1 Normal Ordering

Normal ordering is introduced for the convenience of using Wick's theorem. The reference state for normal ordering and contractions here is the Fermi vacuum. The pseudo-creation and pseudo-annihilation operators are introduced for the sake of normal ordering:

$$\begin{aligned} \hat{b}_i^\dagger &= \hat{i} & \hat{b}_i &= \hat{i}^\dagger \\ \hat{b}_a^\dagger &= \hat{a}^\dagger & \hat{b}_a &= \hat{a} \end{aligned} \tag{1}$$

The normal ordering is satisfied if all pseudo-creation operators are left to all pseudo-annihilation operators, i.e.:

$$\{\hat{A}\hat{B}\hat{C}\dots\} = (-1)^\sigma \hat{b}_p^\dagger \hat{b}_q^\dagger \dots \hat{b}_u \hat{b}_v \tag{2}$$

This is defined such that:

$$\hat{b}_p|0\rangle = \hat{b}_p|ijk\dots\rangle = 0 \tag{3}$$

$$\langle 0|\hat{b}^\dagger = \langle ijk\dots|\hat{b}_p^\dagger = 0 \tag{4}$$

For example, a typical normal ordered string of operators looks like:

$$\hat{a}^\dagger \hat{b}^\dagger \hat{i}\hat{j}\hat{j}^\dagger \hat{i}^\dagger \hat{b}\hat{a} \tag{5}$$

Contractions w.r.t Fermi vacuum are defined as:

$$\overbracket{\hat{A}\hat{B}} = \hat{A}\hat{B} - \{\hat{A}\hat{B}\} \tag{6}$$

and this rearranges to gives the simplest case of Wick's theorem:

$$\hat{A}\hat{B} = \{\hat{A}\hat{B}\} + \{\overbracket{\hat{A}\hat{B}}\} \tag{7}$$

Note that: $\{\overbracket{\hat{A}\hat{B}}\} = \overbracket{\hat{A}\hat{B}}$, since:

$$\{\hat{A}\hat{B}\hat{C}\dots\hat{R}\dots\hat{S}\dots\hat{T}\dots\hat{U}\} = (-1)^{\hat{\sigma}}\overbracket{\hat{R}\hat{T}}\overbracket{\hat{S}\hat{U}}\{\hat{A}\hat{B}\hat{C}\dots\} \tag{8}$$

The anti-commutation relations are satisfied between annihilation operators and between creation operators. However, this is not true between annihilation and creation operators:

$$[\hat{p},\hat{q}]_+ = \hat{p}\hat{q} + \hat{q}\hat{p} = 0 \tag{9}$$

$$[\hat{p}^\dagger\hat{q}^\dagger]_+ = \hat{p}^\dagger\hat{q}^\dagger + \hat{q}^\dagger\hat{p}^\dagger = 0 \tag{10}$$

$$[\hat{p}^\dagger,\hat{q}]_+ = [\hat{q},\hat{p}^\dagger]_+ = \hat{p}^\dagger\hat{q} + \hat{q}\hat{p}^\dagger = \hat{\delta}_{pq} \tag{11}$$

This comes from the permutation relation of slater determinant:

$$|pqijk\dots\rangle = -|qpijk\dots\rangle \tag{12}$$

This means it's free to swap between annihilation operators and between creation annihilation operators, as long as the corresponding sign are assigned:

$$\hat{p}\hat{q} = -\hat{q}\hat{p} \tag{13}$$

$$\hat{p}^\dagger\hat{q}^\dagger = -\hat{q}^\dagger\hat{p}^\dagger \tag{14}$$

Also, we know that contractions between virtual and occupied space is 0 as $\delta_{occ,vir} = 0$. By this we know that only non-zero contractions are:

$$\overbracket{\hat{i}^\dagger\hat{j}} = \delta_{ij} \tag{15}$$

$$\overbracket{\hat{a}\hat{b}^\dagger} = \delta_{ab} \tag{16}$$

1.1 Normal Ordered Hamiltonian

Generally, the Hamiltonian could be written as:

$$\begin{aligned}\hat{H} &= \sum_{pq}\langle p|\hat{h}|q\rangle \hat{p}^\dagger\hat{q} + \frac{1}{4}\sum_{pqrs}\langle pq||rs\rangle \hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r} \\ &= \sum_{pq} h_{pq}\hat{p}^\dagger\hat{q} + \frac{1}{2}\sum_{pqrs}\langle pq|rs\rangle \hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r} \end{aligned} \tag{17}$$

Evaluating the product strings:

$$\begin{aligned}\hat{p}^\dagger\hat{q} =& \{\hat{p}^\dagger\hat{q}\} + \{\hat{p}^\dagger\hat{q}\} \\ =& \{\hat{p}^\dagger\hat{q}\} + \delta_{pq}\delta_{p\in \mathrm{occ}}\end{aligned} \tag{18}$$

$$\begin{aligned}\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r} =& \{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\} + \{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\} + \{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\} + \{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\} \\ &+ \{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\} + \{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\} + \{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\} \\ =& \{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\} + \delta_{pr}\delta_{qs}\delta_{p\in\mathrm{occ}}\delta_{q\in\mathrm{occ}} - \delta_{ps}\delta_{qr}\delta_{p\in\mathrm{occ}}\delta_{q\in\mathrm{occ}} \\ &- \delta_{ps}\delta_{p\in\mathrm{occ}}\{\hat{q}^\dagger\hat{r}\} + \delta_{pr}\delta_{p\in\mathrm{occ}}\{\hat{q}^\dagger\hat{s}\} + \delta_{qs}\delta_{q\in\mathrm{occ}}\{\hat{p}^\dagger\hat{s}\} \\ &- \delta_{qs}\delta_{q\in\mathrm{occ}}\{\hat{p}^\dagger\hat{s}\}\end{aligned} \tag{19}$$

Substitute these back into the expression of Hamiltonian, and the one-body part looks like:

$$\begin{aligned}\sum_{pq} h_{pq}\hat{p}^\dagger\hat{q} &= \sum_{pq} h_{pq}(\{\hat{p}^\dagger\hat{q}\} + \delta_{pq}\delta_{p\in\mathrm{occ}}) \\ &= \sum_{pq} h_{pq}\{\hat{p}^\dagger\hat{q}\} + \sum_i h_{ii}\end{aligned} \tag{20}$$

and the two-body part:

$$\begin{aligned}\frac{1}{4}\sum_{pqrs}\langle pq||rs\rangle\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r} =& \frac{1}{4}(\sum_{pqrs}\langle pq||rs\rangle\{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\} + \sum_{pqrs}\langle pq||rs\rangle\delta_{pr}\delta_{qs}\delta_{p\in\mathrm{occ}}\delta_{q\in\mathrm{occ}} \\ &- \sum_{pqrs}\langle pq||rs\rangle\delta_{ps}\delta_{qr}\delta_{p\in\mathrm{occ}}\delta_{q\in\mathrm{occ}} - \sum_{pqrs}\langle pq||rs\rangle\delta_{ps}\delta_{p\in\mathrm{occ}}\{\hat{q}^\dagger\hat{r}\} \\ &+ \sum_{pqrs}\langle pq||rs\rangle\delta_{pr}\delta_{p\in\mathrm{occ}}\{\hat{q}^\dagger\hat{s}\} + \sum_{pqrs}\langle pq||rs\rangle\delta_{qs}\delta_{q\in\mathrm{occ}}\{\hat{p}^\dagger\hat{r}\} \\ &- \sum_{pqrs}\langle pq||rs\rangle\delta_{qr}\delta_{q\in\mathrm{occ}}\{\hat{p}^\dagger\hat{s}\}) \\ =& \frac{1}{4}(\sum_{pqrs}\langle pq||rs\rangle\{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\} + \sum_{ij}\langle ij||ij\rangle - \sum_{ij}\langle ij||ji\rangle \\ &- \sum_{pri}\langle iq||ri\rangle\{\hat{q}^\dagger\hat{r}\} + \sum_{qsi}\langle iq||is\rangle\{\hat{q}^\dagger\hat{s}\} \\ &+ \sum_{pri}\langle pi||ri\rangle\{\hat{p}^\dagger\hat{r}\} - \sum_{psi}\langle pi||is\rangle\{\hat{p}^\dagger\hat{s}\}) \\ =& \frac{1}{4}\sum_{pqrs}\langle pq||rs\rangle + \frac{1}{2}\sum_{ij}\langle ij||ij\rangle + \sum_{pqi}\langle pi||qi\rangle\{\hat{p}^\dagger\hat{q}\}\end{aligned} \tag{21}$$

Combine and rearrange we obtain the Hamiltonian as:

$$\hat{H} = \sum_i h_{ii} + \frac{1}{2}\sum_{ij}\langle ij||ij\rangle + \sum_{pq} h_{pq}\{\hat{p}^\dagger\hat{q}\} + \sum_{pqi}\langle pi||qi\rangle\{\hat{p}^\dagger\hat{q}\} + \frac{1}{4}\sum_{pqrs}\langle pq||rs\rangle$$

$$= \langle\Phi_0|\hat{H}|\Phi_0\rangle + \sum_{pq} f_{pq}\{\hat{p}^\dagger\hat{q}\} + \frac{1}{4}\sum_{pqrs}\langle pq||rs\rangle\{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\} \tag{22}$$

since we have:

$$E_{\text{HF}} = \langle\Phi_0|\hat{H}|\Phi_0\rangle = \sum_i h_{ii} + \frac{1}{2}\sum_{ij}\langle ij||ij\rangle \tag{23}$$

$$f_{pq} = h_{pq} + \sum_i \langle pi||qi\rangle \tag{24}$$

where f_{pq} is Fock matrix element.
Now taking away the Hartree-Fock energy, we obtain the normal-ordered Hamiltonian w.r.t the Fermi vacuum:

$$\begin{aligned}\hat{H}_{\text{N}} =& \hat{H} - \langle\Phi_0|\hat{H}|\Phi_0\rangle \\ =& \sum_{pq} f_{pq}\{\hat{p}^\dagger\hat{q}\} + \frac{1}{4}\sum_{pqrs}\langle pq||rs\rangle\{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\} \\ =& \hat{F}_{\text{N}} + \hat{W}\end{aligned} \tag{25}$$

This $\hat{H}_{\text{N}}$ operator could be seen as the correlation operator.

1.2 Effective Hamiltonian

From BCH expansion, we can write the effective Hamiltonian as:

$$\begin{aligned}\hat{\mathcal{H}} =& e^{-\hat{T}}\hat{H}_{\text{N}}e^{\hat{T}} \\ =& \hat{H}_{\text{N}} + [\hat{H}_{\text{N}}, \hat{T}] + \frac{1}{2!}[[\hat{H}_{\text{N}}, \hat{T}], \hat{T}] + \frac{1}{3!}[[[\hat{H}_{\text{N}}, \hat{T}], \hat{T}], \hat{T}] \\ &+ \frac{1}{4!}[[[[\hat{H}_{\text{N}}, \hat{T}], \hat{T}], \hat{T}], \hat{T}] + \dots\end{aligned} \tag{26}$$

Note that the cluster operators $\hat{T}_m$ commute with each other, i.e.:

$$[\hat{T}_m, \hat{T}_n] = 0 \tag{27}$$

since:

$$\begin{aligned}[\hat{T}_m, \hat{T}_n] =& \sum_{ai}\sum_{bj}\hat{T}_m\hat{T}_n - \sum_{bj}\sum_{ai}\hat{T}_n\hat{T}m \\ =& \sum_{ai}\sum_{bj}\frac{1}{(m!)^2}t_{i\dots}^{a\dots}\{\hat{a}^\dagger\hat{i}\dots\}\frac{1}{(n!)^2}t_{j\dots}^{b\dots}\{\hat{b}^\dagger\hat{j}\dots\} \\ &- \sum_{bj}\sum_{ai}\frac{1}{(n!)^2}t_{j\dots}^{b\dots}\{\hat{b}^\dagger\hat{j}\dots\}\frac{1}{(m!)^2}t_{i\dots}^{a\dots}\{\hat{a}^\dagger\hat{i}\dots\} \\ =& \sum_{ai}\sum_{bj}\frac{1}{(m!)^2(n!)^2}t_{i\dots}^{a\dots}t_{j\dots}^{b\dots}\{\hat{a}^\dagger\hat{i}\dots\hat{b}^\dagger\hat{j}^\dagger\dots\} \\ &- \sum_{bj}\sum_{ai}\frac{1}{(m!)^2(n!)^2}t_{j\dots}^{b\dots}t_{i\dots}^{a\dots}\{\hat{b}^\dagger\hat{j}\dots\hat{a}^\dagger\hat{i}\dots\} \\ =& 0\end{aligned} \tag{28}$$

as $\{\hat{a}^\dagger\hat{i}\dots\}$ could never make non-zero contractions to its right. Therefore: $\hat{T}_m\hat{T}_n = \hat{T}_n\hat{T}_m$, while the same conclusion could not be drawn between $\hat{T}$ and $\hat{H}$.

Now consider about the infinite sum of commutators in the effective Hamiltonian. It could be reduced significantly using Wick's theorem and properties of operators. Let's give the result at first and then explain and rationalise it:

$$
\begin{aligned}
\hat{\mathcal{H}} =& e^{-\hat{T}}\hat{H}_{\mathrm{N}}e\hat{T} \\
=& \hat{H}_{\mathrm{N}} + \frac{1}{2!}[[\hat{H}_{\mathrm{N}},\hat{T}],\hat{T}] + \frac{1}{3!}[[[\hat{H}_{\mathrm{N}},\hat{T}],\hat{T}],\hat{T}] \\
&+ \frac{1}{4!}[[[[\hat{H}_{\mathrm{N}},\hat{T}],\hat{T}],\hat{T}],\hat{T}] \\
=& \hat{H}_{\mathrm{N}} + (\hat{H}_{\mathrm{N}}\hat{T})_{\mathrm{C}} + \frac{1}{2!}(\hat{H}_{\mathrm{N}}\hat{T}^2)_{\mathrm{C}} + \frac{1}{3!}(\hat{H}_{\mathrm{N}}\hat{T}^3)_{\mathrm{C}} + \frac{1}{4!}(\hat{H}_{\mathrm{N}}\hat{T}^4)_{\mathrm{C}} \\
=& (\hat{H}_{\mathrm{N}}e^{\hat{T}})_{\mathrm{C}}
\end{aligned}
\tag{29}
$$

This means that the effective Hamiltonian only contains terms in which all cluster operators on the right to $\hat{H}_{\mathrm{N}}$ contracts at least once with $\hat{H}_{\mathrm{N}}$. For example, in the expansion of $\hat{W}\hat{T}_2^2 = \{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\}\{\hat{a}^\dagger\hat{b}^\dagger\hat{j}\hat{i}\}\{\hat{c}^\dagger\hat{d}^\dagger\hat{l}\hat{k}\}$:
$\{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\hat{a}^\dagger\hat{b}^\dagger\hat{j}\hat{i}\hat{c}^\dagger\hat{d}^\dagger\hat{l}\hat{k}\}$ will remain, while $\{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\hat{a}^\dagger\hat{b}^\dagger\hat{j}\hat{i}\hat{c}^\dagger\hat{d}^\dagger\hat{l}\hat{k}\}$ will be cancelled.

As a direct result of this connected form combined with the fact that $\hat{H}_{\mathrm{N}}$ contain at most two-body operators (i.e. 4 creation/annihilation operators), the infinite sum of commutators in effective Hamiltonian terminates at four-fold. To rationalise the connected form of $\hat{\mathcal{H}}$, we start by stating some facts:
1. Terms in which all cluster operators are to the left of $\hat{H}_{\mathrm{N}}$, e.g. $\hat{T}\hat{T}\hat{T}\hat{H}_{\mathrm{N}}$, contains only an uncontracted term in the expansion. This is because cluster operator $\hat{T}$ could never make contractions to its right, as the only non-zero contractions are of the forms $\hat{a}\hat{b}^\dagger$ and $\hat{i}^\dagger\hat{j}$.
2. Uncontracted terms in the commutator expansion always cancel out. E.g. $[\hat{H}_{\mathrm{N}},\hat{T}]$ generates two uncontracted terms $\{\hat{p}^\dagger\hat{q}\ldots\}\{\hat{a}^\dagger\hat{i}\ldots\}$ and $-\{\hat{a}^\dagger\hat{i}\ldots\}\{\hat{p}^\dagger\hat{q}\ldots\}$ which cancel out to be zero. Generally this comes from the fact that number of creation/annihilation operators in any term of $\hat{\mathcal{H}}$ is even, hence the permutation $\begin{pmatrix}\{\hat{p}^\dagger\hat{q}\ldots\}\{\hat{a}^\dagger\hat{i}\ldots\} \\ \{\hat{a}^\dagger\hat{i}\ldots\}\{\hat{p}^\dagger\hat{q}\ldots\}\end{pmatrix}$ always have even parity.
3. Any terms which are not in the connected form, i.e. in which there are uncontracted cluster operator $\hat{T}$, will cancel out with each other. This comes from the fact that uncontracted $\hat{T}$ could be moved around in the normal ordering with even parity, and it is free to swap the dummy summation index. We will see this more clearly with an example:
In the expansion of the commutator $[[\hat{W},\hat{T}_1],\hat{T}_1]$:

$$
[[\hat{W},\hat{T}_1],\hat{T}_1] = \hat{W}\hat{T}_1^2 - 2\hat{T}_1\hat{W}\hat{T}_1 + \hat{T}_1^2\hat{W}
\tag{30}
$$

All the uncontracted terms vanish. $\hat{T}_1^2\hat{W}$ has no any other contribution. $\hat{T}_1\hat{W}\hat{T}_1$ term does not satisfy the connected form, hence all the contracted terms will be cancelled out with contracted terms in $\hat{W}\hat{T}_1^2$ which don't satisfy connected rule. More specifically:

$$
\begin{aligned}
\hat{T}_1\hat{W}\hat{T}_1 =& \sum_{ai}\sum_{pqrs}\sum_{bj}\frac{1}{4}t_i^a t_j^b\langle pq||rs\rangle\{\hat{a}^\dagger\hat{i}\}\{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\}\{\hat{b}^\dagger\hat{j}\} \\
=& \frac{1}{4}\sum_{ai}\sum_{pqrs}\sum_{bj}t_i^a t_j^b\langle pq||rs\rangle\Big(\{\hat{a}^\dagger\hat{i}\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\hat{b}^\dagger\hat{j}\} + \{\hat{a}^\dagger\hat{i}\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\hat{b}^\dagger\hat{j}\} \\
&+ \{\hat{a}^\dagger\hat{i}\hat{p}^\dagger\hat{q}\hat{s}\hat{r}\hat{b}^\dagger\hat{j}\} + \{\hat{a}^\dagger\hat{i}\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\hat{b}^\dagger\hat{j}\} + \{\hat{a}^\dagger\hat{i}\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\hat{b}^\dagger\hat{j}\} \\
&+ \{\hat{a}^\dagger\hat{i}\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\hat{b}^\dagger\hat{j}\} + \{\hat{a}^\dagger\hat{i}\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\hat{b}^\dagger\hat{j}\} + \{\hat{a}^\dagger\hat{i}\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\hat{b}^\dagger\hat{j}\}\Big)
\end{aligned}
\tag{31}
$$

If we expand $\hat{W}\hat{T}_1^2 = \sum\limits_{pqrs}\sum\limits_{ai}\sum\limits_{bj}\frac{1}{4}t_i^a t_j^b\langle pq||rs\rangle\{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\}\{\hat{a}^\dagger\hat{i}\}\{\hat{b}^\dagger\hat{j}\}$, we can find the terms in which there are uncontrated $\hat{T}_1$ operators to the right of $\hat{W}$, match exactly with the terms above:

$$\begin{aligned}
&\{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\hat{a}^\dagger\hat{i}\hat{b}^\dagger\hat{j}\} + \{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\hat{a}^\dagger\hat{i}\hat{b}^\dagger\hat{i}\} + \{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\hat{a}^\dagger\hat{i}\hat{b}^\dagger\hat{j}\} + \{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\hat{a}^\dagger\hat{i}\hat{b}^\dagger\hat{j}\}\\
&\{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\hat{a}^\dagger\hat{i}\hat{b}^\dagger\hat{j}\} + \{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\hat{a}^\dagger\hat{i}\hat{b}^\dagger\hat{j}\} + \{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\hat{a}^\dagger\hat{i}\hat{b}^\dagger\hat{j}\} + \{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\hat{a}^\dagger\hat{i}\hat{b}^\dagger\hat{j}\}\\
&\{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\hat{a}^\dagger\hat{i}\hat{b}^\dagger\hat{j}\} + \{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\hat{a}^\dagger\hat{i}\hat{b}^\dagger\hat{j}\} + \{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\hat{a}^\dagger\hat{i}\hat{b}^\dagger\hat{j}\} + \{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\hat{a}^\dagger\hat{i}\hat{b}^\dagger\hat{j}\}\\
&\{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\hat{a}^\dagger\hat{i}\hat{b}^\dagger\hat{j}\} + \{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\hat{a}^\dagger\hat{i}\hat{b}^\dagger\hat{j}\} + \{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\hat{a}^\dagger\hat{i}\hat{b}^\dagger\hat{i}\} + \{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\hat{a}^\dagger\hat{i}\hat{b}^\dagger\hat{j}\}
\end{aligned}\tag{32}$$

After we manipulate these sums with permutation and swapping some dummy indices, we can find that these are exactly twice of the terms in $\hat{T}_1\hat{W}\hat{T}_1$. Since $\hat{T}_1\hat{W}\hat{T}_1$ has a coefficient of -2 in the expansion of the commutator, they cancel each other out exactly.

Combining the rule of connected form and the fact that $\hat{H}_\mathrm{N}$ has at most 4 creation/annihilation operators, the BCH expansion of effective Hamiltonian terminates at four fold, as stated in eqn.29.

1.3 Vacuum Expectation Value

By design of normal ordering, the Fermi vacuum expectation value of any product string in normal ordering w.r.t. Fermin level is 0 unless the product string is fully contracted:

$$\langle 0|\{\hat{A}_1\hat{A}_2\ldots\}\{\hat{B}_1\hat{B}_2\ldots\}\{\hat{C}_1\hat{C}_2\ldots\}|0\rangle = \sum_{\substack{\text{fully}\\ \text{contracted}}}{}^{'}\ \{\hat{A}1\hat{A}_2\ldots\hat{B}_1\hat{B}_2\ldots\hat{C}_1\hat{C}_2\ldots\}\tag{33}$$