Week 48: Coupled cluster theory and summary of course

Morten Hjorth-Jensen[1]

Department of Physics and Center for Computing in Science Education, University of Oslo, Norway[1]

November 25-29, 2024

Week 48, November 25-29, 2024

1. Thursday:
   1.1 Short repetition from last week
   1.2 How to write your own coupled-cluster theory code, pairing model example
   1.3 Coupled cluster theory, singles and doubles excitations, diagrammatic expansion
   1.4 Video of lecture at https://youtu.be/wVbJ82zpHsU
   1.5 Whiteboard notes at https://github.com/ManyBodyPhysics/FYS4480/blob/master/doc/HandwrittenNotes/2024/NotesNovember28.pdf
2. Friday:
   2.1 Coupled cluster theory for singles and doubles excitations using a diagrammatic derivation
   2.2 Summary of course and discussion of final oral exam
3. Lecture material: Lecture notes and Shavitt and Bartlett chapters 9 and 10. See also slides at https://github.com/ManyBodyPhysics/FYS4480/blob/master/doc/pub/week48/pdf/cc.pdf

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

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

where (often used notations, see also Shavitt and Bartlett chapters 3-4)

$$
f_q^p = \langle p|\widehat{h}_0|q\rangle + \sum_i \langle pi|\widehat{v}|qi\rangle
$$

$$
\langle pq||rs\rangle = \langle pq|\widehat{v}|rs\rangle
$$

$$
\mathrm{E}_0 = \sum_i \langle i|\widehat{h}_0|i\rangle + \frac{1}{2} \sum_{ij} \langle ij|\widehat{v}|ij\rangle
$$

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.

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.

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.

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.

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.

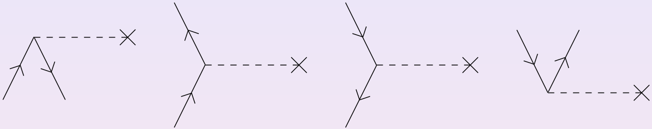
Diagram elements - Directed lines

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.

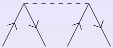
Diagram elements - Onebody Hamiltonian



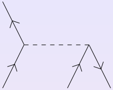
Level: -1 Level: 0 Level: 0 Level: +1

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

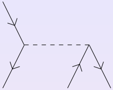
Diagram elements - Twobody Hamiltonian



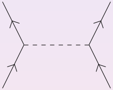
Level: -2



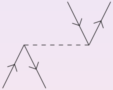
Level: -1



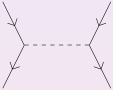
Level: -1



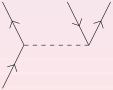
Level: 0



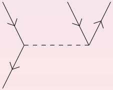
Level: 0



Level: 0



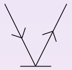
Level: +1



Level: +1

Level: +2

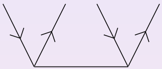
Diagram elements - Onebody cluster operator



Level: +1

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

Diagram elements - Twobody cluster operator



Level: +2

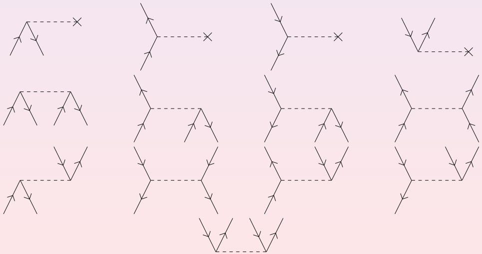
- Horisontal line segment with two vertices.
- Excitation level of +2.

CCSD energy equation - Derivation

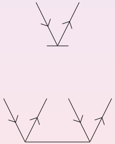
$$\mathrm{E}_{\mathrm{CCSD}} = \langle \Phi_0 | \quad | \Phi_0 \rangle$$

- No external lines.
- Final excitation level: 0

Elements: $\widehat{H}_N$



Elements: $\widehat{T}$



CCSD energy equation

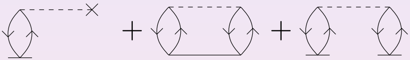
$E_{CCSD} =$ 

Diagram rules

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

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.

Diagram rules

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

Diagram rules

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

Diagram rules

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

Diagram rules

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

CCSD energy equation

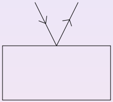
$$E_{CCSD} = f_a^i t_i^a + \frac{1}{4}\langle ij||ab\rangle t_{ij}^{ab} + \frac{1}{2}\langle ij||ab\rangle t_i^a t_j^b$$

Note the implicit sum over repeated indices.

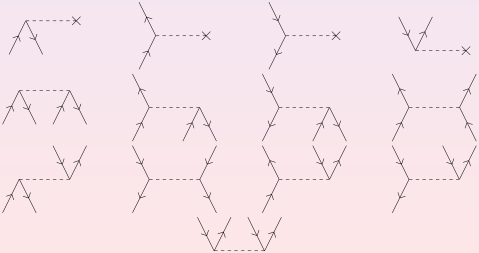
CCSD $\widehat{T}_1$ amplitude equation - Derivation

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

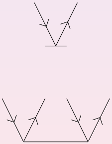
- One pair of particle/hole external lines.
- Final excitation level: +1



Elements: $\widehat{H}_N$



Elements: $\widehat{T}$



CCSD $\widehat{T}_1$ amplitude equation

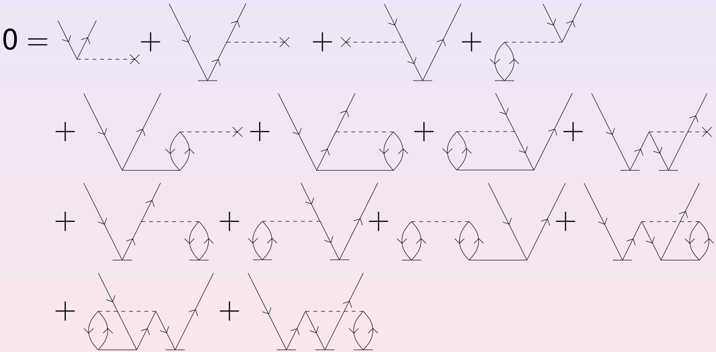


Diagram rules

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

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. ($t_{\text{in}}^{\text{out}}$, $t_{\text{lin,rin}}^{\text{lout,rout}}$)
- Calculate the phase: $(-1)^{\text{holelines}+\text{loops}}$
- Multiply by a factor of $\frac{1}{2}$ for each equivalent line and each ecuivalent vertex.

Diagram rules

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

Diagram rules

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

Diagram rules

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

Diagram rules

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

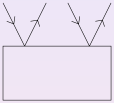
CCSD $\widehat{T}_1$ amplitude equation

$$
\begin{aligned}
0 = {} & f_i^a + f_e^a t_i^e - f_i^m t_m^a + \langle ma||ei\rangle t_m^e + f_e^m t_{im}^{ae} + \frac{1}{2}\langle am||ef\rangle t_{im}^{ef} \\
& - \frac{1}{2}\langle mn||ei\rangle t_{mn}^{ea} - f_e^m t_i^e t_m^a + \langle am||ef\rangle t_i^e t_m^f - \langle mn||ei\rangle t_m^e t_n^a \\
& + \langle mn||ef\rangle t_m^e t_{ni}^{fa} - \frac{1}{2}\langle mn||ef\rangle t_i^e t_{mn}^{af} - \frac{1}{2}\langle mn||ef\rangle t_n^a t_{mi}^{ef} \\
& - \langle mn||ef\rangle t_i^e t_m^a t_n^f
\end{aligned}
$$

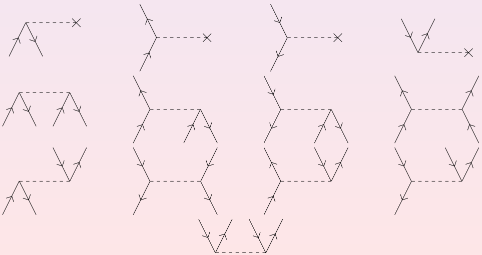
CCSD $\widehat{T}_2$ amplitude equation - Derivation

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

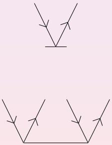
- Two pairs of particle/hole external lines.
- Final excitation level: +2



Elements: $\widehat{H}_N$



Elements: $\widehat{T}$



CCSD $\widehat{T}_2$ amplitude equation

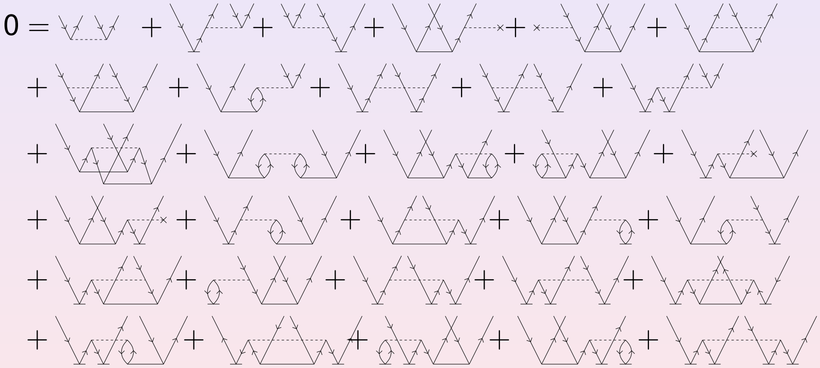


Diagram rules

- Label all lines.
- Sum over all internal indices.
- Extract matrix elements. ($f_{\mathrm{in}}^{\mathrm{out}}$, $\langle \mathrm{lout}, \mathrm{rout} || \mathrm{lin}, \mathrm{rin} \rangle$)
- Extract cluster amplitudes with indices in the order left to right. Incoming lines are subscripts, while outgoing lines are superscripts. ($t_{\mathrm{in}}^{\mathrm{out}}$, $t_{\mathrm{lin,rin}}^{\mathrm{lout,rout}}$)
- Calculate the phase: $(-1)^{\mathrm{holelines+loops}}$
- 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.

CCSD $\widehat{T}_2$ amplitude equation

$$
\begin{aligned}
0 = &\langle ab||ij\rangle + P(ij)\langle ab||ej\rangle t_i^e - P(ab)\langle am||ij\rangle t_m^b + P(ab) f_e^b t_{ij}^{ae} - P(ij) f_i^m t_{mj}^{ab} \\
&+ \frac{1}{2}\langle ab||ef\rangle t_{ij}^{ef} + \frac{1}{2}\langle mn||ij\rangle t_{mn}^{ab} + P(ij)P(ab)\langle mb||ej\rangle t_{im}^{ae} \\
&+ \frac{1}{2}P(ij)\langle ab||ef\rangle t_i^e t_j^f + \frac{1}{2}P(ab)\langle mn||ij\rangle t_m^a t_n^b - P(ij)P(ab)\langle mb||ej\rangle t_i^e t_m^a \\
&+ \frac{1}{4}\langle mn||ef\rangle t_{ij}^{ef} t_{mn}^{ab} + \frac{1}{2}P(ij)P(ab)\langle mn||ef\rangle t_{im}^{ae} t_{nj}^{fb} - \frac{1}{2}P(ab)\langle mn||ef\rangle t_{ij}^{ae} t_{mn}^{bf} \\
&- \frac{1}{2}P(ij)\langle mn||ef\rangle t_{mi}^{ef} t_{nj}^{ab} - P(ij) f_e^m t_i^e t_{mj}^{ab} - P(ab) f_e^m t_{ij}^{ae} t_m^b \\
&+ P(ij)P(ab)\langle am||ef\rangle t_i^e t_{mj}^{fb} - \frac{1}{2}P(ab)\langle am||ef\rangle t_{ij}^{ef} t_m^b + P(ab)\langle bm||ef\rangle t_{ij}^{ae} t_m^f \\
&- P(ij)P(ab)\langle mn||ej\rangle t_{im}^{ae} t_n^b + \frac{1}{2}P(ij)\langle mn||ej\rangle t_i^e t_{mn}^{ab} - P(ij)\langle mn||ei\rangle t_m^e t_{nj}^{ab} \\
&- \frac{1}{2}P(ij)P(ab)\langle am||ef\rangle t_i^e t_j^f t_m^b + \frac{1}{2}P(ij)P(ab)\langle mn||ej\rangle t_i^e t_m^a t_n^b \\
&+ \frac{1}{4}P(ij)\langle mn||ef\rangle t_i^e t_{mn}^{ab} t_j^f - P(ij)P(ab)\langle mn||ef\rangle t_i^e t_m^a t_{nj}^{fb} \\
&+ \frac{1}{4}P(ab)\langle mn||ef\rangle t_m^a t_{ij}^{ef} t_n^b - P(ij)\langle mn||ef\rangle t_m^e t_i^f t_{nj}^{ab} - P(ab)\langle mn||ef\rangle t_{ij}^{ae} t_m^b t_n^f \\
&+ \frac{1}{4}P(ij)P(ab)\langle mn||ef\rangle t_i^e t_m^a t_j^f t_n^b
\end{aligned}
$$

The expansion

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

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

The CCSD energy equation revisited

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$
\begin{aligned}
\left\{ a_a^\dagger a_i \right\} \left\{ a_p^\dagger a_q \right\} &= a_a^\dagger a_i a_p^\dagger a_q = a_p^\dagger a_q a_a^\dagger a_i \\
a_p^\dagger a_q a_a^\dagger a_i &= a_p^\dagger a_q a_a^\dagger a_i \\
&\quad + \wick{\c1 a_p^\dagger a_q a_a^\dagger \c1 a_i} + \wick{a_p^\dagger \c1 a_q \c1 a_a^\dagger a_i} \\
&\quad + \wick{\c1 a_p^\dagger \c2 a_q \c2 a_a^\dagger \c1 a_i} \\
&= a_p^\dagger a_q a_a^\dagger a_i + \delta_{qa} a_p^\dagger a_i + \delta_{pi} a_q a_a^\dagger + \delta_{qa} \delta_{pi}
\end{aligned}
$$

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

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

$$= \frac{1}{4}\sum_{\substack{pq\\ijab}} \left[a_p^\dagger a_q, a_a^\dagger a_b^\dagger a_j a_i\right]$$

$$= \frac{1}{4}\sum_{\substack{pq\\ijab}} f_q^p t_{ij}^{ab} \left(a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i - a_a^\dagger a_b^\dagger a_j a_i a_p^\dagger a_q\right)$$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$= -\frac{1}{2} 2 \sum_{abij} f_b^j t_j^a t_i^b a_a^\dagger a_i$$

$$= -\sum_{abij} f_b^j t_j^a t_i^b a_a^\dagger a_i$$

$$= \frac{1}{2}\left(\widehat{F}_N \widehat{T}_1^2\right)_c$$

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

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

The CCSD energy equation revisited

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

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.

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.

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.

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.

The CCSD energy equation revisited

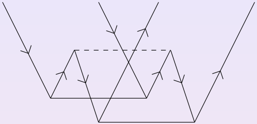
- No contractions possible between cluster operators.
- Cluster operators need to contract with free indices to the left.
- Disconnected parts automatically cancel in the commutator.
- Onebody operators can connect to maximum two cluster operators.
- Twobody operators can connect to maximum four cluster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

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.

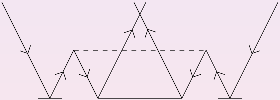
Factoring, motivation

Diagram (2.12)



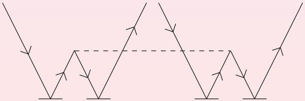
$$= \frac{1}{4}\langle mn|\widehat{v}|ef\rangle t_{ij}^{ef} t_{mn}^{ab}$$

Diagram (2.26)



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

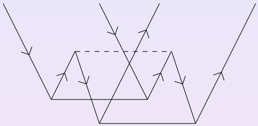
Diagram (2.31)



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

Factoring, motivation

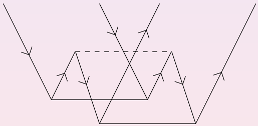
Diagram (2.12)



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

Diagram cost: $n_p^4 n_h^4$

Diagram (2.12) - Factored



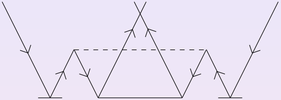
$$= \frac{1}{4}\langle mn|\widehat{v}|ef\rangle t_{ij}^{ef} t_{mn}^{ab}$$

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

$$= \frac{1}{4} X_{ij}^{mn} t_{mn}^{ab}$$

Factoring, motivation

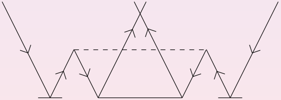
Diagram (2.26)



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

Diagram cost: $n_p^4 n_h^4$

Diagram (2.26) - Factored



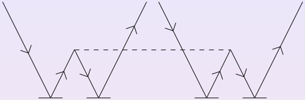
$$= \frac{1}{4} P(ij) \langle mn | \widehat{v} | ef \rangle t_i^e t_{mn}^{ab} t_j^f$$

$$= \frac{1}{4} P(ij) t_{mn}^{ab} t_i^e X_{ej}^{mn}$$

$$= \frac{1}{4} P(ij) t_{mn}^{ab} Y_{ij}^{mn}$$

Factoring, motivation

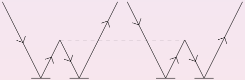
Diagram (2.31)



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

Diagram cost: $n_p^4 n_h^4$

Diagram (2.31) - Factored



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

$$= \frac{1}{4} P(ij)P(ab) t_m^a t_n^b t_i^e X_{ej}^{mn}$$

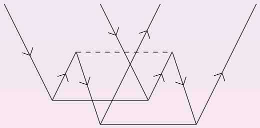
$$= \frac{1}{4} P(ij)P(ab) t_m^a t_n^b Y_{ij}^{mn}$$

$$= \frac{1}{4} P(ij)P(ab) t_m^a Z_{ij}^{mb}$$

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

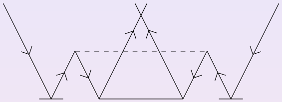


$$= \frac{1}{4}\langle mn|\widehat{v}|ef\rangle t_{ij}^{ef} t_{mn}^{ab}$$

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

Factoring, Classification

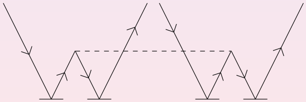
Diagram (2.26)



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

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

Diagram (2.31)



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

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

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

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

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

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

Coupled Cluster algorithm

7.7cm Setup modelspace

Calculate f and v amplitudes

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

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

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

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

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

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

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

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

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

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

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

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

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