Second Quantization

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May 18-22 2015

Second quantization

We introduce the time-independent operators $a_\alpha^\dagger$ and a_α which create and annihilate, respectively, a particle in the single-particle state φ_α. We define the fermion creation operator $a_\alpha^\dagger$

$$a_\alpha^\dagger|0\rangle \equiv |\alpha\rangle, \tag{1}$$

and

$$a_\alpha^\dagger|\alpha_1\dots\alpha_n\rangle_{\mathrm{AS}} \equiv |\alpha\alpha_1\dots\alpha_n\rangle_{\mathrm{AS}} \tag{2}$$

Second quantization

In Eq. (**??**) 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. (**??**) $a_\alpha^\dagger$ acts on an antisymmetric n-particle state and creates an antisymmetric $(n+1)$-particle state, where the one-body state φ_α is occupied, under the condition that $\alpha \neq \alpha_1, \alpha_2, \dots, \alpha_n$. It follows that we can express an antisymmetric state as the product of the creation operators acting on the vacuum state.

$$|\alpha_1\dots\alpha_n\rangle_{\mathrm{AS}} = a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger \dots a_{\alpha_n}^\dagger|0\rangle \tag{3}$$

Second quantization

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

$$|\alpha_1\dots\alpha_i\dots\alpha_k\dots\alpha_n\rangle_{\mathrm{AS}} = -|\alpha_1\dots\alpha_k\dots\alpha_i\dots\alpha_n\rangle_{\mathrm{AS}} \tag{4}$$

we obtain

$$a_{\alpha_i}^\dagger a_{\alpha_k}^\dagger = -a_{\alpha_k}^\dagger a_{\alpha_i}^\dagger \tag{5}$$

Second quantization

Using the Pauli principle

$$|\alpha_1 \dots \alpha_i \dots \alpha_i \dots \alpha_n\rangle_{\text{AS}} = 0 \tag{6}$$

it follows that

$$a^\dagger_{\alpha_i} a^\dagger_{\alpha_i} = 0. \tag{7}$$

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

$$a^\dagger_\alpha a^\dagger_\beta + a^\dagger_\beta a^\dagger_\alpha \equiv \{a^\dagger_\alpha, a^\dagger_\beta\} = 0 \tag{8}$$

Second quantization

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

$$a_\alpha = (a^\dagger_\alpha)^\dagger \tag{9}$$

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

$$\{a_\alpha, a_\beta\} = 0 \tag{10}$$

Second quantization

What is the physical interpretation of the operator a_α and what is the effect of a_α on a given state $|\alpha_1\alpha_2 \dots \alpha_n\rangle_{\text{AS}}$? Consider the following matrix element

$$\langle\alpha_1\alpha_2 \dots \alpha_n|a_\alpha|\alpha'_1\alpha'_2 \dots \alpha'_m\rangle \tag{11}$$

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

$$\langle\alpha_1\alpha_2 \dots \alpha_n|a_\alpha = 0 \tag{12}$$

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

$$\langle\alpha_1\alpha_2 \dots \alpha_n|a_\alpha = \langle\alpha\alpha_1\alpha_2 \dots \alpha_n| \tag{13}$$

Second quantization

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

$$\langle\alpha_1\alpha_2 \dots \alpha_n|a_\alpha|\alpha'_1\alpha'_2 \dots \alpha'_m\rangle = \langle\alpha_1\alpha_2 \dots \alpha_n|\alpha\alpha'_1\alpha'_2 \dots \alpha'_m\rangle \tag{14}$$

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

Second quantization

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

$$\langle \alpha_1\alpha_2 \dots \alpha_n | a_\alpha | \alpha'_1\alpha'_2 \dots \alpha'_{n+1}\rangle = 0 \tag{15}$$

when $\alpha \in \{\alpha'_i\}$. If $\alpha \notin \{\alpha'_i\}$, we obtain

$$a_\alpha \underbrace{|\alpha'_1\alpha'_2 \dots \alpha'_{n+1}\rangle}_{\neq\alpha} = 0 \tag{16}$$

and in particular

$$a_\alpha|0\rangle = 0 \tag{17}$$

Second quantization

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

$$\langle \alpha_1\alpha_2 \dots \alpha_n | a_\alpha | \alpha\alpha_1\alpha_2 \dots \alpha_n\rangle = 1 \tag{18}$$

and thus

$$a_\alpha|\alpha\alpha_1\alpha_2 \dots \alpha_n\rangle = |\alpha_1\alpha_2 \dots \alpha_n\rangle \tag{19}$$

Second quantization

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

The next step is to establish the commutator algebra of $a^\dagger_\alpha$ and a_β.

Second quantization

The action of the anti-commutator $\{a^\dagger_\alpha,a_\alpha\}$ on a given n-particle state is

$$\begin{aligned} a^\dagger_\alpha a_\alpha \underbrace{|\alpha_1\alpha_2 \dots \alpha_n\rangle}_{\neq\alpha} &= 0 \\ a_\alpha a^\dagger_\alpha \underbrace{|\alpha_1\alpha_2 \dots \alpha_n\rangle}_{\neq\alpha} &= a_\alpha \underbrace{|\alpha\alpha_1\alpha_2 \dots \alpha_n\rangle}_{\neq\alpha} = \underbrace{|\alpha_1\alpha_2 \dots \alpha_n\rangle}_{\neq\alpha} \end{aligned} \tag{20}$$

if the single-particle state α is not contained in the state.

Second quantization

If it is present we arrive at

$$\begin{aligned}
a_\alpha^\dagger a_\alpha|\alpha_1\alpha_2\dots\alpha_k\alpha\alpha_{k+1}\dots\alpha_{n-1}\rangle &= a_\alpha^\dagger a_\alpha(-1)^k|\alpha\alpha_1\alpha_2\dots\alpha_{n-1}\rangle \\
&= (-1)^k|\alpha\alpha_1\alpha_2\dots\alpha_{n-1}\rangle = |\alpha_1\alpha_2\dots\alpha_k\alpha\alpha_{k+1}\dots\alpha_{n-1}\rangle \\
a_\alpha a_\alpha^\dagger|\alpha_1\alpha_2\dots\alpha_k\alpha\alpha_{k+1}\dots\alpha_{n-1}\rangle &= 0 \qquad (21)
\end{aligned}$$

From Eqs. (**??**) and (**??**) we arrive at

$$\{a_\alpha^\dagger, a_\alpha\} = a_\alpha^\dagger a_\alpha + a_\alpha a_\alpha^\dagger = 1 \qquad (22)$$

Second quantization

The action of $\left\{a_\alpha^\dagger, a_\beta\right\}$, with $\alpha \neq \beta$ on a given state yields three possibilities. The first case is a state vector which contains both α and β, then either α or β and finally none of them.

Second quantization

The first case results in

$$\begin{aligned}
a_\alpha^\dagger a_\beta|\alpha\beta\alpha_1\alpha_2\dots\alpha_{n-2}\rangle &= 0 \\
a_\beta a_\alpha^\dagger|\alpha\beta\alpha_1\alpha_2\dots\alpha_{n-2}\rangle &= 0 \qquad (23)
\end{aligned}$$

while the second case gives

$$\begin{aligned}
a_\alpha^\dagger a_\beta|\beta\underbrace{\alpha_1\alpha_2\dots\alpha_{n-1}}_{\neq\alpha}\rangle &= |\alpha\underbrace{\alpha_1\alpha_2\dots\alpha_{n-1}}_{\neq\alpha}\rangle \\
a_\beta a_\alpha^\dagger|\beta\underbrace{\alpha_1\alpha_2\dots\alpha_{n-1}}_{\neq\alpha}\rangle &= a_\beta|\alpha\beta\underbrace{\beta\alpha_1\alpha_2\dots\alpha_{n-1}}_{\neq\alpha}\rangle \\
&= -|\alpha\underbrace{\alpha_1\alpha_2\dots\alpha_{n-1}}_{\neq\alpha}\rangle \qquad (24)
\end{aligned}$$

Second quantization

Finally if the state vector does not contain α and β

$$\begin{aligned}
a_\alpha^\dagger a_\beta|\underbrace{\alpha_1\alpha_2\dots\alpha_n}_{\neq\alpha,\beta}\rangle &= 0 \\
a_\beta a_\alpha^\dagger|\underbrace{\alpha_1\alpha_2\dots\alpha_n}_{\neq\alpha,\beta}\rangle &= a_\beta|\alpha\underbrace{\alpha_1\alpha_2\dots\alpha_n}_{\neq\alpha,\beta}\rangle = 0 \qquad (25)
\end{aligned}$$

For all three cases we have

$$\{a_\alpha^\dagger, a_\beta\} = a_\alpha^\dagger a_\beta + a_\beta a_\alpha^\dagger = 0, \quad \alpha \neq \beta \qquad (26)$$

Second quantization

We can summarize our findings in Eqs. (**??**) and (**??**) as

$$\{a_\alpha^\dagger, a_\beta\} = \delta_{\alpha\beta} \tag{27}$$

with $\delta_{\alpha\beta}$ is the Kroenecker δ-symbol.

The properties of the creation and annihilation operators can be summarized as (for fermions)

$$a_\alpha^\dagger|0\rangle \equiv |\alpha\rangle,$$

and

$$a_\alpha^\dagger|\alpha_1 \dots \alpha_n\rangle_{\mathrm{AS}} \equiv |\alpha\alpha_1 \dots \alpha_n\rangle_{\mathrm{AS}}.$$

from which follows

$$|\alpha_1 \dots \alpha_n\rangle_{\mathrm{AS}} = a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger \dots a_{\alpha_n}^\dagger |0\rangle.$$

Second quantization

The hermitian conjugate has the folowing properties

$$a_\alpha = (a_\alpha^\dagger)^\dagger.$$

Finally we found

$$a_\alpha \underbrace{|\alpha_1'\alpha_2' \dots \alpha_{n+1}'}\rangle_{\neq\alpha} = 0, \quad \text{in particular } a_\alpha|0\rangle = 0,$$

and

$$a_\alpha|\alpha\alpha_1\alpha_2 \dots \alpha_n\rangle = |\alpha_1\alpha_2 \dots \alpha_n\rangle,$$

and the corresponding commutator algebra

$$\{a_\alpha^\dagger, a_\beta^\dagger\} = \{a_\alpha, a_\beta\} = 0 \qquad \{a_\alpha^\dagger, a_\beta\} = \delta_{\alpha\beta}.$$

Second quantization

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 $a_\alpha^\dagger$ adds one particle to the single-particle state α of a give many-body state vector, while an annihilation operator a_α removes a particle from a single-particle state α.

Second quantization

Let us consider an operator proportional with $a^\dagger_\alpha a_\beta$ and $\alpha = \beta$. It acts on an n-particle state resulting in

$$a^\dagger_\alpha a_\alpha|\alpha_1\alpha_2\dots\alpha_n\rangle = \begin{cases} 0 & \alpha \notin \{\alpha_i\} \\ \\ |\alpha_1\alpha_2\dots\alpha_n\rangle & \alpha \in \{\alpha_i\} \end{cases} \tag{28}$$

Summing over all possible one-particle states we arrive at

$$\left(\sum_\alpha a^\dagger_\alpha a_\alpha\right)|\alpha_1\alpha_2\dots\alpha_n\rangle = n|\alpha_1\alpha_2\dots\alpha_n\rangle \tag{29}$$

Second quantization

The operator

$$\hat{N} = \sum_\alpha a^\dagger_\alpha a_\alpha \tag{30}$$

is called the number operator since it counts the number of particles in a give state vector when it acts on the different single-particle states. It acts on one single-particle state at the time and falls therefore under category one-body operators. Next we look at another important one-body operator, namely $\hat{H}_0$ and study its operator form in the occupation number representation.

Second quantization

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-body state with its pertinent expectation value has already been studied in coordinate space. In coordinate space the operator reads

$$\hat{H}_0 = \sum_i \hat{h}_0(x_i) \tag{31}$$

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

$$\Phi(x_1, x_2, \dots, x_n, \alpha_1, \alpha_2, \dots, \alpha_n) = \frac{1}{\sqrt{n!}}\sum_p (-1)^p \hat{P}\psi_{\alpha_1}(x_1)\psi_{\alpha_2}(x_2)\dots\psi_{\alpha_n}(x_n).$$

Second quantization

Defining

$$\hat{h}_0(x_i)\psi_{\alpha_i}(x_i) = \sum_{\alpha'_k}\psi_{\alpha'_k}(x_i)\langle\alpha'_k|\hat{h}_0|\alpha_k\rangle \tag{32}$$

we can easily evaluate the action of $\hat{H}_0$ on each product of one-particle functions in Slater determinant. From Eq. (**??**) we obtain the following result without permuting any particle pair

$$
\begin{aligned}
& \left(\sum_i \hat{h}_0(x_i)\right)\psi_{\alpha_1}(x_1)\psi_{\alpha_2}(x_2)\dots\psi_{\alpha_n}(x_n) \\
= & \sum_{\alpha_1'}\langle\alpha_1'|\hat{h}_0|\alpha_1\rangle\psi_{\alpha_1'}(x_1)\psi_{\alpha_2}(x_2)\dots\psi_{\alpha_n}(x_n) \\
+ & \sum_{\alpha_2'}\langle\alpha_2'|\hat{h}_0|\alpha_2\rangle\psi_{\alpha_1}(x_1)\psi_{\alpha_2'}(x_2)\dots\psi_{\alpha_n}(x_n) \\
+ & \dots \\
+ & \sum_{\alpha_n'}\langle\alpha_n'|\hat{h}_0|\alpha_n\rangle\psi_{\alpha_1}(x_1)\psi_{\alpha_2}(x_2)\dots\psi_{\alpha_n'}(x_n)
\end{aligned}
\tag{33}
$$

Second quantization

If we interchange particles 1 and 2 we obtain

$$
\begin{aligned}
& \left(\sum_i \hat{h}_0(x_i)\right)\psi_{\alpha_1}(x_2)\psi_{\alpha_1}(x_2)\dots\psi_{\alpha_n}(x_n) \\
= & \sum_{\alpha_2'}\langle\alpha_2'|\hat{h}_0|\alpha_2\rangle\psi_{\alpha_1}(x_2)\psi_{\alpha_2'}(x_1)\dots\psi_{\alpha_n}(x_n) \\
+ & \sum_{\alpha_1'}\langle\alpha_1'|\hat{h}_0|\alpha_1\rangle\psi_{\alpha_1'}(x_2)\psi_{\alpha_2}(x_1)\dots\psi_{\alpha_n}(x_n) \\
+ & \dots \\
+ & \sum_{\alpha_n'}\langle\alpha_n'|\hat{h}_0|\alpha_n\rangle\psi_{\alpha_1}(x_2)\psi_{\alpha_1}(x_2)\dots\psi_{\alpha_n'}(x_n)
\end{aligned}
\tag{34}
$$

Second quantization

We can continue by computing all possible permutations. We rewrite also our Slater determinant in its second quantized form and skip the dependence on the quantum numbers x_i. Summing up all contributions and taking care of all phases $(-1)^p$ we arrive at

$$
\begin{aligned}
\hat{H}_0|\alpha_1,\alpha_2,\dots,\alpha_n\rangle &= \sum_{\alpha_1'}\langle\alpha_1'|\hat{h}_0|\alpha_1\rangle|\alpha_1'\alpha_2\dots\alpha_n\rangle \\
&+ \sum_{\alpha_2'}\langle\alpha_2'|\hat{h}_0|\alpha_2\rangle|\alpha_1\alpha_2'\dots\alpha_n\rangle \\
&+ \dots \\
&+ \sum_{\alpha_n'}\langle\alpha_n'|\hat{h}_0|\alpha_n\rangle|\alpha_1\alpha_2\dots\alpha_n'\rangle
\end{aligned}
\tag{35}
$$

Second quantization

In Eq. (**??**) we have expressed the action of the one-body operator of Eq. (**??**) on the n-body state in its second quantized form. This equation can be further manipulated if we use the properties of the creation and annihilation operator on each primed quantum number, that is

$$|\alpha_1\alpha_2\dots\alpha_k'\dots\alpha_n\rangle = a^\dagger_{\alpha_k'}a_{\alpha_k}|\alpha_1\alpha_2\dots\alpha_k\dots\alpha_n\rangle \tag{36}$$

Inserting this in the right-hand side of Eq. (**??**) results in

$$\begin{aligned}
\hat{H}_0|\alpha_1\alpha_2\dots\alpha_n\rangle &= \sum_{\alpha_1'}\langle\alpha_1'|\hat{h}_0|\alpha_1\rangle a^\dagger_{\alpha_1'}a_{\alpha_1}|\alpha_1\alpha_2\dots\alpha_n\rangle \\
&+ \sum_{\alpha_2'}\langle\alpha_2'|\hat{h}_0|\alpha_2\rangle a^\dagger_{\alpha_2'}a_{\alpha_2}|\alpha_1\alpha_2\dots\alpha_n\rangle \\
&+ \dots \\
&+ \sum_{\alpha_n'}\langle\alpha_n'|\hat{h}_0|\alpha_n\rangle a^\dagger_{\alpha_n'}a_{\alpha_n}|\alpha_1\alpha_2\dots\alpha_n\rangle \\
&= \sum_{\alpha,\beta}\langle\alpha|\hat{h}_0|\beta\rangle a^\dagger_\alpha a_\beta|\alpha_1\alpha_2\dots\alpha_n\rangle \qquad (37)
\end{aligned}$$

Second quantization

In the number occupation representation or second quantization we get the following expression for a one-body operator which conserves the number of particles

$$\hat{H}_0 = \sum_{\alpha\beta}\langle\alpha|\hat{h}_0|\beta\rangle a^\dagger_\alpha a_\beta \tag{38}$$

Obviously, $\hat{H}_0$ can be replaced by any other one-body operator which preserved the number of particles. The stucture of the operator is therefore not limited to say the kinetic or single-particle energy only.

The opearator $\hat{H}_0$ takes a particle from the single-particle state β to the single-particle state α with a probability for the transition given by the expectation value $\langle\alpha|\hat{h}_0|\beta\rangle$.

Second quantization

It is instructive to verify Eq. (**??**) by computing the expectation value of $\hat{H}_0$ between two single-particle states

$$\langle\alpha_1|\hat{h}_0|\alpha_2\rangle = \sum_{\alpha\beta}\langle\alpha|\hat{h}_0|\beta\rangle\langle 0|a_{\alpha_1}a^\dagger_\alpha a_\beta a^\dagger_{\alpha_2}|0\rangle \tag{39}$$

Second quantization

Using the commutation relations for the creation and annihilation operators we have

$$a_{\alpha_1} a^\dagger_\alpha a_\beta a^\dagger_{\alpha_2} = (\delta_{\alpha\alpha_1} - a^\dagger_\alpha a_{\alpha_1})(\delta_{\beta\alpha_2} - a^\dagger_{\alpha_2} a_\beta), \tag{40}$$

which results in

$$\langle 0|a_{\alpha_1} a^\dagger_\alpha a_\beta a^\dagger_{\alpha_2}|0\rangle = \delta_{\alpha\alpha_1}\delta_{\beta\alpha_2} \tag{41}$$

and

$$\langle \alpha_1|\hat{h}_0|\alpha_2\rangle = \sum_{\alpha\beta} \langle \alpha|\hat{h}_0|\beta\rangle \delta_{\alpha\alpha_1}\delta_{\beta\alpha_2} = \langle \alpha_1|\hat{h}_0|\alpha_2\rangle \tag{42}$$

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

$$\hat{H}_I = \sum_{i<j} V(x_i, x_j) \tag{43}$$

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

$$V(x_i, x_j)\psi_{\alpha_k}(x_i)\psi_{\alpha_l}(x_j) = \sum_{\alpha'_k\alpha'_l} \psi'_{\alpha_k}(x_i)\psi'_{\alpha_l}(x_j)\langle \alpha'_k\alpha'_l|\hat{v}|\alpha_k\alpha_l\rangle \tag{44}$$

Operators in second quantization

We can now let $\hat{H}_I$ act on all terms in the linear combination for $|\alpha_1\alpha_2\dots\alpha_n\rangle$. Without any permutations we have

$$\begin{aligned}
& \left(\sum_{i<j} V(x_i, x_j)\right)\psi_{\alpha_1}(x_1)\psi_{\alpha_2}(x_2)\dots\psi_{\alpha_n}(x_n) \\
= & \sum_{\alpha'_1\alpha'_2} \langle \alpha'_1\alpha'_2|\hat{v}|\alpha_1\alpha_2\rangle \psi'_{\alpha_1}(x_1)\psi'_{\alpha_2}(x_2)\dots\psi_{\alpha_n}(x_n) \\
+ & \dots \\
+ & \sum_{\alpha'_1\alpha'_n} \langle \alpha'_1\alpha'_n|\hat{v}|\alpha_1\alpha_n\rangle \psi'_{\alpha_1}(x_1)\psi_{\alpha_2}(x_2)\dots\psi'_{\alpha_n}(x_n) \\
+ & \dots \\
+ & \sum_{\alpha'_2\alpha'_n} \langle \alpha'_2\alpha'_n|\hat{v}|\alpha_2\alpha_n\rangle \psi_{\alpha_1}(x_1)\psi'_{\alpha_2}(x_2)\dots\psi'_{\alpha_n}(x_n) \\
+ & \dots
\end{aligned} \tag{45}$$

where on the rhs we have a term for each distinct pairs.

Operators in second quantization

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

$$
\begin{aligned}
H_I|\alpha_1\alpha_2\dots\alpha_n\rangle &= \sum_{\alpha_1',\alpha_2'}\langle\alpha_1'\alpha_2'|\hat{v}|\alpha_1\alpha_2\rangle|\alpha_1'\alpha_2'\dots\alpha_n\rangle \\
&+ \dots \\
&+ \sum_{\alpha_1',\alpha_n'}\langle\alpha_1'\alpha_n'|\hat{v}|\alpha_1\alpha_n\rangle|\alpha_1'\alpha_2\dots\alpha_n'\rangle \\
&+ \dots \\
&+ \sum_{\alpha_2',\alpha_n'}\langle\alpha_2'\alpha_n'|\hat{v}|\alpha_2\alpha_n\rangle|\alpha_1\alpha_2'\dots\alpha_n'\rangle \\
&+ \dots
\end{aligned}
\tag{46}
$$

Operators in second quantization

We introduce second quantization via the relation

$$
\begin{aligned}
& a^\dagger_{\alpha_k'} a^\dagger_{\alpha_l'} a_{\alpha_l} a_{\alpha_k}|\alpha_1\alpha_2\dots\alpha_k\dots\alpha_l\dots\alpha_n\rangle \\
=\ & (-1)^{k-1}(-1)^{l-2} a^\dagger_{\alpha_k'} a^\dagger_{\alpha_l'} a_{\alpha_l} a_{\alpha_k}|\alpha_k\alpha_l\underbrace{\alpha_1\alpha_2\dots\alpha_n}_{\neq\alpha_k,\alpha_l}\rangle \\
=\ & (-1)^{k-1}(-1)^{l-2}|\alpha_k'\alpha_l'\underbrace{\alpha_1\alpha_2\dots\alpha_n}_{\neq\alpha_k',\alpha_l'}\rangle \\
=\ & |\alpha_1\alpha_2\dots\alpha_k'\dots\alpha_l'\dots\alpha_n\rangle
\end{aligned}
\tag{47}
$$

Operators in second quantization

Inserting this in (**??**) gives

$$
\begin{aligned}
H_I|\alpha_1\alpha_2\dots\alpha_n\rangle &= \sum_{\alpha_1',\alpha_2'}\langle\alpha_1'\alpha_2'|\hat{v}|\alpha_1\alpha_2\rangle a^\dagger_{\alpha_1'} a^\dagger_{\alpha_2'} a_{\alpha_2} a_{\alpha_1}|\alpha_1\alpha_2\dots\alpha_n\rangle \\
&+ \dots \\
&= \sum_{\alpha_1',\alpha_n'}\langle\alpha_1'\alpha_n'|\hat{v}|\alpha_1\alpha_n\rangle a^\dagger_{\alpha_1'} a^\dagger_{\alpha_n'} a_{\alpha_n} a_{\alpha_1}|\alpha_1\alpha_2\dots\alpha_n\rangle \\
&+ \dots \\
&= \sum_{\alpha_2',\alpha_n'}\langle\alpha_2'\alpha_n'|\hat{v}|\alpha_2\alpha_n\rangle a^\dagger_{\alpha_2'} a^\dagger_{\alpha_n'} a_{\alpha_n} a_{\alpha_2}|\alpha_1\alpha_2\dots\alpha_n\rangle \\
&+ \dots \\
&= {\sum_{\alpha,\beta,\gamma,\delta}}' \langle\alpha\beta|\hat{v}|\gamma\delta\rangle a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma|\alpha_1\alpha_2\dots\alpha_n\rangle
\end{aligned}
\tag{48}
$$

Operators in second quantization

Here we let $\sum'$ indicate that the sums running over α and β run over all single-particle states, while the summations γ and δ run over all pairs of single-particle states. We wish to remove this restriction and since

$$\langle \alpha\beta|\hat{v}|\gamma\delta\rangle = \langle \beta\alpha|\hat{v}|\delta\gamma\rangle \tag{49}$$

we get

$$\sum_{\alpha\beta} \langle \alpha\beta|\hat{v}|\gamma\delta\rangle a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma = \sum_{\alpha\beta} \langle \beta\alpha|\hat{v}|\delta\gamma\rangle a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma \tag{50}$$

$$= \sum_{\alpha\beta} \langle \beta\alpha|\hat{v}|\delta\gamma\rangle a^\dagger_\beta a^\dagger_\alpha a_\gamma a_\delta \tag{51}$$

where we have used the anti-commutation rules.

Operators in second quantization

Changing the summation indices α and β in (**??**) we obtain

$$\sum_{\alpha\beta} \langle \alpha\beta|\hat{v}|\gamma\delta\rangle a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma = \sum_{\alpha\beta} \langle \alpha\beta|\hat{v}|\delta\gamma\rangle a^\dagger_\alpha a^\dagger_\beta a_\gamma a_\delta \tag{52}$$

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

$$\hat{H}_I = \frac{1}{2}\sum_{\alpha\beta\gamma\delta} \langle \alpha\beta|\hat{v}|\gamma\delta\rangle a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma \tag{53}$$

where we sum freely over all single-particle states α, β, γ og δ.

Operators in second quantization

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

$$\langle \alpha_1\alpha_2|\hat{H}_I|\beta_1\beta_2\rangle = \frac{1}{2}\sum_{\alpha\beta\gamma\delta} \langle \alpha\beta|\hat{v}|\gamma\delta\rangle \langle 0|a_{\alpha_2}a_{\alpha_1} a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma a^\dagger_{\beta_1} a^\dagger_{\beta_2}|0\rangle. \tag{54}$$

Operators in second quantization

Using the commutation relations we get

$$
\begin{aligned}
& a_{\alpha_2}a_{\alpha_1}a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma a^\dagger_{\beta_1}a^\dagger_{\beta_2} \\
= \; & a_{\alpha_2}a_{\alpha_1}a^\dagger_\alpha a^\dagger_\beta (a_\delta \delta_{\gamma\beta_1} a^\dagger_{\beta_2} - a_\delta a^\dagger_{\beta_1} a_\gamma a^\dagger_{\beta_2}) \\
= \; & a_{\alpha_2}a_{\alpha_1}a^\dagger_\alpha a^\dagger_\beta (\delta_{\gamma\beta_1}\delta_{\delta\beta_2} - \delta_{\gamma\beta_1}a^\dagger_{\beta_2}a_\delta - a_\delta a^\dagger_{\beta_1}\delta_{\gamma\beta_2} + a_\delta a^\dagger_{\beta_1}a^\dagger_{\beta_2}a_\gamma) \\
= \; & a_{\alpha_2}a_{\alpha_1}a^\dagger_\alpha a^\dagger_\beta (\delta_{\gamma\beta_1}\delta_{\delta\beta_2} - \delta_{\gamma\beta_1}a^\dagger_{\beta_2}a_\delta \\
& \quad -\delta_{\delta\beta_1}\delta_{\gamma\beta_2} + \delta_{\gamma\beta_2}a^\dagger_{\beta_1}a_\delta + a_\delta a^\dagger_{\beta_1}a^\dagger_{\beta_2}a_\gamma)
\end{aligned}
\tag{55}
$$

Operators in second quantization

The vacuum expectation value of this product of operators becomes

$$
\begin{aligned}
& \langle 0|a_{\alpha_2}a_{\alpha_1}a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma a^\dagger_{\beta_1}a^\dagger_{\beta_2}|0\rangle \\
= \; & (\delta_{\gamma\beta_1}\delta_{\delta\beta_2} - \delta_{\delta\beta_1}\delta_{\gamma\beta_2})\langle 0|a_{\alpha_2}a_{\alpha_1}a^\dagger_\alpha a^\dagger_\beta|0\rangle \\
= \; & (\delta_{\gamma\beta_1}\delta_{\delta\beta_2} - \delta_{\delta\beta_1}\delta_{\gamma\beta_2})(\delta_{\alpha\alpha_1}\delta_{\beta\alpha_2} - \delta_{\beta\alpha_1}\delta_{\alpha\alpha_2})
\end{aligned}
\tag{56}
$$

Operators in second quantization

Insertion of Eq. (**??**) in Eq. (**??**) results in

$$
\begin{aligned}
\langle \alpha_1\alpha_2|\hat{H}_I|\beta_1\beta_2\rangle &= \frac{1}{2}\big[\langle \alpha_1\alpha_2|\hat{v}|\beta_1\beta_2\rangle - \langle \alpha_1\alpha_2|\hat{v}|\beta_2\beta_1\rangle \\
& \quad -\langle \alpha_2\alpha_1|\hat{v}|\beta_1\beta_2\rangle + \langle \alpha_2\alpha_1|\hat{v}|\beta_2\beta_1\rangle\big] \\
&= \langle \alpha_1\alpha_2|\hat{v}|\beta_1\beta_2\rangle - \langle \alpha_1\alpha_2|\hat{v}|\beta_2\beta_1\rangle \\
&= \langle \alpha_1\alpha_2|\hat{v}|\beta_1\beta_2\rangle_{\mathrm{AS}}.
\end{aligned}
\tag{57}
$$

Operators in second quantization

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

$$
\begin{aligned}
\hat{H}_I &= \frac{1}{2}\sum_{\alpha\beta\gamma\delta}\langle \alpha\beta|\hat{v}|\gamma\delta\rangle a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma \\
&= \frac{1}{4}\sum_{\alpha\beta\gamma\delta}\left[\langle \alpha\beta|\hat{v}|\gamma\delta\rangle - \langle \alpha\beta|\hat{v}|\delta\gamma\rangle\right] a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma \\
&= \frac{1}{4}\sum_{\alpha\beta\gamma\delta}\langle \alpha\beta|\hat{v}|\gamma\delta\rangle_{\mathrm{AS}} a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma
\end{aligned}
\tag{58}
$$

Operators in second quantization

The factors in front of the operator, either $\frac{1}{4}$ or $\frac{1}{2}$ 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

$$H = \sum_{\alpha,\beta} \langle \alpha | \hat{t} + \hat{u}_{\mathrm{ext}} | \beta \rangle a_\alpha^\dagger a_\beta + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | \hat{v} | \gamma\delta \rangle a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma. \tag{59}$$

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. Expecation 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 Schroedinger'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 Schroedinger'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 pure vacuum $|0\rangle$, where all single-particle states are active. With many particles present it is often useful to introduce another reference state than the vacuum state$|0\rangle$. We will label this state $|c\rangle$ (c for core) and as we will see it can reduce considerably the complexity and thereby the dimensionality of the many-body problem. It allows us to sum up to infinite order specific many-body correlations. The particle-hole representation is one of these handy representations.

Particle-hole formalism

In the original particle representation these states are products of the creation operators $a_{\alpha_i}^\dagger$ acting on the true vacuum $|0\rangle$. Following Eq. (**??**) we have

$$|\alpha_1\alpha_2\dots\alpha_{n-1}\alpha_n\rangle = a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger \dots a_{\alpha_{n-1}}^\dagger a_{\alpha_n}^\dagger |0\rangle \tag{60}$$

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

$$|\alpha_1\alpha_2\dots\alpha_{n-1}\rangle = a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger \dots a_{\alpha_{n-1}}^\dagger |0\rangle \tag{62}$$

Particle-hole formalism

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

$$|c\rangle \equiv |\alpha_1\alpha_2 \dots \alpha_{n-1}\alpha_n\rangle = a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} \dots a^\dagger_{\alpha_{n-1}} a^\dagger_{\alpha_n} |0\rangle \tag{63}$$

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

$$|\alpha_1\alpha_2 \dots \alpha_{n-1}\alpha_n\alpha_{n+1}\rangle = (-1)^n a^\dagger_{\alpha_{n+1}}|c\rangle \equiv (-1)^n|\alpha_{n+1}\rangle_c \tag{64}$$

$$|\alpha_1\alpha_2 \dots \alpha_{n-1}\rangle = (-1)^{n-1} a_{\alpha_n}|c\rangle \equiv (-1)^{n-1}|\alpha_{n-1}\rangle_c \tag{65}$$

Particle-hole formalism

The first state has one additional particle with respect to the new vacuum state $|c\rangle$ 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 $|c\rangle$ 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. (**??**)

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

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

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

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

$$\{b^\dagger_\alpha, b^\dagger_\beta\} = \{b_\alpha, b_\beta\} = 0$$

$$\{b^\dagger_\alpha, b_\beta\} = \delta_{\alpha\beta} \tag{68}$$

We assume also that the new reference state is properly normalized

$$\langle c|c\rangle = 1 \tag{69}$$

Particle-hole formalism

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 $|c\rangle$ may not necesseraly be interpreted as one particle coupled to a core. We define now new creation operators that act on a state α creating a new quasiparticle state

$$b^\dagger_\alpha|c\rangle = \left\{ \begin{array}{ll} a^\dagger_\alpha|c\rangle = |\alpha\rangle, & \alpha > F \\ \\ a_\alpha|c\rangle = |\alpha^{-1}\rangle, & \alpha \leq F \end{array} \right. \tag{70}$$

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

The annihilation is the hermitian conjugate of the creation operator

$$b_\alpha = (b_\alpha^\dagger)^\dagger,$$

resulting in

$$b_\alpha^\dagger = \begin{cases} a_\alpha^\dagger & \alpha > F \\ \\ a_\alpha & \alpha \le F \end{cases} \qquad b_\alpha = \begin{cases} a_\alpha & \alpha > F \\ \\ a_\alpha^\dagger & \alpha \le F \end{cases} \tag{71}$$

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

$$|\beta_1\beta_2\dots\beta_{n_p}\gamma_1^{-1}\gamma_2^{-1}\dots\gamma_{n_h}^{-1}\rangle \equiv \underbrace{b_{\beta_1}^\dagger b_{\beta_2}^\dagger \dots b_{\beta_{n_p}}^\dagger}_{>F}\underbrace{b_{\gamma_1}^\dagger b_{\gamma_2}^\dagger \dots b_{\gamma_{n_h}}^\dagger}_{\le F}|c\rangle \tag{72}$$

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

$$\hat{N} = \sum_\alpha a_\alpha^\dagger a_\alpha = \sum_{\alpha > F} b_\alpha^\dagger b_\alpha + n_c - \sum_{\alpha \le F} b_\alpha^\dagger b_\alpha \tag{73}$$

where n_c is the number of particle in the new vacuum state $|c\rangle$. The action of $\hat{N}$ on a many-body state results in

$$N|\beta_1\beta_2\dots\beta_{n_p}\gamma_1^{-1}\gamma_2^{-1}\dots\gamma_{n_h}^{-1}\rangle = (n_p + n_c - n_h)|\beta_1\beta_2\dots\beta_{n_p}\gamma_1^{-1}\gamma_2^{-1}\dots\gamma_{n_h}^{-1}\rangle \tag{74}$$

Here $n = n_p + n_c - n_h$ is the total number of particles in the quasi-particle state of Eq. (**??**). Note that $\hat{N}$ counts the total number of particles present

$$N_{qp} = \sum_\alpha b_\alpha^\dagger b_\alpha, \tag{75}$$

gives us the number of quasi-particles as can be seen by computing

$$N_{qp} = |\beta_1\beta_2\dots\beta_{n_p}\gamma_1^{-1}\gamma_2^{-1}\dots\gamma_{n_h}^{-1}\rangle = (n_p + n_h)|\beta_1\beta_2\dots\beta_{n_p}\gamma_1^{-1}\gamma_2^{-1}\dots\gamma_{n_h}^{-1}\rangle \tag{76}$$

where $n_{qp} = n_p + n_h$ is the total number of quasi-particles.

Particle-hole formalism

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

$$\begin{aligned} \hat{H}_0 &= \sum_{\alpha\beta>F} \langle\alpha|\hat{h}_0|\beta\rangle b_\alpha^\dagger b_\beta + \sum_{\substack{\alpha>F \\ \beta\leq F}} \left[\langle\alpha|\hat{h}_0|\beta\rangle b_\alpha^\dagger b_\beta^\dagger + \langle\beta|\hat{h}_0|\alpha\rangle b_\beta b_\alpha\right] \\ &+ \sum_{\alpha\leq F} \langle\alpha|\hat{h}_0|\alpha\rangle - \sum_{\alpha\beta\leq F} \langle\beta|\hat{h}_0|\alpha\rangle b_\alpha^\dagger b_\beta \end{aligned} \tag{77}$$

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

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 $i, j, k, \ldots$ for hole states and $a, b, c, \ldots$ for states above F, viz. particle states. This means also that we will skip the constraint $\leq F$ or $> F$ in the summation symbols. Our operator $\hat{H}_0$ reads now

$$\begin{aligned} \hat{H}_0 &= \sum_{ab} \langle a|\hat{h}|b\rangle b_a^\dagger b_b + \sum_{ai} \left[\langle a|\hat{h}|i\rangle b_a^\dagger b_i^\dagger + \langle i|\hat{h}|a\rangle b_i b_a\right] \\ &+ \sum_{i} \langle i|\hat{h}|i\rangle - \sum_{ij} \langle j|\hat{h}|i\rangle b_i^\dagger b_j \end{aligned} \tag{78}$$

Particle-hole formalism

The two-particle 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

$$\hat{H}_I = \hat{H}_I^{(a)} + \hat{H}_I^{(b)} + \hat{H}_I^{(c)} + \hat{H}_I^{(d)} + \hat{H}_I^{(e)} \tag{79}$$

Using anti-symmetrized matrix elements, bthe term $\hat{H}_I^{(a)}$ is

$$\hat{H}_I^{(a)} = \frac{1}{4} \sum_{abcd} \langle ab|\hat{V}|cd\rangle b_a^\dagger b_b^\dagger b_d b_c \tag{80}$$

Particle-hole formalism

The next term $\hat{H}_I^{(b)}$ reads

$$\hat{H}_I^{(b)} = \frac{1}{4} \sum_{abci} \left(\langle ab|\hat{V}|ci\rangle b_a^\dagger b_b^\dagger b_i^\dagger b_c + \langle ai|\hat{V}|cb\rangle b_a^\dagger b_i b_b b_c\right) \tag{81}$$

This term conserves the number of quasiparticles but creates or removes a three-particle-one-hole state. For $\hat{H}_I^{(c)}$ we have

$$\begin{aligned}\hat{H}_I^{(c)} &= \frac{1}{4}\sum_{abij}\left(\langle ab|\hat{V}|ij\rangle b_a^\dagger b_b^\dagger b_j^\dagger b_i^\dagger + \langle ij|\hat{V}|ab\rangle b_a b_b b_j b_i\right) + \\ & \frac{1}{2}\sum_{abij}\langle ai|\hat{V}|bj\rangle b_a^\dagger b_j^\dagger b_b b_i + \frac{1}{2}\sum_{abi}\langle ai|\hat{V}|bi\rangle b_a^\dagger b_b. \end{aligned} \tag{82}$$

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

$$\begin{aligned}\hat{H}_I^{(d)} &= \frac{1}{4}\sum_{aijk}\left(\langle ai|\hat{V}|jk\rangle b_a^\dagger b_k^\dagger b_j^\dagger b_i + \langle ji|\hat{V}|ak\rangle b_k^\dagger b_j b_i b_a\right) + \\ & \frac{1}{4}\sum_{aij}\left(\langle ai|\hat{V}|ji\rangle b_a^\dagger b_j^\dagger + \langle ji|\hat{V}|ai\rangle - \langle ji|\hat{V}|ia\rangle b_j b_a\right). \end{aligned} \tag{83}$$

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

$$\hat{H}_I^{(e)} = \frac{1}{4}\sum_{ijkl}\langle kl|\hat{V}|ij\rangle b_i^\dagger b_j^\dagger b_l b_k + \frac{1}{2}\sum_{ijk}\langle ij|\hat{V}|kj\rangle b_k^\dagger b_i + \frac{1}{2}\sum_{ij}\langle ij|\hat{V}|ij\rangle \tag{84}$$

The first terms represents the interaction between two holes while the second stands for the interaction between a hole and the remaining holes in the vacuum state. It represents a contribution to single-hole energy to first order. The last term collects all contributions to the energy of the ground state of a closed-shell system arising from hole-hole correlations.

Summarizing and defining a normal-ordered Hamiltonian

$$\Phi_{AS}(\alpha_1,\dots,\alpha_A;x_1,\dots x_A) = \frac{1}{\sqrt{A}}\sum_{\hat{P}}(-1)^P\hat{P}\prod_{i=1}^{A}\psi_{\alpha_i}(x_i),$$

which is equivalent with $|\alpha_1\dots\alpha_A\rangle = a_{\alpha_1}^\dagger\dots a_{\alpha_A}^\dagger|0\rangle$. We have also

$$a_p^\dagger|0\rangle = |p\rangle, \quad a_p|q\rangle = \delta_{pq}|0\rangle$$

$$\delta_{pq} = \left\{a_p, a_q^\dagger\right\},$$

and

$$0 = \left\{a_p^\dagger, a_q\right\} = \left\{a_p, a_q\right\} = \left\{a_p^\dagger, a_q^\dagger\right\}$$
$$|\Phi_0\rangle = |\alpha_1 \dots \alpha_A\rangle, \quad \alpha_1, \dots, \alpha_A \leq \alpha_F$$

Summarizing and defining a normal-ordered Hamiltonian

$$\left\{a_p^\dagger, a_q\right\} = \delta_{pq}, p, q \leq \alpha_F$$
$$\left\{a_p, a_q^\dagger\right\} = \delta_{pq}, p, q > \alpha_F$$

with $i, j, \dots \leq \alpha_F, \quad a, b, \dots > \alpha_F, \quad p, q, \dots -$ any

$$a_i|\Phi_0\rangle = |\Phi_i\rangle, \qquad a_a^\dagger|\Phi_0\rangle = |\Phi^a\rangle$$

and

$$a_i^\dagger|\Phi_0\rangle = 0 \qquad a_a|\Phi_0\rangle = 0$$

Summarizing and defining a normal-ordered Hamiltonian

One- and two-body operators. The one-body operator is defined as

$$\hat{F} = \sum_{pq} \langle p|\hat{f}|q\rangle a_p^\dagger a_q$$

while the two-body opreator is defined as

$$\hat{V} = \frac{1}{4} \sum_{pqrs} \langle pq|\hat{v}|rs\rangle_{AS} a_p^\dagger a_q^\dagger a_s a_r$$

where we have defined the antisymmetric matrix elements

$$\langle pq|\hat{v}|rs\rangle_{AS} = \langle pq|\hat{v}|rs\rangle - \langle pq|\hat{v}|sr\rangle.$$

Summarizing and defining a normal-ordered Hamiltonian

We can also define a three-body operator

$$\hat{V}_3 = \frac{1}{36} \sum_{pqrstu} \langle pqr|\hat{v}_3|stu\rangle_{AS} a_p^\dagger a_q^\dagger a_r^\dagger a_u a_t a_s$$

with the antisymmetrized matrix element

$$\langle pqr|\hat{v}_3|stu\rangle_{AS} = \langle pqr|\hat{v}_3|stu\rangle + \langle pqr|\hat{v}_3|tus\rangle + \langle pqr|\hat{v}_3|ust\rangle - \langle pqr|\hat{v}_3|sut\rangle - \langle pqr|\hat{v}_3|tsu\rangle - \langle pqr|\hat{v}_3|uts\rangle. \tag{85}$$

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)

$$|\Phi_0\rangle = |c\rangle = a_i^\dagger a_j^\dagger \dots a_l^\dagger |0\rangle.$$

We wish to determine $\hat{u}^{HF}$ so that $E_0^{HF} = \langle c|\hat{H}|c\rangle$ 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 $|c\rangle = \prod_{i=1}^{n} a_{\alpha_i}^\dagger |0\rangle$, can be written as

$$|c'\rangle = exp\left\{\sum_{a>F}\sum_{i\le F} C_{ai} a_a^\dagger a_i\right\}|c\rangle$$

Hartree-Fock in second quantization and Thouless' theorem

Let us give a simple proof of Thouless' theorem. The theorem states that we can make a linear combination av 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 $\exp \hat{A} \times \exp \hat{B}$ is equal to $\exp(\hat{A} + \hat{B})$ only if the two operators commute, that is

$$[\hat{A}, \hat{B}] = 0.$$

Thouless' theorem

If the operators do not commute, we need to resort to the Baker-Campbell-Hauersdorf. This relation states that

$$\exp \hat{C} = \exp \hat{A} \exp \hat{B},$$

with

$$\hat{C} = \hat{A} + \hat{B} + \frac{1}{2}[\hat{A}, \hat{B}] + \frac{1}{12}[[\hat{A}, \hat{B}], \hat{B}] - \frac{1}{12}[[\hat{A}, \hat{B}], \hat{A}] + \dots$$

From these relations, we note that in our expression for $|c'\rangle$ we have commutators of the type

$$[a_a^\dagger a_i, a_b^\dagger a_j],$$

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

$$|c'\rangle = exp\left\{\sum_{a>F}\sum_{i\le F} C_{ai}a_a^\dagger a_i\right\}|c\rangle = \prod_i\left\{1+\sum_{a>F} C_{ai}a_a^\dagger a_i + \left(\sum_{a>F} C_{ai}a_a^\dagger a_i\right)^2 + \dots\right\}|c\rangle$$

Thouless' theorem

We note that

$$\prod_i \sum_{a>F} C_{ai}a_a^\dagger a_i \sum_{b>F} C_{bi}a_b^\dagger a_i|c\rangle = 0,$$

and all higher-order powers of these combinations of creation and annihilation operators disappear due to the fact that $(a_i)^n|c\rangle = 0$ when $n > 1$. This allows us to rewrite the expression for $|c'\rangle$ as

$$|c'\rangle = \prod_i\left\{1+\sum_{a>F} C_{ai}a_a^\dagger a_i\right\}|c\rangle,$$

which we can rewrite as

$$|c'\rangle = \prod_i\left\{1+\sum_{a>F} C_{ai}a_a^\dagger a_i\right\}|a_{i_1}^\dagger a_{i_2}^\dagger \dots a_{i_n}^\dagger|0\rangle.$$

The last equation can be written as

$$|c'\rangle = \prod_i\left\{1+\sum_{a>F} C_{ai}a_a^\dagger a_i\right\}|a_{i_1}^\dagger a_{i_2}^\dagger \dots a_{i_n}^\dagger|0\rangle = \left(1+\sum_{a>F} C_{ai_1}a_a^\dagger a_{i_1}\right)a_{i_1}^\dagger \quad (86)$$

$$\times\left(1+\sum_{a>F} C_{ai_2}a_a^\dagger a_{i_2}\right)a_{i_2}^\dagger \dots |0\rangle = \prod_i\left(a_i^\dagger + \sum_{a>F} C_{ai}a_a^\dagger\right)|0\rangle. \quad (87)$$

New operators

If we define a new creation operator

$$b_i^\dagger = a_i^\dagger + \sum_{a>F} C_{ai}a_a^\dagger, \quad (88)$$

we have

$$|c'\rangle = \prod_i b_i^\dagger|0\rangle = \prod_i\left(a_i^\dagger + \sum_{a>F} C_{ai}a_a^\dagger\right)|0\rangle,$$

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. (**??**). The single-particle states have all 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

$$\tilde{b}_i^\dagger = \sum_p f_{ip} a_p^\dagger,$$

where f_{ip} is a matrix element of a unitary matrix which transforms our creation and annihilation operators $a^\dagger$ and a to $\tilde{b}^\dagger$ and $\tilde{b}$. These new operators define a new representation of a Slater determinant as

$$|\tilde{c}\rangle = \prod_i \tilde{b}_i^\dagger |0\rangle.$$

Showing that $|\tilde{c}\rangle = |c'\rangle$

We need to show that $|\tilde{c}\rangle = |c'\rangle$. We need also to assume that the new state is not orthogonal to $|c\rangle$, that is $\langle c|\tilde{c}\rangle \neq 0$. From this it follows that

$$\langle c|\tilde{c}\rangle = \langle 0|a_{i_n} \dots a_{i_1} \left(\sum_{p=i_1}^{i_n} f_{i_1 p} a_p^\dagger\right) \left(\sum_{q=i_1}^{i_n} f_{i_2 q} a_q^\dagger\right) \dots \left(\sum_{t=i_1}^{i_n} f_{i_n t} a_t^\dagger\right) |0\rangle,$$

which is nothing but the determinant $det(f_{ip})$ which we can, using the intermediate normalization condition, normalize to one, that is

$$det(f_{ip}) = 1,$$

meaning that f has an inverse defined as (since we are dealing with orthogonal, and in our case unitary as well, transformations)

$$\sum_k f_{ik} f_{kj}^{-1} = \delta_{ij},$$

and

$$\sum_j f_{ij}^{-1} f_{jk} = \delta_{ik}.$$

Wrapping it up

Using these relations we can then define the linear combination of creation (and annihilation as well) operators as

$$\sum_i f_{ki}^{-1} \tilde{b}_i^\dagger = \sum_i f_{ki}^{-1} \sum_{p=i_1}^{\infty} f_{ip} a_p^\dagger = a_k^\dagger + \sum_i \sum_{p=i_{n+1}}^{\infty} f_{ki}^{-1} f_{ip} a_p^\dagger.$$

Defining

$$c_{kp} = \sum_{i \leq F} f_{ki}^{-1} f_{ip},$$

we can redefine

$$a_k^\dagger + \sum_i \sum_{p=i_{n+1}}^{\infty} f_{ki}^{-1} f_{ip} a_p^\dagger = a_k^\dagger + \sum_{p=i_{n+1}}^{\infty} c_{kp} a_p^\dagger = b_k^\dagger,$$

our starting point. We have shown that our general representation of a Slater determinant

$$|\tilde{c}\rangle = \prod_i \tilde{b}_i^\dagger |0\rangle = |c'\rangle = \prod_i b_i^\dagger |0\rangle,$$

with

$$b_k^\dagger = a_k^\dagger + \sum_{p=i_{n+1}}^{\infty} c_{kp} a_p^\dagger.$$

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

$$|c'\rangle = |c\rangle + |\delta c\rangle,$$

where $|\delta c\rangle$ 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

$$|c'\rangle = \left(1 + \sum_{ai} \delta C_{ai} a_a^\dagger a_i\right) |c\rangle.$$

In our derivation of the Hartree-Fock equations we have shown that

$$\langle \delta c|\hat{H}|c\rangle = 0,$$

which means that we have to satisfy

$$\langle c| \sum_{ai} \delta C_{ai} \left\{ a_a^\dagger a_i \right\} \hat{H}|c\rangle = 0.$$

With this as a background, we are now ready to study the stability of the Hartree-Fock equations.

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 $\langle c|\hat{H}|c\rangle$ 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

$$\frac{\langle c'|\hat{H}|c'\rangle}{\langle c'|c'\rangle} \ge \langle c|\hat{H}|c\rangle = E_0,$$

with

$$|c'\rangle = |c\rangle + |\delta c\rangle.$$

Using Thouless' theorem we can write out $|c'\rangle$ as

$$|c'\rangle = \exp\left\{\sum_{a>F}\sum_{i\le F}\delta C_{ai}a_a^\dagger a_i\right\}|c\rangle \tag{89}$$

$$= \left\{1 + \sum_{a>F}\sum_{i\le F}\delta C_{ai}a_a^\dagger a_i + \frac{1}{2!}\sum_{ab>F}\sum_{ij\le F}\delta C_{ai}\delta C_{bj}a_a^\dagger a_i a_b^\dagger a_j + \dots\right\} \tag{90}$$

where the amplitudes δC are small.

Hartree-Fock in second quantization and stability of HF solution

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

$$\langle c'|c'\rangle = 1 + \sum_{a>F}\sum_{i\le F}|\delta C_{ai}|^2 + O(\delta C_{ai}^3).$$

The expectation value for the energy is now given by (using the Hartree-Fock condition)

$$\langle c'|\hat{H}|c'\rangle = \langle c|\hat{H}|c\rangle + \sum_{ab>F}\sum_{ij\le F}\delta C_{ai}^*\delta C_{bj}\langle c|a_i^\dagger a_a\hat{H}a_b^\dagger a_j|c\rangle +$$

$$\frac{1}{2!}\sum_{ab>F}\sum_{ij\le F}\delta C_{ai}\delta C_{bj}\langle c|\hat{H}a_a^\dagger a_i a_b^\dagger a_j|c\rangle + \frac{1}{2!}\sum_{ab>F}\sum_{ij\le F}\delta C_{ai}^*\delta C_{bj}^*\langle c|a_j^\dagger a_b a_i^\dagger a_a\hat{H}|c\rangle + \dots$$

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

$$\langle c|\left(\{a_i^\dagger a_a\}\hat{H}\{a_b^\dagger a_j\}\right)|c\rangle = \sum_{pq}\sum_{ijab}\delta C_{ai}^*\delta C_{bj}\langle p|\hat{h}_0|q\rangle\langle c|\left(\{a_i^\dagger a_a\}\{a_p^\dagger a_q\}\{a_b^\dagger a_j\}\right)|c\rangle \tag{91}$$

$$+ \frac{1}{4}\sum_{pqrs}\sum_{ijab}\delta C_{ai}^*\delta C_{bj}\langle pq|\hat{v}|rs\rangle\langle c|\left(\{a_i^\dagger a_a\}\{a_p^\dagger a_q^\dagger a_s a_r\}\{a_b^\dagger a_j\}\right)|c\rangle, \tag{92}$$

resulting in

$$E_0 \sum_{ai} |\delta C_{ai}|^2 + \sum_{ai} |\delta C_{ai}|^2 (\varepsilon_a - \varepsilon_i) - \sum_{ijab} \langle aj|\hat{v}|bi\rangle \delta C_{ai}^* \delta C_{bj}.$$

Hartree-Fock in second quantization and stability of HF solution

$$\frac{1}{2!}\langle c| \left(\{a_j^\dagger a_b\}\{a_i^\dagger a_a\}\hat{V}_N\right)|c\rangle = \frac{1}{2!}\langle c| \left(\hat{V}_N\{a_a^\dagger a_i\}\{a_b^\dagger a_j\}\right)^\dagger |c\rangle$$

which is nothing but

$$\frac{1}{2!}\langle c| \left(\hat{V}_N\{a_a^\dagger a_i\}\{a_b^\dagger a_j\}\right)|c\rangle^* = \frac{1}{2}\sum_{ijab} (\langle ij|\hat{v}|ab\rangle)^* \delta C_{ai}^* \delta C_{bj}^*$$

or

$$\frac{1}{2}\sum_{ijab} (\langle ab|\hat{v}|ij\rangle) \delta C_{ai}^* \delta C_{bj}^*$$

where we have used the relation

$$\langle a|\hat{A}|b\rangle = (\langle b|\hat{A}^\dagger|a\rangle)^*$$

due to the hermiticity of $\hat{H}$ and $\hat{V}$.

Hartree-Fock in second quantization and stability of HF solution

We define two matrix elements

$$A_{ai,bj} = -\langle aj|\hat{v}bi\rangle$$

and

$$B_{ai,bj} = \langle ab|\hat{v}|ij\rangle$$

both being anti-symmetrized.

Hartree-Fock in second quantization and stability of HF solution

With these definitions we write out the energy as

$$\langle c'|H|c'\rangle = \left(1 + \sum_{ai} |\delta C_{ai}|^2\right)\langle c|H|c\rangle + \sum_{ai} |\delta C_{ai}|^2 (\varepsilon_a^{HF} - \varepsilon_i^{HF}) + \sum_{ijab} A_{ai,bj}\delta C_{ai}^* \delta C_{bj} + \tag{93}$$

$$\frac{1}{2}\sum_{ijab} B_{ai,bj}^* \delta C_{ai}\delta C_{bj} + \frac{1}{2}\sum_{ijab} B_{ai,bj}\delta C_{ai}^* \delta C_{bj}^* + O(\delta C_{ai}^3), \tag{94}$$

which can be rewritten as

$$\langle c'|H|c'\rangle = \left(1+\sum_{ai}|\delta C_{ai}|^2\right)\langle c|H|c\rangle + \Delta E + O(\delta C_{ai}^3),$$

and skipping higher-order terms we arrived

$$\frac{\langle c'|\hat{H}|c'\rangle}{\langle c'|c'\rangle} = E_0 + \frac{\Delta E}{(1+\sum_{ai}|\delta C_{ai}|^2)}.$$

Hartree-Fock in second quantization and stability of HF solution

We have defined

$$\Delta E = \frac{1}{2}\langle\chi|\hat{M}|\chi\rangle$$

with the vectors

$$\chi = [\delta C \;\; \delta C^*]^T$$

and the matrix

$$\hat{M} = \left(\begin{array}{cc} \Delta + A & B \\ B^* & \Delta + A^* \end{array}\right),$$

with $\Delta_{ai,bj} = (\varepsilon_a - \varepsilon_i)\delta_{ab}\delta_{ij}$.

Hartree-Fock in second quantization and stability of HF solution

The condition

$$\Delta E = \frac{1}{2}\langle\chi|\hat{M}|\chi\rangle \geq 0$$

for an arbitrary vector

$$\chi = [\delta C \;\; \delta C^*]^T$$

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 ai)

$$(\varepsilon_a - \varepsilon_i)\delta_{ab}\delta_{ij} + A_{ai,bj} \geq 0.$$

This equation can be used as a first test of the stability of the Hartree-Fock equation.

Operators in second quantization

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

$$|\alpha_1 \dots \alpha_n\rangle = a_{\alpha_1}^{\dagger} a_{\alpha_2}^{\dagger} \dots a_{\alpha_n}^{\dagger}|0\rangle.$$

The time consuming part stems from the action of the Hamiltonian on the above determinant,

$$\left(\sum_{\alpha\beta}\langle\alpha|t+u|\beta\rangle a_\alpha^\dagger a_\beta + \frac{1}{4}\sum_{\alpha\beta\gamma\delta}\langle\alpha\beta|\hat{v}|\gamma\delta\rangle a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma\right) a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger \dots a_{\alpha_n}^\dagger|0\rangle.$$

A practically useful way to implement this action is to encode a Slater determinant as a bit pattern.

Operators in second quantization

Assume that we have at our disposal n different single-particle orbits $\alpha_0, \alpha_2, \dots, \alpha_{n-1}$ and that we can distribute among these orbits $N \le n$ 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 $\alpha_0, \alpha_1, \dots, \alpha_{15}$ and $N = 4$ fermions occupying the states α_3, α_6, α_{10} and α_{13} we could write this Slater determinant as

$$\Phi_\Lambda = a_{\alpha_3}^\dagger a_{\alpha_6}^\dagger a_{\alpha_{10}}^\dagger a_{\alpha_{13}}^\dagger|0\rangle.$$

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

α_0	α_1	α_2	α_3	α_4	α_5	α_6	α_7	α_8	α_9	α_{10}	α_{11}	α_{12}	α_{13}	α_{14}	α_{15}
0	0	0	1	0	0	1	0	0	0	1	0	0	1	0	0

which translates into the decimal number

$$2^3 + 2^6 + 2^{10} + 2^{13} = 9288.$$

We can thus encode a Slater determinant as a bit pattern.

Operators in second quantization

With N particles that can be distributed over n single-particle states, the total number of Slater determinats (and defining thereby the dimensionality of the system) is

$$\dim(\mathcal{H}) = \left(\begin{array}{c} n \\ N \end{array}\right).$$

The total number of bit patterns is 2^n.

Operators in second quantization

We assume again that we have at our disposal n different single-particle orbits $\alpha_0, \alpha_2, \dots, \alpha_{n-1}$ and that we can distribute among these orbits $N \le n$ particles.

The ordering among these states is important as it defines the order of the creation operators. We will write the determinant

$$\Phi_\Lambda = a^\dagger_{\alpha_3} a^\dagger_{\alpha_6} a^\dagger_{\alpha_{10}} a^\dagger_{\alpha_{13}} |0\rangle,$$

in a more compact way as

$$\Phi_{3,6,10,13} = |0001001000100100\rangle.$$

The action of a creation operator is thus

$$a^\dagger_{\alpha_4} \Phi_{3,6,10,13} = a^\dagger_{\alpha_4} |0001001000100100\rangle = a^\dagger_{\alpha_4} a^\dagger_{\alpha_3} a^\dagger_{\alpha_6} a^\dagger_{\alpha_{10}} a^\dagger_{\alpha_{13}} |0\rangle,$$

which becomes

$$-a^\dagger_{\alpha_3} a^\dagger_{\alpha_4} a^\dagger_{\alpha_6} a^\dagger_{\alpha_{10}} a^\dagger_{\alpha_{13}} |0\rangle = -|0001101000100100\rangle.$$

Operators in second quantization

Similarly

$$a^\dagger_{\alpha_6} \Phi_{3,6,10,13} = a^\dagger_{\alpha_6} |0001001000100100\rangle = a^\dagger_{\alpha_6} a^\dagger_{\alpha_3} a^\dagger_{\alpha_6} a^\dagger_{\alpha_{10}} a^\dagger_{\alpha_{13}} |0\rangle,$$

which becomes

$$-a^\dagger_{\alpha_4} (a^\dagger_{\alpha_6})^2 a^\dagger_{\alpha_{10}} a^\dagger_{\alpha_{13}} |0\rangle = 0!$$

This gives a simple recipe:

- If one of the bits b_j is 1 and we act with a creation operator on this bit, we return a null vector
- If $b_j = 0$, 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

Consider the action of $a^\dagger_{\alpha_2}$ on various slater determinants:

$$\begin{array}{lll}
a^\dagger_{\alpha_2}\Phi_{00111} & = a^\dagger_{\alpha_2}|00111\rangle & = 0 \times |00111\rangle \\
a^\dagger_{\alpha_2}\Phi_{01011} & = a^\dagger_{\alpha_2}|01011\rangle & = (-1) \times |01111\rangle \\
a^\dagger_{\alpha_2}\Phi_{01101} & = a^\dagger_{\alpha_2}|01101\rangle & = 0 \times |01101\rangle \\
a^\dagger_{\alpha_2}\Phi_{01110} & = a^\dagger_{\alpha_2}|01110\rangle & = 0 \times |01110\rangle \\
a^\dagger_{\alpha_2}\Phi_{10011} & = a^\dagger_{\alpha_2}|10011\rangle & = (-1) \times |10111\rangle \\
a^\dagger_{\alpha_2}\Phi_{10101} & = a^\dagger_{\alpha_2}|10101\rangle & = 0 \times |10101\rangle \\
a^\dagger_{\alpha_2}\Phi_{10110} & = a^\dagger_{\alpha_2}|10110\rangle & = 0 \times |10110\rangle \\
a^\dagger_{\alpha_2}\Phi_{11001} & = a^\dagger_{\alpha_2}|11001\rangle & = (+1) \times |11101\rangle \\
a^\dagger_{\alpha_2}\Phi_{11010} & = a^\dagger_{\alpha_2}|11010\rangle & = (+1) \times |11110\rangle
\end{array}$$

What is the simplest way to obtain the phase when we act with one annihilation(creation) operator on the given Slater determinant representation?

Operators in second quantization

We have an SD representation

$$\Phi_\Lambda = a^\dagger_{\alpha_0} a^\dagger_{\alpha_3} a^\dagger_{\alpha_6} a^\dagger_{\alpha_{10}} a^\dagger_{\alpha_{13}} |0\rangle,$$

in a more compact way as

$$\Phi_{0,3,6,10,13} = |1001001000100100\rangle.$$

The action of

$$a^\dagger_{\alpha_4} a_{\alpha_0} \Phi_{0,3,6,10,13} = a^\dagger_{\alpha_4} |0001001000100100\rangle = a^\dagger_{\alpha_4} a^\dagger_{\alpha_3} a^\dagger_{\alpha_6} a^\dagger_{\alpha_{10}} a^\dagger_{\alpha_{13}} |0\rangle,$$

which becomes

$$-a^\dagger_{\alpha_3} a^\dagger_{\alpha_4} a^\dagger_{\alpha_6} a^\dagger_{\alpha_{10}} a^\dagger_{\alpha_{13}} |0\rangle = -|0001101000100100\rangle.$$

Operators in second quantization

The action

$$a_{\alpha_0} \Phi_{0,3,6,10,13} = |0001001000100100\rangle,$$

can be obtained by subtracting the logical sum (AND operation) of $\Phi_{0,3,6,10,13}$ and a word which represents only α_0, that is

$$|1000000000000000\rangle,$$

from $\Phi_{0,3,6,10,13} = |1001001000100100\rangle$.

This operation gives $|0001001000100100\rangle$.

Similarly, we can form $a^\dagger_{\alpha_4} a_{\alpha_0} \Phi_{0,3,6,10,13}$, say, by adding $|0000100000000000\rangle$ to $a_{\alpha_0} \Phi_{0,3,6,10,13}$, first checking that their logical sum is zero in order to make sure that orbital α_4 is not already occupied.

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 $S_1 = |1000000000000000\rangle$

- Define S_2 as the similar word that represents the bit to be added, that is in our case

$S_2 = |0000100000000000\rangle$.

- 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

$$\Phi_{0,3,6,10,13} = |1001001000100100\rangle,$$

which results in $|0001000000000000\rangle$. Counting the number of 1−bits gives the phase. Here you need however an algorithm for bitcounting. Several efficient ones available.

Exercises

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 ψ_λ, with $\lambda = 1, 2, \ldots, A$. The unitary transformation

$$\psi_a = \sum_\lambda C_{a\lambda}\phi_\lambda,$$

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

$$\Phi_0 = \prod_{i=1}^{n} a^\dagger_{\alpha_i}|0\rangle,$$

use Wick's theorem to compute the normalization integral $\langle\Phi_0|\Phi_0\rangle$.

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

$$|\alpha_1\alpha_2\rangle = a^\dagger_{\alpha_1}a^\dagger_{\alpha_2}|0\rangle,$$

$$\hat{F} = \sum_{\alpha\beta}\langle\alpha|\hat{f}|\beta\rangle a^\dagger_\alpha a_\beta,$$

$$\langle\alpha|\hat{f}|\beta\rangle = \int \psi^*_\alpha(x)f(x)\psi_\beta(x)dx,$$

$$\hat{G} = \frac{1}{2}\sum_{\alpha\beta\gamma\delta}\langle\alpha\beta|\hat{g}|\gamma\delta\rangle a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma,$$

and

$$\langle\alpha\beta|\hat{g}|\gamma\delta\rangle = \int\int \psi_\alpha^*(x_1)\psi_\beta^*(x_2)g(x_1,x_2)\psi_\gamma(x_1)\psi_\delta(x_2)dx_1dx_2$$

Compare these results with those from exercise 3c).

Exercises

Exercise 3. Show that the onebody 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

$$\hat{H}_0 = \sum_{pq}\langle p|\hat{h}_0|q\rangle \left\{a_p^\dagger a_q\right\} + \sum_i \langle i|\hat{h}_0|i\rangle.$$

Explain the meaning of the various symbols. Which reference vacuum has been used?

Exercises

Exercise 4. Show that the twobody part of the Hamiltonian

$$\hat{H}_I = \frac{1}{4}\sum_{pqrs}\langle pq|\hat{v}|rs\rangle a_p^\dagger a_q^\dagger a_s a_r,$$

can be written, using standard annihilation and creation operators, in normal-ordered form as

$$\hat{H}_I = \frac{1}{4}\sum_{pqrs}\langle pq|\hat{v}|rs\rangle \left\{a_p^\dagger a_q^\dagger a_s a_r\right\} + \sum_{pqi}\langle pi|\hat{v}|qi\rangle \left\{a_p^\dagger a_q\right\} + \frac{1}{2}\sum_{ij}\langle ij|\hat{v}|ij\rangle.$$

Explain again the meaning of the various symbols.

This exercise is optional: Derive the normal-ordered form of the threebody part of the Hamiltonian.

$$\hat{H}_3 = \frac{1}{36}\sum_{\substack{pqr\\stu}}\langle pqr|\hat{v}_3|stu\rangle a_p^\dagger a_q^\dagger a_r^\dagger a_u a_t a_s,$$

and specify the contributions to the twobody, onebody and the scalar part.

Exercises

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 three N-particle Slater determinants $|\Phi_0$, $|\Phi_i^a\rangle$ and $|\Phi_{ij}^{ab}\rangle$, where the notation means that Slater determinant $|\Phi_i^a\rangle$ differs from $|\Phi_0\rangle$ by one single-particle state, that is a single-particle state ψ_i is replaced by a single-particle state ψ_a. It is often interpreted as a so-called one-particle-one-hole excitation. Similarly, the Slater determinant $|\Phi_{ij}^{ab}\rangle$ 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 $ijk\dots$ represent single-particle states below the Fermi level and $abc\dots$ represent states above the Fermi level, so-called particle states. We define thereafter a general onebody normal-ordered (with respect to the new vacuum state) operator as

$$\hat{F}_N = \sum_{pq} \langle p|f|\beta\rangle \left\{a_p^\dagger a_q\right\},$$

with

$$\langle p|f|q\rangle = \int \psi_p^*(x) f(x)\psi_q(x)dx,$$

and a general normal-ordered two-body operator

$$\hat{G}_N = \frac{1}{4}\sum_{pqrs} \langle pq|g|rs\rangle_{AS} \left\{a_p^\dagger a_q^\dagger a_s a_r\right\},$$

with for example the direct matrix element given as

$$\langle pq|g|rs\rangle = \int\int \psi_p^*(x_1)\psi_q^*(x_2) g(x_1,x_2)\psi_r(x_1)\psi_s(x_2)dx_1 dx_2$$

with g being invariant under the interchange of the coordinates of two particles. The single-particle states ψ_i are not necessarily eigenstates of $\hat{f}$. The curly brackets mean that the operators are normal-ordered with respect to the new vacuum reference state.

How would you write the above Slater determinants in a second quantization formalism, utilizing the fact that we have defined a new reference state?

Use thereafter Wick's theorem to find the expectation values of

$$\langle \Phi_0|\hat{F}_N|\Phi_0\rangle,$$

and

$$\langle \Phi_0 \hat{G}_N|\Phi_0\rangle.$$

Find thereafter

$$\langle \Phi_0|\hat{F}_N|\Phi_i^a\rangle,$$

and

$$\langle\Phi_0|\hat{G}_N|\Phi_i^a\rangle,$$

Finally, find

$$\langle\Phi_0|\hat{F}_N|\Phi_{ij}^{ab}\rangle,$$

and

$$\langle\Phi_0|\hat{G}_N|\Phi_{ij}^{ab}\rangle.$$

What happens with the two-body operator if we have a transition probability of the type

$$\langle\Phi_0|\hat{G}_N|\Phi_{ijk}^{abc}\rangle,$$

where the Slater determinant to the right of the operator differs by more than two single-particle states?

Exercises

Exercise 6. Write a program which sets up all possible Slater determinants given $N = 4$ eletrons 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 bits set in integer """
    count = 0
    while(int_type):
        int_type &= int_type - 1
        count += 1
    return(count)


# testBit() returns a nonzero result, 2**offset, if the bit at 'offset' is one.

def testBit(int_type, offset):
    mask = 1 << offset
    return(int_type & mask) >> offset

# setBit() returns an integer with the bit at 'offset' set to 1.

def setBit(int_type, offset):
    mask = 1 << offset
    return(int_type | mask)
```

```python
# clearBit() returns an integer with the bit at 'offset' cleared.

def clearBit(int_type, offset):
    mask = ~(1 << offset)
    return(int_type & mask)

# toggleBit() returns an integer with the bit at 'offset' inverted, 0 -> 1 and 1 -> 0.

def toggleBit(int_type, offset):
    mask = 1 << offset
    return(int_type ^ mask)

# binary string made from number

def bin0(s):
    return str(s) if s<=1 else bin0(s>>1) + str(s&1)

def bin(s, L = 0):
    ss = bin0(s)
    if L > 0:
        return '0'*(L-len(ss)) + ss
    else:
        return ss



class Slater:
    """ Class for Slater determinants """
    def __init__(self):
        self.word = int(0)

    def create(self, j):
        print "c^+_" + str(j) + " |" + bin(self.word) + ">  = ",
        # Assume bit j is set, then we return zero.
        s = 0
        # Check if bit j is set.
        isset = testBit(self.word, j)
        if isset == 0:
            bits = bitCount(self.word & ((1<<j)-1))
            s = pow(-1, bits)
            self.word = setBit(self.word, j)

        print str(s) + " x |" + bin(self.word) + ">"
        return s

    def annihilate(self, j):
        print "c_" + str(j) + " |" + bin(self.word) + ">  = ",
        # Assume bit j is not set, then we return zero.
        s = 0
        # Check if bit j is set.
        isset = testBit(self.word, j)
        if isset == 1:
            bits = bitCount(self.word & ((1<<j)-1))
            s = pow(-1, bits)
            self.word = clearBit(self.word, j)

        print str(s) + " x |" + bin(self.word) + ">"
        return s
```

Do some testing:

```
# Do some testing:

phi = Slater()
phi.create(0)
phi.create(1)
phi.create(2)
phi.create(3)

print


s = phi.annihilate(2)
s = phi.create(7)
s = phi.annihilate(0)
s = phi.create(200)
```

Exercises: Using sympy to compute matrix elements

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.

```
from sympy import *
from sympy.physics.secondquant import *

i, j = symbols('i,j', below_fermi=True)
a, b = symbols('a,b', above_fermi=True)
p, q = symbols('p,q')
print simplify(wicks(Fd(i)*F(a)*Fd(p)*F(q)*Fd(b)*F(j), keep_only_fully_contracted=True))
```

The code defines single-particle states above and below the Fermi level, in addition to the genereal symbols pq which can refer to any type of state below or above the Fermi level. Wick's theorem is implemented between the creation and annihilation operators Fd and F, respectively. Using the simplify option, one can lump together several Kronecker-δ functions.

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

```
# This code sets up a two-body Hamiltonian for fermions
from sympy import symbols, latex, WildFunction, collect, Rational
from sympy.physics.secondquant import F, Fd, wicks, AntiSymmetricTensor, substitute_dummies, NO

# setup hamiltonian
p,q,r,s = symbols('p q r s',dummy=True)
f = AntiSymmetricTensor('f',(p,),(q,))
pr = NO((Fd(p)*F(q)))
v = AntiSymmetricTensor('v',(p,q),(r,s))
pqsr = NO(Fd(p)*Fd(q)*F(s)*F(r))
Hamiltonian=f*pr + Rational(1)/Rational(4)*v*pqsr
print "Hamiltonian defined as:", latex(Hamiltonian)
```

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

$$f^p_q \left\{a^\dagger_p a_q\right\} - \frac{1}{4} v^{qp}_{sr} \left\{a^\dagger_p a^\dagger_q a_r a_s\right\}$$

Exercises: Using sympy to compute matrix elements

We can now use this code to compute the matrix elements between two two-body Slater determinants using Wick's theorem.

```
from sympy import symbols, latex, WildFunction, collect, Rational, simplify
from sympy.physics.secondquant import F, Fd, wicks, AntiSymmetricTensor, substitute_dummies, NO, evalua
# setup hamiltonian
p,q,r,s = symbols('p q r s',dummy=True)
f = AntiSymmetricTensor('f',(p,),(q,))
pr = NO((Fd(p)*F(q)))
v = AntiSymmetricTensor('v',(p,q),(r,s))
pqsr = NO(Fd(p)*Fd(q)*F(s)*F(r))
Hamiltonian=f*pr + Rational(1)/Rational(4)*v*pqsr
c,d = symbols('c, d',above_fermi=True)
a,b = symbols('a, b',above_fermi=True)

expression = wicks(F(b)*F(a)*Hamiltonian*Fd(c)*Fd(d),keep_only_fully_contracted=True, simplify_kronecke
expression = evaluate_deltas(expression)
expression = simplify(expression)
print "Hamiltonian defined as:", latex(expression)
```

The result is as expected,

$$\delta_{ac} f^b_d - \delta_{ad} f^b_c - \delta_{bc} f^a_d + \delta_{bd} f^a_c + v^{ab}_{cd}.$$

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

```
from sympy import symbols, latex, WildFunction, collect, Rational, simplify
from sympy.physics.secondquant import F, Fd, wicks, AntiSymmetricTensor, substitute_dummies, NO, evalua
# setup hamiltonian
p,q,r,s = symbols('p q r s',dummy=True)
```

```
f = AntiSymmetricTensor('f',(p,),(q,))
pr = Fd(p)*F(q)
v = AntiSymmetricTensor('v',(p,q),(r,s))
pqsr = Fd(p)*Fd(q)*F(s)*F(r)
#define the Hamiltonian
Hamiltonian = f*pr + Rational(1)/Rational(4)*v*pqsr
#define indices for states above and below the Fermi level
index_rule = {
     'below':  'kl',
     'above':  'cd',
     'general': 'pqrs'
     }
Hnormal = substitute_dummies(Hamiltonian,new_indices=True, pretty_indices=index_rule)
print "Hamiltonian defined as:", latex(Hnormal)
```

which results in

$$f_p^q a_q^\dagger a_p + \frac{1}{4} v_{qp}^{sr} a_s^\dagger a_r^\dagger a_p a_q$$

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).

```
from sympy import symbols, latex, WildFunction, collect, Rational, simplify
from sympy.physics.secondquant import F, Fd, wicks, AntiSymmetricTensor, substitute_dummies,
# setup hamiltonian
p,q,r,s = symbols('p q r s',dummy=True)
f = AntiSymmetricTensor('f',(p,),(q,))
pr = Fd(p)*F(q)
v = AntiSymmetricTensor('v',(p,q),(r,s))
pqsr = Fd(p)*Fd(q)*F(s)*F(r)
#define the Hamiltonian
Hamiltonian=f*pr + Rational(1)/Rational(4)*v*pqsr
#define indices for states above and below the Fermi level
index_rule = {
     'below':  'kl',
     'above':  'cd',
     'general': 'pqrs'
     }
Hnormal = substitute_dummies(Hamiltonian,new_indices=True, pretty_indices=index_rule)
E0 = wicks(Hnormal,keep_only_fully_contracted=True)
Hnormal = Hnormal-E0
w = WildFunction('w')
Hnormal = collect(Hnormal, NO(w))
Hnormal = evaluate_deltas(Hnormal)
print latex(Hnormal)
```

which gives us

$$-f_i^i + f_p^q a_q^\dagger a_p - \frac{1}{4} v_{ii}^{ii} - \frac{1}{4} v_{ii}^{ii} + \frac{1}{4} v_{qp}^{sr} a_r^\dagger a_s^\dagger a_q a_p,$$

again as expected, with the reference energy to be subtracted.

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.

```
from sympy import symbols, latex, WildFunction, collect, Rational, simplify
from sympy.physics.secondquant import F, Fd, wicks, AntiSymmetricTensor, substitute_dummies, NO, evalua
# setup hamiltonian
p,q,r,s = symbols('p q r s',dummy=True)

v = AntiSymmetricTensor('v',(p,q),(r,s))
pqsr = NO(Fd(p)*Fd(q)*F(s)*F(r))
Hamiltonian=Rational(1)/Rational(4)*v*pqsr
a,b,c,d,e,f = symbols('a,b, c, d, e, f',above_fermi=True)

expression = wicks(F(c)*F(b)*F(a)*Hamiltonian*Fd(d)*Fd(e)*Fd(f),keep_only_fully_contracted=True, simpli
expression = evaluate_deltas(expression)
expression = simplify(expression)
print latex(expression)
```

resulting in nine terms (as expected),

$$-\delta_{ad}v^{cb}_{ef} - \delta_{ae}v^{cb}_{fd} + \delta_{af}v^{cb}_{ed} - \delta_{bd}v^{ac}_{ef} - \delta_{be}v^{ac}_{fd} + \delta_{bf}v^{ac}_{ed} + \delta_{cd}v^{ab}_{ef} + \delta_{ce}v^{ab}_{fd} - \delta_{cf}v^{ab}_{ed}$$

Exercises: Derivation of Hartree-Fock equations

Exercise 8. What is the diagrammatic representation of the HF equation?

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

(Represent $(-u^{HF})$ by the symbol $---$X .)

Exercises: Derivation of Hartree-Fock equations

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 λ and that our system ends in a new state $|\Phi_n\rangle$. Define the energy needed to remove this particle as

$$E_\lambda = \sum_n |\langle\Phi_n|a_\lambda|\Phi\rangle|^2(E_0 - E_n),$$

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

- Show that

$$E_\lambda = \langle\Phi|a_\lambda^\dagger\left[a_\lambda, H\right]|\Phi\rangle,$$

where H is the Hamiltonian of this system.

- If we assume that Φ is the Hartree-Fock result, find the relation between E_λ and the single-particle energy ε_λ for states $\lambda \leq F$ and $\lambda > F$, with

$$\varepsilon_\lambda = \langle\lambda|\hat{t} + \hat{u}|\lambda\rangle,$$

and

$$\langle\lambda|\hat{u}|\lambda\rangle = \sum_{\beta\leq F}\langle\lambda\beta|\hat{v}|\lambda\beta\rangle.$$

We have assumed an antisymmetrized matrix element here. Discuss the result.

The Hamiltonian operator is defined as

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