) is dropped. Denoting by
\[ a_{\kappa \sigma}^\dagger \text{ and } a_{\kappa \sigma} \] the creators and annihilators of electrons in the basis states \( \chi_k(\mathbf{r}) \), the electronic part (2.66) has the second quantized version

\[
\sum_{k, \sigma} \epsilon(k) a_{\kappa \sigma}^\dagger a_{\kappa \sigma} + \frac{1}{2} \sum_{k_1, k_2, k_3, k_4, \sigma, \sigma'} \langle k_1, k_2 | V_{ee} | k_3, k_4 \rangle a_{k_1 \sigma}^\dagger a_{k_2 \sigma'} a_{k_3 \sigma} a_{k_4 \sigma'} \quad (2.67)
\]

where

\[
\langle k_1, k_2 | V_{ee} | k_3, k_4 \rangle = \int d\mathbf{r} \int d\mathbf{r}' \frac{\chi_{k_1}(\mathbf{r}) \chi_{k_2}(\mathbf{r}')}{\chi_{k_3}(\mathbf{r}) \chi_{k_4}(\mathbf{r}')} V_{ee}(\mathbf{r} - \mathbf{r}') \quad (2.68)
\]

Bloch’s theorem, that is \( \chi_k(\mathbf{r} + \mathbf{R}) = e^{ik \cdot \mathbf{R}} \chi_k(\mathbf{r}) \), implies that (2.68) is non-zero only for

\[
(k_1 + k_2) - (k_3 + k_4) = \mathbf{G}
\]

where \( \mathbf{G} \) is a vector of the dual lattice, i.e. satisfying \( e^{i\mathbf{G} \cdot \mathbf{R}} = 1 \). Physically this means that in a collision process between electrons their momentum is conserved modulo a vector of the dual lattice. In the Jellium model where the effect of a periodic potential is not taken into account this condition is not present (or in other words \( \mathbf{G} = 0 \) and momentum is conserved \( (k_1 + k_2) = (k_3 + k_4) \)).

The second term in (2.65) is the interaction of the electrons with lattice deformations, to lowest order. This term leads to the standard electron-phonon interaction. From (2.61) we have

\[
\sum_j \delta \mathbf{R}_j \cdot \nabla V_{ei}(\mathbf{r} - \mathbf{R}_j^0) = \frac{1}{\sqrt{NM}} \sum_{q, \lambda} Q_{q \lambda} \epsilon_{\lambda}(\mathbf{q}) \cdot \sum_j e^{i\mathbf{q} \mathbf{R}_j^0} \nabla V_{ei}(\mathbf{r} - \mathbf{R}_j^0). \quad (2.70)
\]

The matrix elements of the sum over \( j \) between two Bloch wave functions are

\[
\sum_j e^{i\mathbf{q} \mathbf{R}^0_j} \int d\mathbf{r} \chi_{k}(\mathbf{r}) \nabla V_{ei}(\mathbf{r} - \mathbf{R}_j^0) \chi_{k'}(\mathbf{r})
\]

\[
= \sum_j e^{i(\mathbf{k}' - \mathbf{k} + \mathbf{q}) \cdot \mathbf{R}^0_j} \int d\mathbf{r} \chi_{k}(\mathbf{r}) \nabla V_{ei}(\mathbf{r}) \chi_{k'}(\mathbf{r})
\]

\[
= N \sum_G \delta_{\mathbf{k}' - \mathbf{k} + \mathbf{q}, \mathbf{G}} \langle \mathbf{k} | \nabla V_{ei} | \mathbf{k}' \rangle. \quad (2.71)
\]

To obtain the last equality the Poisson summation formula is used. It follows from (2.71) and (2.70) that the electron-phonon interaction takes the form

\[
\sum_{k, k', q, \sigma, G} g_{k, k'}(\mathbf{q}) \delta_{\mathbf{k}' - \mathbf{k} + \mathbf{q}, \mathbf{G}} (b_{q \lambda} + b_{-q \lambda}^\dagger) a_{k \sigma}^\dagger a_{k' \sigma} \quad (2.72)
\]

with the function \( g_{k, k'}(\mathbf{q}) \) describing the electron-phonon coupling:

\[
g_{k, k'}(\mathbf{q}) = \left( \frac{\hbar N}{2 \omega_{q \lambda} M} \right)^{\frac{1}{2}} \langle \mathbf{k} | \nabla V_{ei} | \mathbf{k}' \rangle \cdot \epsilon_{\lambda}(\mathbf{q}) \quad (2.73)
\]
In summary the total Hamiltonian of the system is given by the sum of three expressions (2.64), (2.67) and (3.1). This is a very complicated Hamiltonian, and in practice the matrix elements involved in the interactions are not well known.

All our further discussions of electron-phonon coupling will be based on the Jellium model where the ionic density is assumed to be spread uniformly in space. In other words the Bloch functions $\chi_{\lambda}(r)$ are replaced by plane waves $L^{-\frac{2}{3}} \exp(i\mathbf{k} \cdot \mathbf{r})$, $\epsilon(\mathbf{k}) = \frac{\hbar^2 |\mathbf{k}|^2}{2m}$, and only the term $G = 0$ remains. Then (3.1) becomes

$$\sum_{\mathbf{k}, \mathbf{q}, \sigma} g_{\mathbf{q}, \lambda}(b_{\mathbf{q}, \lambda}^\dagger + b_{-\mathbf{q}, \lambda}^\dagger) a_{\mathbf{k} + \mathbf{q}, \sigma}^\dagger a_{\mathbf{k}, \sigma}$$

with

$$g_{\mathbf{q}, \lambda} = \left( \frac{\hbar N}{2\omega_{\mathbf{q}, \lambda}^2 M L^3} \right)^\frac{1}{2} \mathbf{q} \cdot \epsilon_{\lambda}(\mathbf{q}) \tilde{V}_{ei}(\mathbf{q}).$$

We see on this formula that the electron-phonon coupling is purely longitudinal within the Jellium model. In order to estimate $g_{\mathbf{q}, \lambda}$ we take the bare electron-ion potential

$$\tilde{V}_{ei}(\mathbf{q}) = \frac{Z^2 e^2}{\epsilon_0 |\mathbf{q}|^2}$$

and for $\omega_{\mathbf{q}, \lambda}^2$ the bare ion frequency

$$\omega_{\mathbf{q}, \lambda}^2 = \omega_{\text{plasma-ions}}^2 = \frac{N Z^2 e^2}{L^3 \epsilon_0 M}.$$

Then one finds

$$g_{\mathbf{q}, \lambda} = \frac{\hbar \omega_{\text{plasma-ions}} Z^2}{2 \omega_{\mathbf{q}, \lambda}^2 M \epsilon_0 |\mathbf{q}|^2}. \quad \text{(2.74)}$$

One also notes the following identity

$$\frac{2g_{\mathbf{q}, \lambda}^2}{\hbar \omega_{\text{plasma-ions}}} = \frac{e^2}{\epsilon_0 |\mathbf{q}|^2} \text{ (2.75)}$$

which means that the energy scales of the bare electron-phonon and electron-electron interactions are of the same order. Therefore a consistent treatment of a metal has to take into account both (see chapter 5).

Finally note that $(b_{\mathbf{q}, \lambda} + b_{-\mathbf{q}, \lambda}^\dagger) a_{\mathbf{k} + \mathbf{q}, \sigma}^\dagger a_{\mathbf{k}, \sigma}$ represents absorption and emission processes of phonons by electrons.

Absorption process : $g_{\mathbf{q}, \lambda} b_{\mathbf{q}, \lambda}^\dagger a_{\mathbf{k} + \mathbf{q}, \sigma}^\dagger a_{\mathbf{k}, \sigma}$

\[ \begin{array}{c}
\textbf{q} \\
\textbf{k} \rightarrow \textbf{k} + \textbf{q}
\end{array} \]
Emission process: \( g_{q\lambda} b_{-q\lambda}^\dagger a_{k+q\sigma}^\dagger a_k \)

**Literature**