1 Energy Derivation

$$
\begin{aligned}
E_{\mathrm{CC}} =& \langle 0|\hat{\mathcal{H}}|0\rangle \\
=& \langle 0|\hat{H}_{\mathrm{N}} e^{\hat{T}}|0\rangle_{\mathrm{C}} \\
=& \langle 0|\hat{H}_{\mathrm{N}}(1+\hat{T}+\frac{1}{2!}\hat{T}^2+\frac{1}{3!}\hat{T}^3+\dots)|0\rangle_{\mathrm{C}}
\end{aligned} \tag{1}
$$

By Slater-Condon rule, since $\hat{H}_{\mathrm{N}}$ has at most two-body operators, the exponential series truncates to 2nd order:

$$
\begin{aligned}
E_{\mathrm{CC}} &= \langle 0|\hat{H}_{\mathrm{N}}(1+\hat{T}+\frac{1}{2}\hat{T}^2)|0\rangle_{\mathrm{C}} \\
&= \langle 0|\hat{H}_{\mathrm{N}}|0\rangle + \langle 0|\hat{H}_{\mathrm{N}}\hat{T}|0\rangle_{\mathrm{C}} + \frac{1}{2}\langle 0|\hat{H}_{\mathrm{N}}\hat{T}^2|0\rangle_{\mathrm{C}}
\end{aligned} \tag{2}
$$

The term $\hat{H}_{\mathrm{N}}$ is automatically zero by the definition of Fermi level. The linear term could be expanded as:

$$
\begin{aligned}
\langle 0|\hat{H}_{\mathrm{N}}\hat{T}|0\rangle =& \langle 0|(\hat{F}_{\mathrm{N}}+\hat{W})(\hat{T}_1+\hat{T}_2)|0\rangle_{\mathrm{C}} \\
=& \langle 0|\hat{F}_{\mathrm{N}}\hat{T}_1|0\rangle_{\mathrm{C}} + \langle 0|\hat{F}_{\mathrm{N}}\hat{T}_2|0\rangle_{\mathrm{C}} + \langle 0|\hat{W}\hat{T}_1|0\rangle_{\mathrm{C}} + \langle 0|\hat{W}\hat{T}_2|0\rangle_{\mathrm{C}}
\end{aligned} \tag{3}
$$

The second and third terms are zero by Slater-Condon rule. This can also be rationalised as these terms cannot fully contract. The one-body term expands as:

$$
\begin{aligned}
\langle 0|\hat{F}_{\mathrm{N}}\hat{T}_1|0\rangle_{\mathrm{C}} &= \sum_{pq}\sum_{ai} f_{pq} t_i^a \langle 0|\{\hat{p}^\dagger\hat{q}\}\{\hat{a}^\dagger\hat{i}\}|0\rangle \\
&= \sum_{pq}\sum_{ai} f_{pq} t_i^a \langle 0|\hat{p}^\dagger\hat{q}\hat{a}^\dagger\hat{i}|0\rangle \\
&= \sum_{pq}\sum_{ai} f_{pq} t_i^a \delta_{pi}\delta_{qa} \\
&= \sum_{ai} f_{ia} t_i^a
\end{aligned} \tag{4}
$$

and the two-body term expands in the same way:

$$
\begin{aligned}
\langle 0|\hat{W}\hat{T}_2|0\rangle_{\mathrm{C}} = \sum_{pqrs}\sum_{abij} \frac{1}{4}\langle pq||rs\rangle \frac{1}{4} t_{ij}^{ab} \Big(& \langle 0|\{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\hat{a}^\dagger\hat{b}^\dagger\hat{j}\hat{i}\}|0\rangle + \langle 0|\{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\hat{a}^\dagger\hat{b}^\dagger\hat{j}\hat{i}\}|0\rangle \\
& + \langle 0|\{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\hat{a}^\dagger\hat{b}^\dagger\hat{j}\hat{i}\}|0\rangle + \langle 0|\{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\hat{a}^\dagger\hat{b}^\dagger\hat{j}\hat{i}\}|0\rangle \Big) \\
=& \frac{1}{16}\sum_{pqrs}\sum_{abij}\langle pq||rs\rangle t_{ij}^{ab}(\delta_{pi}\delta_{qj}\delta_{sb}\delta_{ra} - \delta_{pi}\delta_{qj}\delta_{sa}\delta_{rb} - \delta_{pj}\delta_{qi}\delta_{sb}\delta_{ra} + \delta_{pj}\delta_{qi}\delta_{sa}\delta_{rb}) \\
=& \frac{1}{16}\sum_{abij} t_{ij}^{ab}(\langle ij||ab\rangle - \langle ij||ba\rangle - \langle ji||ab\rangle + \langle ji||ba\rangle) \\
=& \frac{1}{4}\sum_{abij} t_{ij}^{ab}\langle ij||ab\rangle
\end{aligned} \tag{5}
$$

Then let's look at the quadratic term in eqn(?):

$$
\langle 0|\hat{H}_{\mathrm{N}}\hat{T}^2|0\rangle_{\mathrm{C}} = \langle 0|(\hat{F}_{\mathrm{N}}+\hat{W})(\hat{T}_1^2+2\hat{T}_1\hat{T}_2+\hat{T}_2^2)|0\rangle_{\mathrm{C}}
$$

$$
\begin{aligned}
=&\langle 0|\hat{F}_{\mathrm{N}}\hat{T}_1^2|0\rangle_{\mathrm{C}} + 2\langle 0|\hat{F}_{\mathrm{N}}\hat{T}_1\hat{T}_2|0\rangle_{\mathrm{C}} + \langle 0|\hat{F}_{\mathrm{N}}\hat{T}_2^2|0\rangle_{\mathrm{C}} \\
&+ \langle 0|\hat{W}\hat{T}_1^2|0\rangle_{\mathrm{C}} + 2\langle 0|\hat{W}\hat{T}_1\hat{T}_2|0\rangle_{\mathrm{C}} + \langle 0|\hat{W}\hat{T}_2^2|0\rangle_{\mathrm{C}}
\end{aligned} \tag{6}
$$

Again, by Slater-Condon rule, or by counting excitation levels, only one term remains:

$$
\begin{aligned}
\langle 0|\hat{H}_{\mathrm{N}}\hat{T}^2|0\rangle_{\mathrm{C}} =&\langle 0|\hat{W}\hat{T}_1^2|0\rangle_{\mathrm{C}} \\
=&\sum_{pqrs}\sum_{ai}\sum_{bj}\frac{1}{4}\langle pq||rs\rangle t_i^a t_j^b \langle 0|\{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\}\{\hat{a}^\dagger\hat{i}\}\{\hat{b}^\dagger\hat{i}\}|0\rangle \\
=&\frac{1}{4}\sum_{pqrs}\sum_{abij}\langle pq||rs\rangle t_i^a t_j^b \Big(\langle 0|\{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\hat{a}^\dagger\hat{i}\hat{b}^\dagger\hat{j}\}|0\rangle + \langle 0|\{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\hat{a}^\dagger\hat{i}\hat{b}^\dagger\hat{j}\}|0\rangle \\
&+ \langle 0|\{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\hat{a}^\dagger\hat{i}\hat{b}^\dagger b\hat{j}\}|0\rangle + \langle 0|\{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\hat{a}^\dagger\hat{i}\hat{b}^\dagger\hat{j}\}|0\rangle\Big) \\
=&\frac{1}{4}\sum_{pqrs}\sum_{abij}\langle pq||rs\rangle t_i^a t_j^b (\delta_{pj}\delta_{qi}\delta_{sa}\delta_{rb} - \delta_{pj}\delta_{qi}\delta_{sb}\delta_{ra} + \delta_{pi}\delta_{qj}\delta_{sb}\delta_{ra} - \delta_{pi}\delta_{qj}\delta_{sa}\delta_{rb}) \\
=&\frac{1}{4}\sum_{abij} t_i^a t_j^b (\langle ji||ba\rangle - \langle ji||ab\rangle + \langle ij||ab\rangle - \langle ij||ba\rangle) \\
=&\sum_{abij} t_i^a t_j^b \langle ij||ab\rangle
\end{aligned} \tag{7}
$$

Therefore, the CCSD energy is obtained as:

$$
\begin{aligned}
E_{\mathrm{CCSD}} =&\langle 0|\hat{H}_{\mathrm{N}}\hat{T}|0\rangle_{\mathrm{C}} + \frac{1}{2}\langle 0|\hat{H}_{\mathrm{N}}\hat{T}^2|0\rangle_{\mathrm{C}} \\
=&\sum_{ai} f_{ia} t_i^a + \frac{1}{4}\sum_{ijab} t_{ij}^{ab}\langle ij||ab\rangle + \frac{1}{2}\sum_{ijab} t_i^a t_j^b \langle ij||ab\rangle
\end{aligned} \tag{8}
$$