Slides from FYS-KJM4480/9480 Lectures

Morten Hjorth-Jensen

Department of Physics and Center of Mathematics for Applications
University of Oslo, N-0316 Oslo, Norway

Week 48, November 25-29

Plans for week 48: coupled-cluster theory and summary of course

- Short repetition from last week
- How to write your own coupled-cluster theory code, pairing model example
- Coupled-cluster theory for singles and doubles excitations using a diagrammatic derivation
- Summary and discussion of final oral exam
- Suggested literature: Shavitt and Bartlett chapters 9 and 10

CCSD with twobody Hamiltonian

Truncating the cluster operator $\widehat{T}$ at the $n = 2$ level, defines CCSD approximation to the Coupled Cluster wavefunction. The coupled cluster wavefunction is now given by

$$|\Psi_{CC}\rangle = e^{\widehat{T}_1 + \widehat{T}_2}|\Phi_0\rangle$$

where

$$\hat{T}_1 = \sum_{ia} t_i^a a_a^\dagger a_i$$
$$\hat{T}_2 = \frac{1}{4}\sum_{ijab} t_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i.$$

CCSD with twobody Hamiltonian cont.

Normal ordered Hamiltonian

$$
\begin{aligned}
\widehat{H} &= \sum_{pq} f_q^p \left\{ a_p^\dagger a_q \right\} + \frac{1}{4} \sum_{pqrs} \langle pq||rs\rangle \left\{ a_p^\dagger a_q^\dagger a_s a_r \right\} \\
&\quad + \mathrm{E}_0 \\
&= \widehat{F}_N + \widehat{V}_N + \mathrm{E}_0 = \widehat{H}_N + \mathrm{E}_0
\end{aligned}
$$

where

$$
\begin{aligned}
f_q^p &= \langle p|\widehat{t}|q\rangle + \sum_i \langle pi|\widehat{v}|qi\rangle \\
\langle pq||rs\rangle &= \langle pq|\widehat{v}|rs\rangle \\
\mathrm{E}_0 &= \sum_i \langle i|\widehat{t}|i\rangle + \frac{1}{2} \sum_{ij} \langle ij|\widehat{v}|ij\rangle
\end{aligned}
$$

Diagram equations - Derivation

Contract $\widehat{H}_N$ with $\widehat{T}$ in all possible unique combinations that satisfy a given form. The diagram equation is the sum of all these diagrams.

- Contract one $\widehat{H}_N$ element with $0, 1$ or multiple $\widehat{T}$ elements.
- All $\widehat{T}$ elements must have atleast one contraction with $\widehat{H}_N$.
- No contractions between $\widehat{T}$ elements are allowed.
- A single $\widehat{T}$ element can contract with a single element of $\widehat{H}_N$ in different ways.

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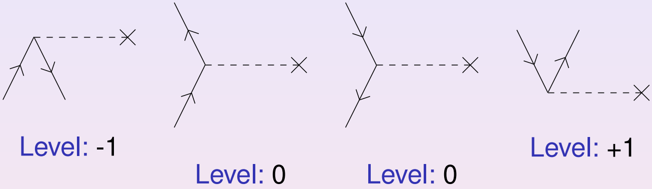
Diagram elements - Directed lines

Figure: Particle line

Figure: Hole line

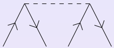
- Represents a contraction between second quantized operators.
- External lines are connected to one operator vertex and infinity.
- Internal lines are connected to operator vertices in both ends.

Diagram elements - Onebody Hamiltonian



- Horisontal dashed line segment with one vertex.
- Excitation level identify the number of particle/hole pairs created by the operator.

Diagram elements - Twobody Hamiltonian



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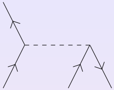

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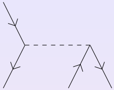

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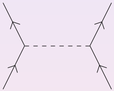

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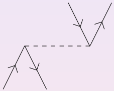

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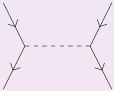

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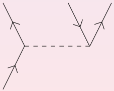

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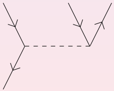

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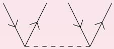
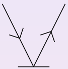


Level: +2

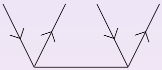
Diagram elements - Onebody cluster operator



Level: +1

- Horisontal line segment with one vertex.
- Excitation level of +1.

Diagram elements - Twobody cluster operator



Level: +2

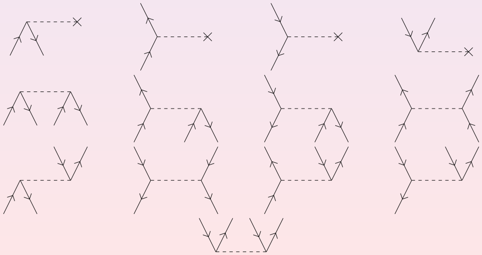
- Horisontal line segment with two vertices.
- Excitation level of +2.

CCSD energy equation - Derivation

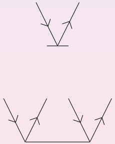
$$\mathrm{E}_{\mathrm{CCSD}} = \langle \Phi_0 | | \Phi_0 \rangle$$

- No external lines.
- Final excitation level: 0

Elements: $\widehat{H}_N$



Elements: $\widehat{T}$



CCSD energy equation

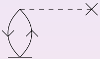
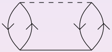
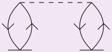
$E_{CCSD} =$  $+$  $+$ 

Diagram rules

- Label all lines.
- Sum over all internal indices.
- Extract matrix elements. ($f_{\text{in}}^{\text{out}}$, $\langle \text{lout}, \text{rout} || \text{lin}, \text{rin} \rangle$)
- Extract cluster amplitudes with indices in the order left to right. Incoming lines are subscripts, while outgoing lines are superscripts. ($t_{\text{in}}^{\text{out}}$, $t_{\text{lin},\text{rin}}^{\text{lout},\text{rout}}$)
- Calculate the phase: $(-1)^{\text{holelines}+\text{loops}}$
- Multiply by a factor of $\frac{1}{2}$ for each equivalent line and each ecuivalent vertex.

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CCSD energy equation

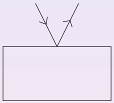
$$E_{CCSD} = f^i_a t^a_i + \frac{1}{4}\langle ij||ab\rangle t^{ab}_{ij} + \frac{1}{2}\langle ij||ab\rangle t^a_i t^b_j$$

Note the implicit sum over repeated indices.

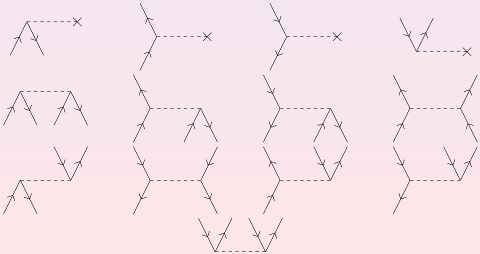
CCSD $\widehat{T}_1$ amplitude equation - Derivation

$$0 = \langle \Phi_i^a | | \Phi_0 \rangle$$

- One pair of particle/hole external lines.
- Final excitation level: +1



Elements: $\widehat{H}_N$



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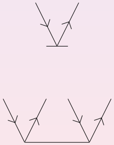
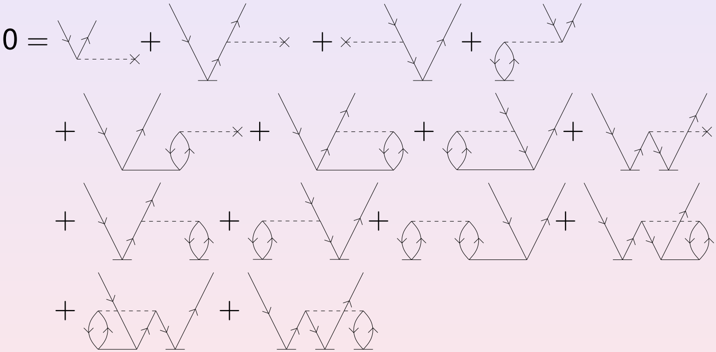


CCSD $\widehat{T}_1$ amplitude equation



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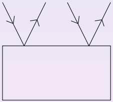
CCSD $\widehat{T}_1$ amplitude equation

$$0 = f_i^a + f_e^a t_i^e - f_i^m t_m^a + \langle ma||ei\rangle t_m^e + f_e^m t_{im}^{ae} + \frac{1}{2}\langle am||ef\rangle t_{im}^{ef} \quad -\frac{1}{2}\langle mn||e$$

CCSD $\widehat{T}_2$ amplitude equation - Derivation

$$0 = \langle \Phi_{ij}^{ab} | | \Phi_0 \rangle$$

- Two pairs of particle/hole external lines.
- Final excitation level: +2



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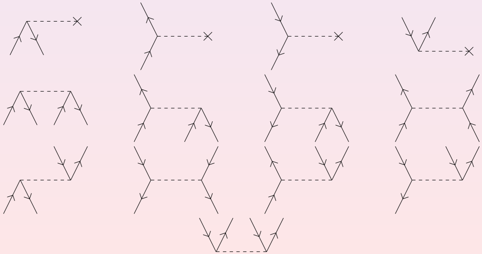
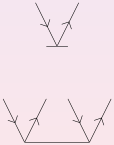


Elements: $\widehat{T}$



CCSD $\widehat{T}_2$ amplitude equation

$0 =$ 

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- Calculate the phase: $(-1)^{\text{holelines+loops}}$
- Multiply by a factor of $\frac{1}{2}$ for each equivalent line and each ecuivalent vertex.
- Antisymmetrize a pair of external particle/hole line that does not connect to the same operator.

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CCSD $\widehat{T}_2$ amplitude equation

$$0 = \langle ab||ij\rangle + P(ij)\langle ab||ej\rangle t_i^e - P(ab)\langle am||ij\rangle t_m^b + P(ab) f_e^b t_{ij}^{ae} - P(ij) f_i^m t_{mj}^{ab} \quad + \frac{1}{2}\langle ab||ef\rangle t_{ij}^{ef} +$$

The expansion

$$E_{CC} = \langle\Psi_0|\Big(\hat{H}_N + \left[\hat{H}_N, \hat{T}\right] + \frac{1}{2}\left[\left[\hat{H}_N, \hat{T}\right], \hat{T}\right] + \frac{1}{3!}\left[\left[\left[\hat{H}_N, \hat{T}\right], \hat{T}\right], \hat{T}\right] + \frac{1}{4!}\left[\left[\left[\left[\hat{H}_N, \hat{T}\right], \hat{T}\right], \hat{T}\right], \hat{T}\right] + +\Big)|\Psi_0\rangle$$

$$0 = \langle\Psi_{ij\dots}^{ab\dots}|\Big(\hat{H}_N + \left[\hat{H}_N, \hat{T}\right] + \frac{1}{2}\left[\left[\hat{H}_N, \hat{T}\right], \hat{T}\right] + \frac{1}{3!}\left[\left[\left[\hat{H}_N, \hat{T}\right], \hat{T}\right], \hat{T}\right] + \frac{1}{4!}\left[\left[\left[\left[\hat{H}_N, \hat{T}\right], \hat{T}\right], \hat{T}\right], \hat{T}\right] + +\Big)|\Psi_0\rangle$$

The CCSD energy equation revisited

The expanded CC energy equation involves an infinite sum over nested commutators

$$
\begin{aligned}
E_{CC} = \langle\Psi_0|\Big(\hat{H}_N + \left[\hat{H}_N, \hat{T}\right] + \frac{1}{2}\left[\left[\hat{H}_N, \hat{T}\right], \hat{T}\right] \\
+ \frac{1}{3!}\left[\left[\left[\hat{H}_N, \hat{T}\right], \hat{T}\right], \hat{T}\right] \\
+ \frac{1}{4!}\left[\left[\left[\left[\hat{H}_N, \hat{T}\right], \hat{T}\right], \hat{T}\right], \hat{T}\right] + + \Big)|\Psi_0\rangle,
\end{aligned}
$$

but fortunately we can show that it truncates naturally, depending on the Hamiltonian.

The first term is zero by construction.

$$
\langle\Psi_0|\widehat{H}_N|\Psi_0\rangle = 0
$$

The CCSD energy equation revisited.

The second term can be split up into different pieces

$$\langle\Psi_0|\left[\hat{H}_N, \hat{T}\right]|\Psi_0\rangle = \langle\Psi_0|\Big(\left[\hat{F}_N, \hat{T}_1\right] + \left[\hat{F}_N, \hat{T}_2\right] + \left[\hat{V}_N, \hat{T}_1\right] + \left[\hat{V}_N, \hat{T}_2\right]\Big)|\Psi_0\rangle$$

Since we need the explicit expressions for the commutators both in the next term and in the amplitude equations, we calculate them separately.

The expansion - $\left[\hat{F}_N, \hat{T}_1\right]$

$$
\begin{aligned}
\left[\hat{F}_N, \hat{T}_1\right] &= \sum_{pqia} \left(f_q^p a_p^\dagger a_q t_i^a a_a^\dagger a_i - t_i^a a_a^\dagger a_i f_q^p a_p^\dagger a_q \right) \\
&= \sum_{pqia} f_q^p t_i^a \left(a_p^\dagger a_q a_a^\dagger a_i - a_a^\dagger a_i a_p^\dagger a_q \right)
\end{aligned}
$$

$$
\left\{a_a^\dagger a_i\right\}\left\{a_p^\dagger a_q\right\} = a_a^\dagger a_i a_p^\dagger a_q = a_p^\dagger a_q a_a^\dagger a_i
$$

$$
\begin{aligned}
a_p^\dagger a_q a_a^\dagger a_i = {} & a_p^\dagger a_q a_a^\dagger a_i \\
& + a_p^\dagger a_q a_a^\dagger a_i + a_p^\dagger a_q a_a^\dagger a_i \\
& + a_p^\dagger a_q a_a^\dagger a_i \\
= {} & a_p^\dagger a_q a_a^\dagger a_i + \delta_{qa} a_p^\dagger a_i + \delta_{pi} a_q a_a^\dagger + \delta_{qa}\delta_{pi}
\end{aligned}
$$

The expansion - $\left[\hat{F}_N, \hat{T}_1\right]$

$$\begin{aligned}
\left[\hat{F}_N, \hat{T}_1\right] &= \sum_{pqia} \left(f^p_q a^\dagger_p a_q t^a_i a^\dagger_a a_i - t^a_i a^\dagger_a a_i f^p_q a^\dagger_p a_q \right) \\
&= \sum_{pqia} f^p_q t^a_i \left(a^\dagger_p a_q a^\dagger_a a_i - a^\dagger_a a_i a^\dagger_p a_q \right)
\end{aligned}$$

$$\left\{ a^\dagger_a a_i \right\} \left\{ a^\dagger_p a_q \right\} = a^\dagger_a a_i a^\dagger_p a_q = a^\dagger_p a_q a^\dagger_a a_i$$

$$\begin{aligned}
a^\dagger_p a_q a^\dagger_a a_i &= a^\dagger_p a_q a^\dagger_a a_i \\
&\quad + a^\dagger_p a_q a^\dagger_a a_i + a^\dagger_p a_q a^\dagger_a a_i \\
&\quad + a^\dagger_p a_q a^\dagger_a a_i \\
&= a^\dagger_p a_q a^\dagger_a a_i + \delta_{qa} a^\dagger_p a_i + \delta_{pi} a_q a^\dagger_a + \delta_{qa} \delta_{pi}
\end{aligned}$$

The expansion - $\left[\hat{F}_N, \hat{T}_1\right]$

$$
\begin{aligned}
\left[\hat{F}_N, \hat{T}_1\right] &= \sum_{pqia} \left(f_q^p a_p^\dagger a_q t_i^a a_a^\dagger a_i - t_i^a a_a^\dagger a_i f_q^p a_p^\dagger a_q \right) \\
&= \sum_{pqia} f_q^p t_i^a \left(a_p^\dagger a_q a_a^\dagger a_i - a_a^\dagger a_i a_p^\dagger a_q \right)
\end{aligned}
$$

$$
\left\{a_a^\dagger a_i\right\} \left\{a_p^\dagger a_q\right\} = a_a^\dagger a_i a_p^\dagger a_q = a_p^\dagger a_q a_a^\dagger a_i
$$

$$
\begin{aligned}
a_p^\dagger a_q a_a^\dagger a_i &= a_p^\dagger a_q a_a^\dagger a_i \\
&\quad + a_p^\dagger a_q a_a^\dagger a_i + a_p^\dagger a_q a_a^\dagger a_i \\
&\quad + a_p^\dagger a_q a_a^\dagger a_i \\
&= a_p^\dagger a_q a_a^\dagger a_i + \delta_{qa} a_p^\dagger a_i + \delta_{pi} a_q a_a^\dagger + \delta_{qa}\delta_{pi}
\end{aligned}
$$

The expansion - $\left[\hat{F}_N, \hat{T}_1\right]$

$$
\begin{aligned}
\left[\hat{F}_N, \hat{T}_1\right] &= \sum_{pqia} \left(f_q^p a_p^\dagger a_q t_i^a a_a^\dagger a_i - t_i^a a_a^\dagger a_i f_q^p a_p^\dagger a_q \right) \\
&= \sum_{pqia} f_q^p t_i^a \left(a_p^\dagger a_q a_a^\dagger a_i - a_a^\dagger a_i a_p^\dagger a_q \right)
\end{aligned}
$$

$$
\left\{ a_a^\dagger a_i \right\} \left\{ a_p^\dagger a_q \right\} = a_a^\dagger a_i a_p^\dagger a_q = a_p^\dagger a_q a_a^\dagger a_i
$$

$$
\begin{aligned}
a_p^\dagger a_q a_a^\dagger a_i &= a_p^\dagger a_q a_a^\dagger a_i \\
&\quad + a_p^\dagger a_q a_a^\dagger a_i + a_p^\dagger a_q a_a^\dagger a_i \\
&\quad + a_p^\dagger a_q a_a^\dagger a_i \\
&= a_p^\dagger a_q a_a^\dagger a_i + \delta_{qa} a_p^\dagger a_i + \delta_{pi} a_q a_a^\dagger + \delta_{qa} \delta_{pi}
\end{aligned}
$$

The expansion - $\left[\hat{F}_N, \hat{T}_1\right]$

$$\left[\hat{F}_N, \hat{T}_1\right] = \sum_{pqia} \left(f_q^p a_p^\dagger a_q t_i^a a_a^\dagger a_i - t_i^a a_a^\dagger a_i f_q^p a_p^\dagger a_q \right)$$

$$= \sum_{pqia} f_q^p t_i^a \left(a_p^\dagger a_q a_a^\dagger a_i - a_a^\dagger a_i a_p^\dagger a_q \right)$$

$$\left\{ a_a^\dagger a_i \right\} \left\{ a_p^\dagger a_q \right\} = a_a^\dagger a_i a_p^\dagger a_q = a_p^\dagger a_q a_a^\dagger a_i$$

$$a_p^\dagger a_q a_a^\dagger a_i = a_p^\dagger a_q a_a^\dagger a_i$$

$$+ a_p^\dagger a_q a_a^\dagger a_i + a_p^\dagger a_q a_a^\dagger a_i$$

$$+ a_p^\dagger a_q a_a^\dagger a_i$$

$$= a_p^\dagger a_q a_a^\dagger a_i + \delta_{qa} a_p^\dagger a_i + \delta_{pi} a_q a_a^\dagger + \delta_{qa}\delta_{pi}$$

The expansion - $\left[\hat{F}_N, \hat{T}_1\right]$

$$
\begin{aligned}
\left[\hat{F}_N, \hat{T}_1\right] &= \sum_{pqia} \left(f_q^p a_p^\dagger a_q t_i^a a_a^\dagger a_i - t_i^a a_a^\dagger a_i f_q^p a_p^\dagger a_q \right) \\
&= \sum_{pqia} f_q^p t_i^a \left(a_p^\dagger a_q a_a^\dagger a_i - a_a^\dagger a_i a_p^\dagger a_q \right)
\end{aligned}
$$

$$
\begin{aligned}
\left\{ a_a^\dagger a_i \right\} \left\{ a_p^\dagger a_q \right\} &= a_a^\dagger a_i a_p^\dagger a_q = a_p^\dagger a_q a_a^\dagger a_i \\
a_p^\dagger a_q a_a^\dagger a_i &= a_p^\dagger a_q a_a^\dagger a_i \\
&\quad + a_p^\dagger a_q a_a^\dagger a_i + a_p^\dagger a_q a_a^\dagger a_i \\
&\quad + a_p^\dagger a_q a_a^\dagger a_i \\
&= a_p^\dagger a_q a_a^\dagger a_i + \delta_{qa} a_p^\dagger a_i + \delta_{pi} a_q a_a^\dagger + \delta_{qa} \delta_{pi}
\end{aligned}
$$

The expansion - $\left[\hat{F}_N, \hat{T}_1\right]$

$$
\begin{aligned}
\left[\hat{F}_N, \hat{T}_1\right] &= \sum_{pqia} \left(f_q^p a_p^\dagger a_q t_i^a a_a^\dagger a_i - t_i^a a_a^\dagger a_i f_q^p a_p^\dagger a_q \right) \\
&= \sum_{pqia} f_q^p t_i^a \left(a_p^\dagger a_q a_a^\dagger a_i - a_a^\dagger a_i a_p^\dagger a_q \right)
\end{aligned}
$$

$$
\begin{aligned}
\left\{ a_a^\dagger a_i \right\} \left\{ a_p^\dagger a_q \right\} = a_a^\dagger a_i a_p^\dagger a_q &= a_p^\dagger a_q a_a^\dagger a_i \\
a_p^\dagger a_q a_a^\dagger a_i &= a_p^\dagger a_q a_a^\dagger a_i \\
&\quad + a_p^\dagger a_q a_a^\dagger a_i + a_p^\dagger a_q a_a^\dagger a_i \\
&\quad + a_p^\dagger a_q a_a^\dagger a_i \\
&= a_p^\dagger a_q a_a^\dagger a_i + \delta_{qa} a_p^\dagger a_i + \delta_{pi} a_q a_a^\dagger + \delta_{qa} \delta_{pi}
\end{aligned}
$$

The expansion - $\left[\hat{F}_N, \hat{T}_1\right]$

Wicks theorem gives us

$$\left\{a_p^\dagger a_q\right\}\left\{a_a^\dagger a_i\right\} - \left\{a_a^\dagger a_i\right\}\left\{a_p^\dagger a_q\right\} = \delta_{qa}\left\{a_p^\dagger a_i\right\} + \delta_{pi}\left\{a_q a_a^\dagger\right\} + \delta_{qa}\delta_{pi}.$$

Inserted into the original expression, we arrive at the explicit value of the commutator

$$\begin{aligned}\left[\hat{F}_N, \hat{T}_1\right] &= \sum_{pai} f_a^p t_i^a a_p^\dagger a_i + \sum_{qai} f_q^i t_i^a a_q a_a^\dagger + \sum_{ai} f_a^i t_i^a \\ &= \left(\widehat{F}_N \widehat{T}_1\right)_c.\end{aligned}$$

The subscript means that the product only includes terms where the operators are connected by atleast one shared index.

The expansion - $\left[\hat{F}_N, \hat{T}_2\right]$

$$
\begin{aligned}
\left[\hat{F}_N, \hat{T}_2\right] &= \left[\sum_{pq} f_q^p a_p^\dagger a_q, \frac{1}{4}\sum_{ijab} t_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i\right] \\
&= \frac{1}{4}\sum_{\substack{pq\\ijab}} \left[a_p^\dagger a_q, a_a^\dagger a_b^\dagger a_j a_i\right] \\
&= \frac{1}{4}\sum_{\substack{pq\\ijab}} f_q^p t_{ij}^{ab} \left(a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i - a_a^\dagger a_b^\dagger a_j a_i a_p^\dagger a_q\right)
\end{aligned}
$$

The expansion - $\left[\hat{F}_N, \hat{T}_2\right]$

$$
\begin{aligned}
a_a^\dagger a_b^\dagger a_j a_i a_p^\dagger a_q &= a_a^\dagger a_b^\dagger a_j a_i a_p^\dagger a_q \\
&= a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i
\end{aligned}
$$

$$
\begin{aligned}
a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i &= a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i + \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} + \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} \\
&\quad + \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} + \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} + \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} \\
&\quad + \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} + \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} + \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} \\
&= a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i - \delta_{pj} a_q a_a^\dagger a_b^\dagger a_i + \delta_{pi} a_q a_a^\dagger a_b^\dagger a_j \\
&\quad + \delta_{qa} a_p^\dagger a_b^\dagger a_j a_i - \delta_{qb} a_p^\dagger a_a^\dagger a_j a_i - \delta_{pj}\delta_{qa} a_b^\dagger a_i \\
&\quad + \delta_{pi}\delta_{qa} a_b^\dagger a_j + \delta_{pj}\delta_{qb} a_a^\dagger a_i - \delta_{pi}\delta_{qb} a_a^\dagger a_j
\end{aligned}
$$

The expansion - $\left[\hat{F}_N, \hat{T}_2\right]$

$$
\begin{aligned}
a_a^\dagger a_b^\dagger a_j a_i a_p^\dagger a_q &= a_a^\dagger a_b^\dagger a_j a_i a_p^\dagger a_q \\
&= a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i
\end{aligned}
$$

$$
\begin{aligned}
a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i = a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i &+ \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} + \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} \\
&+ \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} + \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} + \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} \\
&+ \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} + \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} + \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} \\
&= a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i - \delta_{pj} a_q a_a^\dagger a_b^\dagger a_i + \delta_{pi} a_q a_a^\dagger a_b^\dagger a_j \\
&+ \delta_{qa} a_p^\dagger a_b^\dagger a_j a_i - \delta_{qb} a_p^\dagger a_a^\dagger a_j a_i - \delta_{pj}\delta_{qa} a_b^\dagger a_i \\
&+ \delta_{pi}\delta_{qa} a_b^\dagger a_j + \delta_{pj}\delta_{qb} a_a^\dagger a_i - \delta_{pi}\delta_{qb} a_a^\dagger a_j
\end{aligned}
$$

The expansion - $\left[\hat{F}_N, \hat{T}_2\right]$

$$
\begin{aligned}
a_a^\dagger a_b^\dagger a_j a_i a_p^\dagger a_q &= a_a^\dagger a_b^\dagger a_j a_i a_p^\dagger a_q \\
&= a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i
\end{aligned}
$$

$$
\begin{aligned}
a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i &= a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i + \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} + \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} \\
&\quad + \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} + \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} + \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} \\
&\quad + \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} + \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} + \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} \\
&= a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i - \delta_{pj} a_q a_a^\dagger a_b^\dagger a_i + \delta_{pi} a_q a_a^\dagger a_b^\dagger a_j \\
&\quad + \delta_{qa} a_p^\dagger a_b^\dagger a_j a_i - \delta_{qb} a_p^\dagger a_a^\dagger a_j a_i - \delta_{pj}\delta_{qa} a_b^\dagger a_i \\
&\quad + \delta_{pi}\delta_{qa} a_b^\dagger a_j + \delta_{pj}\delta_{qb} a_a^\dagger a_i - \delta_{pi}\delta_{qb} a_a^\dagger a_j
\end{aligned}
$$

The expansion - $\left[\hat{F}_N, \hat{T}_2\right]$

$$
\begin{aligned}
a_a^\dagger a_b^\dagger a_j a_i a_p^\dagger a_q &= a_a^\dagger a_b^\dagger a_j a_i a_p^\dagger a_q \\
&= a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i
\end{aligned}
$$

$$
\begin{aligned}
a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i &= a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i + \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} + \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} \\
&+ \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} + \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} + \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} \\
&+ \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} + \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} + \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} \\
&= a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i - \delta_{pj} a_q a_a^\dagger a_b^\dagger a_i + \delta_{pi} a_q a_a^\dagger a_b^\dagger a_j \\
&+ \delta_{qa} a_p^\dagger a_b^\dagger a_j a_i - \delta_{qb} a_p^\dagger a_a^\dagger a_j a_i - \delta_{pj}\delta_{qa} a_b^\dagger a_i \\
&+ \delta_{pi}\delta_{qa} a_b^\dagger a_j + \delta_{pj}\delta_{qb} a_a^\dagger a_i - \delta_{pi}\delta_{qb} a_a^\dagger a_j
\end{aligned}
$$

The expansion - $\left[\hat{F}_N, \hat{T}_2\right]$

$$
\begin{aligned}
a_a^\dagger a_b^\dagger a_j a_i a_p^\dagger a_q &= a_a^\dagger a_b^\dagger a_j a_i a_p^\dagger a_q \\
&= a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \\
a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i &= a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i + \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} + \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} \\
&\quad + \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} + \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} + \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} \\
&\quad + \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} + \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} + \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} \\
&= a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i - \delta_{pj} a_q a_a^\dagger a_b^\dagger a_i + \delta_{pi} a_q a_a^\dagger a_b^\dagger a_j \\
&\quad + \delta_{qa} a_p^\dagger a_b^\dagger a_j a_i - \delta_{qb} a_p^\dagger a_a^\dagger a_j a_i - \delta_{pj}\delta_{qa} a_b^\dagger a_i \\
&\quad + \delta_{pi}\delta_{qa} a_b^\dagger a_j + \delta_{pj}\delta_{qb} a_a^\dagger a_i - \delta_{pi}\delta_{qb} a_a^\dagger a_j
\end{aligned}
$$

The expansion - $\left[\hat{F}_N, \hat{T}_2\right]$

$$
\begin{aligned}
a_a^\dagger a_b^\dagger a_j a_i a_p^\dagger a_q &= a_a^\dagger a_b^\dagger a_j a_i a_p^\dagger a_q \\
&= a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \\
a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i &= a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i + \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} + \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} \\
&\quad + \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} + \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} + \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} \\
&\quad + \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} + \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} + \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} \\
&= a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i - \delta_{pj} a_q a_a^\dagger a_b^\dagger a_i + \delta_{pi} a_q a_a^\dagger a_b^\dagger a_j \\
&\quad + \delta_{qa} a_p^\dagger a_b^\dagger a_j a_i - \delta_{qb} a_p^\dagger a_a^\dagger a_j a_i - \delta_{pj}\delta_{qa} a_b^\dagger a_i \\
&\quad + \delta_{pi}\delta_{qa} a_b^\dagger a_j + \delta_{pj}\delta_{qb} a_a^\dagger a_i - \delta_{pi}\delta_{qb} a_a^\dagger a_j
\end{aligned}
$$

The expansion - $\left[\hat{F}_N, \hat{T}_2\right]$

Wicks theorem gives us

$$\left(a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i - a_a^\dagger a_b^\dagger a_j a_i a_p^\dagger a_q\right) =$$
$$- \delta_{pj} a_q a_a^\dagger a_b^\dagger a_i + \delta_{pi} a_q a_a^\dagger a_b^\dagger a_j + \delta_{qa} a_p^\dagger a_b^\dagger a_j a_i$$
$$- \delta_{qb} a_p^\dagger a_a^\dagger a_j a_i - \delta_{pj}\delta_{qa} a_b^\dagger a_i + \delta_{pi}\delta_{qa} a_b^\dagger a_j + \delta_{pj}\delta_{qb} a_a^\dagger a_i$$
$$- \delta_{pi}\delta_{qb} a_a^\dagger a_j$$

Inserted into the original expression, we arrive at

$$\left[\hat{F}_N, \hat{T}_2\right] = \frac{1}{4} \sum_{\substack{pq \\ abij}} f_q^p t_{ij}^{ab} \Big(-\delta_{pj} a_q a_a^\dagger a_b^\dagger a_i + \delta_{pi} a_q a_a^\dagger a_b^\dagger a_j$$
$$+ \delta_{qa} a_p^\dagger a_b^\dagger a_j a_i - \delta_{qb} a_p^\dagger a_a^\dagger a_j a_i - \delta_{pj}\delta_{qa} a_b^\dagger a_i$$
$$+ \delta_{pi}\delta_{qa} a_b^\dagger a_j + \delta_{pj}\delta_{qb} a_a^\dagger a_i - \delta_{pi}\delta_{qb} a_a^\dagger a_j\Big).$$

The expansion - $\left[\hat{F}_N, \hat{T}_2\right]$

Wicks theorem gives us

$$
\begin{aligned}
&\left(a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i - a_a^\dagger a_b^\dagger a_j a_i a_p^\dagger a_q\right) = \\
&\quad - \delta_{pj} a_q a_a^\dagger a_b^\dagger a_i + \delta_{pi} a_q a_a^\dagger a_b^\dagger a_j + \delta_{qa} a_p^\dagger a_b^\dagger a_j a_i \\
&\quad - \delta_{qb} a_p^\dagger a_a^\dagger a_j a_i - \delta_{pj}\delta_{qa} a_b^\dagger a_i + \delta_{pi}\delta_{qa} a_b^\dagger a_j + \delta_{pj}\delta_{qb} a_a^\dagger a_i \\
&\quad - \delta_{pi}\delta_{qb} a_a^\dagger a_j
\end{aligned}
$$

Inserted into the original expression, we arrive at

$$
\begin{aligned}
\left[\widehat{F}_N, \widehat{T}_2\right] = \frac{1}{4} \sum_{\substack{pq \\ abij}} f_q^p t_{ij}^{ab} \Big(& -\delta_{pj} a_q a_a^\dagger a_b^\dagger a_i + \delta_{pi} a_q a_a^\dagger a_b^\dagger a_j \\
& + \delta_{qa} a_p^\dagger a_b^\dagger a_j a_i - \delta_{qb} a_p^\dagger a_a^\dagger a_j a_i - \delta_{pj}\delta_{qa} a_b^\dagger a_i \\
& + \delta_{pi}\delta_{qa} a_b^\dagger a_j + \delta_{pj}\delta_{qb} a_a^\dagger a_i - \delta_{pi}\delta_{qb} a_a^\dagger a_j \Big).
\end{aligned}
$$

The expansion - $\left[\hat{F}_N, \hat{T}_2\right]$

After renaming indices and changing the order of operators, we arrive at the explicit expression

$$\begin{aligned}\left[\widehat{F}_N, \widehat{T}_2\right] &= \frac{1}{2}\sum_{qijab} f_q^i t_{ij}^{ab} a_q a_a^\dagger a_b^\dagger a_j + \frac{1}{2}\sum_{pijab} f_a^p t_{ij}^{ab} a_p^\dagger a_b^\dagger a_j a_i \\ &\quad + \sum_{ijab} f_a^i t_{ij}^{ab} a_b^\dagger a_j \\ &= \left(\widehat{F}_N \widehat{T}_2\right)_c .\end{aligned}$$

The subscript implies that only the connected terms from the product contribute.

The expansion - $\frac{1}{2}\left[\left[\widehat{F}_N, \widehat{T}_1\right], \widehat{T}_1\right]$

$$\left[\hat{F}_N, \hat{T}_1\right] = \sum_{pai} f_a^p t_i^a a_p^\dagger a_i + \sum_{qai} f_q^i t_i^a a_q a_a^\dagger + \sum_{ai} f_a^i t_i^a$$

$$\begin{aligned}
\left[\left[\widehat{F}_N, \widehat{T}_1\right], \widehat{T}_1\right] &= \left[\sum_{pai} f_a^p t_i^a a_p^\dagger a_i + \sum_{qai} f_q^i t_i^a a_q a_a^\dagger + \sum_{ai} f_a^i t_i^a, \sum_{jb} t_j^b a_b^\dagger a_j\right. \\
&= \left[\sum_{pai} f_a^p t_i^a a_p^\dagger a_i + \sum_{qai} f_q^i t_i^a a_q a_a^\dagger, \sum_{jb} t_j^b a_b^\dagger a_j\right. \\
&= \sum_{pabij} f_a^p t_i^a t_j^b \left[a_p^\dagger a_i, a_b^\dagger a_j\right] + \sum_{qabij} f_q^i t_i^a t_j^b \left[a_q a_a^\dagger, a_b^\dagger a_j\right]
\end{aligned}$$

$$a_b^\dagger a_j a_p^\dagger a_i = a_b^\dagger a_j a_p^\dagger a_i = a_p^\dagger a_i a_b^\dagger a_j$$

$$a_b^\dagger a_j a_q a_a^\dagger = a_b^\dagger a_j a_q a_a^\dagger = a_q a_a^\dagger a_b^\dagger a_j$$

The expansion - $\frac{1}{2}\left[\left[\widehat{F}_N, \widehat{T}_1\right], \widehat{T}_1\right]$

$$\left[\hat{F}_N, \hat{T}_1\right] = \sum_{pai} f_a^p t_i^a a_p^\dagger a_i + \sum_{qai} f_q^i t_i^a a_q a_a^\dagger + \sum_{ai} f_a^i t_i^a$$

$$\begin{aligned}
\left[\left[\widehat{F}_N, \widehat{T}_1\right], \widehat{T}_1\right] &= \left[\sum_{pai} f_a^p t_i^a a_p^\dagger a_i + \sum_{qai} f_q^i t_i^a a_q a_a^\dagger + \sum_{ai} f_a^i t_i^a, \sum_{jb} t_j^b a_b^\dagger a_j\right] \\
&= \left[\sum_{pai} f_a^p t_i^a a_p^\dagger a_i + \sum_{qai} f_q^i t_i^a a_q a_a^\dagger, \sum_{jb} t_j^b a_b^\dagger a_j\right] \\
&= \sum_{pabij} f_a^p t_i^a t_j^b \left[a_p^\dagger a_i, a_b^\dagger a_j\right] + \sum_{qabij} f_q^i t_i^a t_j^b \left[a_q a_a^\dagger, a_b^\dagger a_j\right]
\end{aligned}$$

$$a_b^\dagger a_j a_p^\dagger a_i = a_b^\dagger a_j a_p^\dagger a_i = a_p^\dagger a_i a_b^\dagger a_j$$

$$a_b^\dagger a_j a_q a_a^\dagger = a_b^\dagger a_j a_q a_a^\dagger = a_q a_a^\dagger a_b^\dagger a_j$$

The expansion - $\frac{1}{2}\left[\left[\widehat{F}_N, \widehat{T}_1\right], \widehat{T}_1\right]$

$$\left[\hat{F}_N, \hat{T}_1\right] = \sum_{pai} f_a^p t_i^a a_p^\dagger a_i + \sum_{qai} f_q^i t_i^a a_q a_a^\dagger + \sum_{ai} f_a^i t_i^a$$

$$\begin{aligned}
\left[\left[\widehat{F}_N, \widehat{T}_1\right], \widehat{T}_1\right] &= \left[\sum_{pai} f_a^p t_i^a a_p^\dagger a_i + \sum_{qai} f_q^i t_i^a a_q a_a^\dagger + \sum_{ai} f_a^i t_i^a, \sum_{jb} t_j^b a_b^\dagger a_j\right. \\
&= \left[\sum_{pai} f_a^p t_i^a a_p^\dagger a_i + \sum_{qai} f_q^i t_i^a a_q a_a^\dagger, \sum_{jb} t_j^b a_b^\dagger a_j\right. \\
&= \sum_{pabij} f_a^p t_i^a t_j^b \left[a_p^\dagger a_i, a_b^\dagger a_j\right] + \sum_{qabij} f_q^i t_i^a t_j^b \left[a_q a_a^\dagger, a_b^\dagger a_j\right]
\end{aligned}$$

$$a_b^\dagger a_j a_p^\dagger a_i = a_b^\dagger a_j a_p^\dagger a_i = a_p^\dagger a_i a_b^\dagger a_j$$

$$a_b^\dagger a_j a_q a_a^\dagger = a_b^\dagger a_j a_q a_a^\dagger = a_q a_a^\dagger a_b^\dagger a_j$$

The expansion - $\frac{1}{2}\left[\left[\widehat{F}_N, \widehat{T}_1\right], \widehat{T}_1\right]$

$$\left[\hat{F}_N, \hat{T}_1\right] = \sum_{pai} f^p_a t^a_i a^\dagger_p a_i + \sum_{qai} f^i_q t^a_i a_q a^\dagger_a + \sum_{ai} f^i_a t^a_i$$

$$\begin{aligned}
\left[\left[\widehat{F}_N, \widehat{T}_1\right], \widehat{T}_1\right] &= \left[\sum_{pai} f^p_a t^a_i a^\dagger_p a_i + \sum_{qai} f^i_q t^a_i a_q a^\dagger_a + \sum_{ai} f^i_a t^a_i, \sum_{jb} t^b_j a^\dagger_b a_j\right. \\
&= \left[\sum_{pai} f^p_a t^a_i a^\dagger_p a_i + \sum_{qai} f^i_q t^a_i a_q a^\dagger_a, \sum_{jb} t^b_j a^\dagger_b a_j\right. \\
&= \sum_{pabij} f^p_a t^a_i t^b_j \left[a^\dagger_p a_i, a^\dagger_b a_j\right] + \sum_{qabij} f^i_q t^a_i t^b_j \left[a_q a^\dagger_a, a^\dagger_b a_j\right]
\end{aligned}$$

$$a^\dagger_b a_j a^\dagger_p a_i = a^\dagger_b a_j a^\dagger_p a_i = a^\dagger_p a_i a^\dagger_b a_j$$
$$a^\dagger_b a_j a_q a^\dagger_a = a^\dagger_b a_j a_q a^\dagger_a = a_q a^\dagger_a a^\dagger_b a_j$$

The expansion - $\left[\left[\widehat{F}_N, \widehat{T}_1\right], \widehat{T}_1\right]$

$$\begin{aligned}
\frac{1}{2}\left[\left[\widehat{F}_N, \widehat{T}_1\right], \widehat{T}_1\right] &= \frac{1}{2}\left(\sum_{pabij} f_a^p t_i^a t_j^b \delta_{pj} a_i a_b^\dagger - \sum_{qabij} f_q^i t_i^a t_j^b \delta_{qb} a_a^\dagger a_j\right) \\
&= -\frac{1}{2} 2 \sum_{abij} f_b^j t_j^a t_i^b a_a^\dagger a_i \\
&= -\sum_{abij} f_b^j t_j^a t_i^b a_a^\dagger a_i \\
&= \frac{1}{2}\left(\widehat{F}_N \widehat{T}_1^2\right)_c
\end{aligned}$$

The CCSD energy equation revisited

$$\langle\Phi_0|\left[\hat{V}_N,\hat{T}_1\right]|\Phi_0\rangle = \langle\Phi_0|\left[\frac{1}{4}\sum_{pqrs}\langle pq||rs\rangle a_p^\dagger a_q^\dagger a_s a_r, \sum_{ia} t_i^a a_a^\dagger a_i\right]|\Phi_0\rangle$$

$$= \frac{1}{4}\sum_{\substack{pqr\\sia}}\langle pq||rs\rangle t_i^a \langle\Phi_0|\left[a_p^\dagger a_q^\dagger a_s a_r, a_a^\dagger a_i\right]|\Phi_0\rangle$$

$$= 0$$

The CCSD energy equation revisited

$$
\begin{aligned}
\langle\Phi_0|\left[\hat{V}_N, \hat{T}_1\right]|\Phi_0\rangle &= \langle\Phi_0|\left[\frac{1}{4}\sum_{pqrs}\langle pq||rs\rangle a_p^\dagger a_q^\dagger a_s a_r, \sum_{ia} t_i^a a_a^\dagger a_i\right]|\Phi_0\rangle \\
&= \frac{1}{4}\sum_{\substack{pqr\\sia}}\langle pq||rs\rangle t_i^a \langle\Phi_0|\left[a_p^\dagger a_q^\dagger a_s a_r, a_a^\dagger a_i\right]|\Phi_0\rangle \\
&= 0
\end{aligned}
$$

The CCSD energy equation revisited

$$
\begin{aligned}
\langle\Phi_0|\left[\hat{V}_N, \hat{T}_1\right]|\Phi_0\rangle &= \langle\Phi_0|\left[\frac{1}{4}\sum_{pqrs}\langle pq||rs\rangle a_p^\dagger a_q^\dagger a_s a_r, \sum_{ia} t_i^a a_a^\dagger a_i\right]|\Phi_0\rangle \\
&= \frac{1}{4}\sum_{\substack{pqr\\sia}}\langle pq||rs\rangle t_i^a \langle\Phi_0|\left[a_p^\dagger a_q^\dagger a_s a_r, a_a^\dagger a_i\right]|\Phi_0\rangle \\
&= 0
\end{aligned}
$$

The CCSD energy equation revisited

$$\langle\Phi_0|\left[\hat{V}_N, \hat{T}_2\right]|\Phi_0\rangle =$$

$$\langle\Phi_0|\left[\frac{1}{4}\sum_{pqrs}\langle pq||rs\rangle a_p^\dagger a_q^\dagger a_s a_r, \frac{1}{4}\sum_{ijab} t_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i\right]|\Phi_0\rangle$$

$$= \frac{1}{16}\sum_{\substack{pqr\\sijab}}\langle pq||rs\rangle t_{ij}^{ab}\langle\Phi_0|\left[a_p^\dagger a_q^\dagger a_s a_r, a_a^\dagger a_b^\dagger a_j a_i\right]|\Phi_0\rangle$$

$$= \frac{1}{16}\sum_{\substack{pqr\\sijab}}\langle pq||rs\rangle t_{ij}^{ab}\langle\Phi_0|\Big(\left\{a_p^\dagger a_q^\dagger a_s a_r a_a^\dagger a_b^\dagger a_j a_i\right\} + \left\{a_p^\dagger a_q^\dagger a_s a_r a_a^\dagger a_b^\dagger a_j a_i\right\}$$

$$\left\{a_p^\dagger a_q^\dagger a_s a_r a_a^\dagger a_b^\dagger a_j a_i\right\} + \left\{a_p^\dagger a_q^\dagger a_s a_r a_a^\dagger a_b^\dagger a_j a_i\right\}\Big)|\Phi_0\rangle$$

$$= \frac{1}{4}\sum_{ijab}\langle ij||ab\rangle t_{ij}^{ab}$$

The CCSD energy equation revisited

$$\langle\Phi_0|\left[\hat{V}_N, \hat{T}_2\right]|\Phi_0\rangle =$$

$$\langle\Phi_0|\left[\frac{1}{4}\sum_{pqrs}\langle pq||rs\rangle a_p^\dagger a_q^\dagger a_s a_r, \frac{1}{4}\sum_{ijab} t_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i\right]|\Phi_0\rangle$$

$$= \frac{1}{16}\sum_{\substack{pqr\\sijab}}\langle pq||rs\rangle t_{ij}^{ab}\langle\Phi_0|\left[a_p^\dagger a_q^\dagger a_s a_r, a_a^\dagger a_b^\dagger a_j a_i\right]|\Phi_0\rangle$$

$$= \frac{1}{16}\sum_{\substack{pqr\\sijab}}\langle pq||rs\rangle t_{ij}^{ab}\langle\Phi_0|\Big(\left\{a_p^\dagger a_q^\dagger a_s a_r a_a^\dagger a_b^\dagger a_j a_i\right\} + \left\{a_p^\dagger a_q^\dagger a_s a_r a_a^\dagger a_b^\dagger a_j a_i\right\}$$

$$\left\{a_p^\dagger a_q^\dagger a_s a_r a_a^\dagger a_b^\dagger a_j a_i\right\} + \left\{a_p^\dagger a_q^\dagger a_s a_r a_a^\dagger a_b^\dagger a_j a_i\right\}\Big)|\Phi_0\rangle$$

$$= \frac{1}{4}\sum_{ijab}\langle ij||ab\rangle t_{ij}^{ab}$$

The CCSD energy equation revisited

$$\langle\Phi_0|\left[\hat{V}_N, \hat{T}_2\right]|\Phi_0\rangle =$$

$$\langle\Phi_0|\left[\frac{1}{4}\sum_{pqrs}\langle pq||rs\rangle a_p^\dagger a_q^\dagger a_s a_r, \frac{1}{4}\sum_{ijab} t_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i\right]|\Phi_0\rangle$$

$$= \frac{1}{16}\sum_{\substack{pqr\\sijab}}\langle pq||rs\rangle t_{ij}^{ab}\langle\Phi_0|\left[a_p^\dagger a_q^\dagger a_s a_r, a_a^\dagger a_b^\dagger a_j a_i\right]|\Phi_0\rangle$$

$$= \frac{1}{16}\sum_{\substack{pqr\\sijab}}\langle pq||rs\rangle t_{ij}^{ab}\langle\Phi_0|\Big(\left\{a_p^\dagger a_q^\dagger a_s a_r a_a^\dagger a_b^\dagger a_j a_i\right\} + \left\{a_p^\dagger a_q^\dagger a_s a_r a_a^\dagger a_b^\dagger a_j a_i\right\}$$

$$\left\{a_p^\dagger a_q^\dagger a_s a_r a_a^\dagger a_b^\dagger a_j a_i\right\} + \left\{a_p^\dagger a_q^\dagger a_s a_r a_a^\dagger a_b^\dagger a_j a_i\right\}\Big)|\Phi_0\rangle$$

$$= \frac{1}{4}\sum_{ijab}\langle ij||ab\rangle t_{ij}^{ab}$$

The CCSD energy equation revisited

$$
\begin{aligned}
&\langle\Phi_0|\left[\hat{V}_N, \hat{T}_2\right]|\Phi_0\rangle = \\
&\quad \langle\Phi_0|\left[\frac{1}{4}\sum_{pqrs}\langle pq||rs\rangle a_p^\dagger a_q^\dagger a_s a_r, \frac{1}{4}\sum_{ijab} t_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i\right]|\Phi_0\rangle \\
&= \frac{1}{16}\sum_{\substack{pqr\\sijab}}\langle pq||rs\rangle t_{ij}^{ab}\langle\Phi_0|\left[a_p^\dagger a_q^\dagger a_s a_r, a_a^\dagger a_b^\dagger a_j a_i\right]|\Phi_0\rangle \\
&= \frac{1}{16}\sum_{\substack{pqr\\sijab}}\langle pq||rs\rangle t_{ij}^{ab}\langle\Phi_0|\Big(\left\{a_p^\dagger a_q^\dagger a_s a_r a_a^\dagger a_b^\dagger a_j a_i\right\} + \left\{a_p^\dagger a_q^\dagger a_s a_r a_a^\dagger a_b^\dagger a_j a_i\right\} \\
&\quad \left\{a_p^\dagger a_q^\dagger a_s a_r a_a^\dagger a_b^\dagger a_j a_i\right\} + \left\{a_p^\dagger a_q^\dagger a_s a_r a_a^\dagger a_b^\dagger a_j a_i\right\}\Big)|\Phi_0\rangle \\
&= \frac{1}{4}\sum_{ijab}\langle ij||ab\rangle t_{ij}^{ab}
\end{aligned}
$$

The CCSD energy equation revisited

The CCSD energy get two contributions from $\left(\widehat{H}_N\widehat{T}\right)_c$

$$
\begin{aligned}
E_{CC} &\Leftarrow \langle\Phi_0|\left[\hat{H}_N, \hat{T}\right]|\Phi_0\rangle \\
&= \sum_{ia} f_a^i t_i^a + \frac{1}{4}\sum_{ijab}\langle ij||ab\rangle t_{ij}^{ab}
\end{aligned}
$$

The CCSD energy equation revisited

$$E_{CC} \Leftarrow \langle\Phi_0|\frac{1}{2}\left(\widehat{H}_N\widehat{T}^2\right)_c|\Phi_0\rangle$$

$$\langle\Phi_0|\frac{1}{2}\left(\widehat{V}_N\widehat{T}_1^2\right)_c|\Phi_0\rangle =$$

$$\frac{1}{8}\sum_{pqrs}\sum_{ijab}\langle pq||rs\rangle t_i^a t_j^b \langle\Phi_0|\left(a_p^\dagger a_q^\dagger a_s a_r a_a^\dagger a_i a_b^\dagger a_j\right)_c|\Phi_0\rangle$$

$$= \frac{1}{8}\sum_{pqrs}\sum_{ijab}\langle pq||rs\rangle t_i^a t_j^b \langle\Phi_0|$$

$$\left(\left\{a_p^\dagger a_q^\dagger a_s a_r a_a^\dagger a_i a_b^\dagger a_j\right\} + \left\{a_p^\dagger a_q^\dagger a_s a_r a_a^\dagger a_i a_b^\dagger a_j\right\} + \left\{a_p^\dagger a_q^\dagger a_s a_r a_a^\dagger a_i a_b^\dagger a_j\right\}\right.$$

$$\left. + \left\{a_p^\dagger a_q^\dagger a_s a_r a_a^\dagger a_i a_b^\dagger a_j\right\}\right)|\Phi_0\rangle$$

$$= \frac{1}{2}\sum_{ijab}\langle ij||ab\rangle t_i^a t_j^b$$

The CCSD energy equation revisited

$$E_{CC} \Leftarrow \langle\Phi_0|\frac{1}{2}\left(\widehat{H}_N\widehat{T}^2\right)_c|\Phi_0\rangle$$

$$\langle\Phi_0|\frac{1}{2}\left(\widehat{V}_N\widehat{T}_1^2\right)_c|\Phi_0\rangle =$$

$$\frac{1}{8}\sum_{pqrs}\sum_{ijab}\langle pq||rs\rangle t_i^a t_j^b\langle\Phi_0|\left(a_p^\dagger a_q^\dagger a_s a_r a_a^\dagger a_i a_b^\dagger a_j\right)_c|\Phi_0\rangle$$

$$= \frac{1}{8}\sum_{pqrs}\sum_{ijab}\langle pq||rs\rangle t_i^a t_j^b\langle\Phi_0|$$

$$\left(\left\{a_p^\dagger a_q^\dagger a_s a_r a_a^\dagger a_i a_b^\dagger a_j\right\} + \left\{a_p^\dagger a_q^\dagger a_s a_r a_a^\dagger a_i a_b^\dagger a_j\right\} + \left\{a_p^\dagger a_q^\dagger a_s a_r a_a^\dagger a_i a_b^\dagger a_j\right\}\right.$$

$$\left. + \left\{a_p^\dagger a_q^\dagger a_s a_r a_a^\dagger a_i a_b^\dagger a_j\right\}\right)|\Phi_0\rangle$$

$$= \frac{1}{2}\sum_{ijab}\langle ij||ab\rangle t_i^a t_j^b$$

The CCSD energy equation revisited

$$E_{CC} \Leftarrow \langle\Phi_0|\frac{1}{2}\left(\widehat{H}_N\widehat{T}^2\right)_c|\Phi_0\rangle$$

$$\langle\Phi_0|\frac{1}{2}\left(\widehat{V}_N\widehat{T}_1^2\right)_c|\Phi_0\rangle =$$

$$\frac{1}{8}\sum_{pqrs}\sum_{ijab}\langle pq||rs\rangle t_i^a t_j^b \langle\Phi_0|\left(a_p^\dagger a_q^\dagger a_s a_r a_a^\dagger a_i a_b^\dagger a_j\right)_c|\Phi_0\rangle$$

$$= \frac{1}{8}\sum_{pqrs}\sum_{ijab}\langle pq||rs\rangle t_i^a t_j^b \langle\Phi_0|$$

$$\left(\left\{a_p^\dagger a_q^\dagger a_s a_r a_a^\dagger a_i a_b^\dagger a_j\right\} + \left\{a_p^\dagger a_q^\dagger a_s a_r a_a^\dagger a_i a_b^\dagger a_j\right\} + \left\{a_p^\dagger a_q^\dagger a_s a_r a_a^\dagger a_i a_b^\dagger a_j\right\}\right.$$

$$\left. + \left\{a_p^\dagger a_q^\dagger a_s a_r a_a^\dagger a_i a_b^\dagger a_j\right\}\right)|\Phi_0\rangle$$

$$= \frac{1}{2}\sum_{ijab}\langle ij||ab\rangle t_i^a t_j^b$$

The CCSD energy equation revisited

$$E_{CC} \Leftarrow \langle \Phi_0 | \frac{1}{2} \left(\widehat{H}_N \widehat{T}^2 \right)_c | \Phi_0 \rangle$$

$$\langle \Phi_0 | \frac{1}{2} \left(\widehat{V}_N \widehat{T}_1^2 \right)_c | \Phi_0 \rangle =$$

$$\frac{1}{8} \sum_{pqrs} \sum_{ijab} \langle pq||rs \rangle t_i^a t_j^b \langle \Phi_0 | \left(a_p^\dagger a_q^\dagger a_s a_r a_a^\dagger a_i a_b^\dagger a_j \right)_c | \Phi_0 \rangle$$

$$= \frac{1}{8} \sum_{pqrs} \sum_{ijab} \langle pq||rs \rangle t_i^a t_j^b \langle \Phi_0 |$$

$$\left(\left\{ a_p^\dagger a_q^\dagger a_s a_r a_a^\dagger a_i a_b^\dagger a_j \right\} + \left\{ a_p^\dagger a_q^\dagger a_s a_r a_a^\dagger a_i a_b^\dagger a_j \right\} + \left\{ a_p^\dagger a_q^\dagger a_s a_r a_a^\dagger a_i a_b^\dagger a_j \right\} \right.$$

$$\left. + \left\{ a_p^\dagger a_q^\dagger a_s a_r a_a^\dagger a_i a_b^\dagger a_j \right\} \right) | \Phi_0 \rangle$$

$$= \frac{1}{2} \sum_{ijab} \langle ij||ab \rangle t_i^a t_j^b$$

The CCSD energy equation revisited

- No contractions possible between cluster operators.
- Cluster operators need to contract with free indices to the left.
- Disconnected parts automatically cancel in the commutator.
- Onebody operators can connect to maximum two cluster operators.
- Twobody operators can connect to maximum four cluster operators.
- Different terms in the expansion contributes to different equations.

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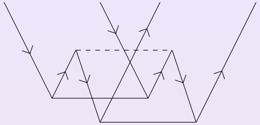
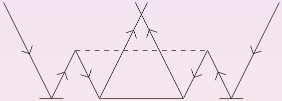
Factoring, motivation

Diagram (2.12)



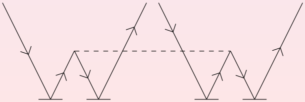
$$= \frac{1}{4}\langle mn||ef\rangle t_{ij}^{ef} t_{mn}^{ab}$$

Diagram (2.26)



$$= \frac{1}{4}P(ij)\langle mn||ef\rangle t_i^e t_{mn}^{ab} t_j^f$$

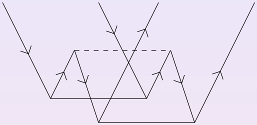
Diagram (2.31)



$$= \frac{1}{4}P(ij)P(ab)\langle mn||ef\rangle t_i^e t_m^a t_j^f t_n^b$$

Factoring, motivation

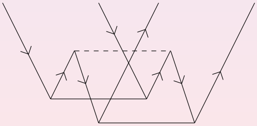
Diagram (2.12)



$$= \frac{1}{4}\langle mn||ef\rangle t_{ij}^{ef} t_{mn}^{ab}$$

Diagram cost: $n_p^4 n_h^4$

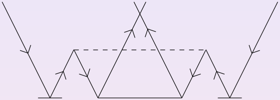
Diagram (2.13) - Factored



$$= \frac{1}{4}\langle mn||ef\rangle t_{ij}^{ef} t_{mn}^{ab} \quad = \frac{1}{4}\left(\langle mn||ef\rangle t_{ij}^{ef}\right) t_{mn}^{ab} = \frac{1}{4}X_{ij}^{m}$$

Factoring, motivation

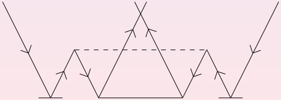
Diagram (2.26)



$$= \frac{1}{4} P(ij) \langle mn || ef \rangle t_i^e t_{mn}^{ab} t_j^f$$

Diagram cost: $n_p^4 n_h^4$

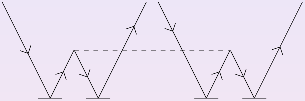
Diagram (2.26) - Factored



$$= \frac{1}{4} P(ij) \langle mn || ef \rangle t_i^e t_{mn}^{ab} t_j^f \quad = \frac{1}{4} P(ij) t_{mn}^{ab} t_i^e X_{ej}^{mn} = \frac{1}{4} P$$

Factoring, motivation

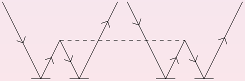
Diagram (2.31)



$$= \frac{1}{4} P(ij)P(ab)\langle mn||ef\rangle t_i^e t_m^a t_j^f t_n^b$$

Diagram cost: $n_p^4 n_h^4$

Diagram (2.31) - Factored

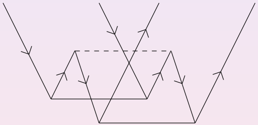


$$= \frac{1}{4} P(ij)P(ab)\langle mn||ef\rangle t_i^e t_m^a t_j^f t_n^b \quad = \frac{1}{4} P(ij)P(ab) t_m^a t_n^b t_i^e X_{ej}^{mn} =$$

Factoring, Classification

A diagram is classified by how many hole and particle lines between a $\hat{T}_i$ operator and the interaction ($T_i(p^{np}h^{nh})$).

Diagram (2.12) Classification

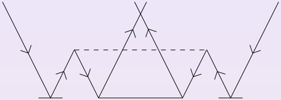


$$= \frac{1}{4}\langle mn||ef\rangle t_{ij}^{ef} t_{mn}^{ab}$$

This diagram is classified as $T_2(p^2) \times T_2(h^2)$

Factoring, Classification

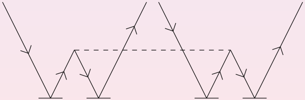
Diagram (2.26)



$$= \frac{1}{4} P(ij) \langle mn||ef \rangle t_i^e t_{mn}^{ab} t_j^f$$

This diagram is classified as $T_2(h^2) \times T_1(p) \times T_1(p)$

Diagram (2.31)



$$= \frac{1}{4} P(ij) P(ab) \langle mn||ef \rangle t_i^e t_m^a t_j^f t_n^b$$

This diagram is classified as $T_1(p) \times T_1(p) \times T_1(h) \times T_1(h)$

Factoring, Classification

Cost of making intermediates

Object	CPU cost	Memory cost
$T_2(h)$	$n_p^2 n_h$	n_p^2
$T_2(h^2)$	n_p^2	$n_h^{-2} n_p^2$
$T_2(p)$	$n_p n_h^2$	n_h^2
$T_2(ph)$	$n_p n_h$	1
$T_1(h)$	n_p	$n_h^{-1} n_p$
$T_2(ph^2)$	n_p	n_h^{-2}
$T_2(p^2)$	n_h^2	$n_p^{-2} n_h^2$
$T_1(p)$	n_h	$n_p^{-1} n_h$
$T_2(p^2 h)$	n_h	n_p^{-2}
$T_1(ph)$	1	$n_p^{-1} n_h^{-1}$

Factoring, Classification

Classification of $\hat{T}_1$ diagrams

Object	Expression id
$T_2(ph)$	5, 11
$T_1(h)$	3, 8, 10, 13, 14
$T_2(ph^2)$	7, 12
$T_1(p)$	2, 8, 9, 12, 14
$T_2(p^2h)$	6, 13
$T_1(ph)$	4, 9, 10, 11, 14

Factoring, Classification

Classification of $\hat{T}_2$ diagrams

Object	Expression id
$T_2(h)$	5, 15, 16, 23, 29
$T_2(h^2)$	7, 12, 22, 26
$T_2(p)$	4, 14, 17, 20, 30
$T_2(ph)$	8, 13, 13, 18, 21, 27
$T_1(h)$	3, 10, 10, 11, 17, 19, 21, 24, 25, 25, 27, 28, 28, 30, 31, 31
$T_2(ph^2)$	14
$T_2(p^2)$	6, 12, 19, 28
$T_1(p)$	2, 9, 9, 11, 16, 18, 22, 24, 24, 25, 26, 26, 27, 29, 31, 31
$T_2(p^2h)$	15
$T_1(ph)$	20, 23, 29, 30

Factoring, $T_2(h)$

Contribution to the $\hat{T}_2$ amplitude equation from $T_2(h)$

$$T_2(h) \Leftarrow -P(ij) f_i^m t_{mj}^{ab} - \frac{1}{2} P(ij) \langle mn || ef \rangle t_{mi}^{ef} t_{nj}^{ab} - P(ij) f_e^m t_i^e t_{mj}^{ab} \qquad -P(ij)\langle$$

Factoring, $T_2(h^2)$

Contribution to the $\hat{T}_2$ amplitude equation from $T_2(h^2)$

$$T_2(h^2) \Leftarrow \frac{1}{2}\langle mn||ij\rangle t_{mn}^{ab} + \frac{1}{4}\langle mn||ef\rangle t_{ij}^{ef} t_{mn}^{ab} + \frac{1}{2}P(ij)\langle mn||ej\rangle t_i^e t_{mn}^{ab} \quad +$$

Factored T_1 amplitude equations

$$0 = f_i^a + \langle ma||ei\rangle t_m^e + \frac{1}{2}\langle am||ef\rangle t_{im}^{ef} + t_i^e(\mathrm{I2a})_e^a - t_m^a(\bar{\mathrm{H}}3)_i^m \qquad + \frac{1}{2} t_{mn}^{ea}(\bar{\mathrm{H}}$$

Can be solved by

1. Matrix inversion for each iteration ($n_p^3 n_h^3$)
2. Extracting diagonal elements ($n_p^3 n_h^2$)

Factored T_1 amplitude equations

$$0 = f_i^a + \langle ma||ei\rangle t_m^e + \frac{1}{2}\langle am||ef\rangle t_{im}^{ef} + t_i^e(\mathrm{I2a})_e^a - t_m^a(\bar{\mathrm{H}}3)_i^m \qquad + \frac{1}{2} t_{mn}^{ea}(\bar{\mathrm{H}}$$

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Factored T_1 amplitude equations

Define

$$D_i^a = (\bar{\mathrm{H}}3)_i^i - (\mathrm{I2a})_a^a,$$

and we get the T_1 amplitude equations

$$D_i^a t_i^a = f_i^a + \langle ma||ei\rangle t_m^e + (1-\delta_{ea}) t_i^e (\mathrm{I2a})_e^a$$
$$- (1-\delta_{mi}) t_m^a (\bar{\mathrm{H}}3)_i^m + \frac{1}{2}\langle am||ef\rangle t_{im}^{ef} \qquad + \frac{1}{2} t_{mn}^{ea} (\bar{\mathrm{H}}7)_{ie}^{mn} + t_{im}^{ae} (\bar{\mathrm{H}}1$$

Factored T_2 amplitude equations

$$
\begin{aligned}
0 = \langle ab||ij\rangle + \frac{1}{2}\langle ab||ef\rangle t_{ij}^{ef} - P(ij)t_{im}^{ab}(\bar{\mathrm{H}}3)_j^m + \frac{1}{2}t_{mn}^{ab}(\bar{\mathrm{H}}9)_{ij}^{mn} \\
+ P(ab)t_{ij}^{ae}(\bar{\mathrm{H}}2)_e^b + P(ij)P(ab)t_{im}^{ae}(\mathrm{I}10\mathrm{c})_{ej}^{mb} - P(ab)t_m^a(\mathrm{I}12\mathrm{a})_{ij}^{mb} \\
+ P(ij)t_i^e(\mathrm{I}11a)_{ej}^{ab}
\end{aligned}
$$

Can be solved by

1. Matrix inversion for each iteration ($n_p^6 n_h^6$)
2. Extracting diagonal elements ($n_p^4 n_h^2$)

Factored T_2 amplitude equations

Similarily we define

$$D_{ij}^{ab} = (\bar{\mathrm{H}}3)_i^i + (\bar{\mathrm{H}}3)_j^j - (\bar{\mathrm{H}}2)_a^a - (\bar{\mathrm{H}}2)_b^b$$

and get the T_2 amplitude equations

$$\begin{aligned} D_{ij}^{ab} t_{ij}^{ab} = \langle ab||ij\rangle + \frac{1}{2}\langle ab||ef\rangle t_{ij}^{ef} - P(ij)(1-\delta_{jm}) t_{im}^{ab} (\bar{\mathrm{H}}3)_j^m \\ + \frac{1}{2} t_{mn}^{ab} (\bar{\mathrm{H}}9)_{ij}^{mn} + P(ab)(1-\delta_{be}) t_{ij}^{ae} (\bar{\mathrm{H}}2)_e^b \\ + P(ij)P(ab) t_{im}^{ae} (\mathrm{I10c})_{ej}^{mb} - P(ab) t_m^a (\mathrm{I12a})_{ij}^{mb} \\ + P(ij) t_i^e (\mathrm{I11}a)_{ej}^{ab} \end{aligned}$$

Coupled Cluster algorithm

7.7cm Setup modelspace

Calculate f and v amplitudes

$t_i^a \leftarrow 0;\ t_{ij}^{ab} \leftarrow 0$

$E \leftarrow 1;\ E_{old} \leftarrow 0$

$E_{ref} \leftarrow \sum_i \langle i|\widehat{t}|i\rangle + \frac{1}{2}\sum_{ij}\langle ij|\widehat{v}|ij\rangle$

while not converged ($E - E_{old} > \epsilon$)

Calculate intermediates

$t_i^a \leftarrow$ calculated value

$t_{ij}^{ab} \leftarrow$ calculated value

$E_{old} \leftarrow E$

$E \leftarrow f_a^i t_i^a + \frac{1}{4}\langle ij||ab\rangle t_{ij}^{ab} + \frac{1}{2}\langle ij||ab\rangle t_i^a t_j^b$

end while

$E_{GS} \leftarrow E_{ref} + E$

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