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Notation

Antisymmetrized wavefunction

$$\Phi_{AS}(\alpha_1, \ldots, \alpha_A; \mathbf{x}_1, \ldots \mathbf{x}_A) = \frac{1}{\sqrt{A}} \sum_{\hat{P}} (-1)^P \hat{P} \prod_{i=1}^{A} \psi_{\alpha_i}(\mathbf{x}_i)$$

$$\equiv |\alpha_1 \ldots \alpha_A\rangle$$

$$= a_{\alpha_1}^\dagger \ldots a_{\alpha_A}^\dagger |0\rangle$$

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

$$\delta_{pq} = \left\{ a_p, a_q^\dagger \right\}$$

$$0 = \left\{ a_p^\dagger, a_q \right\} = \{a_p, a_q\} = \left\{ a_p^\dagger, a_q^\dagger \right\}$$

Notation
Second quantization, quasiparticles

Reference state

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

Creation and annihilation operators

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

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

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

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

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

Notation
Second quantization, operators

Normal ordered operators

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

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

$$\hat{H}_N = \frac{1}{36} \sum_{\substack{pqr \\ stu}} \langle pqr|\hat{v}_3|stu\rangle a_p^\dagger a_q^\dagger a_r^\dagger a_u a_t a_s \qquad + \frac{1}{4} \sum_{pqrs} \langle pq||rs\rangle a_p^\dagger a_q^\dagger a_s a_r + \sum_{pq} f_q^p a_p^\dagger$$

$$= \hat{H}_3^N + \hat{V}_N + \hat{F}_N$$

where

$$\hat{F}_N = \sum_{pq} f_q^p a_p^\dagger a_q \qquad \hat{V}_N = \frac{1}{4} \sum_{pqrs} \langle pq||rs\rangle a_p^\dagger a_q^\dagger a_s a_r$$

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

Definitions

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

$$\hat{H}_N = \hat{H} - E_0$$

$$E_0 = \langle\Phi_0|\hat{H}|\Phi_0\rangle$$

$$= \sum_i \langle i|\hat{h}_0|i\rangle + \frac{1}{2}\sum_{ij}\langle ij|\hat{v}|ij\rangle + \frac{1}{6}\sum_{ijk}\langle ijk|\hat{v}_3|ijk\rangle,$$

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

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

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

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

Derivation, onebody part

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

$$a_p^\dagger a_q = \left\{ a_p^\dagger a_q \right\} + \left\{ \overline{a_p^\dagger a_q} \right\} \qquad = \left\{ a_p^\dagger a_q \right\} + \delta_{pq\in i}$$

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

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

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

Derivation, twobody part

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

$$a_p^\dagger a_q^\dagger a_s a_r = a_p^\dagger a_q^\dagger a_s a_r \quad\quad + a_p^\dagger \overbrace{a_q^\dagger a_s} a_r + a_p^\dagger \overbrace{a_q^\dagger a_s a_r} + \overbrace{a_p^\dagger a_q^\dagger} a_s a_r \quad + \overbrace{a_p^\dagger a_q^\dagger a_s} a_r +$$

Derivation, twobody part

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

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Derivation, twobody part

$$\hat{H}_I = \frac{1}{4} \sum_{pqrs} \langle pq|\hat{v}|rs \rangle a_p^\dagger a_q^\dagger a_s a_r \quad = \frac{1}{4} \sum_{pqrs} \langle pq|\hat{v}|rs \rangle a_p^\dagger a_q^\dagger a_s a_r + \quad \frac{1}{4} \sum_{pqrs} \Big(\delta_{qs \in i} \langle pq$$

Derivation, twobody part

$$= \frac{1}{4} \sum_{pqrs} \langle pq|\hat{v}|rs\rangle a_p^\dagger a_q^\dagger a_s a_r \qquad + \frac{1}{4} \sum_{pqi} \Big(\langle pi|\hat{v}|qi\rangle - \langle pi|\hat{v}|iq\rangle - \langle ip|\hat{v}|qi\rangle + \langle ip|$$

Definitions
The basics, Normal ordered Hamiltonian

Derivation, twobody part
A twobody part

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

A onebody part

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

and a scalar part

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

Definitions

Twobody Hamiltonian

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

where

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

Definitions

Twobody Hamiltonian

The amplitudes are given by

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$$\hat{H}_N = \hat{H} - E_0$$

$$E_0 = \langle \Phi_0|\hat{H}|\Phi_0\rangle$$

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

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

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

$$E_{CCSD} = \qquad + \qquad +$$

Diagram rules

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

$$0 = \quad + \quad + \quad +$$
$$+ \quad + \quad + \quad +$$
$$+ \quad + \quad + \quad +$$
$$+ \quad +$$

Diagram rules

▶ Label all lines.

▶ Sum over all internal indices.

▶ Extract matrix elements. (f_{in}^{out}, $\langle lout, rout||lin, rin\rangle$)

▶ Extract cluster amplitudes with indices in the order left to right. Incoming lines are subscripts, while outgoing lines are superscripts. (t_{in}^{out}, $t_{lin,rin}^{lout,rout}$)

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

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

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- ▶ Calculate the phase: $(-1)^{\text{holelines+loops}}$
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CCSD $\widehat{T}_1$ amplitude equation

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

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

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

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

Elements: $\widehat{H}_N$

Elements: $\widehat{T}$

CCSD $\widehat{T}_2$ amplitude equation

$$0 = \qquad + \qquad + \qquad + \qquad + \qquad + \qquad +$$

Diagram rules

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

Diagram rules

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CCSD $\widehat{T}_2$ amplitude equation

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

The expansion

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$+ \overset{\frown}{a_p^\dagger a_q a_a^\dagger} a_i + a_p^\dagger \overset{\frown}{a_q a_a^\dagger} a_i$$

$$+ \overset{\frown}{a_p^\dagger a_q} \overset{\frown}{a_a^\dagger a_i}$$

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

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

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

Wicks theorem gives us

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Wicks theorem gives us

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

Inserted into the original expression, we arrive at

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

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

Wicks theorem gives us

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

Inserted into the original expression, we arrive at

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

The CCSD energy equation revisited

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

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

$$= 0$$

The CCSD energy equation revisited

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

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

$$= 0$$

The CCSD energy equation revisited

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

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

$$= 0$$

The CCSD energy equation revisited

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

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

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

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

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

$= \dfrac{1}{4} \sum\limits_{ijab} \langle ij||ab\rangle t_{ij}^{ab}$

The CCSD energy equation revisited

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

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

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

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

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

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

The CCSD energy equation revisited

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

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

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

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

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

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

The CCSD energy equation revisited

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

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

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

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

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

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

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

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

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

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

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

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

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

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

The CCSD energy equation revisited

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

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

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

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

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

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

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The CCSD energy equation revisited

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

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

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The CCSD energy equation revisited

▶ No contractions possible between cluster operators.

▶ Cluster operators need to contract with free indices to the left.

▶ Disconnected parts automatically cancel in the commutator.

▶ Onebody operators can connect to maximum two cluster operators.

▶ Twobody operators can connect to maximum four cluster operators.

▶ Different terms in the expansion contributes to different equations.

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Factoring, motivation

Diagram (2.12)

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

Diagram (2.26)

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

Diagram (2.31)

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

Factoring, motivation

Diagram (2.12)

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

Diagram cost: $n_p^4 n_h^4$

Diagram (2.13) - Factored

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

Factoring, motivation

Diagram (2.26)

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

Diagram cost: $n_p^4 n_h^4$

Diagram (2.26) - Factored

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

Factoring, motivation

Diagram (2.31)

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

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Diagram (2.31) - Factored

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

Factoring, Classification

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

Diagram (2.12) Classification

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

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

Factoring, Classification

Diagram (2.26)

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

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

Diagram (2.31)

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

Factoring, Classification

Cost of making intermediates

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

Factoring, Classification

Classification of $\hat{T}_1$ diagrams

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

Factoring, Classification

Classification of $\hat{T}_2$ diagrams

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

Factoring, $T_2(h)$

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

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

Factoring, $T_2(h^2)$

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

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

Factored T_1 amplitude equations

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

Can be solved by

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

Factored T_1 amplitude equations

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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

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

Factored T_2 amplitude equations

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

Can be solved by

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

Factored T_2 amplitude equations

Similarily we define

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

and get the T_2 amplitude equations

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

Coupled Cluster algorithm

7.7cm   Setup modelspace
Calculate f and v amplitudes
$$t_i^a \leftarrow 0; \; t_{ij}^{ab} \leftarrow 0$$
$$E \leftarrow 1; \; E_{old} \leftarrow 0$$
$$E_{ref} \leftarrow \sum_i \langle i | \hat{f} | i \rangle + \frac{1}{2} \sum_{ij} \langle ij | \hat{v} | ij \rangle$$
while not converged $(E - E_{old} > \epsilon)$
Calculate intermediates
$$t_i^a \leftarrow \text{calculated value}$$
$$t_{ij}^{ab} \leftarrow \text{calculated value}$$
$$E_{old} \leftarrow E$$
$$E \leftarrow f_a^i t_i^a + \frac{1}{4} \langle ij || ab \rangle t_{ij}^{ab} + \frac{1}{2} \langle ij || ab \rangle t_i^a t_j^b$$
end while
$$E_{GS} \leftarrow E_{ref} + E$$

Coupled Cluster algorithm

7.7cm   Setup modelspace

Calculate f and v amplitudes

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

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

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

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

     Calculate intermediates

     $t_i^a \leftarrow$ calculated value

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

     $E_{old} \leftarrow E$

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

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Coupled Cluster algorithm

Typical convergence of the T_2 amplitudes