Slides from FYS-KJM4480/9480 Lectures

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Configuration interaction (CI) theory

An alternative way to derive the last equation is to start from

$$(\hat{H} - E)|\Psi_0\rangle = (\hat{H} - E)\sum_{P'H'} C_{H'}^{P'}|\Phi_{H'}^{P'}\rangle = 0,$$

and if this equation is successively projected against all Φ_H^P in the expansion of Ψ, then the last equation on the previous slide results. As stated previously, one solves this equation normally by diagonalization. If we are able to solve this equation exactly (that is numerically exactly) in a large Hilbert space (it will be truncated in terms of the number of single-particle states included in the definition of Slater determinants), it can then serve as a benchmark for other many-body methods which approximate the correlation operator $\hat{C}$.

For reasons to come (link with Coupled-Cluster theory and Many-Body perturbation theory), we will rewrite Eq. (**??**) as a set of coupled non-linear equations in terms of the unknown coefficients C_H^P.

Configuration interaction (CI) theory

To see this, we look at $\langle \Phi_H^P| = \langle \Phi_0|$ in Eq. (**??**), that is we multiply with $\langle \Phi_0|$ from the left in

$$(\hat{H} - E) \sum_{P'H'} C_{H'}^{P'} |\Phi_{H'}^{P'}\rangle = 0,$$

and we assume that we have a two-body operator at most. Using Slater's rule gives then and equation for the correlation energy in terms of C_i^a and C_{ij}^{ab}. We get then

$$\langle \Phi_0|\hat{H} - E|\Phi_0\rangle + \sum_{ai} \langle \Phi_0|\hat{H} - E|\Phi_i^a\rangle C_i^a + \sum_{abij} \langle \Phi_0|\hat{H} - E|\Phi_{ij}^{ab}\rangle C_{ij}^{ab} = 0,$$

or

$$E - E_0 = \Delta E = \sum_{ai} \langle \Phi_0|\hat{H}|\Phi_i^a\rangle C_i^a + \sum_{abij} \langle \Phi_0|\hat{H}|\Phi_{ij}^{ab}\rangle C_{ij}^{ab},$$

where the E_0 is the reference energy and ΔE becomes the correlation energy. We have already computed the expectation values $\langle \Phi_0|\hat{H}|\Phi_i^a$ and $\langle \Phi_0|\hat{H}|\Phi_{ij}^{ab}\rangle$.

Configuration interaction (CI) theory

We can rewrite

$$E - E_0 = \Delta E = \sum_{ai} \langle \Phi_0 | \hat{H} | \Phi_i^a \rangle C_i^a + \sum_{abij} \langle \Phi_0 | \hat{H} | \Phi_{ij}^{ab} \rangle C_{ij}^{ab},$$

as

$$\Delta E = \sum_{ai} \langle i | \hat{f} | a \rangle C_i^a + \sum_{abij} \langle ij | \hat{v} | ab \rangle C_{ij}^{ab}.$$

This equation determines the correlation energy but not the coefficients C. We need more equations. Our next step is to set up

$$\langle \Phi_i^a | \hat{H} - E | \Phi_0 \rangle + \sum_{bj} \langle \Phi_i^a | \hat{H} - E | \Phi_j^b \rangle C_j^b + \sum_{bcjk} \langle \Phi_i^a | \hat{H} - E | \Phi_{jk}^{bc} \rangle C_{jk}^{bc} + \sum_{bcdjkl} \langle \Phi_i^a | \hat{H} - E | \Phi_{jkl}^{bcd} \rangle C_{jkl}^{bcd} = 0,$$

as this equation will allow us to find an expression for the coefficents C_i^a since we can rewrite this equation as

$$\langle i | \hat{f} | a \rangle + \langle \Phi_i^a | \hat{H} - E | \Phi_i^a \rangle C_i^a + \sum_{bj \neq ai} \langle \Phi_i^a | \hat{H} | \Phi_j^b \rangle C_j^b + \sum_{bcjk} \langle \Phi_i^a | \hat{H} | \Phi_{jk}^{bc} \rangle C_{jk}^{bc} + \sum_{bcdjkl} \langle \Phi_i^a | \hat{H} | \Phi_{jkl}^{bcd} \rangle C_{jkl}^{bcd} = 0.$$

Configuration interaction (CI) theory

We rewrite this equation as

$$C_i^a = -(\langle\Phi_i^a|\hat{H}-E|\Phi_i^a\rangle)^{-1}\left(\langle i|\hat{f}|a\rangle + \sum_{bj\neq ai}\langle\Phi_i^a|\hat{H}|\Phi_j^b\rangle C_j^b + \dots\right.$$

$$\left.\dots\sum_{bcjk}\langle\Phi_i^a|\hat{H}|\Phi_{jk}^{bc}\rangle C_{jk}^{bc} + \sum_{bcdjkl}\langle\Phi_i^a|\hat{H}|\Phi_{jkl}^{bcd}\rangle C_{jkl}^{bcd}\right).$$

Since these equations are solved iteratively (that is we can start with a guess for the coefficients C_i^a), it is common to start the iteration by setting

$$C_i^a = -\frac{\langle i|\hat{f}|a\rangle}{\langle\Phi_i^a|\hat{H}-E|\Phi_i^a\rangle},$$

and the denominator can be written as

$$C_i^a = \frac{\langle i|\hat{f}|a\rangle}{\langle i|\hat{f}|i\rangle - \langle a|\hat{f}|a\rangle + \langle ai|\hat{v}|ai\rangle - E}.$$

The observant reader will however see that we need an equation for C_{jk}^{bc} and C_{jkl}^{bcd} as well. To find equations for these coefficients we need then to continue our multiplications from the left with the various Φ_H^P terms.

Configuration interaction (CI) theory

For C_{jk}^{bc} we need then

$$\langle\Phi_{ij}^{ab}|\hat{H}-E|\Phi_0\rangle+\sum_{kc}\langle\Phi_{ij}^{ab}|\hat{H}-E|\Phi_k^c\rangle C_k^c+\sum_{cdkl}\langle\Phi_{ij}^{ab}|\hat{H}-E|\Phi_{kl}^{cd}\rangle C_{kl}^{cd}+$$

$$\sum_{cdeklm}\langle\Phi_{ij}^{ab}|\hat{H}-E|\Phi_{klm}^{cde}\rangle C_{klm}^{cde}+\sum_{cdefklmn}\langle\Phi_{ij}^{ab}|\hat{H}-E|\Phi_{klmn}^{cdef}\rangle C_{klmn}^{cdef}=0,$$

and we can isolate the coefficients C_{kl}^{cd} in a similar way as we did for the coefficients C_i^a. At the end we can rewrite our solution of the Schrödinger equation in terms of n coupled equations for the coefficients C_H^P. This is a very cumbersome way of solving the equation. However, by using this iterative scheme we can illustrate how we can compute the various terms in the wave operator or correlation operator $\hat{C}$. We will later identify the calculation of the various terms C_H^P as parts of different many-body approximations to full CI. In particular, we will relate this non-linear scheme with Coupled Cluster theory and many-body perturbation theory.

Configuration interaction (CI) theory

If we use a Hartree-Fock basis, how can one simplify the equation

$$\Delta E = \sum_{ai} \langle i|\hat{f}|a\rangle C_i^a + \sum_{abij} \langle ij|\hat{v}|ab\rangle C_{ij}^{ab}?$$

And what about

$$\langle \Phi_i^a|\hat{H}-E|\Phi_0\rangle + \sum_{bj} \langle \Phi_i^a|\hat{H}-E|\Phi_j^b\rangle C_j^b + \sum_{bcjk} \langle \Phi_i^a|\hat{H}-E|\Phi_{jk}^{bc}\rangle C_{jk}^{bc} + \sum_{bcdjkl} \langle \Phi_i^a|\hat{H}-E|\Phi_{jkl}^{bcd}\rangle C_{jkl}^{bcd} = 0,$$

and

$$\langle \Phi_{ij}^{ab}|\hat{H}-E|\Phi_0\rangle + \sum_{kc} \langle \Phi_{ij}^{ab}|\hat{H}-E|\Phi_k^c\rangle C_k^c + \sum_{cdkl} \langle \Phi_{ij}^{ab}|\hat{H}-E|\Phi_{kl}^{cd}\rangle C_{kl}^{cd} +$$

$$\sum_{cdeklm} \langle \Phi_{ij}^{ab}|\hat{H}-E|\Phi_{klm}^{cde}\rangle C_{klm}^{cde} + \sum_{cdefklmn} \langle \Phi_{ij}^{ab}|\hat{H}-E|\Phi_{klmn}^{cdef}\rangle C_{klmn}^{cdef} = 0?$$

Diagram rules

- Draw all topologically distinct diagrams by linking up particle and hole lines with various interaction vertices. Two diagrams can be made topologically equivalent by deformation of fermion lines under the restriction that the ordering of the vertices is not changed and particle lines and hole lines remain particle and hole lines.
- For the explicit evaluation of a diagram: Sum freely over all internal indices and label all lines.
- Extract matrix elements for the one-body operators (if present) as $\langle \mathrm{out}|\hat{f}|\mathrm{in}\rangle$ and for the two-body operator (if present) as $\langle \mathrm{left\ out}, \mathrm{right\ out}||\hat{v}||\mathrm{left\ in}, \mathrm{right\ in}\rangle$.

Diagram rules

- Calculate the phase factor: $(-1)^{\mathrm{holelines}+\mathrm{loops}}$
- Multiply by a factor of $\frac{1}{2}$ for each equivalent pair of lines (particle lines or hole lines) that begin at the same interaction vertex and end at the same (yet different from the first) interaction vertex.
- For each interval between successive interaction vertices with minimum one single-particle state above the Fermi level with n hole states and m particle states there is a factor

$$\frac{1}{\sum_i^n \epsilon_i - \sum_a^m \epsilon_a}.$$

CCSD with twobody Hamiltonian

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

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

where

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

CCSD with twobody Hamiltonian cont.

Normal ordered Hamiltonian

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

where

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

Diagram equations - Derivation

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

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

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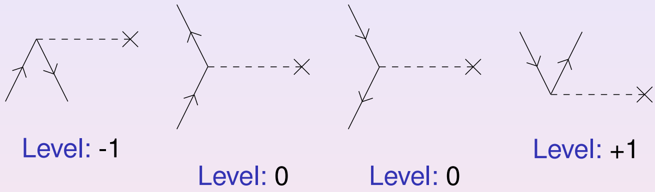
Diagram elements - Directed lines

Figure: Particle line

Figure: Hole line

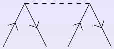
- Represents a contraction between second quantized operators.
- External lines are connected to one operator vertex and infinity.
- Internal lines are connected to operator vertices in both ends.

Diagram elements - Onebody Hamiltonian



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

Diagram elements - Twobody Hamiltonian



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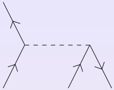

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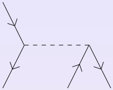

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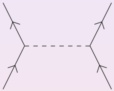

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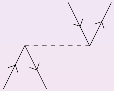

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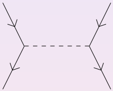

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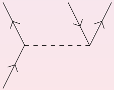
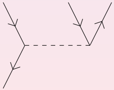


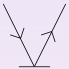
Level: +1



Level: +1

Level: +2

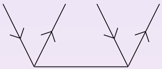
Diagram elements - Onebody cluster operator



Level: +1

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

Diagram elements - Twobody cluster operator



Level: +2

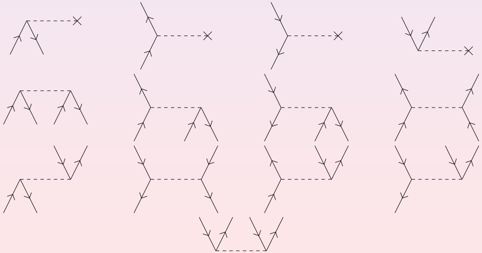
- Horisontal line segment with two vertices.
- Excitation level of +2.

CCSD energy equation - Derivation

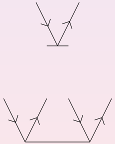
$$\mathrm{E}_{\mathrm{CCSD}} = \langle \Phi_0 | | \Phi_0 \rangle$$

- No external lines.
- Final excitation level: 0

Elements: $\widehat{H}_N$



Elements: $\widehat{T}$



CCSD energy equation

$$E_{CCSD} =$$

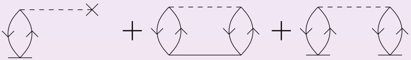


Diagram rules

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

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CCSD energy equation

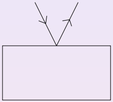
$$E_{CCSD} = f_a^i t_i^a + \frac{1}{4}\langle ij||ab\rangle t_{ij}^{ab} + \frac{1}{2}\langle ij||ab\rangle t_i^a t_j^b$$

Note the implicit sum over repeated indices.

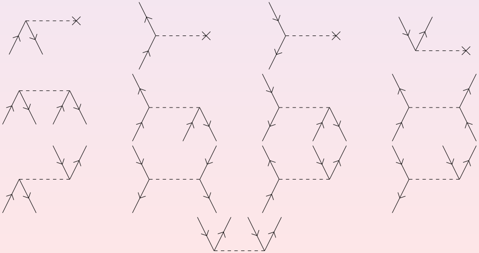
CCSD $\widehat{T}_1$ amplitude equation - Derivation

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

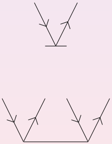
- One pair of particle/hole external lines.
- Final excitation level: +1



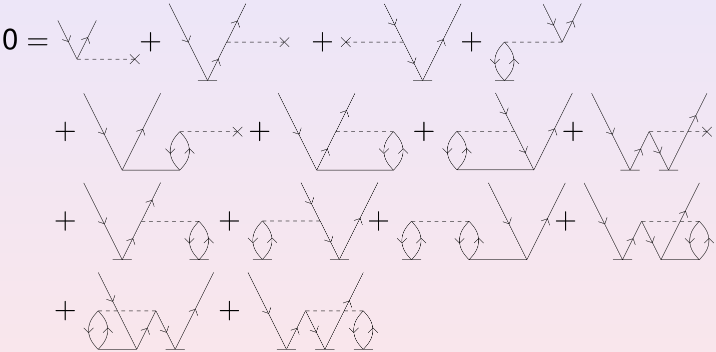
Elements: $\widehat{H}_N$



Elements: $\widehat{T}$



CCSD $\widehat{T}_1$ amplitude equation



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- Calculate the phase: $(-1)^{\mathrm{holelines+loops}}$
- Multiply by a factor of $\frac{1}{2}$ for each equivalent line and each ecuivalent vertex.

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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.

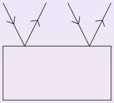
CCSD $\widehat{T}_1$ amplitude equation

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

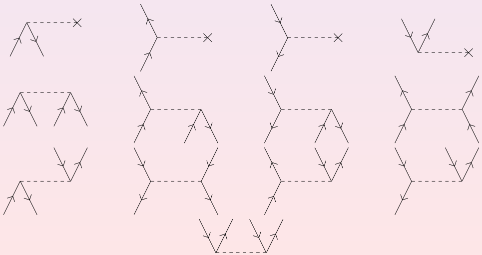
CCSD $\widehat{T}_2$ amplitude equation - Derivation

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

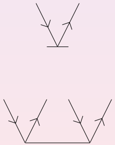
- Two pairs of particle/hole external lines.
- Final excitation level: +2



Elements: $\widehat{H}_N$



Elements: $\widehat{T}$



CCSD $\widehat{T}_2$ amplitude equation

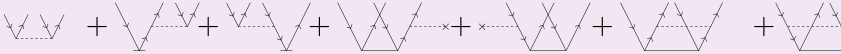
$0 =$ 

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

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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.
- Antisymmetrize a pair of external particle/hole line that does not connect to the same operator.

CCSD $\widehat{T}_2$ amplitude equation

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

The expansion

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

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

The CCSD energy equation revisited

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

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

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

The first term is zero by construction.

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

The CCSD energy equation revisited.

The second term can be split up into different pieces

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Wicks theorem gives us

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Wicks theorem gives us

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

Inserted into the original expression, we arrive at

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

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

Wicks theorem gives us

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

Inserted into the original expression, we arrive at

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

The CCSD energy equation revisited

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

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

$$= 0$$

The CCSD energy equation revisited

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

The CCSD energy equation revisited

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

The CCSD energy equation revisited

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

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

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

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

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

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

The CCSD energy equation revisited

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

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

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

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

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

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

The CCSD energy equation revisited

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

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

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

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

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

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

The CCSD energy equation revisited

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

The CCSD energy equation revisited

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

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

The CCSD energy equation revisited

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

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

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

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

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

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

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

The CCSD energy equation revisited

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

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

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

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

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

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

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The CCSD energy equation revisited

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

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The CCSD energy equation revisited

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

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

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

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

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

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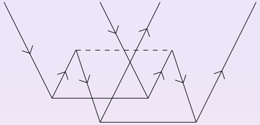
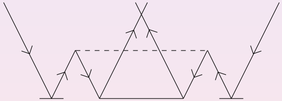
Factoring, motivation

Diagram (2.12)



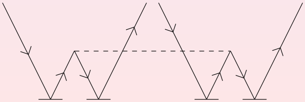
$$= \frac{1}{4}\langle mn||ef\rangle t_{ij}^{ef} t_{mn}^{ab}$$

Diagram (2.26)



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

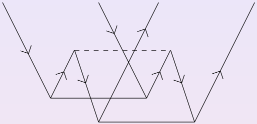
Diagram (2.31)



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

Factoring, motivation

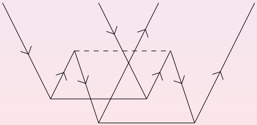
Diagram (2.12)



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

Diagram cost: $n_p^4 n_h^4$

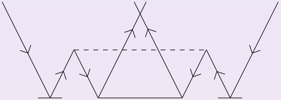
Diagram (2.13) - Factored



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

Factoring, motivation

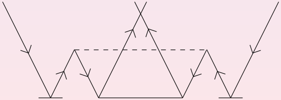
Diagram (2.26)



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

Diagram cost: $n_p^4 n_h^4$

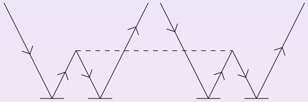
Diagram (2.26) - Factored



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

Factoring, motivation

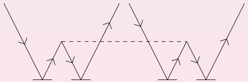
Diagram (2.31)



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

Diagram cost: $n_p^4 n_h^4$

Diagram (2.31) - Factored

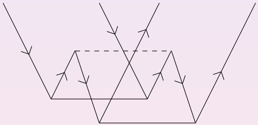


$$= \frac{1}{4} P(ij)P(ab)\langle mn||ef\rangle t_i^e t_m^a t_j^f t_n^b \quad = \frac{1}{4} P(ij)P(ab) t_m^a t_n^b t_i^e X_{ej}^{mn} =$$

Factoring, Classification

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

Diagram (2.12) Classification

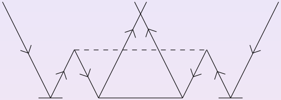


$$= \frac{1}{4}\langle mn||ef\rangle t_{ij}^{ef} t_{mn}^{ab}$$

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

Factoring, Classification

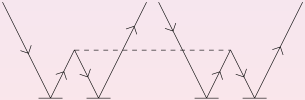
Diagram (2.26)



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

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

Diagram (2.31)



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

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

Factoring, Classification

Cost of making intermediates

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

Factoring, Classification

Classification of $\hat{T}_1$ diagrams

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

Factoring, Classification

Classification of $\hat{T}_2$ diagrams

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

Factoring, $T_2(h)$

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

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

Factoring, $T_2(h^2)$

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

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

Factored T_1 amplitude equations

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

Can be solved by

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

Factored T_1 amplitude equations

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

Factored T_1 amplitude equations

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Factored T_1 amplitude equations

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Factored T_1 amplitude equations

Define

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

and we get the T_1 amplitude equations

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

Factored T_2 amplitude equations

$$
\begin{aligned}
0 = {} & \langle ab||ij\rangle + \frac{1}{2}\langle ab||ef\rangle t_{ij}^{ef} - P(ij)t_{im}^{ab}(\bar{\mathrm{H}}3)_j^m + \frac{1}{2}t_{mn}^{ab}(\bar{\mathrm{H}}9)_{ij}^{mn} \\
& + P(ab)t_{ij}^{ae}(\bar{\mathrm{H}}2)_e^b + P(ij)P(ab)t_{im}^{ae}(\mathrm{I10c})_{ej}^{mb} - P(ab)t_m^a(\mathrm{I12a})_{ij}^{mb} \\
& + P(ij)t_i^e(\mathrm{I}11a)_{ej}^{ab}
\end{aligned}
$$

Can be solved by

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

Factored T_2 amplitude equations

Similarily we define

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

and get the T_2 amplitude equations

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

Coupled Cluster algorithm

7.7cm Setup modelspace

Calculate f and v amplitudes

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

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

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

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

Calculate intermediates

$t_i^a \leftarrow$ calculated value

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

$E_{old} \leftarrow E$

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

end while

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

Coupled Cluster algorithm

7.7cm Setup modelspace

Calculate f and v amplitudes

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

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

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

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Calculate intermediates

$t_i^a \leftarrow$ calculated value

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$E_{old} \leftarrow E$

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

end while

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Coupled Cluster algorithm

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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

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

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

Calculate intermediates

$t_i^a \leftarrow$ calculated value

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

$E_{old} \leftarrow E$

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

end while

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

Coupled Cluster algorithm

7.7cm Setup modelspace

Calculate f and v amplitudes

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

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

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

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

Calculate intermediates

$t_i^a \leftarrow$ calculated value

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

$E_{old} \leftarrow E$

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

end while

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

Coupled Cluster algorithm

7.7cm Setup modelspace

Calculate f and v amplitudes

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

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

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

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

Calculate intermediates

$t_i^a \leftarrow$ calculated value

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

$E_{old} \leftarrow E$

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

end while

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

Coupled Cluster algorithm

7.7cm Setup modelspace

Calculate f and v amplitudes

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

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

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

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

Calculate intermediates

$t_i^a \leftarrow$ calculated value

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

$E_{old} \leftarrow E$

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

end while

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

Coupled Cluster algorithm

Typical convergence of the T_2 amplitudes