Second quantization

We introduce the time-independent operators $a_\alpha^\dagger$ and $a_\alpha$, which create and annihilate, respectively, a particle in the single-particle state $\phi_\alpha$. We define the fermion creation operator $a_\alpha^\dagger a_\alpha^\dagger |0\rangle = |\alpha\rangle$, (1)

and $a_\alpha^\dagger |\alpha_1...\alpha_n\rangle_{AS} = |\alpha_1...\alpha_n\rangle_{AS}$ (2)

In Eq. (1) the operator $a_\alpha^\dagger$ acts on the vacuum state $|0\rangle$, which does not contain any particles. Alternatively, we could define a closed-shell nucleus or atom as our new vacuum, but then we need to introduce the particle-hole formalism, see the discussion to come. In Eq. (2) $a_\alpha^\dagger$ acts on an antisymmetric $n$-particle state and creates an antisymmetric $(n+1)$-particle state, where the one-body state $\phi_\alpha$ is occupied, under the condition that $\alpha \neq \alpha_1, \alpha_2, ..., \alpha_n$. It follows that we can express an antisymmetric state as the product of the creation operators acting on the vacuum state.

$|\alpha_1...\alpha_n\rangle_{AS} = a_\alpha^\dagger a_\alpha^\dagger ... a_\alpha^\dagger |0\rangle$ (3)

It is easy to derive the commutation and anticommutation rules for the fermionic creation operators $a_\alpha^\dagger$. Using the antisymmetry of the states (3)

$|\alpha_1...\alpha_2...\alpha_k...\alpha_n\rangle_{AS} = -|\alpha_1...\alpha_k...\alpha_2...\alpha_n\rangle_{AS}$ (4)

we obtain

$a_\alpha^\dagger a_\alpha^\dagger = -a_\alpha^\dagger a_\alpha^\dagger$ (5)

Using the Pauli principle

$|\alpha_1...\alpha_2...\alpha_3...\alpha_4\rangle_{AS} = 0$ (6)

it follows that

$a_\alpha^\dagger a_\alpha^\dagger = 0$ (7)

If we combine Eqs. (5) and (7), we obtain the well-known anti-commutation rule

$a_\alpha^\dagger a_\beta^\dagger + a_\beta^\dagger a_\alpha^\dagger = \{a_\alpha^\dagger, a_\beta^\dagger\} = 0$ (8)
What is the physical interpretation of the operator $a_\alpha$ and what is the effect of $a_\alpha$ on a given state $|\alpha_1\alpha_2\ldots\alpha_n\rangle$? Consider the following matrix element

$$\langle \alpha_1\alpha_2\ldots\alpha_n|a_\alpha|\alpha_{i_1}\alpha_{i_2}\ldots\alpha_m\rangle$$

where both sides are antisymmetric. We distinguish between two cases. The first (1) is when $n \in \{\alpha_i\}$. Using the Pauli principle of Eq. (6) it follows

$$\langle \alpha_1\alpha_2\ldots\alpha_n|a_\alpha|\alpha_{i_1}\alpha_{i_2}\ldots\alpha_m\rangle = 0$$

The second (2) case is when $n \notin \{\alpha_i\}$. It follows that an hermitian conjugation

$$\langle \alpha_1\alpha_2\ldots\alpha_n|a_\alpha = \langle \alpha_{i_1}\alpha_{i_2}\ldots\alpha_m| (13)$$

For the last case, the minus and plus signs apply when the sequence $\alpha, \alpha_1, \alpha_2, \ldots, \alpha_n$ and $\alpha'_1, \alpha'_2, \ldots, \alpha'_{m+1}$ are related to each other via even and odd permutations. If we assume that $\alpha \notin \{\alpha_i\}$ we obtain

$$\langle \alpha_1\alpha_2\ldots\alpha_n|a_\alpha|\alpha_{i_1}\alpha_{i_2}\ldots\alpha_{i_{m+1}}\rangle = 0$$

and in particular

$$a_\alpha|0\rangle = 0$$

The action of the operator $a_\alpha$ from the left on a state vector is to remove one particle in the state $\alpha$. If the state vector does not contain the single-particle state $\alpha$, the outcome of the operation is zero. The operator $a_\alpha$ is normally called for a destruction or annihilation operator.

The next step is to establish the commutator algebra of $a_\alpha$ and $a^\dagger_\alpha$. Consider the matrix element

$$\langle \alpha_1\alpha_2\ldots\alpha_n|a^\dagger_\alpha|\alpha_{i_1}\alpha_{i_2}\ldots\alpha_m\rangle$$

If $\{\alpha_i\} = \{\alpha\}$, performing the right permutations, the sequence $\alpha, \alpha_1, \alpha_2, \ldots, \alpha_n$ is identical with the sequence $\alpha'_1, \alpha'_2, \ldots, \alpha'_{n+1}$. This results in

$$\langle \alpha_1\alpha_2\ldots\alpha_n|a^\dagger_\alpha|\alpha_{i_1}\alpha_{i_2}\ldots\alpha_m\rangle = 1$$

and thus

$$a^\dagger_\alpha|\alpha_1\alpha_2\ldots\alpha_n\rangle = |\alpha_1\alpha_2\ldots\alpha_n\rangle$$

Second quantization

The hermitian conjugate of $a^\dagger_\alpha$ is

$$a_\alpha = (a^\dagger_\alpha)^\dagger$$

If we take the hermitian conjugate of Eq. (8), we arrive at

$${a_\alpha, a_\beta} = 0$$

This results in

$$\langle \alpha_1\alpha_2\ldots\alpha_n|a_\alpha = \langle \alpha\alpha_1\alpha_2\ldots\alpha_n\rangle$$

Second quantization

Eq. (13) holds for case (1) since the lefthand side is zero due to the Pauli principle. We write Eq. (11) as

$$\langle \alpha_1\alpha_2\ldots\alpha_n|a_\alpha = \langle \alpha\alpha_1\alpha_2\ldots\alpha_n\rangle$$

Here we must have $m = n + 1$ if Eq. (14) has to be trivially different from zero.

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$$\langle \alpha_1\alpha_2\ldots\alpha_n|a_\alpha = \langle \alpha\alpha_1\alpha_2\ldots\alpha_n\rangle$$

Here we must have $m = n + 1$ if Eq. (14) has to be trivially different from zero.
From Eqs. (20) and (21) we arrive at
\begin{align*}
\{a_\alpha^\dagger, a_\alpha\} = 0 & \quad (20) \\
\{a_\alpha^\dagger, a_\beta\} = a_\alpha a_\beta & \quad (23)
\end{align*}
while the second case gives
\begin{align*}
\{a_\alpha a_\beta, a_\lambda \} = a_\alpha a_\lambda & \quad (24)
\end{align*}
From Eqs. (20) and (21) we arrive at
\begin{align*}
\{a_\alpha^\dagger, a_\alpha\} = a_\alpha a_\alpha - 1 & \quad (22)
\end{align*}
Finally if the state vector does not contain \(\alpha\) and \(\beta\)
\begin{align*}
\{a_\alpha^\dagger, a_\beta\} = a_\alpha a_\beta & = 0 \quad (25)
\end{align*}
For all three cases we have
\begin{align*}
\{a_\alpha^\dagger, a_\beta\} = a_\alpha^\dagger a_\beta + a_\beta a_\alpha^\dagger & = 0, \quad \alpha \neq \beta \quad (26)
\end{align*}
We can summarize our findings in Eqs. (22) and (26) as
\begin{align*}
\{a_\alpha^\dagger, a_\beta\} = \delta_{\alpha\beta} \quad (27)
\end{align*}
with \(\delta_{\alpha\beta}\) is the Kronecker \(\delta\)-symbol.
The properties of the creation and annihilation operators can be summarized as (for fermions)
\begin{align*}
a_\alpha^\dagger |\alpha\rangle &= |\alpha\rangle, \\
a_\alpha |\alpha\rangle &= 0
\end{align*}
and
\begin{align*}
a_\alpha^\dagger |\alpha_1 \ldots \alpha_k\rangle_{AS} &= |\alpha_1 \ldots \alpha_k\rangle_{AS},
\end{align*}
from which follows
\begin{align*}
|\alpha_1 \ldots \alpha_k\rangle_{AS} &= a_\alpha^\dagger a_\alpha |\alpha_\alpha_1 \ldots \alpha_k\rangle_{0},
\end{align*}
We want to obtain an expression for a one-body operator which conserves the number of particles. Here we study the one-body operator for the kinetic energy plus an eventual external one-body potential. The action of this operator on a particular \( n \)-particle state with its pertinent expectation value has already been studied in coordinate space. In coordinate space the operator reads

\[
\hat{H}_0 = \sum_i \hat{h}_0(x_i)
\]

and the anti-symmetric \( n \)-particle Slater determinant is defined as

\[
\Phi(x_1,x_2,\ldots,x_n,\alpha_1,\alpha_2,\ldots,\alpha_n) = \frac{1}{\sqrt{n!}} \sum_{p} (-1)^p \hat{P}_{\{\alpha\}} \psi_{\alpha_1}(x_1) \psi_{\alpha_2}(x_2) \cdots \psi_{\alpha_n}(x_n)
\]

Finally we found

\[
\hat{a}_\alpha|\alpha_1\alpha_2\ldots\alpha_n\rangle = |\alpha_1\alpha_2\ldots\alpha_n\rangle,
\]

and the corresponding commutator algebra

\[
\{\hat{a}_\alpha^\dagger, \hat{a}_\beta\} = \{\hat{a}_\alpha, \hat{a}_\beta\} = 0 \quad \{\hat{a}_\alpha^\dagger, \hat{a}_\beta\} = \delta_{\alpha\beta}.
\]

Let us consider an operator proportional with \( \hat{a}_\alpha^\dagger \) and \( \alpha = \beta \). It acts on an \( n \)-particle state resulting in

\[
a_{\alpha}^\dagger a_{\alpha} \mid \alpha_1\alpha_2\ldots\alpha_n \rangle = \begin{cases} 0 & \alpha \notin \{\alpha\} \\ |\alpha_1\alpha_2\ldots\alpha_n \rangle & \alpha \in \{\alpha\} \end{cases}
\]

Summing over all possible one-particle states we arrive at

\[
\sum_{\alpha} a_{\alpha}^\dagger a_{\alpha} |\alpha_1\alpha_2\ldots\alpha_n\rangle = \pi |\alpha_1\alpha_2\ldots\alpha_n\rangle
\]

A very useful operator is the so-called number-operator. Most physics cases we will study in this text conserve the total number of particles. The number operator is therefore a useful quantity which allows us to test that our many-body formalism conserves the number of particles. In for example \((d, p)\) or \((p, d)\) reactions it is important to be able to describe quantum mechanical states where particles get added or removed. A creation operator \( \hat{a}_\alpha^\dagger \) adds one particle to the single-particle state \( \alpha \) of a given many-body state vector, while an annihilation operator \( \hat{a}_\alpha \) removes a particle from a single-particle state \( \alpha \).

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Second quantization

If we interchange particles 1 and 2 we obtain
\[ \sum_n \langle \alpha | H_0 | \alpha \rangle a^{\dagger}_{\alpha_1} a_{\alpha_2 ...} \]
\[ = \sum_n \langle \alpha | H_0 | \alpha \rangle a^{\dagger}_{\alpha_1} a_{\alpha_2 ...} \]
\[ + \sum_n \langle \alpha | H_0 | \alpha \rangle a^{\dagger}_{\alpha_2} a_{\alpha_1 ...} \]
\[ + \cdots \]
\[ + \sum_n \langle \alpha | H_0 | \alpha \rangle a^{\dagger}_{\alpha_n} a_{\alpha_{n-1} ...} \]
\[ \sum_n \langle \alpha | H_0 | \alpha \rangle a^{\dagger}_{\alpha_n} a_{\alpha_{n-1} ...} \]
\[ = \sum_n \langle \alpha | H_0 | \alpha \rangle a^{\dagger}_{\alpha_1} a_{\alpha_2 ...} \]
\[ + \sum_n \langle \alpha | H_0 | \alpha \rangle a^{\dagger}_{\alpha_2} a_{\alpha_1 ...} \]
\[ + \cdots \]
\[ + \sum_n \langle \alpha | H_0 | \alpha \rangle a^{\dagger}_{\alpha_n} a_{\alpha_{n-1} ...} \]
\[ \sum_n \langle \alpha | H_0 | \alpha \rangle a^{\dagger}_{\alpha_n} a_{\alpha_{n-1} ...} \]
\[ = \sum_n \langle \alpha | H_0 | \alpha \rangle a^{\dagger}_{\alpha_1} a_{\alpha_2 ...} \]
\[ + \sum_n \langle \alpha | H_0 | \alpha \rangle a^{\dagger}_{\alpha_2} a_{\alpha_1 ...} \]
\[ + \cdots \]
\[ + \sum_n \langle \alpha | H_0 | \alpha \rangle a^{\dagger}_{\alpha_n} a_{\alpha_{n-1} ...} \]
\[ \sum_n \langle \alpha | H_0 | \alpha \rangle a^{\dagger}_{\alpha_n} a_{\alpha_{n-1} ...} \]
\[ = \sum_n \langle \alpha | H_0 | \alpha \rangle a^{\dagger}_{\alpha_1} a_{\alpha_2 ...} \]
\[ + \sum_n \langle \alpha | H_0 | \alpha \rangle a^{\dagger}_{\alpha_2} a_{\alpha_1 ...} \]
\[ + \cdots \]
\[ + \sum_n \langle \alpha | H_0 | \alpha \rangle a^{\dagger}_{\alpha_n} a_{\alpha_{n-1} ...} \]
\[ \sum_n \langle \alpha | H_0 | \alpha \rangle a^{\dagger}_{\alpha_n} a_{\alpha_{n-1} ...} \]
\[ = \sum_n \langle \alpha | H_0 | \alpha \rangle a^{\dagger}_{\alpha_1} a_{\alpha_2 ...} \]
\[ + \sum_n \langle \alpha | H_0 | \alpha \rangle a^{\dagger}_{\alpha_2} a_{\alpha_1 ...} \]
\[ + \cdots \]
\[ + \sum_n \langle \alpha | H_0 | \alpha \rangle a^{\dagger}_{\alpha_n} a_{\alpha_{n-1} ...} \]
\[ \sum_n \langle \alpha | H_0 | \alpha \rangle a^{\dagger}_{\alpha_n} a_{\alpha_{n-1} ...} \]
\[ = \sum_n \langle \alpha | H_0 | \alpha \rangle a^{\dagger}_{\alpha_1} a_{\alpha_2 ...} \]
\[ + \sum_n \langle \alpha | H_0 | \alpha \rangle a^{\dagger}_{\alpha_2} a_{\alpha_1 ...} \]
\[ + \cdots \]
\[ + \sum_n \langle \alpha | H_0 | \alpha \rangle a^{\dagger}_{\alpha_n} a_{\alpha_{n-1} ...} \]
\[ \sum_n \langle \alpha | H_0 | \alpha \rangle a^{\dagger}_{\alpha_n} a_{\alpha_{n-1} ...} \]
\[ = \sum_n \langle \alpha | H_0 | \alpha \rangle a^{\dagger}_{\alpha_1} a_{\alpha_2 ...} \]
\[ + \sum_n \langle \alpha | H_0 | \alpha \rangle a^{\dagger}_{\alpha_2} a_{\alpha_1 ...} \]
\[ + \cdots \]
\[ + \sum_n \langle \alpha | H_0 | \alpha \rangle a^{\dagger}_{\alpha_n} a_{\alpha_{n-1} ...} \]
\[ \sum_n \langle \alpha | H_0 | \alpha \rangle a^{\dagger}_{\alpha_n} a_{\alpha_{n-1} ...} \]
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\[ + \sum_n \langle \alpha | H_0 | \alpha \rangle a^{\dagger}_{\alpha_2} a_{\alpha_1 ...} \]
\[ + \cdots \]
\[ + \sum_n \langle \alpha | H_0 | \alpha \rangle a^{\dagger}_{\alpha_n} a_{\alpha_{n-1} ...} \]
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\[ = \sum_n \langle \alpha | H_0 | \alpha \rangle a^{\dagger}_{\alpha_1} a_{\alpha_2 ...} \]
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\[ + \cdots \]
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\[ + \sum_n \langle \alpha | H_0 | \alpha \rangle a^{\dagger}_{\alpha_2} a_{\alpha_1 ...} \]
\[ + \cdots \]
\[ + \sum_n \langle \alpha | H_0 | \alpha \rangle a^{\dagger}_{\alpha_n} a_{\alpha_{n-1} ...} \]
\[ \sum_n \langle \alpha | H_0 | \alpha \rangle a^{\dagger}_{\alpha_n} a_{\alpha_{n-1} ...} \]
Two-body operators in second quantization

Let us now derive the expression for our two-body interaction part, which also conserves the number of particles. We can proceed in exactly the same way as for the one-body operator. In the coordinate representation our two-body interaction part takes the following expression

$$H_I = \sum_{ij} V(x_i, x_j)$$

where the summation runs over distinct pairs. The term $V$ can be an interaction model for the nucleon-nucleon interaction or the interaction between two electrons. It can also include additional two-body interaction terms.

The action of this operator on a product of two single-particle functions is defined as

$$V(x_i, x_j)|\psi_i(x_i)\psi_j(x_j)\rangle = \sum_{\alpha, \beta} \langle \alpha_i | V | \beta_i \rangle \psi^{\dagger}_\beta(x_i)\psi_\alpha(x_j)$$

where on the rhs we have a term for each distinct pairs. The term following expression our two-body interaction part takes the

Summing over all terms we obtain

$$\sum_k a^{\dagger}_\alpha a_\gamma a_\alpha a_\delta |\alpha_1\alpha_2 \ldots \alpha_n\rangle = ( -1)^{k-1}( -1)^{l-2} |\alpha_1\alpha_2 \ldots \alpha_n\rangle$$

where $\sum^{'}$ indicates that the sums running over $\alpha$ and $\beta$ run over all single-particle states, while the summations run over all single-particle states, while the summations run over all single-particle states.

For the other terms on the rhs we obtain similar expressions and summing over all terms we obtain

$$\sum_k a^{\dagger}_\alpha a_\gamma a_\alpha a_\delta |\alpha_1\alpha_2 \ldots \alpha_n\rangle = ( -1)^{k-1}( -1)^{l-2} |\alpha_1\alpha_2 \ldots \alpha_n\rangle$$

where we have used the anti-commutation rules.

Inserting this in (46) gives

$$H_I |\alpha_1\alpha_2 \ldots \alpha_n\rangle = \sum \langle \alpha_i | V | \beta_i \rangle \sum_{\alpha, \beta} \langle \beta_i | V | \gamma_i \rangle \psi^{\dagger}_\gamma(x_i)\psi_\alpha(x_j)$$

Here we let $\sum^{'}$ indicate that the sums running over $\alpha$ and $\beta$ run over all single-particle states, while the summations run over all pairs of single-particle states. We wish to remove this restriction and since

$$\langle \alpha | V | \beta \rangle = \langle \beta | V | \alpha \rangle$$

we get

$$\sum \langle \alpha_i | V | \beta_i \rangle \sum_{\alpha, \beta} \langle \beta_i | V | \gamma_i \rangle \psi^{\dagger}_\gamma(x_i)\psi_\alpha(x_j)$$

where we have used the anti-commutation rules.
Operators in second quantization

Changing the summation indices $\alpha$ and $\beta$ in (51) we obtain

$$\sum_{\alpha\beta\gamma\delta} (|\alpha\beta\gamma\delta|\hat{v}|\gamma\delta\alpha\beta\rangle - |\alpha\beta\gamma\delta|\hat{v}|\gamma\delta\beta\alpha\rangle)$$

(52)

From this it follows that the restriction on the summation over $\gamma$ and $\delta$ can be removed if we multiply with a factor $\frac{1}{2}$ resulting in

$$\hat{H}_B = \frac{1}{2} \sum_{\alpha\beta\gamma\delta} (|\alpha\beta\gamma\delta|\hat{v}|\gamma\delta\alpha\beta\rangle - |\alpha\beta\gamma\delta|\hat{v}|\gamma\delta\beta\alpha\rangle)$$

(53)

where we sum freely over all single-particle states $\alpha$, $\beta$, $\gamma$ og $\delta$.

Operators in second quantization

Using the commutation relations we get

$$a_{\alpha_1\beta_1} a_{\alpha_2\beta_2} a_{\alpha_1\beta_1} a_{\alpha_2\beta_2}$$

$$- a_{\alpha_1\beta_1} a_{\alpha_2\beta_2} (a_{\alpha_1\beta_2} a_{\alpha_2\beta_1} - a_{\alpha_2\beta_1} a_{\alpha_1\beta_2})$$

$$- a_{\alpha_1\beta_1} a_{\alpha_2\beta_2} (a_{\alpha_1\beta_2} a_{\alpha_2\beta_1} - a_{\alpha_2\beta_1} a_{\alpha_1\beta_2})$$

$$- a_{\alpha_1\beta_1} a_{\alpha_2\beta_2} (a_{\alpha_1\beta_2} a_{\alpha_2\beta_1} - a_{\alpha_2\beta_1} a_{\alpha_1\beta_2})$$

$$- a_{\alpha_1\beta_1} a_{\alpha_2\beta_2} (a_{\alpha_1\beta_2} a_{\alpha_2\beta_1} - a_{\alpha_2\beta_1} a_{\alpha_1\beta_2})$$

(55)

Operators in second quantization

Insertion of Eq. (56) in Eq. (54) results in

$$\langle \alpha_1\alpha_2 | \hat{H}_B | \beta_1\beta_2 \rangle \Rightarrow \frac{1}{2} \sum_{\alpha\beta\gamma\delta} (|\alpha\beta|\hat{v}|\gamma\delta\rangle |\beta_1\beta_2\rangle - |\alpha\beta|\hat{v}|\gamma\delta\rangle |\beta_2\beta_1\rangle$$

$$- |\alpha\beta|\hat{v}|\gamma\delta\rangle |\beta_1\beta_2\rangle + |\alpha\beta|\hat{v}|\gamma\delta\rangle |\beta_2\beta_1\rangle$$

(56)

Operators in second quantization

With this expression we can now verify that the second quantization form of $\hat{H}_B$ in Eq. (53) results in the same matrix between two anti-symmetrized two-particle states as its corresponding coordinate space representation. We have

$$\langle \alpha_1\alpha_2 | \hat{H}_B | \beta_1\beta_2 \rangle \Rightarrow \frac{1}{2} \sum_{\alpha\beta\gamma\delta} (|\alpha\beta|\hat{v}|\gamma\delta\rangle |\beta_1\beta_2\rangle - |\alpha\beta|\hat{v}|\gamma\delta\rangle |\beta_2\beta_1\rangle$$

(57)

Operators in second quantization

The vacuum expectation value of this product of operators becomes

$$\langle 0 | a_{\alpha_2} a_{\alpha_1} a_{\alpha_1} a_{\beta_2} | 0 \rangle$$

$$\Rightarrow (\delta_{\gamma\beta_1} \delta_{\delta\beta_2} - \delta_{\delta\beta_1} \delta_{\gamma\beta_2})$$

$$\langle 0 | a_{\alpha_2} a_{\alpha_1} a_{\alpha_1} a_{\beta_2} | 0 \rangle$$

$$\Rightarrow (\delta_{\gamma\beta_1} \delta_{\delta\beta_2} - \delta_{\delta\beta_1} \delta_{\gamma\beta_2})$$

(58)

Operators in second quantization

The two-body operator can also be expressed in terms of the anti-symmetrized matrix elements we discussed previously as

$$\hat{H}_B = \frac{1}{2} \sum_{\alpha\beta\gamma\delta} (|\alpha\beta\gamma\delta|\hat{v}|\gamma\delta\alpha\beta\rangle - |\alpha\beta\gamma\delta|\hat{v}|\gamma\delta\beta\alpha\rangle)$$

(59)
Operators in second quantization

The factors in front of the operator, either \(\frac{1}{2}\) or \(\frac{1}{4}\), tells whether we use antisymmetrized matrix elements or not. We can now express the Hamiltonian operator for a many-fermion system in the occupation basis representation as

\[
H = \sum_{\alpha} \langle \alpha | H_{\text{ext}} | \alpha \rangle a_\alpha^\dagger a_\alpha + \frac{1}{4} \sum_{\alpha<\beta} \langle \alpha | H_{\text{int}} | \beta \rangle a_\alpha^\dagger a_\beta^\dagger a_\beta a_\alpha. \tag{59}
\]

This is the form we will use in the rest of these lectures, assuming that we work with anti-symmetrized two-body matrix elements.

Particle-hole formalism

Second quantization is a useful and elegant formalism for constructing many-body states and quantum mechanical operators. One can express and translate many physical processes into simple pictures such as Feynman diagrams. Expectation values of many-body states are also easily calculated. However, although the equations are seemingly easy to set up, from a practical point of view, that is the solution of Schrödinger’s equation, there is no particular gain. The many-body equation is equally hard to solve, irrespective of representation. The cliche that there is no free lunch brings us down to earth again. Note however that a transformation to a particular basis, for cases where the interaction obeys specific symmetries, can ease the solution of Schrödinger’s equation. But there is at least one important case where second quantization comes to our rescue. It is namely easy to introduce another representation of this state but there is at least one important case where second quantization comes to our rescue. It is namely easy to introduce another reference state than the vacuum state, where all single-particle states are active. With many particles present it is often useful to introduce another reference state than the vacuum state. We will label this state |c⟩ for core) as and as we will see it can reduce considerably the representation of this state.

In the original particle representation these states are products of the creation operators \(a_\alpha^\dagger\) acting on the true vacuum \(|0\rangle\). Following Eq. (3) we have

\[
|\alpha_1\alpha_2...\alpha_{n-1}\alpha_n\rangle = a_\alpha^\dagger a_\beta^\dagger ... a_{\alpha_{n-1}}^\dagger a_{\alpha_n}^\dagger |0\rangle \tag{60}
\]

\[
|\alpha_1\alpha_2...\alpha_{n-1}\alpha_{n+1}\rangle = a_{\alpha_{n+1}}^\dagger a_{\alpha_n}^\dagger ... a_{\alpha_{n-1}}^\dagger |0\rangle \tag{61}
\]

\[
|\alpha_1\alpha_2...\alpha_{n-1}\rangle = a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger ... a_{\alpha_{n-1}}^\dagger |0\rangle \tag{62}
\]

Particle-hole formalism

Second quantization is a useful and elegant formalism for constructing many-body states and quantum mechanical operators. One can express and translate many physical processes into simple pictures such as Feynman diagrams. Expectation values of many-body states are also easily calculated. However, although the equations are seemingly easy to set up, from a practical point of view, that is the solution of Schrödinger’s equation, there is no particular gain. The many-body equation is equally hard to solve, irrespective of representation. The cliche that there is no free lunch brings us down to earth again. Note however that a transformation to a particular basis, for cases where the interaction obeys specific symmetries, can ease the solution of Schrödinger’s equation. But there is at least one important case where second quantization comes to our rescue. It is namely easy to introduce another reference state than the vacuum state, where all single-particle states are active. With many particles present it is often useful to introduce another reference state than the vacuum state. We will label this state |c⟩ for core) as and as we will see it can reduce considerably the representation of this state.

If we use Eq. (60) as our new reference state, we can simplify considerably the representation of this state

\[
|c\rangle \equiv |\alpha_1\alpha_2...\alpha_{n-1}\rangle = a_{\alpha_{n+1}}^\dagger a_{\alpha_n}^\dagger ... a_{\alpha_{n-1}}^\dagger |0\rangle \tag{63}
\]

The new reference states for the \(n+1\) and \(n-1\) states can then be written as

\[
|\alpha_1\alpha_2...\alpha_{n-1}\alpha_{n+1}\rangle = (-1)^n a_{\alpha_{n+1}}^\dagger |c\rangle = (-1)^n |\alpha_1\alpha_2...\alpha_{n-1}\rangle \tag{64}
\]

\[
|\alpha_1\alpha_2...\alpha_{n-1}\rangle = (-1)^{n-1} a_{\alpha_{n-1}}^\dagger |c\rangle = (-1)^{n-1} |\alpha_1\alpha_2...\alpha_{n-2}\rangle \tag{65}
\]

Particle-hole formalism

The first state has one additional particle with respect to the new vacuum state |c⟩ and is normally referred to as a one-particle state or one particle added to the many-body reference state. The second state has one particle less than the reference vacuum state |c⟩ and is referred to as a one-hole state. When dealing with a new reference state it is often convenient to introduce new creation and annihilation operators since we have from Eq. (65)

\[
a_\alpha |c\rangle \neq 0 \tag{66}
\]

since \(\alpha\) is contained in |c⟩, while for the true vacuum we have \(a_\alpha |0\rangle = 0\) for all \(\alpha\).

The new reference state leads to the definition of new creation and annihilation operators which satisfy the following relations

\[
b_\alpha |c\rangle = 0 \tag{67}
\]

\[
\{b_\alpha^\dagger, b_\beta\} = \{a_\alpha, a_\beta\} = 0 \tag{68}
\]

The physical interpretation of these new operators is that of so-called quasiparticle states. This means that a state defined by the addition of one extra particle to a reference state |c⟩ may not necessarily be interpreted as one particle coupled to a core. We define now new creation operators that act on a state \(\alpha\) creating a new quasiparticle state

\[
b_\alpha^\dagger |c\rangle \equiv \begin{cases} a_\alpha^\dagger |c\rangle, & \alpha > F \\ a_\alpha^\dagger |c\rangle, & \alpha \leq F \end{cases} \tag{70}
\]

where \(F\) is the Fermi level representing the last occupied single-particle orbit of the new reference state |c⟩.

The annihilation is the hermitian conjugate of the creation operator

\[
b_\alpha = (b_\alpha^\dagger)^\dagger, \tag{71}
\]

resulting in

\[
\langle \alpha | c \rangle = \langle c | \alpha \rangle \tag{72}
\]
Particle-hole formalism

With the new creation and annihilation operator we can now construct many-body quasiparticle states, with one-particle-one-hole states, two-particle-two-hole states etc. in the same fashion as we previously constructed many-particle states. We can write a general particle-hole state as

\[ |\alpha_1\beta_1...\alpha_n\beta_n\rangle = \hat{b}_{\alpha_1}^{\dagger}\hat{b}_{\alpha_2}\hat{b}_{\alpha_3}^{\dagger}...\hat{b}_{\alpha_n}^{\dagger}|\beta_1\beta_2...\beta_n\rangle \]  

(72)

We can now rewrite our one-body and two-body operators in terms of the new creation and annihilation operators. The number operator becomes

\[ \hat{N} = \sum_{\alpha \in F} \hat{n}_\alpha \]  

(73)

where \( n_\alpha \) is the number of particle in the new vacuum state \( |c\rangle \).

The action of \( \hat{N} \) on a many-body state results in

\[ \hat{N}|\psi\rangle = \sum_{\alpha \in F} n_\alpha |\psi\rangle \hat{b}_\alpha^{\dagger}\hat{b}_\alpha |\psi\rangle \]

Particle-hole formalism

Before we continue with the expressions for the two-body operator, we introduce a nomenclature we will use for the rest of this text. It is inspired by the notation used in quantum chemistry. We reserve the labels \( i, j, k... \) for hole states and \( \alpha, \beta, \gamma... \) for states above \( F \), viz. particle states. This means that we will skip the constraint \( \leq F \) or \( > F \) in the summation symbols. Our operator \( \hat{H}_0 \) reads now

\[ \hat{H}_0 = \sum_{\alpha \beta} \langle \alpha | \hat{H} | \beta \rangle \hat{b}_\alpha^{\dagger}\hat{b}_\beta + \frac{1}{4} \sum_{\alpha \beta \gamma \delta} \langle \alpha | \hat{V} | \beta \rangle \hat{b}_\alpha^{\dagger}\hat{b}_\beta \hat{b}_\gamma^{\dagger}\hat{b}_\delta + \frac{1}{4} \sum_{\alpha \beta \gamma \delta} \langle \beta | \hat{V} | \alpha \rangle \hat{b}_\alpha^{\dagger}\hat{b}_\beta \hat{b}_\gamma^{\dagger}\hat{b}_\delta \]

(78)

The two-body operator in the particle-hole formalism is more complicated since we have to translate four indices \( \alpha, \beta, \gamma, \delta \) to the possible combinations of particle and hole states. When performing the commutator algebra we can regroup the operator in five different terms

\[ \hat{H}_0 = \hat{H}_0^{(4)} + \hat{H}_0^{(3)} + \hat{H}_0^{(2)} + \hat{H}_0^{(1)} + \hat{H}_0^{(0)} \]  

(79)

Using anti-symmetrized matrix elements, bthe term \( \hat{H}_0^{(4)} \) is

\[ \hat{H}_0^{(4)} = \frac{1}{4} \sum_{\alpha \beta \gamma \delta} \langle \alpha | \hat{V} | \beta \rangle \hat{b}_\alpha^{\dagger}\hat{b}_\beta \hat{b}_\gamma^{\dagger}\hat{b}_\delta + \frac{1}{4} \sum_{\alpha \beta \gamma \delta} \langle \beta | \hat{V} | \alpha \rangle \hat{b}_\alpha^{\dagger}\hat{b}_\beta \hat{b}_\gamma^{\dagger}\hat{b}_\delta \]

(80)

Particle-hole formalism

We express the one-body operator \( \hat{H}_0 \) in terms of the quasi-particle creation and annihilation operators, resulting in

\[ \hat{H}_0 = \sum_{\alpha \beta} \langle \alpha | \hat{H} | \beta \rangle \hat{b}_\alpha^{\dagger}\hat{b}_\beta + \frac{1}{4} \sum_{\alpha \beta \gamma \delta} \langle \alpha | \hat{V} | \beta \rangle \hat{b}_\alpha^{\dagger}\hat{b}_\beta \hat{b}_\gamma^{\dagger}\hat{b}_\delta + \frac{1}{4} \sum_{\alpha \beta \gamma \delta} \langle \beta | \hat{V} | \alpha \rangle \hat{b}_\alpha^{\dagger}\hat{b}_\beta \hat{b}_\gamma^{\dagger}\hat{b}_\delta \]

(77)

The first term gives contribution only for particle states, while the last one contributes only for holestates. The second term can create or destroy a set of quasi-particles and the third term is the contribution from the vacuum state \( |c\rangle \).

Particle-hole formalism

The first line stands for the creation of a two-particle-two-hole state, while the second line represents the creation to two one-particle-one-hole pairs while the last term represents a contribution to the particle single-particle energy from the hole states, that is an interaction between the particle states and the hole states within the new vacuum state. The fourth term reads

\[ \hat{H}_0^{(4)} = \frac{1}{4} \sum_{\alpha \beta \gamma \delta} \langle \alpha | \hat{V} | \beta \rangle \hat{b}_\alpha^{\dagger}\hat{b}_\beta \hat{b}_\gamma^{\dagger}\hat{b}_\delta + \frac{1}{4} \sum_{\alpha \beta \gamma \delta} \langle \beta | \hat{V} | \alpha \rangle \hat{b}_\alpha^{\dagger}\hat{b}_\beta \hat{b}_\gamma^{\dagger}\hat{b}_\delta \]

(83)

The terms in the first line stand for the creation of a particle-hole state interacting with hole states, we will label this as a two-hole-one-particle contribution. The remaining terms are a particle-hole state interacting with the holes in the vacuum state. Finally we have

\[ \hat{H}_0^{(0)} = \frac{1}{4} \sum_{\alpha \beta \gamma \delta} \langle \alpha | \hat{V} | \beta \rangle \hat{b}_\alpha^{\dagger}\hat{b}_\beta \hat{b}_\gamma^{\dagger}\hat{b}_\delta + \frac{1}{4} \sum_{\alpha \beta \gamma \delta} \langle \beta | \hat{V} | \alpha \rangle \hat{b}_\alpha^{\dagger}\hat{b}_\beta \hat{b}_\gamma^{\dagger}\hat{b}_\delta \]

(84)
Summarizing and defining a normal-ordered Hamiltonian

The one-body operator is defined as
\[ \hat{f} = \sum_{pq} (\hat{P}^f_q) a_p^\dagger a_q, \]
while the two-body operator is defined as
\[ \hat{V} = \frac{1}{2} \sum_{pqrs} (\hat{P}^V_{rs}) a_p^\dagger a_q a_r^\dagger a_s, \]
where we have defined the antisymmetric matrix elements
\[ (\hat{P}^V_{rs}) = (\hat{P}^V_{rs}) = (\hat{P}^V_{ts}), \quad (\hat{P}^V_{q}) = (\hat{P}^V_{q}), \quad (\hat{P}^V_{q}) = (\hat{P}^V_{q}), \]
with \( i, j, \ldots \leq \alpha_F \), \( a, b, \ldots > \alpha_F \), \( p, q, \ldots = \) any.

\[ a_i |\Phi_0\rangle = |\Phi_i \rangle, \quad a_i^\dagger |\Phi_0\rangle = |\Phi_a \rangle \]
and
\[ a_i^\dagger |\Phi_0\rangle = 0, \quad a_a |\Phi_0\rangle = 0. \]

One- and two-body operators

The one-body operator is defined as
\[ \hat{f} = \sum_{pq} (\hat{P}^f_q) a_p^\dagger a_q \]
while the two-body operator is defined as
\[ \hat{V} = \frac{1}{2} \sum_{pqrs} (\hat{P}^V_{rs}) a_p^\dagger a_q a_r^\dagger a_s, \]
where we have defined the antisymmetric matrix elements
\[ (\hat{P}^V_{rs}) = (\hat{P}^V_{rs}) = (\hat{P}^V_{ts}), \quad (\hat{P}^V_{q}) = (\hat{P}^V_{q}), \quad (\hat{P}^V_{q}) = (\hat{P}^V_{q}), \]
with \( i, j, \ldots \leq \alpha_F \), \( a, b, \ldots > \alpha_F \), \( p, q, \ldots = \) any.

We can also define a three-body operator
\[ \hat{V}_3 = \frac{1}{2} \sum_{pqrs} (\hat{P}^V_{rs}) a_p^\dagger a_q a_r^\dagger a_s, \]
with the antisymmetric matrix element
\[ (\hat{P}^V_{rs}) = (\hat{P}^V_{rs}) = (\hat{P}^V_{ts}), \quad (\hat{P}^V_{q}) = (\hat{P}^V_{q}), \quad (\hat{P}^V_{q}) = (\hat{P}^V_{q}), \]
(85)

Hartree-Fock in second quantization and stability of HF solution

We wish now to derive the Hartree-Fock equations using our second-quantized formalism and study the stability of the equations. Our ansatz for the ground state of the system is approximated as (this is our representation of a Slater determinant in second quantization)
\[ |\Psi_0\rangle = |c\rangle = a_1^\dagger \ldots a_n^\dagger |\Phi_0\rangle. \]

We wish to determine \( n^{HF} \) so that \( E^{HF} = \langle c | \hat{H} | c \rangle \) becomes a local minimum. In our analysis here we will need Thouless’ theorem, which states that an arbitrary Slater determinant \( |c\rangle \) which is not orthogonal to a determinant \( |c\rangle = \prod_{i=1}^n a_i^\dagger |\Phi_0\rangle \), can be written as
\[ |c\rangle = \exp \left( \sum_{i<j} C_{ij} a_i^\dagger a_j \right) |c\rangle. \]

Let us give a simple proof of Thouless’ theorem. The theorem states that we can make a linear combination of particle-hole excitations with respect to a given reference state \( |c\rangle \). With this linear combination, we can make a new Slater determinant \( |c'\rangle \) which is not orthogonal to \( |c\rangle \), that is
\[ \langle c | c' \rangle \neq 0. \]

To show this we need some intermediate steps. The exponential product of two operators \( \exp A \times \exp B \) is equal to \( \exp (A + B) \) only if the two operators commute, that is
\[ [A, B] = 0. \]
Thouless' theorem

If the operators do not commute, we need to resort to the Baker-Campbell-Hauersdorf. This relation states that
\[
\exp \mathcal{C} = \exp \mathcal{A} \exp \mathcal{B},
\]
with
\[
\mathcal{C} = \mathcal{A} + \mathcal{B} + \frac{1}{2}[\mathcal{A}, \mathcal{B}] + \frac{1}{12}[[\mathcal{A}, \mathcal{B}], \mathcal{B}] - \frac{1}{12}[[\mathcal{A}, \mathcal{B}], \mathcal{A}] + \ldots
\]
From these relations, we note that in our expression for \(|c\rangle\) we have commutators of the type
\[
[a_i a_j^\dagger, a_k a_l^\dagger],
\]
and it is easy to convince oneself that these commutators, or higher powers thereof, are all zero. This means that we can write out our new representation of a Slater determinant as
\[
|\pi\rangle = \left\{ \prod_{i} \sum_{a_F} C_{a_F} a_i^\dagger a_{a_F}^\dagger \right\} |c\rangle.
\]

New operators

If we define a new creation operator
\[
b_i^\dagger = a_i^\dagger + \sum_{a_F} C_{a_F} a_i^\dagger,
\]
we have
\[
|c\rangle = \prod_i (b_i^\dagger |0\rangle) = \prod_i \left( a_i^\dagger + \sum_{a_F} C_{a_F} a_i^\dagger \right) |0\rangle,
\]
meaning that the new representation of the Slater determinant in second quantization, \(|c\rangle\), looks like our previous ones. However, this representation is not general enough since we have a restriction on the sum over single-particle states in Eq. (88). The single-particle states have to be above the Fermi level. The question then is whether we can construct a general representation of a Slater determinant with a creation operator
\[
b_i^\dagger = \sum_{a_F} C_{a_F} a_i^\dagger,
\]

Wrapping it up

Using these relations we can then define the linear combination of creation (and annihilation as well) operators as
\[
\sum_{i} c_{i,j}^{-1} b_{j} = \sum_{i} c_{i,j} a_{j}^\dagger - a_{j}^\dagger + \sum_{i,j \neq k, l} c_{i,j}^{-1} c_{k,l} a_{k}^\dagger a_{l}^\dagger.
\]
Defining
\[
c_{i,j} = \sum_{c_{i,j}^{-1}} c_{i,j}^{-1} b_{j},
\]
we can redefine
\[
a_{j}^\dagger = \sum_{i} \sum_{c_{i,j}^{-1}} c_{i,j}^{-1} a_{i}^\dagger - a_{i}^\dagger + \sum_{i,j} c_{i,j} c_{j,i}^\dagger b_{i}^\dagger - b_{i}^\dagger,
\]
our starting point. We have shown that our general representation of a Slater determinant
\[
|\pi\rangle = \left\{ \prod_{i} b_i^\dagger |0\rangle \right\} - |c\rangle = \prod_{i} b_i^\dagger |0\rangle - |c\rangle.
\]

Showing that \(|\pi\rangle = |c\rangle\)

We need to show that \(|\pi\rangle = |c\rangle\). We need also to assume that the new state is not orthogonal to \(|c\rangle\), that is \langle c | c \rangle \neq 0. From this it follows that
\[
\langle c | c \rangle = \langle 0 | a_i \ldots a_l \left( \sum_{i,k} f_i a_i^\dagger \right) \left( \sum_{i,j} f_i a_i^\dagger \right) \ldots \left( \sum_{i,k} f_i a_i^\dagger \right) |0\rangle = 0,
\]
which is nothing but the determinant \(\det(f)\) which we can, using the intermediate normalization condition, normalize to one, that is
\[
\det(f) = 1.
\]
meaning that \(f\) has an inverse defined as (since we are dealing with orthogonal, and in our case unitary as well, transformations)
\[
\sum_k f_k f_k^{-1} = \delta_k,
\]
and

Thouless' theorem

This means that we can actually write an ansatz for the ground state of the system as a linear combination of terms which contain the ansatz itself \(|c\rangle\) with an admixture from an infinity of one-particle-one-hole states. The latter has important consequences when we wish to interpret the Hartree-Fock equations and their stability. We can rewrite the new representation as
\[
|c\rangle = |c\rangle + |c\rangle_f.
\]
where \(|c\rangle_f\) can now be interpreted as a small variation. If we approximate this term with contributions from one-particle-one-hole (1p-1h) states only, we arrive at
\[
|c\rangle = \left( 1 + \sum_{\alpha} \delta_{\alpha} a_{\alpha}^\dagger \right) |c\rangle.
\]
In our derivation of the Hartree-Fock equations we have shown that
\[
\langle c | H | c \rangle = 0.
\]
Hartree-Fock in second quantization and stability of HF solution

The variational condition for deriving the Hartree-Fock equations guarantees only that the expectation value \( \langle \hat{H} | c \rangle \) has an extreme value, not necessarily a minimum. To figure out whether the extreme value we have found is a minimum, we can use second quantization to analyze our results and find a criterion for the above expectation value to a local minimum. We will use Thouless' theorem and show that

\[
|c'| = |c| + |\delta C|
\]

resulting in

\[
E_0 = \sum a \delta C_{a}^2 + \sum a \delta C_{a}^2 (\epsilon_a - \epsilon_i) - \sum ij ab \langle a|\hat{V}|b \rangle \delta C_{a}^* \delta C_{b}.
\]

Hartree-Fock in second quantization and stability of HF solution

We have already calculated the second term on the right-hand side of the previous equation

\[
\langle c| (a|a\rangle \hat{H} (a|a\rangle)|c\rangle = \sum a b \delta C_{a} \delta C_{b} (a|a\rangle \hat{H} (a|a\rangle)|c\rangle + \frac{1}{2} \sum a b \delta C_{a} \delta C_{b} (a|a\rangle \hat{H} (a|a\rangle)|c\rangle
\]

resulting in

\[
E_0 = \sum a \delta C_{a}^2 + \sum a \delta C_{a}^2 (\epsilon_a - \epsilon_i) - \sum ij ab \langle a|\hat{V}|b \rangle \delta C_{a}^* \delta C_{b}.
\]

Hartree-Fock in second quantization and stability of HF solution

We define two matrix elements

\[
A_{i,j} = \langle a|\hat{V}|b \rangle
\]

and

\[
B_{i,j} = \langle ab|\hat{V}|ij \rangle
\]

both being anti-symmetrized.

Hartree-Fock in second quantization and stability of HF solution

The expectation value for the energy is now given by (using the intermediate normalization condition \( |c'\rangle = 1 \))

\[
\langle c'|c \rangle = 1 + \sum a b \delta C_{a}^2 (a|a\rangle (a|a\rangle)|c\rangle + \frac{1}{2} \sum a b \delta C_{a}^2 \delta C_{b} (a|a\rangle \hat{H} (a|a\rangle)|c\rangle + \frac{1}{2} \sum a b \delta C_{a}^2 \delta C_{b} (a|a\rangle \hat{H} (a|a\rangle)|c\rangle + O(\delta C_{a}^4).
\]

Hartree-Fock in second quantization and stability of HF solution

The norm of \(|c'|\) is given by (using the intermediate normalization condition \( |c'\rangle = 1 \))

\[
\langle c'|c \rangle = 1 + \sum a b \delta C_{a}^2 (a|a\rangle (a|a\rangle)|c\rangle + \frac{1}{2} \sum a b \delta C_{a}^2 \delta C_{b} (a|a\rangle \hat{H} (a|a\rangle)|c\rangle + \frac{1}{2} \sum a b \delta C_{a}^2 \delta C_{b} (a|a\rangle \hat{H} (a|a\rangle)|c\rangle + O(\delta C_{a}^4).
\]

Hartree-Fock in second quantization and stability of HF solution

With these definitions we write out the energy as

\[
\langle c'|\hat{H}|c \rangle = \left( 1 + \sum a \delta C_{a}^2 \right) \langle c'\rangle \hat{C} \langle c \rangle + \sum a \delta C_{a}^2 (\epsilon_a - \epsilon_i) + \sum a \delta C_{a}^2 (\epsilon_a - \epsilon_i) + \sum a b \delta C_{a}^2 \delta C_{b} (a|a\rangle \hat{H} (a|a\rangle)|c\rangle + \frac{1}{2} \sum a b \delta C_{a}^2 \delta C_{b} (a|a\rangle \hat{H} (a|a\rangle)|c\rangle + O(\delta C_{a}^4).
\]

Hartree-Fock in second quantization and stability of HF solution

The norm of \(|c'|\) is given by (using the intermediate normalization condition \( |c'\rangle = 1 \))

\[
\langle c'|c \rangle = 1 + \sum a b \delta C_{a}^2 (a|a\rangle (a|a\rangle)|c\rangle + \frac{1}{2} \sum a b \delta C_{a}^2 \delta C_{b} (a|a\rangle \hat{H} (a|a\rangle)|c\rangle + \frac{1}{2} \sum a b \delta C_{a}^2 \delta C_{b} (a|a\rangle \hat{H} (a|a\rangle)|c\rangle + O(\delta C_{a}^4).
\]

Hartree-Fock in second quantization and stability of HF solution

The norm of \(|c'|\) is given by (using the intermediate normalization condition \( |c'\rangle = 1 \))

\[
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\]
We have defined
\[ \Delta E = \frac{1}{2} \langle \chi | \hat{M} | \chi \rangle \]
with the vectors
\[ \chi = [\hat{C} \; \hat{C}^\dagger]^T \]
and the matrix
\[ \hat{M} = \begin{pmatrix} \Delta + A & B^\dagger \\ B & \Delta + A^\dagger \end{pmatrix} \]
with \( \Delta_{\alpha \beta} = (\varepsilon_\alpha - \varepsilon_i) \delta_{\alpha \beta} \delta_{ij} \).

The condition
\[ \Delta E = \frac{1}{2} \langle \chi | \hat{M} | \chi \rangle \geq 0 \]
for an arbitrary vector
\[ \chi = [\hat{C} \; \hat{C}^\dagger]^T \]
means that all eigenvalues of the matrix have to be larger than or equal zero. A necessary (but no sufficient) condition is that the matrix elements (for all \( \alpha \))
\[ (\varepsilon_\alpha - \varepsilon_i) \delta_{\alpha \beta} + A_{\alpha \beta} \geq 0 \]
This equation can be used as a first test of the stability of the Hartree-Fock equation.

In the build-up of a shell-model or FCI code that is meant to tackle large dimensionalities is the action of the Hamiltonian \( \hat{H} \) on a Slater determinant represented in second quantization as
\[ \langle \alpha_1 \cdots \alpha_n | \hat{H} | \alpha_1 \cdots \alpha_n \rangle = -\sum_{i<j} (\varepsilon_\alpha - \varepsilon_i) \delta_{\alpha \beta} \delta_{ij} + A_{\alpha \beta} \]
The time consuming part stems from the action of the Hamiltonian on the above determinant,
\[ \left( \sum_{\alpha} a_{\alpha} | \alpha \rangle \langle \alpha | + \frac{1}{2} \sum_{\alpha \beta} a_{\alpha}^\dagger a_{\beta} | \alpha \rangle \langle \alpha | a_{\beta}^\dagger a_{\beta} | \alpha \rangle \right) \left( a_{\alpha}^\dagger a_{\beta} | \alpha \rangle \langle \alpha | - a_{\beta}^\dagger a_{\alpha} | \alpha \rangle \langle \alpha | \right) \]
A practically useful way to implement this action is to encode a Slater determinant as a bit pattern.

Assume that we have at our disposal \( n \) different single-particle orbits \( \nu_1, \nu_2, \ldots, \nu_{N-1} \) and that we can distribute among these orbits \( N \leq n \) particles. A Slater determinant can then be coded as an integer of \( N \) bits. As an example, if we have \( n = 16 \) single-particle states \( \nu_1, \nu_2, \ldots, \nu_{15} \) and \( N = 4 \) fermions occupying the states \( \nu_1, \nu_2, \nu_{13} \) and \( \nu_{14} \) we could write this Slater determinant as
\[ \Phi_A = a_{\nu_1}^\dagger a_{\nu_2}^\dagger a_{\nu_{13}}^\dagger a_{\nu_{14}}^\dagger |0\rangle \]
The unoccupied single-particle states have bit value 0 while the occupied ones are represented by bit state 1. In the binary notation we would write this 16 bits long integer as
\[ 0 \ 0 \ 0 \ 0 \ 1 \ 0 \ 0 \ 1 \ 0 \ 0 \ 0 \ 1 \ 0 \ 0 \ 1 \ 0 \]
which translates into the decimal number
\[ 9288 \]
We assume again that we have at our disposal \( n \) different single-particle orbits \( \nu_1, \nu_2, \ldots, \nu_{N-1} \) and that we can distribute among these orbits \( N \leq n \) particles. The ordering among these states is important as it defines the order of the creation operators.

We will write the determinant
\[ \Phi_A = a_{\nu_1}^\dagger a_{\nu_2}^\dagger a_{\nu_{13}}^\dagger a_{\nu_{14}}^\dagger |0\rangle \]
in a more compact way as
\[ \Phi_{5,10,13} = |0001001000100010\rangle \]
The action of a creation operator is thus
\[ a_{\nu_5}^\dagger a_{\nu_{10}}^\dagger a_{\nu_{13}}^\dagger a_{\nu_{14}}^\dagger |0\rangle = |0001001000100100\rangle \]
which becomes
\[ -a_{\nu_5}^\dagger a_{\nu_6}^\dagger a_{\nu_{13}}^\dagger a_{\nu_{14}}^\dagger |0\rangle = |0001011000101000\rangle \]
Operators in second quantization

Similarly
\[ a'_{\alpha} \Phi_{0,3,6,10,13} = a'_{\alpha} (|0001001000100100\rangle) = a'_{\alpha} |0001000000000000\rangle, \]
which becomes
\[ -a'_{\alpha} a'_{\lambda} a'_{\mu} a'_{\nu} a'_{\xi} |0\rangle = 0. \]
This gives a simple recipe:
- If one of the bits \( b_i \) is 1 and we act with a creation operator on this bit, we return a null vector.
- If \( b_i = 0 \), we set it to 1 and return a sign factor \((-1)^l\), where \( l \) is the number of bits set before bit \( j \).

Operators in second quantization

We have an SD representation
\[ \Phi_{\lambda} = a_{\alpha} a_{\lambda} a_{\mu} a_{\nu} a_{\xi} |0\rangle, \]
in a more compact way as
\[ \Phi_{3,6,10,13} = |0001001000100100\rangle. \]

The action of
\[ a_{\alpha} a_{\lambda} \Phi_{3,6,10,13} = a_{\alpha} (|0001001000100100\rangle) = a_{\alpha} |0001000000000000\rangle, \]
which becomes
\[ -a_{\alpha} a_{\lambda} a_{\mu} a_{\nu} a_{\xi} |0\rangle = -|0001101000100100\rangle. \]

Operators in second quantization

It is trickier however to get the phase \((-1)^l\). One possibility is as follows:
- Let \( S_1 \) be a word that represents the 1-bit to be removed and all others set to zero.
- In the previous example \( S_1 = |00000000000000\rangle \)
- Define \( S_2 \) as the similar word that represents the bit to be added, that is in our case
\[ S_2 = |0001000000000000\rangle. \]
- Compute then \( S = S_1 + S_2 \), which here becomes
\[ S = |0111000000000000\rangle \]
- Perform then the logical AND operation of \( S \) with the word containing \( \Phi_{3,6,10,13} = |0001001000100100\rangle \),
which results in \(|0001000000000000\rangle\). Counting the number of
bits in the above, we get as usual the factor \((-1)^l\).

Operators in second quantization

Consider the action of \( a_{\alpha} \) on various Slater determinants:
\[ a_{\alpha} \Phi_{0011} = a_{\alpha} (|0011\rangle) = 0 \times |0011\rangle \]
\[ a_{\alpha} \Phi_{1011} = a_{\alpha} (|1011\rangle) = (-1) \times |1011\rangle \]

Similarly
\[ a_{\alpha} \Phi_{0110} = a_{\alpha} (|0110\rangle) = 0 \times |0110\rangle \]
\[ a_{\alpha} \Phi_{1010} = a_{\alpha} (|1010\rangle) = (-1) \times |1010\rangle \]

Similar actions can be obtained by subtracting the logical sum (AND operation) of
\[ \Phi_{3,6,10,13} \] and a word which represents only \( n_{\lambda} \), that is
\[ |0000000000000000\rangle. \]

This gives \(|0001001000100100\rangle \).\]

Similarly, we can form \( a_{\alpha} a_{\lambda} \Phi_{3,6,10,13} \), say, by adding \(|0000100000000000\rangle\) to \( a_{\alpha} \Phi_{3,6,10,13} \),
first checking that their logical sum is zero in order to make sure that orbital \( n_{\alpha} \) is not already occupied.

Operators in second quantization

Exercise 1

This exercise serves to convince you about the relation between two different single-particle bases, where one could be our new Hartree-Fock basis and the other a harmonic oscillator basis.

Consider a Slater determinant built up of single-particle orbitals \( \psi_\lambda \),
with \( \lambda = 1, 2, \ldots, A \). The unitary transformation
\[ \psi_\lambda = \sum_\lambda C_\lambda \psi_\lambda, \]

brings us into the new basis. The new basis has quantum numbers
\( a = 1, 2, \ldots, A \). Show that the new basis is orthonormal. Show that
the new Slater determinant constructed from the new single-particle
wave functions can be written as the determinant based on the
previous basis and the determinant of the matrix \( C \). Show that
the old and the new Slater determinants are equal up to a complex
constant with absolute value unity. (Hint: \( C \) is a unitary matrix.)
Starting with the second quantization representation of the Slater
determinant.
Exercises

Exercise 2
Calculate the matrix elements
\[ \langle \alpha_1 \alpha_2 | \hat{F} | \alpha_1 \alpha_2 \rangle \]
and
\[ \langle \alpha_1 \alpha_2 | \hat{G} | \alpha_1 \alpha_2 \rangle \]
with
\[ | \alpha_1 \alpha_2 \rangle = a_\alpha_1 ^\dagger a_\alpha_2 ^\dagger \ldots \int \psi_{\alpha_1}^* (x_1) \psi_{\beta_1}^* (x_2) g(x_1, x_2) \psi_{\gamma_1} (x_1) \psi_{\delta_1} (x_2) dx_1 dx_2 \]

Exercise 3
Show that the one-body part of the Hamiltonian
\[ \hat{H}_0 = \sum_{pq} \langle p | \hat{h}_0 | q \rangle a_p ^\dagger a_q, \]
can be written, using standard annihilation and creation operators, in normal-ordered form as
\[ \hat{H}_0 = \sum_{pq} \langle p | \hat{h}_0 | q \rangle \left\{ a_p ^\dagger a_q \right\} + \sum_i (\hat{h}_i). \]

Exercise 4
Show that the two-body part of the Hamiltonian
\[ \hat{H}_2 = \frac{1}{2} \sum_{pqr} \langle p | \hat{v} | qr \rangle a_p ^\dagger a_q ^\dagger a_r a_s, \]
can be written, using standard annihilation and creation operators, in normal-ordered form as
\[ \hat{H}_2 = \frac{1}{2} \sum_{pqr} \langle p | \hat{v} | qr \rangle \left\{ a_p ^\dagger a_r ^\dagger a_q a_s \right\} + \frac{1}{2} \sum_i (\hat{v}_i). \]

Exercise 5
The aim of this exercise is to set up specific matrix elements that will turn useful when we start our discussions of the nuclear shell model, in particular you will notice, depending on the character of the operator, that many matrix elements will actually be zero. Consider these N-particle Slater determinants \( | \Phi_0 \rangle \) and \( | \Phi_1 \rangle \), where the notation means that Slater determinant \( | \Phi_1 \rangle \) differs from \( | \Phi_0 \rangle \) by one single-particle state, that is a single-particle state \( | \psi_i \rangle \) is replaced by a single-particle state \( | \gamma_i \rangle \). It is often interpreted as a so-called one-particle-one-hole excitation. Similarly, the Slater determinant \( | \Phi_2 \rangle \) differs by two single-particle states from \( | \Phi_0 \rangle \) and is normally thought of as a two-particle-two-hole excitation.

We assume also that \( | \Phi_0 \rangle \) represents our new vacuum reference state and the labels \( jk \ldots \) represent single-particle states below the Fermi level and \( abc \ldots \) represent states above the Fermi level, so-called particle states. We define thereafter a general one-body normal-ordered (with respect to the new vacuum state) operator as
\[ \sum_{ij} G_{ij} \langle i | \hat{a}^\dagger j \rangle, \]

Exercise 6
Write a program which sets up all possible Slater determinants given \( N = 4 \) electrons which can occupy the atomic single-particle states defined by the 1s, 2s2p and 3s3p3d shells. How many single-particle states \( n \) are there in total? Include the spin degrees of freedom as well. We include here a python program which may aid in this direction. It uses bit manipulation functions from http://wiki.python.org/moin/BitManipulation.

```
import math

# A simple Python class for Slater determinant manipulation
# Bit manipulation stolen from:
# http://wiki.python.org/moin/BitManipulation

# bitCount() counts the number of bits set (not an optimal function)
def bitCount(int_type):
    count = 0
    while(int_type):
        int_type &= int_type - 1
        count += 1
    return(count)
```

Exercise 7
Compute the matrix element
\[ \langle \alpha_1 \alpha_2 \alpha_3 | \hat{G} | \alpha'_1 \alpha'_2 \alpha'_3 \rangle, \]
using Wick’s theorem and express the two-body operator \( G \) in the occupation number (second quantization) representation.
Exercises: Using sympy to compute matrix elements

The last exercise can be solved using the symbolic Python package called SymPy. SymPy is a Python package for general purpose symbolic algebra. There is a physics module with several interesting submodules. Among these, the submodule called secondquant, contains several functionalities that allow us to test our algebraic manipulations using Wick’s theorem and operators for second quantization.

```python
from sympy import symbols, WildFunction, collect, Rational, from sympy.physics.secondquant import F, Fd, wicks, AntiSymmetricTensor

# setup Hamiltonian
p, q, r, s = symbols('p q r s', dummy=True)
f = AntiSymmetricTensor('f', (p, q), (r, s))
pr = NO((Fd(p)*F(q)))

# redefine the Hamiltonian
Hamiltonian-Rational()=rppr
# redefine the Hamiltonian
Hamiltonian-Rational()=rppr

# print Hamiltonian defined as
print latex(Hnormal)
```

This program produces the following output:

```
\begin{align*}
\delta_{ab}f_{pq} - \delta_{ab}f_{qp} + \delta_{ac}f_{bd} - \delta_{ad}f_{bc} + c + \frac{1}{4}v_{pqrs}.
\end{align*}
```

Exercises: Using sympy to compute matrix elements

We can expand the above Python code by defining one-body and two-body operators using the following SymPy code:

```python
# This code sets up a two-body Hamiltonian for fermions
from sympy import symbols, WildFunction, collect, Rational, from sympy.physics.secondquant import F, Fd, wicks, AntiSymmetricTensor

# setup Hamiltonian
p, q, r, s = symbols('p q r s', dummy=True)
f = AntiSymmetricTensor('f', (p, q), (r, s))
pr = NO((Fd(p)*F(q)))

# redefine the Hamiltonian
Hamiltonian-Rational()=rppr

# print Hamiltonian defined as
print latex(Hnormal)
```

Here we have used the AntiSymmetricTensor functionality, together with normal-ordering defined by the NO function. Using the latex option, this program produces the following output:

```
\begin{align*}
\delta_{ab}f_{pq} - \frac{1}{2}f_{pq}^{ab}q_{a}p_{b}.
\end{align*}
```

Exercises: Using sympy to compute matrix elements

In our next step we define the reference energy $E_0$ and redefine the Hamiltonian by subtracting the reference energy and collecting the coefficients for all normal-ordered products (given by the NO function).

```python
from sympy import symbols, WildFunction, collect, Rational, from sympy.physics.secondquant import F, Fd, wicks, AntiSymmetricTensor

# setup Hamiltonian
p, q, r, s = symbols('p q r s', dummy=True)
f = AntiSymmetricTensor('f', (p, q), (r, s))
pr = NO((Fd(p)*F(q)))

# redefine the Hamiltonian
Hamiltonian-Rational()=rppr

# print Hamiltonian defined as
print latex(Hnormal)
```

which results in

```
\begin{align*}
\delta_{ab}f_{pq} + 1/2f_{pq}^{ab}q_{a}p_{b}.
\end{align*}
```

Exercises: Using sympy to compute matrix elements

We can continue along these lines and define a normal-ordered Hamiltonian with respect to a given reference state. In our first step we just define the Hamiltonian

```python
from sympy import symbols, WildFunction, collect, Rational, from sympy.physics.secondquant import F, Fd, wicks, AntiSymmetricTensor

# setup Hamiltonian
p, q, r, s = symbols('p q r s', dummy=True)
f = AntiSymmetricTensor('f', (p, q), (r, s))
pr = NO((Fd(p)*F(q)))

# redefine the Hamiltonian
Hamiltonian-Rational()=rppr

# print Hamiltonian defined as
print latex(Hnormal)
```

which in the normal order results:

```
\begin{align*}
\delta_{ab}f_{pq} + 1/2f_{pq}^{ab}q_{a}p_{b}.
\end{align*}
```

Exercises: Using sympy to compute matrix elements

We can now go back to exercise 7 and define the Hamiltonian and the second-quantized representation of a three-body Slater determinant.

```python
from sympy import symbols, WildFunction, collect, Rational, from sympy.physics.secondquant import F, Fd, wicks, AntiSymmetricTensor

# setup Hamiltonian
p, q, r, s = symbols('p q r s', dummy=True)
f = AntiSymmetricTensor('f', (p, q), (r, s))
pr = NO((Fd(p)*F(q)))

# redefine the Hamiltonian
Hamiltonian-Rational()=rppr

# print Hamiltonian defined as
print latex(Hnormal)
```

resulting in nine terms (as expected):

```
\begin{align*}
-\delta_{aa}f_{pq} - \delta_{aa}f_{qp} + \delta_{ac}f_{bd} - \delta_{ad}f_{bc} + c + \frac{1}{4}v_{pqrs}.
\end{align*}
```
Exercise 8
What is the diagrammatic representation of the HF equation?

\[ -\langle \alpha_k | u_{HF} | \alpha_i \rangle + n \sum_{j=1}^{n} \left[ \langle \alpha_k \alpha_j | \hat{v} | \alpha_i \alpha_j \rangle - \langle \alpha_k \alpha_j | v | \alpha_j \alpha_i \rangle \right] = 0 \]

(Represent \(-u_{HF}\) by the symbol \(-\cdots\).)

Exercise 9
Consider the ground state \( |\Phi\rangle \) of a bound many-particle system of fermions. Assume that we remove one particle from the single-particle state \( \lambda \) and that our system ends in a new state \( |\Phi_n\rangle \). Define the energy needed to remove this particle as

\[ E_\lambda = \sum_n |\langle \Phi_n | a_\lambda | \Phi \rangle|^2 \left( E_0 - E_n \right) \]

where \( E_0 \) and \( E_n \) are the ground state energies of the states \( |\Phi\rangle \) and \( |\Phi_n\rangle \), respectively.

- Show that
  \[ E_\lambda = \langle \Phi | [a_\lambda, H] | \Phi \rangle \]

where \( H \) is the Hamiltonian of this system.

- If we assume that \( \Phi \) is the Hartree-Fock result, find the relation between \( E_\lambda \) and the single-particle energy \( \epsilon_\lambda \) for states \( \lambda \leq F \) and \( \lambda > F \), with

\[ H = \sum_{\alpha \beta} \langle \alpha | \hat{t} | \beta \rangle a_\alpha^\dagger a_\beta + \frac{1}{2} \sum_{\alpha \beta \gamma \delta} \langle \alpha \beta | \hat{v} | \gamma \delta \rangle a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma. \]