Slides from FYS-KJM4480/9480 Lectures

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Notation

Second quantization

Antisymmetrized wavefunction

$$\begin{aligned}\Phi_{AS}(\alpha_1, \dots, \alpha_A; \mathbf{x}_1, \dots \mathbf{x}_A) &= \frac{1}{\sqrt{A}} \sum_{\hat{P}} (-1)^P \hat{P} \prod_{i=1}^{A} \psi_{\alpha_i}(\mathbf{x}_i) \\ &\equiv |\alpha_1 \dots \alpha_A\rangle \\ &= a^\dagger_{\alpha_1} \dots a^\dagger_{\alpha_A} |0\rangle\end{aligned}$$

$$a^\dagger_p|0\rangle = |p\rangle, \quad a_p|q\rangle = \delta_{pq}|0\rangle$$

$$\delta_{pq} = \left\{a_p, a^\dagger_q\right\}$$

$$0 = \left\{a^\dagger_p, a_q\right\} = \{a_p, a_q\} = \left\{a^\dagger_p, a^\dagger_q\right\}$$

Notation

Second quantization, quasiparticles

Reference state

$$|\Phi_0\rangle = |\alpha_1 \dots \alpha_A\rangle, \quad \alpha_1, \dots, \alpha_A \leq \alpha_F$$

Creation and annihilation operators

$$\left\{a_p^\dagger, a_q\right\} = \delta_{pq}, p, q \leq \alpha_F \qquad \left\{a_p, a_q^\dagger\right\} = \delta_{pq}, p, q > \alpha_F$$

$$i, j, \ldots \leq \alpha_F, \quad a, b, \ldots > \alpha_F, \quad p, q, \ldots - \text{any}$$

$$a_i|\Phi_0\rangle = |\Phi_i\rangle \qquad a_a^\dagger|\Phi_0\rangle = |\Phi^a\rangle$$

$$a_i^\dagger|\Phi_0\rangle = 0 \qquad a_a|\Phi_0\rangle = 0$$

Notation

Second quantization, operators

Onebody operator

$$\hat{F} = \sum_{pq} \langle p|\hat{f}|q\rangle a_p^\dagger a_q$$

Notation

Second quantization, operators

Twobody operator

$$\hat{V} = \frac{1}{4}\sum_{pqrs}\langle pq|\hat{v}|rs\rangle_{AS} a_p^\dagger a_q^\dagger a_s a_r \equiv \frac{1}{4}\sum_{pqrs}\langle pq|\hat{v}|rs\rangle a_p^\dagger a_q^\dagger a_s a_r$$

where we have defined the antisymmetric matrix elements

$$\langle pq|\hat{v}|rs\rangle_{AS} = \langle pq|\hat{v}|rs\rangle - \langle pq|\hat{v}|sr\rangle.$$

Notation

Second quantization, operators

Threebody operator

$$\hat{V}_3 = \frac{1}{36}\sum_{pqrstu} \langle pqr|\hat{v}_3|stu\rangle_{AS} a_p^\dagger a_q^\dagger a_r^\dagger a_u a_t a_s \equiv \frac{1}{36}\sum_{pqrstu} \langle pqr|\hat{v}_3|stu\rangle a_p^\dagger a_q^\dagger a_r^\dagger a_u a_t a_s$$

where we have defined the antisymmetric matrix elements

$$\begin{aligned}\langle pqr|\hat{v}_3|stu\rangle_{AS} = {} & \langle pqr|\hat{v}_3|stu\rangle + \langle pqr|\hat{v}_3|tus\rangle + \langle pqr|\hat{v}_3|ust\rangle \\ & - \langle pqr|\hat{v}_3|sut\rangle - \langle pqr|\hat{v}_3|tsu\rangle - \langle pqr|\hat{v}_3|uts\rangle.\end{aligned}$$

Notation

Second quantization, operators

Normal ordered operators

$$\left\{a_a a_b \dots a_c^\dagger a_d^\dagger\right\} = (-1)^P a_c^\dagger a_d^\dagger \dots a_a a_b$$

All creation operators to the left and all annihilation operators to the right times a factor determined by how many operators have been switched.

Definitions

The basics, Normal ordered Hamiltonian

Definition

The normal ordered Hamiltonian is given by

$$\hat{H}_N = \frac{1}{36}\sum_{\substack{pqr\\stu}} \langle pqr|\hat{v}_3|stu\rangle \left\{a^\dagger_p a^\dagger_q a^\dagger_r a_u a_t a_s\right\} + \frac{1}{4}\sum_{pqrs}\langle pq||rs\rangle \left\{a^\dagger_p a^\dagger_q a_s a_r\right\} + \sum_{pq} f^p_q \left\{a^\dagger_p a_q\right\}$$

$$= \hat{H}^N_3 + \hat{V}_N + \hat{F}_N$$

where

$$\hat{F}_N = \sum_{pq} f^p_q \left\{a^\dagger_p a_q\right\} \qquad \hat{V}_N = \frac{1}{4}\sum_{pqrs}\langle pq||rs\rangle \left\{a^\dagger_p a^\dagger_q a_s a_r\right\}$$

$$\hat{H}^N_3 = \frac{1}{36}\sum_{\substack{pqr\\stu}} \langle pqr|\hat{v}_3|stu\rangle \left\{a^\dagger_p a^\dagger_q a^\dagger_r a_u a_t a_s\right\}$$

Definitions

The basics, Normal ordered Hamiltonian

Definition

The amplitudes are given by

$$f_q^p = \langle p|\hat{h}_0|q\rangle + \sum_i \langle pi|\hat{v}|qi\rangle + \frac{1}{2}\sum_{ij}\langle pij|\hat{v}_3|qij\rangle$$

$$\langle pq||rs\rangle = \langle pq|\hat{v}|rs\rangle + \sum_i \langle pqi|\hat{v}_3|rsi\rangle,$$

In relation to the Hamiltonian, $\hat{H}_N$ is given by

$$\begin{aligned}\hat{H}_N &= \hat{H} - E_0 \\ E_0 &= \langle\Phi_0|\hat{H}|\Phi_0\rangle \\ &= \sum_i \langle i|\hat{h}_0|i\rangle + \frac{1}{2}\sum_{ij}\langle ij|\hat{v}|ij\rangle + \frac{1}{6}\sum_{ijk}\langle ijk|\hat{v}_3|ijk\rangle,\end{aligned}$$

where E_0 is the energy expectation value between reference states.

Definitions

The basics, Normal ordered Hamiltonian

Derivation

We start with the Hamiltonian

$$\hat{H} = \hat{H}_0 + \hat{H}_I$$

where

$$\hat{H}_0 = \sum_{pq} \langle p|\hat{h}_0|q\rangle a_p^\dagger a_q$$

$$\hat{H}_I = \frac{1}{4} \sum_{pqrs} \langle pq|\hat{v}|rs\rangle a_p^\dagger a_q^\dagger a_s a_r$$

$$\hat{H}_3 = \frac{1}{36} \sum_{\substack{pqr \\ stu}} \langle pqr|\hat{v}_3|stu\rangle a_p^\dagger a_q^\dagger a_r^\dagger a_u a_t a_s$$

Definitions

The basics, Normal ordered Hamiltonian

Derivation, onebody part

$$\hat{H}_0 = \sum_{pq} \langle p|\hat{h}_0|q\rangle a_p^\dagger a_q$$

$$\begin{aligned} a_p^\dagger a_q &= \left\{ a_p^\dagger a_q \right\} + \left\{ \overbrace{a_p^\dagger a_q} \right\} \\ &= \left\{ a_p^\dagger a_q \right\} + \delta_{pq\in i} \end{aligned}$$

$$\begin{aligned} \hat{H}_0 &= \sum_{pq} \langle p|\hat{h}_0|q\rangle a_p^\dagger a_q \\ &= \sum_{pq} \langle p|\hat{h}_0|q\rangle \left\{ a_p^\dagger a_q \right\} + \delta_{pq\in i} \sum_{pq} \langle p|\hat{h}_0|q\rangle \\ &= \sum_{pq} \langle p|\hat{h}_0|q\rangle \left\{ a_p^\dagger a_q \right\} + \sum_{i} \langle i|\hat{h}_0|i\rangle \end{aligned}$$

Definitions

The basics, Normal ordered Hamiltonian

Derivation, onebody part

A onebody part

$$\hat{F}_N \Leftarrow \sum_{pq} \langle p|\hat{h}_0|q\rangle \left\{ a_p^\dagger a_q \right\}$$

and a scalar part

$$E_0 \Leftarrow \sum_i \langle i|\hat{h}_0|i\rangle$$

Definitions

Derivation, twobody part

$$\hat{H}_I = \frac{1}{4}\sum_{pqrs}\langle pq|\hat{v}|rs\rangle a_p^\dagger a_q^\dagger a_s a_r$$

$$\begin{aligned}
a_p^\dagger a_q^\dagger a_s a_r = &\left\{a_p^\dagger a_q^\dagger a_s a_r\right\} \\
&+ \left\{a_p^\dagger a_q^\dagger a_s a_r\right\} + \left\{a_p^\dagger a_q^\dagger a_s a_r\right\} + \left\{a_p^\dagger a_q^\dagger a_s a_r\right\} \\
&+ \left\{a_p^\dagger a_q^\dagger a_s a_r\right\} + \left\{a_p^\dagger a_q^\dagger a_s a_r\right\} + \left\{a_p^\dagger a_q^\dagger a_s a_r\right\} \\
= &\left\{a_p^\dagger a_q^\dagger a_s a_r\right\} \\
&+ \delta_{qs\in i}\left\{a_p^\dagger a_r\right\} - \delta_{qr\in i}\left\{a_p^\dagger a_s\right\} - \delta_{ps\in i}\left\{a_q^\dagger a_r\right\} \\
&+ \delta_{pr\in i}\left\{a_q^\dagger a_s\right\} + \delta_{pr\in i}\delta_{qs\in i} - \delta_{ps\in i}\delta_{qr\in i}
\end{aligned}$$

Definitions

The basics, Normal ordered Hamiltonian

Derivation, twobody part

$$\hat{H}_I = \frac{1}{4}\sum_{pqrs}\langle pq|\hat{v}|rs\rangle a_p^\dagger a_q^\dagger a_s a_r$$

$$\begin{aligned}
a_p^\dagger a_q^\dagger a_s a_r = &\left\{a_p^\dagger a_q^\dagger a_s a_r\right\} \\
&+ \left\{a_p^\dagger a_q^\dagger a_s a_r\right\} + \left\{a_p^\dagger a_q^\dagger a_s a_r\right\} + \left\{a_p^\dagger a_q^\dagger a_s a_r\right\} \\
&+ \left\{a_p^\dagger a_q^\dagger a_s a_r\right\} + \left\{a_p^\dagger a_q^\dagger a_s a_r\right\} + \left\{a_p^\dagger a_q^\dagger a_s a_r\right\} \\
= &\left\{a_p^\dagger a_q^\dagger a_s a_r\right\} \\
&+ \delta_{qs\in i}\left\{a_p^\dagger a_r\right\} - \delta_{qr\in i}\left\{a_p^\dagger a_s\right\} - \delta_{ps\in i}\left\{a_q^\dagger a_r\right\} \\
&+ \delta_{pr\in i}\left\{a_q^\dagger a_s\right\} + \delta_{pr\in i}\delta_{qs\in i} - \delta_{ps\in i}\delta_{qr\in i}
\end{aligned}$$

Definitions

The basics, Normal ordered Hamiltonian

Derivation, twobody part

$$
\begin{aligned}
\hat{H}_I &= \frac{1}{4}\sum_{pqrs}\langle pq|\hat{v}|rs\rangle a_p^\dagger a_q^\dagger a_s a_r \\
&= \frac{1}{4}\sum_{pqrs}\langle pq|\hat{v}|rs\rangle \left\{a_p^\dagger a_q^\dagger a_s a_r\right\} + \quad \frac{1}{4}\sum_{pqrs}\Big(\delta_{qs\in i}\langle pq|\hat{v}|rs\rangle \left\{a_p^\dagger a_r\right\} \\
&\quad - \delta_{qr\in i}\langle pq|\hat{v}|rs\rangle \left\{a_p^\dagger a_s\right\} - \delta_{ps\in i}\langle pq|\hat{v}|rs\rangle \left\{a_q^\dagger a_r\right\} \\
&\quad + \delta_{pr\in i}\langle pq|\hat{v}|rs\rangle \left\{a_q^\dagger a_s\right\} + \delta_{pr\in i}\delta_{qs\in i} - \delta_{ps\in i}\delta_{qr\in i}\Big)
\end{aligned}
$$

Derivation, twobody part

$$
\begin{aligned}
&= \frac{1}{4}\sum_{pqrs}\langle pq|\hat{v}|rs\rangle \left\{a_p^\dagger a_q^\dagger a_s a_r\right\} \\
&\quad + \frac{1}{4}\sum_{pqi}\Big(\langle pi|\hat{v}|qi\rangle - \langle pi|\hat{v}|iq\rangle - \langle ip|\hat{v}|qi\rangle + \langle ip|\hat{v}|iq\rangle\Big)\left\{a_p^\dagger a_q\right\} \\
&\quad + \frac{1}{4}\sum_{ij}\Big(\langle ij|\hat{v}|ij\rangle - \langle ij|\hat{v}|ji\rangle\Big) \\
&= \frac{1}{4}\sum_{pqrs}\langle pq|\hat{v}|rs\rangle \left\{a_p^\dagger a_q^\dagger a_s a_r\right\} + \sum_{pqi}\langle pi|\hat{v}|qi\rangle \left\{a_p^\dagger a_q\right\} + \frac{1}{2}\sum_{ij}\langle ij|\hat{v}|ij\rangle
\end{aligned}
$$

Definitions

The basics, Normal ordered Hamiltonian

Derivation, twobody part

A twobody part

$$\hat{V}_N \Leftarrow \frac{1}{4}\sum_{pqrs}\langle pq|\hat{v}|rs\rangle \left\{a_p^\dagger a_q^\dagger a_s a_r\right\}$$

A onebody part

$$\hat{F}_N \Leftarrow \sum_{pqi}\langle pi|\hat{v}|qi\rangle \left\{a_p^\dagger a_q\right\}$$

and a scalar part

$$E_0 \Leftarrow \frac{1}{2}\sum_{ij}\langle ij|\hat{v}|ij\rangle$$

Definitions

The basics, Normal ordered Hamiltonian

Twobody Hamiltonian

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

where

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

Definitions

The basics, Normal ordered Hamiltonian

Twobody Hamiltonian

The amplitudes are given by

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

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In relation to the Hamiltonian, $\hat{H}_N$ is given by

$$\begin{aligned}
\hat{H}_N &= \hat{H} - E_0 \\
E_0 &= \langle \Phi_0|\hat{H}|\Phi_0\rangle \\
&= \sum_i \langle i|\hat{h}_0|i\rangle + \frac{1}{2}\sum_{ij} \langle ij|\hat{v}|ij\rangle
\end{aligned}$$

where E_0 is the energy expectation value between reference states.

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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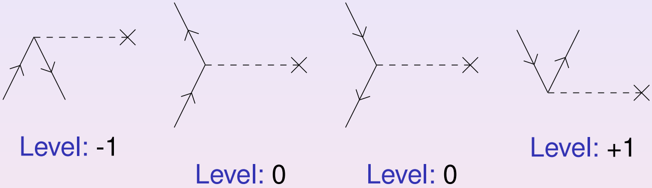
Diagram elements - Directed lines

Figure: Particle line

Figure: Hole line

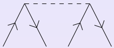
- Represents a contraction between second quantized operators.
- External lines are connected to one operator vertex and infinity.
- Internal lines are connected to operator vertices in both ends.

Diagram elements - Onebody Hamiltonian



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

Diagram elements - Twobody Hamiltonian



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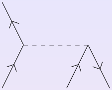

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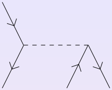

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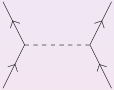
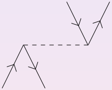
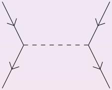


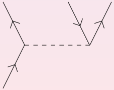
Level: 0



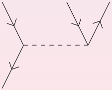
Level: 0



Level: 0



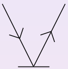
Level: +1



Level: +1

Level: +2

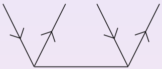
Diagram elements - Onebody cluster operator



Level: +1

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

Diagram elements - Twobody cluster operator



Level: +2

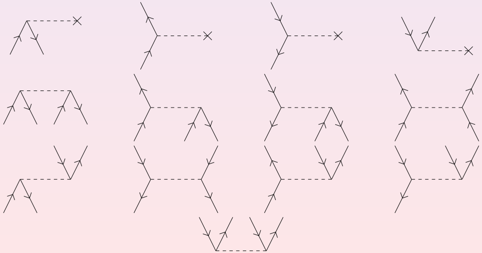
- Horisontal line segment with two vertices.
- Excitation level of +2.

CCSD energy equation - Derivation

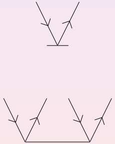
$$E_{\text{CCSD}} = \langle \Phi_0 | | \Phi_0 \rangle$$

- No external lines.
- Final excitation level: 0

Elements: $\widehat{H}_N$



Elements: $\widehat{T}$



CCSD energy equation

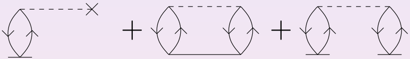
$E_{CCSD} =$ 

Diagram rules

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

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- 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. ($f_{\text{in}}^{\text{out}}$, $\langle \text{lout}, \text{rout} || \text{lin}, \text{rin} \rangle$)
- 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.

CCSD energy equation

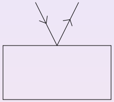
$$E_{CCSD} = f_a^i t_i^a + \frac{1}{4}\langle ij||ab\rangle t_{ij}^{ab} + \frac{1}{2}\langle ij||ab\rangle t_i^a t_j^b$$

Note the implicit sum over repeated indices.

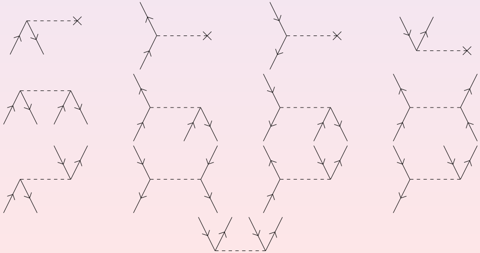
CCSD $\widehat{T}_1$ amplitude equation - Derivation

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

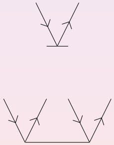
- One pair of particle/hole external lines.
- Final excitation level: +1



Elements: $\widehat{H}_N$



Elements: $\widehat{T}$



CCSD $\widehat{T}_1$ amplitude equation

$0 =$

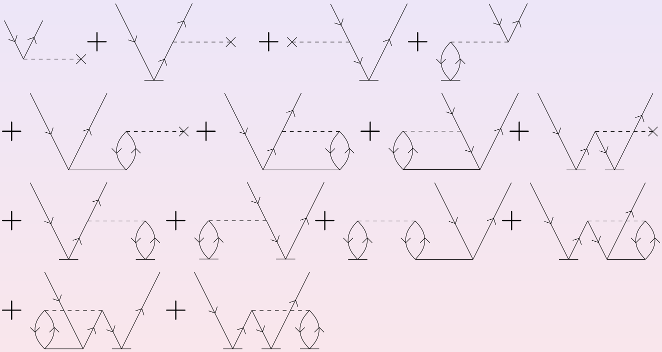


Diagram rules

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

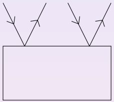
CCSD $\widehat{T}_1$ amplitude equation

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

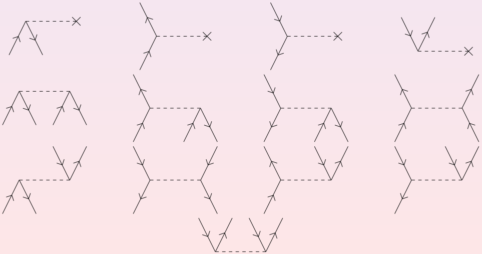
CCSD $\widehat{T}_2$ amplitude equation - Derivation

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

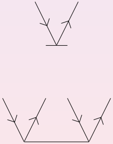
- Two pairs of particle/hole external lines.
- Final excitation level: +2



Elements: $\widehat{H}_N$



Elements: $\widehat{T}$



CCSD $\widehat{T}_2$ amplitude equation

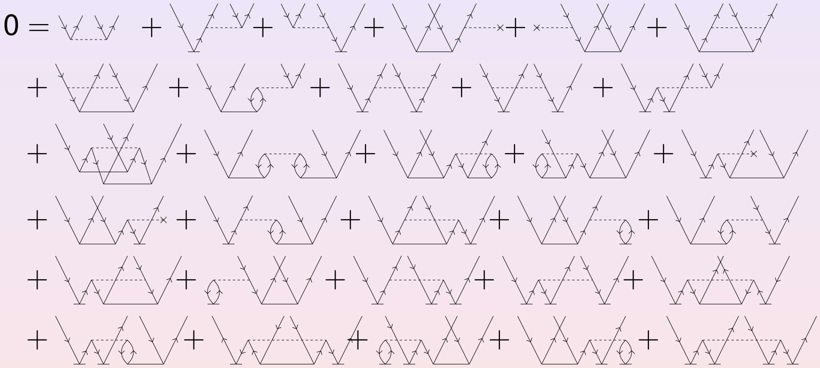


Diagram rules

- Label all lines.
- Sum over all internal indices.
- Extract matrix elements. ($f_{\text{in}}^{\text{out}}$, $\langle \text{lout}, \text{rout} || \text{lin}, \text{rin} \rangle$)
- 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.
- Antisymmetrize a pair of external particle/hole line that does not connect to the same operator.

Diagram rules

- Label all lines.
- Sum over all internal indices.
- Extract matrix elements. ($f_{\mathrm{in}}^{\mathrm{out}}$, $\langle \mathrm{lout}, \mathrm{rout} || \mathrm{lin}, \mathrm{rin} \rangle$)
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Diagram rules

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$- \delta_{pi}\delta_{qb}\left\{a_a^\dagger a_j\right\}$$

Inserted into the original expression, we arrive at

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

The CCSD energy equation revisited

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

The CCSD energy equation revisited

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

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

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

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

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

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

The CCSD energy equation revisited

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

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

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

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

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

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

The CCSD energy equation revisited

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

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

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

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

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

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

The CCSD energy equation revisited

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

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

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

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

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

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

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

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

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

The CCSD energy equation revisited

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

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

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

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

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

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

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

The CCSD energy equation revisited

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

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

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

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

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

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

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

The CCSD energy equation revisited

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

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

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

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

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

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

The CCSD energy equation revisited

- 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.
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The CCSD energy equation revisited

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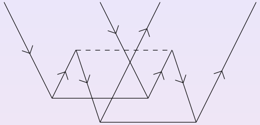
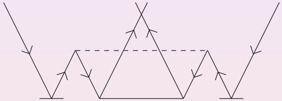
Factoring, motivation

Diagram (2.12)



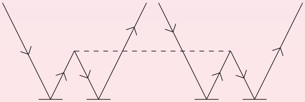
$$= \frac{1}{4}\langle mn||ef\rangle t_{ij}^{ef} t_{mn}^{ab}$$

Diagram (2.26)



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

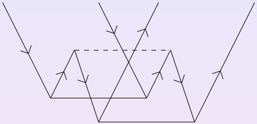
Diagram (2.31)



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

Factoring, motivation

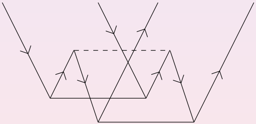
Diagram (2.12)



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

Diagram cost: $n_p^4 n_h^4$

Diagram (2.13) - Factored



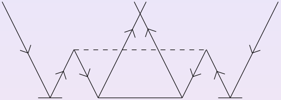
$$= \frac{1}{4}\langle mn||ef\rangle t_{ij}^{ef} t_{mn}^{ab}$$

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

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

Factoring, motivation

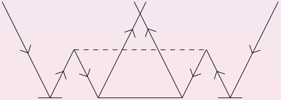
Diagram (2.26)



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

Diagram cost: $n_p^4 n_h^4$

Diagram (2.26) - Factored



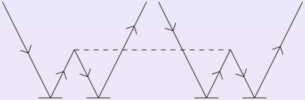
$$= \frac{1}{4} P(ij) \langle mn||ef \rangle t_i^e t_{mn}^{ab} t_j^f$$

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

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

Factoring, motivation

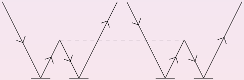
Diagram (2.31)



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

Diagram cost: $n_p^4 n_h^4$

Diagram (2.31) - Factored



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

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

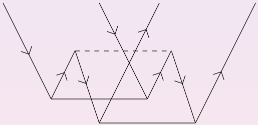
$$= \frac{1}{4} P(ij)P(ab) t_m^a t_n^b Y_{ij}^{mn}$$

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

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

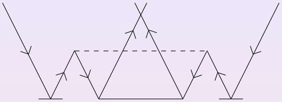


$$= \frac{1}{4}\langle mn||ef\rangle t_{ij}^{ef} t_{mn}^{ab}$$

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

Factoring, Classification

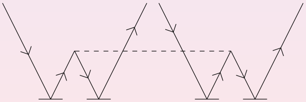
Diagram (2.26)



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

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

Diagram (2.31)



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

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

Factoring, Classification

Cost of making intermediates

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

Factoring, Classification

Classification of $\hat{T}_1$ diagrams

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

Factoring, Classification

Classification of $\hat{T}_2$ diagrams

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

Factoring, $T_2(h)$

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

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

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

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

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

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

Factored T_1 amplitude equations

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

Factored T_1 amplitude equations

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

Factored T_1 amplitude equations

Define

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

and we get the T_1 amplitude equations

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

Factored T_2 amplitude equations

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

Can be solved by

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

Factored T_2 amplitude equations

Similarily we define

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

and get the T_2 amplitude equations

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

Coupled Cluster algorithm

Setup modelspace
Calculate f and v amplitudes
$t_i^a \leftarrow 0$; $t_{ij}^{ab} \leftarrow 0$
$E \leftarrow 1$; $E_{old} \leftarrow 0$
$E_{ref} \leftarrow \sum_i \langle i|\widehat{t}|i\rangle + \frac{1}{2}\sum_{ij}\langle ij|\widehat{v}|ij\rangle$
while not converged ($E - E_{old} > \epsilon$)
  Calculate intermediates
  $t_i^a \leftarrow$ calculated value
  $t_{ij}^{ab} \leftarrow$ calculated value
  $E_{old} \leftarrow E$
  $E \leftarrow f_a^i t_i^a + \frac{1}{4}\langle ij||ab\rangle t_{ij}^{ab} + \frac{1}{2}\langle ij||ab\rangle t_i^a t_j^b$
end while
$E_{GS} \leftarrow E_{ref} + E$

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Coupled Cluster algorithm

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$t_i^a \leftarrow 0$; $t_{ij}^{ab} \leftarrow 0$
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  $t_{ij}^{ab} \leftarrow$ calculated value
  $E_{old} \leftarrow E$
  $E \leftarrow f_a^i t_i^a + \frac{1}{4}\langle ij||ab\rangle t_{ij}^{ab} + \frac{1}{2}\langle ij||ab\rangle t_i^a t_j^b$
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Coupled Cluster algorithm

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Calculate f and v amplitudes
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    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

Typical convergence of the T_2 amplitudes