It is important to recall that the operation of contraction explicitly depends on the state (as it involves $\hat{A}_-$)

If all contractions are numbers, the average value becomes:

$$
\begin{aligned}
\langle\Phi|\hat{A}_1\hat{A}_2\hat{A}_3\ldots\hat{A}_n|\Phi\rangle = {} & \overline{\hat{A}_1}\,\langle\Phi|\hat{A}_2\hat{A}_3\ldots\hat{A}_n|\Phi\rangle + \overline{\hat{A}_1\hat{A}_2}\langle\Phi|\hat{A}_3\ldots\hat{A}_n|\Phi\rangle \\
& + c\,\overline{\hat{A}_1\hat{A}_3}\langle\Phi|\hat{A}_2\ldots\hat{A}_n|\Phi\rangle + \ldots + c^{n-2}\,\overline{\hat{A}_1\hat{A}_n}\langle\Phi|\hat{A}_2\hat{A}_3\ldots|\Phi\rangle,
\end{aligned}
$$

i.e., the average of a product of operators is expressed in terms of products of averages involving <u>less</u> operators. The condition that all contractions are numbers is only fulfilled for certain classes of states $|\Phi\rangle$

Such states are called **product states.**

> Many-body product states are such states in which all contractions of creation and annihilation operators are numbers.

By applying the above recurrence relation, one can formulate the **Wick's theorem:**

> If all the contractions of operators appearing in the product are numbers, then the average of the product becomes a linear combination of products of all possible contractions and self-contractions.

The coefficients appearing in this linear combination are various powers of *c*.

Let us introduce

$$\overbracket{\hat{A}\hat{D}_1\hat{D}_2\dots\hat{D}_k\hat{B}} \equiv c^k\,\overbracket{\hat{A}\hat{B}}\,\hat{D}_1\hat{D}_2\dots\hat{D}_k$$

Using this definition, the expression for the average value of a product, becomes

$$\begin{aligned}\langle\Phi|\hat{A}_1\hat{A}_2\hat{A}_3\dots\hat{A}_n|\Phi\rangle = {}& \overbracket{\hat{A}_1}\,\langle\Phi|\hat{A}_2\hat{A}_3\dots\hat{A}_n|\Phi\rangle + \langle\Phi|\overbracket{\hat{A}_1\hat{A}_2}\hat{A}_3\dots\hat{A}_n|\Phi\rangle \\ &+ \langle\Phi|\overbracket{\hat{A}_1\hat{A}_2\hat{A}_3}\dots\hat{A}_n|\Phi\rangle + \dots + \langle\Phi|\overbracket{\hat{A}_1\hat{A}_2\hat{A}_3\dots\hat{A}_n}|\Phi\rangle.\end{aligned}$$

The coefficient c^k is given by a number of permutations needed to bring the two operators next to each other. In order to calculate the average value of a product, we need to calculate all possible pairwise contractions. Note that for the product states;

$$\overbracket{\hat{A}\hat{B}} = \hat{A}_-\hat{B} - c\hat{B}\hat{A}_- = \langle\Phi|\hat{A}_-\hat{B} - c\hat{B}\hat{A}_-|\Phi\rangle = \langle\Phi|\hat{A}_-\hat{B}|\Phi\rangle$$

That is

$$\overbracket{\hat{A}\hat{B}} = \langle\Phi|\hat{A}\hat{B}|\Phi\rangle - \langle\Phi|\hat{A}|\Phi\rangle\langle\Phi|\hat{B}|\Phi\rangle$$

Deviation of a product average from the product of averages

In practice, we do not need the annihilating part A_-

Example: product of four operators:

$$
\begin{aligned}
\langle\Phi|\hat{A}\hat{B}\hat{C}\hat{D}|\Phi\rangle \quad = \quad & \hat{A}\hat{B}\hat{C}\hat{D} \quad + \quad \overset{c}{\hat{A}\hat{B}\hat{C}\hat{D}} \quad + \quad \overset{c^2}{\hat{A}\hat{B}\hat{C}\hat{D}} \\
+ \quad & \hat{A}\;\hat{B}\;\hat{C}\hat{D} \quad + \quad \hat{A}\;\hat{B}\;\hat{C}\;\hat{D}\;c \quad + \quad \hat{A}\;\hat{B}\hat{C}\;\hat{D} \\
+ \quad & \hat{A}\hat{B}\;\hat{C}\;\hat{D} \quad + \quad \hat{A}\;\hat{B}\;\hat{C}\;\hat{D}\;c \quad + \quad \hat{A}\;\hat{B}\;\hat{C}\;\hat{D}\;c^2 \\
+ \quad & \hat{A}\;\hat{B}\;\hat{C}\;\hat{D}\,.
\end{aligned}
$$

$$
\begin{aligned}
&\langle\Phi|\hat{A}\hat{B}\hat{C}\hat{D}|\Phi\rangle = \\
&\quad =\langle\Phi|\hat{A}\hat{B}|\Phi\rangle\langle\Phi|\hat{C}\hat{D}|\Phi\rangle + c\langle\Phi|\hat{A}\hat{C}|\Phi\rangle\langle\Phi|\hat{B}\hat{D}|\Phi\rangle + \langle\Phi|\hat{A}\hat{D}|\Phi\rangle\langle\Phi|\hat{B}\hat{C}|\Phi\rangle \\
&\quad -(1+c)\langle\Phi|\hat{A}|\Phi\rangle\langle\Phi|\hat{B}|\Phi\rangle\langle\Phi|\hat{C}|\Phi\rangle\langle\Phi|\hat{D}|\Phi\rangle.
\end{aligned}
$$

this term vanishes for Fermions!

Wick's theorem for Slater determinants

$$|\Phi\rangle = a^+_{\mu_1} \ldots a^+_{\mu_A} |0\rangle$$

$$a_{\mu_0} = 0 \qquad (\langle\Phi|a_\mu|\Phi\rangle = 0)$$

$$a_{\mu_-} \quad = \quad \begin{cases} 0 & \text{for} \quad \mu \in \{\mu_i\}, \\ a_\mu & \text{for} \quad \mu \notin \{\mu_i\} \end{cases}$$

$$a_{\mu_+} \quad = \quad \begin{cases} a_\mu & \text{for} \quad \mu \in \{\mu_i\}, \\ 0 & \text{for} \quad \mu \notin \{\mu_i\} \end{cases}$$

$$a^+_{\mu_0} = 0$$

$$a^+_{\mu_-} \quad = \quad \begin{cases} a^+_\mu & \text{for} \quad \mu \in \{\mu_i\}, \\ 0 & \text{for} \quad \mu \notin \{\mu_i\} \end{cases}$$

$$a^+_{\mu_+} \quad = \quad \begin{cases} 0 & \text{for} \quad \mu \in \{\mu_i\}, \\ a^+_\mu & \text{for} \quad \mu \notin \{\mu_i\} \end{cases}$$

Of course, in this case *c=-1.*

Let us now calculate simple contractions:

$$
\begin{aligned}
\overbracket{a_\mu^+ a_\nu} &= \sum_{i=1}^{A} \delta_{\mu\mu_i}\delta_{\nu\mu_i}, \\
\overbracket{a_\mu a_\nu^+} &= \sum_{i=A+1}^{M} \delta_{\mu\mu_i}\delta_{\nu\mu_i}, \\
\overbracket{a_\mu^+ a_\nu^+} &= \overbracket{a_\mu a_\nu} = 0, \\
\overbracket{a_\mu^+} = \overbracket{a_\mu} &= 0.
\end{aligned}
$$

What if Slated determinant is expressed in another basis?

$$|\Phi'\rangle = a'^{+}_{\mu_1} \dots a'^{+}_{\mu_A} |0\rangle$$

$$a'^{+}_{\mu} = \sum_{\nu} U_{\mu\nu} a^{+}_{\nu}$$

$$a_{\mu_0} = 0$$

$$\begin{aligned} a_{\mu_-} &= \sum_{\nu \notin \{\mu_i\}} U^T_{\mu\nu} a'_\nu = \sum_{i=A+1}^{M} \sum_{\nu} U^T_{\mu\nu_i} U^*_{\nu_i\nu} a_\nu, \\ a_{\mu_+} &= \sum_{\nu \in \{\mu_i\}} U^T_{\mu\nu} a'_\nu = \sum_{i=1}^{A} \sum_{\nu} U^T_{\mu\nu_i} U^*_{\nu_i\nu} a_\nu \end{aligned}$$

$$a^{+}_{\mu_0} = 0$$

$$\begin{aligned} a^{+}_{\mu_-} &= \sum_{\nu \in \{\mu_i\}} U^{+}_{\mu\nu} a'^{+}_\nu = \sum_{i=1}^{A} \sum_{\nu} U^{+}_{\mu\nu_i} U_{\nu_i\nu} a^{+}_\nu, \\ a^{+}_{\mu_+} &= \sum_{\nu \notin \{\mu_i\}} U^{+}_{\mu\nu} a'^{+}_\nu = \sum_{i=A+1}^{M} \sum_{\nu} U^{+}_{\mu\nu_i} U_{\nu_i\nu} a^{+}_\nu, \end{aligned}$$

$$
\begin{aligned}
\overbracket{a^{+}_{\mu} a_{\nu}} &= \sum_{i=1}^{A} U^{+}_{\mu\nu_i} U_{\nu_i \nu}; \\
\overbracket{a_{\mu} a^{+}_{\nu}} &= \sum_{i=A+1}^{M} U^{T}_{\mu\nu_i} U^{*}_{\nu_i \nu}; \\
\overbracket{a^{+}_{\mu} a^{+}_{\nu}} &= \overbracket{a_{\mu} a_{\nu}} = 0,
\end{aligned}
$$

… and all self-contractions vanish!