# Summary FYS4480

October 19, 2018

- Slater determinanter
- Kreasjon og annihilasjonsoperatorer
- Antikommutator relasjonene
- Hamilton operatoren i 2. kvantisering
- Matriseelementer, antisymmetrisert
- Vakuumforventingsverdier
- Normal ordning
- Wicks teorem
- Generalisert Wicks teorem
- Normal ordning relativt til HF/Fermi vakuum
- Normal ordnet Hamilton operator (relativt til HF/Fermi vakuum)
- FCI/CI
- Hartree-Fock
- Coupled Cluster
- MPBT

The anticommutator of two operators is defined by

$$\{\hat{A}, \hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}. \tag{1}$$

The creation and annihilation operators satisfy the so-called "fundamental anticommutator" relations

$$\begin{aligned} \{a_p^\dagger, a_q^\dagger\} &= 0 && (2)\\ \{a_p, a_q\} &= 0 && (3)\\ \{a_p, a_q^\dagger\} &= \delta_{pq}. && (4)\\ & && (5) \end{aligned}$$

The matrix representation of a one-body operator, relative to a single particle basis $\{\phi_i\}_{i=1}$, is given by

$$\langle\phi_p|\hat{h}|\phi_q\rangle \equiv \int \phi_p^*(\mathbf{r})\hat{h}\phi_q(\mathbf{r})d\mathbf{r}. \tag{6}$$

Common notations are $\langle\phi_p|\hat{h}|\phi_q\rangle = \langle p|\hat{h}|q\rangle = h_q^p$. The second quantized form a one-body operator is given by

$$\hat{H}_0 = \sum_{pq}\langle p|\hat{h}|q\rangle a_p^\dagger a_q. \tag{7}$$

Likewise the matrix representation of a two-body operator, typically the coulomb interaction, is given by

$$\langle \phi_p \phi_q | \hat{v} | \phi_r \phi_s \rangle = \int \phi_p^*(\mathbf{r_1}) \phi_q^*(\mathbf{r_2}) \hat{v}(\mathbf{r}_1, \mathbf{r}_2) \phi_q(\mathbf{r_1}) \phi_s(\mathbf{r_2}) d\mathbf{r}_1 d\mathbf{r}_2. \tag{8}$$

It is common to write $\langle \phi_p \phi_q | \hat{v} | \phi_r \phi_s \rangle = \langle pq | \hat{v} | rs \rangle = v_{rs}^{pq}$. Furthermore, it is customary to introduce the *anti-symmetric* matrix element

$$\langle pq | \hat{v} | rs \rangle_{AS} \equiv \langle pq | \hat{v} | rs \rangle - \langle pq | \hat{v} | sr \rangle. \tag{9}$$

Here it should be noted that many sources drop the AS subscript, which can be a source of confusion. The second quantized form a two-body operator is given by

$$\hat{W} = \frac{1}{2} \sum_{pqrs} \langle pq | \hat{v} | rs \rangle a_p^\dagger a_q^\dagger a_s a_r \tag{10}$$

$$= \frac{1}{4} \sum_{pqrs} \langle pq | \hat{v} | rs \rangle_{AS} a_p^\dagger a_q^\dagger a_s a_r \tag{11}$$

Thus, the full Hamiltonian $\hat{H} = \hat{H}_0 + \hat{W}$, using anti-symmetric matrix elements is given by

$$\hat{H} = \sum_{pq} \langle p | \hat{h} | q \rangle a_p^\dagger a_q + \frac{1}{4} \sum_{pqrs} \langle pq | \hat{v} | rs \rangle_{AS} a_p^\dagger a_q^\dagger a_s a_r. \tag{12}$$

## Wicks theorem

A sequence of creation and annihilation operators is called an operator string. Generally an operator string of $n$ creation and annihilation operators are on the form

$$A_1 A_2 \cdots A_n, \quad A_i \in \{a_p, a_p^\dagger\} \tag{13}$$

For example

$$A_1 A_2 A_3 A_4 = a_p a_q^\dagger a_r a_s^\dagger,$$

where $A_1 = a_p, A_2 = a_q^\dagger, A_3 = a_r$ and $A_4 = a_s^\dagger$.

Furthermore we refer to the number

$$\langle - | A_1 A_2 \cdots A_n | - \rangle \tag{14}$$

as a vacuum expecatation value, where $A_1 A_2 \cdots A_n$ is an operator string.

The normal-ordered product form of an operator string $A_1 A_2 \cdots A_n$ is defined as a rearrangement,

$$\{A_1 A_2 \cdots A_n\} \equiv (-1)^{|\sigma|} A_{\sigma(1)} A_{\sigma(2)} \cdots A_{\sigma(n)}, \tag{15}$$

where $\sigma$ is a permutation such that all the creation operators in the operator string is to the left of all the annihilation operators, i.e.,

$$\{A_1 A_2 \cdots A_n\} \equiv (-1)^{|\sigma|} [\text{creation operators}] \cdot [\text{annihilation operators}]. \tag{16}$$

The permutation $\sigma$ is in general not be unique, since we may permute the creation and annihilation operators separately without affecting the total expression. For example,

$$\{a_p a_q^\dagger a_r^\dagger a_s\} = a_q^\dagger a_r^\dagger a_p a_s = -a_r^\dagger a_q^\dagger a_p a_s = a_r^\dagger a_q^\dagger a_s a_p = -a_q^\dagger a_r^\dagger a_s a_p \tag{17}$$

To find the permutation $\sigma$ that normal-orders an operator product, it is usually simplest to count the number f of anticommutations necessary to achieve the rearrangement, and set $(-1)^{|\sigma|} = (-1)^f$. Note that the string $A_1 \cdots A_n \neq \{A_1 \cdots A_n\}$ in general, since by reordering creation and annihilation operators we neglect the extra terms arising from the Kronecker delta in the anticommutator relation $\{a_p, a_q^\dagger\} = \delta_{pq}$.

A contraction between to arbitrary creation and annihilation operators $X$ and $Y$ is the number defined by

$$XY = \langle -|XY|-\rangle. \tag{18}$$

We list the possible contractions, relative to the vacuum state $|-\rangle$,

$$a_p^\dagger a_q^\dagger = \langle -|a_p^\dagger a_q^\dagger|-\rangle = 0 \tag{19}$$

$$a_p a_q = \langle -|a_p a_q|-\rangle = 0 \tag{20}$$

$$a_p^\dagger a_q = \langle -|a_p^\dagger a_q|-\rangle = 0 \tag{21}$$

$$a_p a_q^\dagger = \langle -|a_p a_q^\dagger|-\rangle = 0 \tag{22}$$

Wick's theorem states that every string of creation and annihilation operators can be written as a sum of normal-ordered products where we perform every possible contraction. Let $A_1 \cdots A_n$ be an operator string of creation and annihilation operators. Then,

$$A_1 A_2 \cdots A_n = \{A_1 A_2 \cdots A_n\} + \sum_{(1)} \{A_1 \cdots\cdots A_n\} + \sum_{(2)} \{A_1 \cdots\cdots\} + \cdots + \sum_{\lfloor \frac{n}{2} \rfloor} \underbrace{\{A_1 \cdots\cdots\cdots A_n\}}_{\lfloor \frac{n}{2} \rfloor \text{ contractions}}$$

The notation $\sum_{(m)}$ signifies that we sum over all combinations of $m$ contractions. When n is even, the last sum signifies that we sum over $n/2$ contractions, i.e., all operators are contracted. If n is odd, there is one uncontracted operator left in each term of the last sum.

Vacuum expecatation values simplify greatly using Wicks theorem. First note that for any string with at least one factor

$$\langle -|\{A_1 \cdots A_n\}|-\rangle = 0, \tag{23}$$

because in the normal-order product, the annihilation operators are to the right, and the creation operators are on the left. For odd $n$, Wicks theorem gives

$$\langle -|A_1 \cdots A_n|-\rangle = 0, \tag{24}$$

while for even $n$,

$$\langle -|A_1 \cdots A_n|-\rangle = \sum_{\lfloor \frac{n}{2} \rfloor} \underbrace{\{A_1 \cdots\cdots\cdots A_n\}}_{\text{all contracted}}. \tag{25}$$

A useful fact is that the sign of a fully contracted operator product is $(1)^k$, where $k$ is the number of contraction line crossings.