Slides from FYS4480/9480 Lectures

Morten Hjorth-Jensen

Department of Physics and Center for Computing in Science Education
University of Oslo, N-0316 Oslo, Norway and
Facility for Rare Isotope Beams and Department of Physics and Astronomy,
Michigan State University, East Lansing, MI 48824, USA

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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

$$\widehat{H} = \sum_{pq} f_q^p \left\{ a_p^\dagger a_q \right\} + \frac{1}{4} \sum_{pqrs} \langle pq||rs \rangle \left\{ a_p^\dagger a_q^\dagger a_s a_r \right\}$$

$$+ \, \mathrm{E}_0$$

$$= \widehat{F}_N + \widehat{V}_N + \mathrm{E}_0 = \widehat{H}_N + \mathrm{E}_0$$

where

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

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

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

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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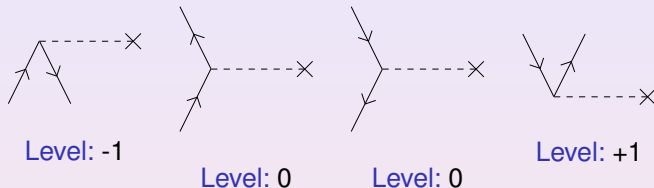
Diagram elements - Directed lines

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

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.

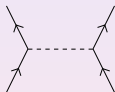# Diagram elements - Twobody Hamiltonian
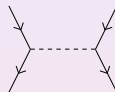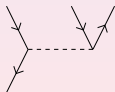

Level: -2

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.
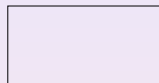
Diagram elements - Twobody cluster operator

Level: +2

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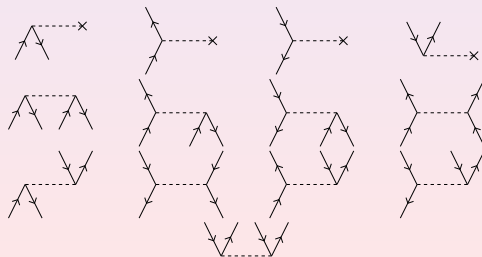- ▶ Excitation level of +2.

CCSD energy equation - Derivation
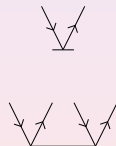
$$E_{CCSD} = \langle \Phi_0 || \Phi_0 \rangle$$

- No external lines.
- Final excitation level: 0

Elements: $\widehat{H}_N$

Elements: $\widehat{T}$

CCSD energy equation

$$E_{CCSD} = \text{<diagram>} + \text{<diagram>} + \text{<diagram>}$$

Diagram rules

▶ **Label all lines.**

▶ Sum over all internal indices.

▶ Extract matrix elements. (f_{in}^{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_{in}^{out}, $t_{\text{lin,rin}}^{\text{lout,rout}}$)

▶ Calculate the phase: $(-1)^{\text{holelines+loops}}$

▶ Multiply by a factor of $\frac{1}{2}$ for each equivalent line and each equivalent vertex.

Diagram rules

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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: $\widehat{H}_N$
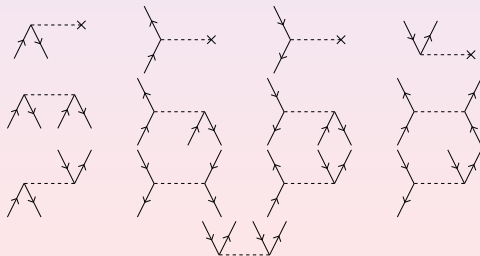
Elements: $\widehat{T}$

CCSD $\widehat{T}_1$ amplitude equation

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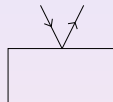- ▶ Multiply by a factor of $\frac{1}{2}$ for each equivalent line and each equivalent vertex.

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CCSD $\widehat{T}_1$ amplitude equation

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

$$- \frac{1}{2}\langle mn||ei\rangle t_{mn}^{ea} - f_e^m t_i^e t_m^a + \langle am||ef\rangle t_i^e t_m^f - \langle mn||ei\rangle t_m^e t_n^a$$

$$+ \langle mn||ef\rangle t_m^e t_{ni}^{fa} - \frac{1}{2}\langle mn||ef\rangle t_i^e t_{mn}^{af} - \frac{1}{2}\langle mn||ef\rangle t_n^a t_{mi}^{ef}$$

$$- \langle mn||ef\rangle t_i^e t_m^a t_n^f$$

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: $\widehat{H}_N$
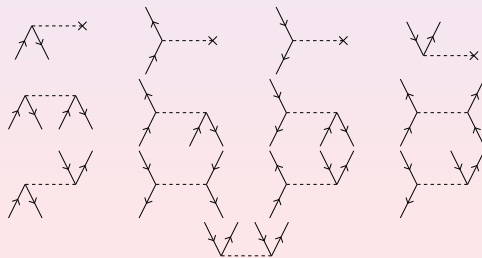
Elements: $\widehat{T}$

CCSD $\widehat{T}_2$ amplitude equation

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- ▶ Multiply by a factor of $\frac{1}{2}$ for each equivalent line and each equivalent vertex.
- ▶ Antisymmetrize a pair of external particle/hole line that does not connect to the same operator.

Diagram rules

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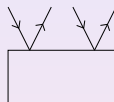- ▶ Multiply by a factor of $\frac{1}{2}$ for each equivalent line and each equivalent vertex.
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- ▶ Antisymmetrize a pair of external particle/hole line that does not connect to the same operator.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$+ \left\{\overbrace{a_p^\dagger \underbrace{a_q a_a^\dagger} a_i}\right\}$$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$
\begin{aligned}
\left[\hat{F}_N, \hat{T}_2\right] &= \left[\sum_{pq} f^p_q \left\{a^\dagger_p a_q\right\}, \frac{1}{4}\sum_{ijab} t^{ab}_{ij} \left\{a^\dagger_a a^\dagger_b a_j a_i\right\}\right] \\
&= \frac{1}{4}\sum_{\substack{pq \\ ijab}} \left[\left\{a^\dagger_p a_q\right\}, \left\{a^\dagger_a a^\dagger_b a_j a_i\right\}\right] \\
&= \frac{1}{4}\sum_{\substack{pq \\ ijab}} f^p_q t^{ab}_{ij} \left(\left\{a^\dagger_p a_q\right\} \left\{a^\dagger_a a^\dagger_b a_j a_i\right\} - \left\{a^\dagger_a a^\dagger_b a_j a_i\right\} \left\{a^\dagger_p a_q\right\}\right)
\end{aligned}
$$

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

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

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

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

$$+ \left\{a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i\right\} + \left\{a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i\right\} + \left\{a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i\right\}$$

$$+ \left\{a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i\right\} + \left\{a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i\right\} + \left\{a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i\right\}$$

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

$$+ \delta_{qa}\left\{a_p^\dagger a_b^\dagger a_j a_i\right\} - \delta_{qb}\left\{a_p^\dagger a_a^\dagger a_j a_i\right\} - \delta_{pi}\delta_{qa}\left\{a_b^\dagger a_i\right\}$$

$$+ \delta_{pi}\delta_{qa}\left\{a_b^\dagger a_i\right\} + \delta_{pi}\delta_{qb}\left\{a_a^\dagger a_i\right\} - \delta_{pi}\delta_{qb}\left\{a_a^\dagger a_i\right\}$$

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

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

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

$+ \left\{a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i\right\} + \left\{a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i\right\} + \left\{a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j\right\}$

$+ \left\{a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i\right\} + \left\{a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i\right\} + \left\{a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j\right\}$

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

$+ \delta_{qa}\left\{a_b^\dagger a_b^\dagger a_j a_i\right\} - \delta_{qb}\left\{a_p^\dagger a_a^\dagger a_j a_i\right\} - \delta_{pi}\delta_{qa}\left\{a_b^\dagger a_i\right\}$

$+ \delta_{pi}\delta_{qa}\left\{a_b^\dagger a_i\right\} + \delta_{pi}\delta_{qb}\left\{a_a^\dagger a_i\right\} - \delta_{pi}\delta_{qb}\left\{a_a^\dagger a_i\right\}$

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

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

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

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

$$+ \left\{a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i\right\} + \left\{a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i\right\} + \left\{a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i\right\}$$

$$+ \left\{a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i\right\} + \left\{a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i\right\} + \left\{a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j\right\}$$

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

$$+ \delta_{qa}\left\{a_p^\dagger a_b^\dagger a_j a_i\right\} - \delta_{qb}\left\{a_p^\dagger a_a^\dagger a_j a_i\right\} - \delta_{pj}\delta_{qa}\left\{a_b^\dagger a_i\right\}$$

$$+ \delta_{pi}\delta_{qa}\left\{a_b^\dagger a_j\right\} + \delta_{pj}\delta_{qb}\left\{a_a^\dagger a_i\right\} - \delta_{pi}\delta_{qb}\left\{a_a^\dagger a_j\right\}$$

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

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

$$\left\{ a_p^\dagger a_q \right\} \left\{ a_a^\dagger a_b^\dagger a_j a_i \right\} = \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} + \left\{ \overline{a_p^\dagger a_q a_a^\dagger a_b^\dagger} a_j a_i \right\} + \left\{ \overline{a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j} a_i \right\}$$

$$+ \left\{ a_p^\dagger \overline{a_q a_a^\dagger} a_b^\dagger a_j a_i \right\} + \left\{ a_p^\dagger \overline{a_q a_a^\dagger a_b^\dagger} a_j a_i \right\} + \left\{ \overline{a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j} a_i \right\}$$

$$+ \left\{ \overline{a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i} \right\} + \left\{ \overline{a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i} \right\} + \left\{ \overline{a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j} \right\}$$

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

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

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

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

$$\left\{ a_p^\dagger a_q \right\} \left\{ a_a^\dagger a_b^\dagger a_j a_i \right\} = \left\{ a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i \right\} + \left\{ \overline{a_p^\dagger a_q a_a^\dagger a_b^\dagger} a_j a_i \right\} + \left\{ \overline{a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j} a_i \right\}$$

$$+ \left\{ a_p^\dagger \overline{a_q a_a^\dagger} a_b^\dagger a_j a_i \right\} + \left\{ a_p^\dagger \overline{a_q a_a^\dagger a_b^\dagger} a_j a_i \right\} + \left\{ \overline{a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j} a_i \right\}$$

$$+ \left\{ \overline{a_p^\dagger a_q a_a^\dagger a_b^\dagger} a_j a_i \right\} + \left\{ \overline{a_p^\dagger a_q a_a^\dagger a_b^\dagger} a_j a_i \right\} + \left\{ \overline{a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j} a_i \right\}$$

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

$$+ \delta_{qa} \left\{ a_p^\dagger a_b^\dagger a_j a_i \right\} - \delta_{qb} \left\{ a_p^\dagger a_a^\dagger a_j a_i \right\} - \delta_{pj}\delta_{qa} \left\{ a_b^\dagger a_i \right\}$$

$$+ \delta_{pi}\delta_{qa} \left\{ a_b^\dagger a_j \right\} + \delta_{pj}\delta_{qb} \left\{ a_a^\dagger a_i \right\} - \delta_{pi}\delta_{qb} \left\{ a_a^\dagger a_j \right\}$$

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

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

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

$$\left\{a_p^\dagger a_q\right\}\left\{a_a^\dagger a_b^\dagger a_j a_i\right\} = \left\{a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i\right\} + \left\{\overline{a_p^\dagger a_q a_a^\dagger} a_b^\dagger a_j a_i\right\} + \left\{\overline{a_p^\dagger a_q a_a^\dagger a_b^\dagger} a_j a_i\right\}$$

$$+ \left\{a_p^\dagger \overline{a_q a_a^\dagger} a_b^\dagger a_j a_i\right\} + \left\{a_p^\dagger \overline{a_q a_a^\dagger a_b^\dagger} a_j a_i\right\} + \left\{\overline{a_p^\dagger a_q a_a^\dagger a_b^\dagger} a_j a_i\right\}$$

$$+ \left\{\overline{a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j a_i}\right\} + \left\{\overline{a_p^\dagger a_q a_a^\dagger a_b^\dagger} a_j a_i\right\} + \left\{\overline{a_p^\dagger a_q a_a^\dagger a_b^\dagger a_j}a_i\right\}$$

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

$$+ \delta_{qa}\left\{a_p^\dagger a_b^\dagger a_j a_i\right\} - \delta_{qb}\left\{a_p^\dagger a_a^\dagger a_j a_i\right\} - \delta_{pj}\delta_{qa}\left\{a_b^\dagger a_i\right\}$$

$$+ \delta_{pi}\delta_{qa}\left\{a_b^\dagger a_j\right\} + \delta_{pj}\delta_{qb}\left\{a_a^\dagger a_i\right\} - \delta_{pi}\delta_{qb}\left\{a_a^\dagger a_j\right\}$$

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

Wicks theorem gives us

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

Inserted into the original expression, we arrive at

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

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

Wicks theorem gives us

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

Inserted into the original expression, we arrive at

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

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

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

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

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

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

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

$$= \left[\sum_{pai} f_a^p t_i^a \left\{a_p^\dagger a_i\right\} + \sum_{qai} f_q^i t_i^a \left\{a_q a_a^\dagger\right\}, \sum_{jb} t_j^b \left\{a_b^\dagger a_j\right\}\right]$$

$$= \sum_{pabij} f_a^p t_i^a t_j^b \left[\left\{a_p^\dagger a_i\right\}, \left\{a_b^\dagger a_j\right\}\right] + \sum_{qabij} f_q^i t_i^a t_j^b \left[\left\{a_q a_a^\dagger\right\}, \left\{a_b^\dagger a_j\right\}\right]$$

$$\left\{a_b^\dagger a_j\right\}\left\{a_p^\dagger a_i\right\} = \left\{a_b^\dagger a_j a_p^\dagger a_i\right\} = \left\{a_p^\dagger a_i a_b^\dagger a_j\right\}$$

$$\left\{a_b^\dagger a_j\right\}\left\{a_q a_a^\dagger\right\} = \left\{a_b^\dagger a_j a_q a_a^\dagger\right\} = \left\{a_q a_a^\dagger a_b^\dagger a_j\right\}$$

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

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

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

$$\left\{a_b^\dagger a_j\right\} \left\{a_p^\dagger a_i\right\} = \left\{a_b^\dagger a_j a_p^\dagger a_i\right\} = \left\{a_p^\dagger a_i a_b^\dagger a_j\right\}$$

$$\left\{a_b^\dagger a_j\right\} \left\{a_q a_a^\dagger\right\} = \left\{a_b^\dagger a_j a_q a_a^\dagger\right\} = \left\{a_q a_a^\dagger a_b^\dagger a_j\right\}$$

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

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

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

$$= \left[\sum_{pai} f_a^p t_i^a \left\{a_p^\dagger a_i\right\} + \sum_{qai} f_q^i t_i^a \left\{a_q a_a^\dagger\right\}, \sum_{jb} t_j^b \left\{a_b^\dagger a_j\right\}\right]$$

$$= \sum_{pabij} f_a^p t_i^a t_j^b \left[\left\{a_p^\dagger a_i\right\}, \left\{a_b^\dagger a_j\right\}\right] + \sum_{qabij} f_q^i t_i^a t_j^b \left[\left\{a_q a_a^\dagger\right\}, \left\{a_b^\dagger a_j\right\}\right]$$

$$\left\{a_b^\dagger a_j\right\} \left\{a_p^\dagger a_i\right\} = \left\{a_b^\dagger a_j a_p^\dagger a_i\right\} = \left\{a_p^\dagger a_i a_b^\dagger a_j\right\}$$

$$\left\{a_b^\dagger a_j\right\} \left\{a_q a_a^\dagger\right\} = \left\{a_b^\dagger a_j a_q a_a^\dagger\right\} = \left\{a_q a_a^\dagger a_b^\dagger a_j\right\}$$

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

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

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

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

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

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

The CCSD energy equation revisited

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

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

$$= 0$$

The CCSD energy equation revisited

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

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

$$= 0$$

The CCSD energy equation revisited

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

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

$$= 0$$

The CCSD energy equation revisited

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

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

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

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

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

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

The CCSD energy equation revisited

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

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

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

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

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

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

The CCSD energy equation revisited

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

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

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

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

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

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

The CCSD energy equation revisited

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

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

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

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

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

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

The CCSD energy equation revisited

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

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

The CCSD energy equation revisited

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

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

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

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

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

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

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

The CCSD energy equation revisited

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

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

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The CCSD energy equation revisited

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

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The CCSD energy equation revisited

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

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

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

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

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

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

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Factoring, motivation
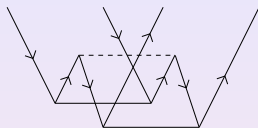
Diagram (2.12)

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

Diagram (2.26)

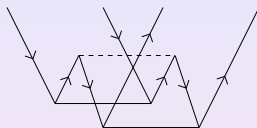$$= \frac{1}{4}P(ij)\langle mn||ef\rangle t_i^e t_{mn}^{ab} t_j^f$$

Diagram (2.31)

$$= \frac{1}{4}P(ij)P(ab)\langle mn||ef\rangle t_i^e t_m^a t_j^f t_n^b$$
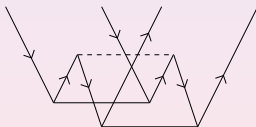
Factoring, motivation
Diagram (2.12)

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

Diagram cost: $n_p^4 n_h^4$

Diagram (2.13) - Factored

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

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

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

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

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

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

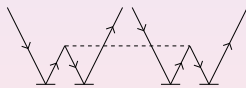$$= \frac{1}{4}P(ij)t_{mn}^{ab} Y_{ij}^{mn}$$

Factoring, motivation
Diagram (2.31)

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

Diagram cost: $n_p^4 n_h^4$

Diagram (2.31) - Factored
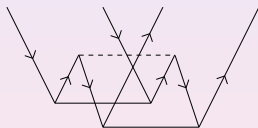

$$= \frac{1}{4} P(ij) P(ab) \langle mn||ef \rangle t_i^e t_m^a t_j^f t_n^b$$

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

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

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

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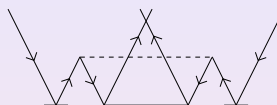
 $= \dfrac{1}{4}\langle mn||ef\rangle t_{ij}^{ef} t_{mn}^{ab}$

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 $T_2(h)$

$$
\begin{aligned}
T_2(h) &\Leftarrow -P(ij)f_i^m t_{mj}^{ab} - \frac{1}{2}P(ij)\langle mn||ef\rangle t_{mi}^{ef} t_{nj}^{ab} - P(ij)f_e^m t_i^e t_{mj}^{ab} \\
&\quad - P(ij)\langle mn||ei\rangle t_m^e t_{nj}^{ab} - P(ij)\langle mn||ef\rangle t_m^e t_i^f t_{nj}^{ab} \\
&= -P(ij)t_{im}^{ab}\Big[f_j^m + \langle mn||je\rangle t_n^e + \frac{1}{2}\langle mn||ef\rangle t_{jn}^{ef} \\
&\quad + t_j^e\Big(f_e^m + \langle mn||ef\rangle t_n^f \Big)\Big] \\
&= -P(ij)t_{im}^{ab}(\bar{\mathrm{H}}3)_j^m
\end{aligned}
$$

Factoring, $T_2(h^2)$

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

$$
\begin{aligned}
T_2(h^2) \Leftarrow &\; \frac{1}{2}\langle mn||ij\rangle t_{mn}^{ab} + \frac{1}{4}\langle mn||ef\rangle t_{ij}^{ef} t_{mn}^{ab} + \frac{1}{2}P(ij)\langle mn||ej\rangle t_i^e t_{mn}^{ab} \\
&+ \frac{1}{4}P(ij)\langle mn||ef\rangle t_i^e t_{mn}^{ab} t_j^f \\
= &\; \frac{1}{2}t_{mn}^{ab}\Big[\langle mn||ij\rangle + \frac{1}{2}\langle mn||ef\rangle t_{ij}^{ef} \\
&+ P(ij)t_j^e\Big(\langle mn||ie\rangle + \frac{1}{2}\langle mn||fe\rangle t_i^f\Big)\Big] \\
= &\; \frac{1}{2}t_{mn}^{ab}(\bar{\mathrm{H}}9)_{ij}^{mn}
\end{aligned}
$$

Factored T_1 amplitude equations

$$0 = f_i^a + \langle ma||ei \rangle t_m^e + \frac{1}{2} \langle am||ef \rangle t_{im}^{ef} + t_i^e (\text{I2a})_e^a - t_m^a (\bar{\text{H}}3)_i^m$$
$$+ \frac{1}{2} t_{mn}^{ea} (\bar{\text{H}}7)_{ie}^{mn} + t_{im}^{ae} (\bar{\text{H}}1)_e^m$$

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

$$0 = f_i^a + \langle ma||ei \rangle t_m^e + \frac{1}{2} \langle am||ef \rangle t_{im}^{ef} + t_i^e (\mathrm{I2a})_e^a - t_m^a (\bar{\mathrm{H}}3)_i^m$$
$$\quad + \frac{1}{2} t_{mn}^{ea} (\bar{\mathrm{H}}7)_{ie}^{mn} + t_{im}^{ae} (\bar{\mathrm{H}}1)_e^m$$

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

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

Factored T_1 amplitude equations

$$
\begin{aligned}
0 &= f_i^a + \langle ma||ei\rangle t_m^e + \frac{1}{2}\langle am||ef\rangle t_{im}^{ef} + t_i^e(\text{I2a})_e^a - t_m^a(\bar{\text{H}}3)_i^m \\
&\quad + \frac{1}{2}t_{mn}^{ea}(\bar{\text{H}}7)_{ie}^{mn} + t_{im}^{ae}(\bar{\text{H}}1)_e^m \\
&= f_i^a + \langle ma||ei\rangle t_m^e + t_i^a(\text{I2a})_a^a + (1-\delta_{ea})t_i^e(\text{I2a})_e^a \\
&\quad - t_i^a(\bar{\text{H}}3)_i^i - (1-\delta_{mi})t_m^a(\bar{\text{H}}3)_i^m + \frac{1}{2}\langle am||ef\rangle t_{im}^{ef} + \frac{1}{2}t_{mn}^{ea}(\bar{\text{H}}7)_{ie}^{mn} \\
&\quad + t_{im}^{ae}(\bar{\text{H}}1)_e^m \\
&= f_i^a + t_i^a\Big((\text{I2a})_a^a - (\bar{\text{H}}3)_i^i\Big) + \langle ma||ei\rangle t_m^e \\
&\quad + (1-\delta_{ea})t_i^e(\text{I2a})_e^a - (1-\delta_{mi})t_m^a(\bar{\text{H}}3)_i^m + \frac{1}{2}\langle am||ef\rangle t_{im}^{ef} \\
&\quad + \frac{1}{2}t_{mn}^{ea}(\bar{\text{H}}7)_{ie}^{mn} + t_{im}^{ae}(\bar{\text{H}}1)_e^m
\end{aligned}
$$

Factored T_1 amplitude equations

$$
\begin{aligned}
0 &= f_i^a + \langle ma||ei\rangle t_m^e + \frac{1}{2}\langle am||ef\rangle t_{im}^{ef} + t_i^e(\text{I2a})_e^a - t_m^a(\bar{\text{H}}3)_i^m \\
&\quad + \frac{1}{2}t_{mn}^{ea}(\bar{\text{H}}7)_{ie}^{mn} + t_{im}^{ae}(\bar{\text{H}}1)_e^m \\
&= f_i^a + \langle ma||ei\rangle t_m^e + t_i^a(\text{I2a})_a^a + (1 - \delta_{ea})t_i^e(\text{I2a})_e^a \\
&\quad - t_i^a(\bar{\text{H}}3)_i^i - (1 - \delta_{mi})t_m^a(\bar{\text{H}}3)_i^m + \frac{1}{2}\langle am||ef\rangle t_{im}^{ef} + \frac{1}{2}t_{mn}^{ea}(\bar{\text{H}}7)_{ie}^{mn} \\
&\quad + t_{im}^{ae}(\bar{\text{H}}1)_e^m \\
&= f_i^a + t_i^a\Big((\text{I2a})_a^a - (\bar{\text{H}}3)_i^i\Big) + \langle ma||ei\rangle t_m^e \\
&\quad + (1 - \delta_{ea})t_i^e(\text{I2a})_e^a - (1 - \delta_{mi})t_m^a(\bar{\text{H}}3)_i^m + \frac{1}{2}\langle am||ef\rangle t_{im}^{ef} \\
&\quad + \frac{1}{2}t_{mn}^{ea}(\bar{\text{H}}7)_{ie}^{mn} + t_{im}^{ae}(\bar{\text{H}}1)_e^m
\end{aligned}
$$

Factored T_1 amplitude equations

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

and we get the T_1 amplitude equations

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

Factored T_2 amplitude equations

$$0 = \langle ab||ij \rangle + \frac{1}{2}\langle ab||ef \rangle t_{ij}^{ef} - P(ij)t_{im}^{ab}(\bar{\text{H}}3)_j^m + \frac{1}{2}t_{mn}^{ab}(\bar{\text{H}}9)_{ij}^{mn}$$
$$+ P(ab)t_{ij}^{ae}(\bar{\text{H}}2)_e^b + P(ij)P(ab)t_{im}^{ae}(\text{I10c})_{ej}^{mb} - P(ab)t_m^a(\text{I12a})_{ij}^{mb}$$
$$+ P(ij)t_i^e(\text{I11a})_{ej}^{ab}$$

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

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

and get the T_2 amplitude equations

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

Coupled Cluster algorithm

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

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

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Calculate f and v amplitudes
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$E \leftarrow 1; \; E_{old} \leftarrow 0$
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Coupled Cluster algorithm

Typical convergence of the T_2 amplitudes