Second Quantization

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- Second quantization and operators, two-body operator with examples
- Wick's theorem (missing in html and ipython notebook but in pdf files)
- Examples on how to use bit representations for Slater determinants

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. (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 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 (3)

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

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

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

it follows that

$$a_{\alpha_i}^\dagger a_{\alpha_i}^\dagger = 0. \tag{7}$$

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

$$a_\alpha^\dagger a_\beta^\dagger + a_\beta^\dagger a_\alpha^\dagger \equiv \{a_\alpha^\dagger, a_\beta^\dagger\} = 0 \tag{8}$$

Second quantization

The hermitian conjugate of $a_\alpha^\dagger$ is

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

If we take the hermitian conjugate of Eq. (8), 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 $|\alpha_1\alpha_2\dots\alpha_n\rangle_{\mathrm{AS}}$? 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. (6) 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. (13) holds for case (1) since the lefthand side is zero due to the Pauli principle. We write Eq. (11) as

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

Here we must have $m = n+1$ if Eq. (14) 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 $a_\alpha^\dagger$ 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

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

From Eqs. (20) and (21) we arrive at

$$\{a^\dagger_\alpha, a_\alpha\} = a^\dagger_\alpha a_\alpha + a_\alpha a^\dagger_\alpha = 1 \tag{22}$$

Second quantization

The action of $\left\{a^\dagger_\alpha, a_\beta\right\}$, 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

$$
\begin{aligned}
a^\dagger_\alpha a_\beta|\alpha\beta\alpha_1\alpha_2\dots\alpha_{n-2}\rangle &= 0 \\
a_\beta a^\dagger_\alpha|\alpha\beta\alpha_1\alpha_2\dots\alpha_{n-2}\rangle &= 0
\end{aligned}
\tag{23}
$$

while the second case gives

$$
\begin{aligned}
a^\dagger_\alpha a_\beta|\beta \underbrace{\alpha_1\alpha_2\dots\alpha_{n-1}}_{\neq\alpha}\rangle &= |\alpha \underbrace{\alpha_1\alpha_2\dots\alpha_{n-1}}_{\neq\alpha}\rangle \\
a_\beta a^\dagger_\alpha|\beta \underbrace{\alpha_1\alpha_2\dots\alpha_{n-1}}_{\neq\alpha}\rangle &= a_\beta|\alpha\beta \underbrace{\beta\alpha_1\alpha_2\dots\alpha_{n-1}}_{\neq\alpha}\rangle \\
&= -|\alpha \underbrace{\alpha_1\alpha_2\dots\alpha_{n-1}}_{\neq\alpha}\rangle
\end{aligned}
\tag{24}
$$

Second quantization

Finally if the state vector does not contain α and β

$$
\begin{aligned}
a^\dagger_\alpha a_\beta| \underbrace{\alpha_1\alpha_2\dots\alpha_n}_{\neq\alpha,\beta}\rangle &= 0 \\
a_\beta a^\dagger_\alpha| \underbrace{\alpha_1\alpha_2\dots\alpha_n}_{\neq\alpha,\beta}\rangle &= a_\beta|\alpha \underbrace{\alpha_1\alpha_2\dots\alpha_n}_{\neq\alpha,\beta}\rangle = 0
\end{aligned}
\tag{25}
$$

For all three cases we have

$$\{a^\dagger_\alpha, a_\beta\} = a^\dagger_\alpha a_\beta + a_\beta a^\dagger_\alpha = 0, \quad \alpha \neq \beta \tag{26}$$

Second quantization

We can summarize our findings in Eqs. (22) and (26) as

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

with $\delta_{\alpha\beta}$ is the Kroenecker δ-symbol.
The properties of the creation and annihilation operators can be summarized as (for fermions)

$$a^\dagger_\alpha|0\rangle \equiv |\alpha\rangle,$$

and

$$a^\dagger_\alpha|\alpha_1\dots\alpha_n\rangle_{\mathrm{AS}} \equiv |\alpha\alpha_1\dots\alpha_n\rangle_{\mathrm{AS}}.$$

from which follows

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

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

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

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.

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

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

Summing over all possible one-particle states we arrive at

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

The operator

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

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.

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

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

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. (32) 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. (35) we have expressed the action of the one-body operator of Eq. (31) 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. (35) results in

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

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. (38) 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 (46) 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.

Changing the summation indices α and β in (51) we obtain

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

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

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

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

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

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

Using the commutation relations we get

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

The vacuum expectation value of this product of operators becomes

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

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

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

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

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

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

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

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

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. (3) we have

$$\begin{aligned}
|\alpha_1\alpha_2\dots\alpha_{n-1}\alpha_n\rangle &= a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger \dots a_{\alpha_{n-1}}^\dagger a_{\alpha_n}^\dagger |0\rangle & (60)\\
|\alpha_1\alpha_2\dots\alpha_{n-1}\alpha_n\alpha_{n+1}\rangle &= a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger \dots a_{\alpha_{n-1}}^\dagger a_{\alpha_n}^\dagger a_{\alpha_{n+1}}^\dagger |0\rangle & (61)\\
|\alpha_1\alpha_2\dots\alpha_{n-1}\rangle &= a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger \dots a_{\alpha_{n-1}}^\dagger |0\rangle & (62)
\end{aligned}$$

Particle-hole formalism

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

$$|c\rangle \equiv |\alpha_1\alpha_2\dots\alpha_{n-1}\alpha_n\rangle = a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger \dots a_{\alpha_{n-1}}^\dagger a_{\alpha_n}^\dagger |0\rangle \quad (63)$$

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

$$\begin{aligned}
|\alpha_1\alpha_2\dots\alpha_{n-1}\alpha_n\alpha_{n+1}\rangle &= (-1)^n a_{\alpha_{n+1}}^\dagger |c\rangle \equiv (-1)^n |\alpha_{n+1}\rangle_c & (64)\\
|\alpha_1\alpha_2\dots\alpha_{n-1}\rangle &= (-1)^{n-1} a_{\alpha_n} |c\rangle \equiv (-1)^{n-1} |\alpha_{n-1}\rangle_c & (65)
\end{aligned}$$

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. (65)

$$a_\alpha |c\rangle \neq 0 \quad (66)$$

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

$$\begin{aligned}
b_\alpha |c\rangle &= 0 & (67)\\
\{b_\alpha^\dagger, b_\beta^\dagger\} = \{b_\alpha, b_\beta\} &= 0 \\
\{b_\alpha^\dagger, b_\beta\} &= \delta_{\alpha\beta} & (68)
\end{aligned}$$

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

$$b_\alpha^\dagger |c\rangle = \begin{cases} a_\alpha^\dagger |c\rangle = |\alpha\rangle, & \alpha > F \\ a_\alpha |c\rangle = |\alpha^{-1}\rangle, & \alpha \leq F \end{cases} \quad (70)$$

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

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

$$|\beta_1\beta_2\dots\beta_{n_p}\gamma_1^{-1}\gamma_2^{-1}\dots\gamma_{n_h}^{-1}\rangle \equiv \underbrace{b^\dagger_{\beta_1}b^\dagger_{\beta_2}\dots b^\dagger_{\beta_{n_p}}}_{>F}\,\underbrace{b^\dagger_{\gamma_1}b^\dagger_{\gamma_2}\dots b^\dagger_{\gamma_{n_h}}}_{\leq F}|c\rangle \tag{72}$$

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

$$\hat{N} = \sum_{\alpha} a^\dagger_\alpha a_\alpha = \sum_{\alpha>F} b^\dagger_\alpha b_\alpha + n_c - \sum_{\alpha\leq F} b^\dagger_\alpha b_\alpha \tag{73}$$

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

Particle-hole formalism

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

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

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 $i, j, k, \dots$ for hole states and $a, b, c, \dots$ 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

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

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

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

Particle-hole formalism

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

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

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

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

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

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

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

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

$$0=\left\{a_p^{\dagger},a_q\right\}=\{a_p,a_q\}=\left\{a_p^{\dagger},a_q^{\dagger}\right\}$$

$$|\Phi_0\rangle=|\alpha_1\dots\alpha_A\rangle,\quad \alpha_1,\dots,\alpha_A\leq\alpha_F$$

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 $i,j,\ldots\leq\alpha_F,\quad a,b,\ldots>\alpha_F,\quad p,q,\ldots-\text{any}$

$$a_i|\Phi_0\rangle=|\Phi_i\rangle,\quad a_a^{\dagger}|\Phi_0\rangle=|\Phi^a\rangle$$

and

$$a_i^{\dagger}|\Phi_0\rangle=0\quad a_a|\Phi_0\rangle=0$$

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

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

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 $\alpha_0,\alpha_2,\ldots,\alpha_{n-1}$ 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 $\alpha_0,\alpha_1,\ldots,\alpha_{15}$ 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_1
0	0	0	1	0	0	1	0	0	0	1	0	0	1	0

which translates into the decimal number

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

$$\dim(\mathcal{H}) = \begin{pmatrix} n \\ N \end{pmatrix}.$$

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 $N \leq n$ particles. The ordering among these states is important as it defines the order of the creation operators. We will write the determinant

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

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:

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

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

Exercises

Exercise 5

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 $\lambda = 1, 2, \dots, A$. The unitary transformation

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

brings us into the new basis. The new basis has quantum numbers $a = 1, 2, \dots, A$. 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 6

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

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

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

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

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

and

Exercises

Exercise 7

Show that the onebody part of the Hamiltonian

$$\hat{H}_0 = \sum_{pq}\langle p|\hat{h}_0|q\rangle a^\dagger_p a_q,$$

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

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

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

Exercises

Exercise 8

Show that the twobody part of the Hamiltonian

$$\hat{H}_I = \frac{1}{4}\sum_{pqrs}\langle pq|\hat{v}|rs\rangle a^\dagger_p a^\dagger_q a_s a_r,$$

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

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

Explain again the meaning of the various symbols.
This exercise is optional: Derive the normal-ordered form of the threebody part of the Hamiltonian.

$$\hat{H}_3 = \frac{1}{36}\sum_{\substack{pqr\\stu}}\langle pqr|\hat{v}_3|stu\rangle a^\dagger_p a^\dagger_q a^\dagger_r a_u a_t a_s,$$

Exercises

Exercise 9

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 $|\Phi_0\rangle$, $|\Phi_i^a\rangle$ 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

Exercises: Using sympy to compute matrix elements

Exercise 11

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
```

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, AntiSymmetricTenso

# 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, sim
from sympy.physics.secondquant import F, Fd, wicks, AntiSymmetricTenso
# 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_c
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, sim
from sympy.physics.secondquant import F, Fd, wicks, AntiSymmetricTenso
# 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_indi
print "Hamiltonian defined as:", latex(Hnormal)
```

which results in

$$f^q_p a^\dagger_q a_p + \frac{1}{4} v^{sr}_{qp} a^\dagger_s a^\dagger_r a_p a_q$$

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, sim
from sympy.physics.secondquant import F, Fd, wicks, AntiSymmetricTenso
# 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_indi
E0 = wicks(Hnormal,keep_only_fully_contracted=True)
Hnormal = Hnormal-E0
w = WildFunction('w')
Hnormal = collect(Hnormal, NO(w))
Hnormal = evaluate_deltas(Hnormal)
```

Exercises: Using sympy to compute matrix elements

We can now go back to exercise 11 and define the Hamiltonian and the second-quantized representation of a three-body Slater determinant.

```
from sympy import symbols, latex, WildFunction, collect, Rational, sim
from sympy.physics.secondquant import F, Fd, wicks, AntiSymmetricTenso
# 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_o
expression = evaluate_deltas(expression)
expression = simplify(expression)
print latex(expression)
```

resulting in nine terms (as expected),

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