

# Week 46: Many-body perturbation theory and start Coupled Cluster theory

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Week 46, November 10-14

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# Week 46, November 10-14, 2025

## Thursday:

1. Linked and unlinked diagrams, Linked diagram theorem and diagram rules, summary

2. Start coupled cluster theory

3. Second midterm at

<https://github.com/ManyBodyPhysics/FYS4480/blob/>

4. Video of lecture at [https://youtu.be/x9kJ\\_o9exLM](https://youtu.be/x9kJ_o9exLM)

5. Whiteboard notes at

<https://github.com/ManyBodyPhysics/FYS4480/blob/>

# Friday's lecture

## Friday:

1. Presentation and discussion of second midterm
2. Coupled Cluster theory
3. Video of lecture at [https://youtu.be/KvM0vCI\\_8HU](https://youtu.be/KvM0vCI_8HU)
4. Whiteboard notes at <https://github.com/ManyBodyPhysics/FYS4480/blob/>
5. Relevant reading for the lectures: Shavitt and Bartlett chapters 6 and 7 on linked and unlinked diagrams. For coupled cluster theory chapter 9 is the most relevant one. The lectures follow to a large extent the material covered in these chapters.

# Definitions

The basics, Normal ordered Hamiltonian

## Twobody Hamiltonian

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

where

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

# Definitions

## The basics, Normal ordered Hamiltonian

### Twobody Hamiltonian

The amplitudes are given by

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

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

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

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

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

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

where  $E_0$  is the energy expectation value between reference states.

# CCSD with twobody Hamiltonian

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

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

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

$$\begin{aligned}\hat{H} &= \sum_{pq} f_q^p \left\{ a_p^\dagger a_q \right\} + \frac{1}{4} \sum_{pqrs} \langle pq | \hat{v} | rs \rangle \left\{ a_p^\dagger a_q^\dagger a_s a_r \right\} \\ &\quad + E_0 \\ &= \hat{F}_N + \hat{V}_N + E_0 = \hat{H}_N + E_0\end{aligned}$$

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

$$\begin{aligned}f_q^p &= \langle p | \hat{h}_0 | q \rangle + \sum_i \langle pi | \hat{v} | qi \rangle \\ \langle pq || rs \rangle &= \langle pq | \hat{v} | rs \rangle \\ E_0 &= \sum_i \langle i | \hat{h}_0 | i \rangle + \frac{1}{2} \sum_{ij} \langle ij | \hat{v} | ij \rangle\end{aligned}$$

# Diagram equations - Derivation

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

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



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# Diagram elements - Directed lines



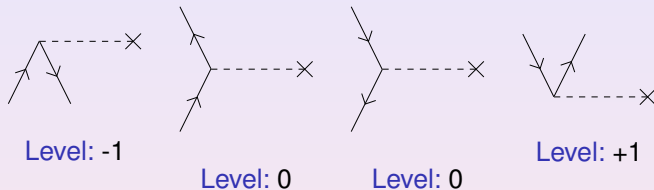
Figure: Particle line



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



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

# Diagram elements - Twobody Hamiltonian



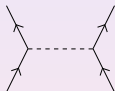
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Level: -1



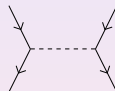
Level: -1



Level: 0



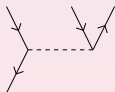
Level: 0



Level: 0



Level: +1



Level: +1



Level: +2

# Diagram elements - Onebody cluster operator



Level: +1

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



# Diagram elements - Twobody cluster operator



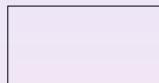
Level: +2

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

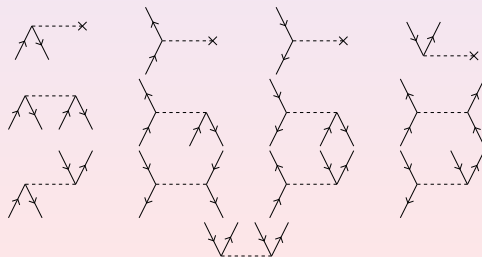
# CCSD energy equation - Derivation

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

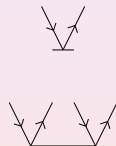
- ▶ No external lines.
- ▶ Final excitation level: 0



Elements:  $\hat{H}_N$



Elements:  $\hat{T}$



# CCSD energy equation

$$E_{CCSD} = \text{[Diagram 1]} + \text{[Diagram 2]} + \text{[Diagram 3]}$$

The equation represents the CCSD energy equation using Feynman diagrams. The first term is a diagram with a horizontal line at the bottom, a vertical line on the left, and a dashed line on the right ending in an 'x'. The second term is a diagram with two vertical lines on the left and two on the right, connected by a horizontal line at the bottom and a dashed line at the top. The third term is a diagram with two vertical lines on the left and two on the right, connected by a dashed line at the top.

# Diagram rules

- ▶ Label all lines.
- ▶ Sum over all internal indices.
- ▶ Extract matrix elements.  $(f_{\text{in}}^{\text{out}}, \langle l_{\text{out}}, r_{\text{out}} || l_{\text{in}}, r_{\text{in}} \rangle)$
- ▶ 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 equivalent vertex.

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# CCSD energy equation

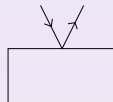
$$E_{CCSD} = f_a^i t_i^a + \frac{1}{4} \langle ij || ab \rangle t_{ij}^{ab} + \frac{1}{2} \langle ij || ab \rangle t_i^a t_j^b$$

Note the implicit sum over repeated indices.

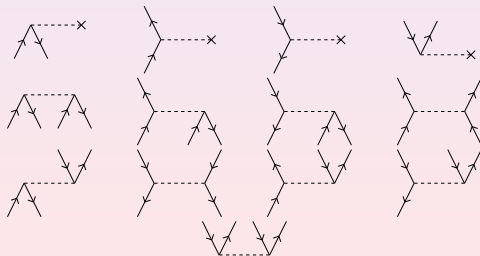
# CCSD $\hat{T}_1$ amplitude equation - Derivation

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

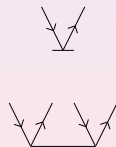
- ▶ One pair of particle/hole external lines.
- ▶ Final excitation level: +1



Elements:  $\hat{H}_N$



Elements:  $\hat{T}$



# CCSD $\hat{T}_1$ amplitude equation

$$0 =$$

The equation is represented as a sum of 16 Feynman diagrams arranged in four rows:

- Row 1: 4 diagrams. The first three show a single excitation (dashed line with 'x') interacting with a double excitation (two solid lines with arrows). The fourth shows a double excitation with a self-energy loop (a dashed line with a circle).
- Row 2: 4 diagrams. The first three show a double excitation with a self-energy loop. The fourth shows a double excitation with a double excitation (two dashed lines with 'x' marks).
- Row 3: 4 diagrams. The first three show a double excitation with a self-energy loop. The fourth shows a double excitation with a double excitation (two dashed lines with 'x' marks).
- Row 4: 2 diagrams. Both show a double excitation with a double excitation (two dashed lines with 'x' marks).

# Diagram rules

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

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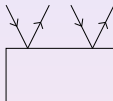
# CCSD $\hat{T}_1$ amplitude equation

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

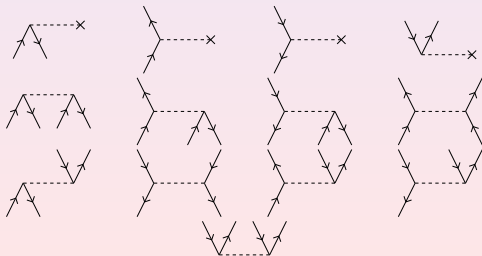
# CCSD $\hat{T}_2$ amplitude equation - Derivation

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

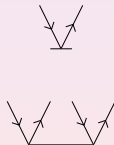
- ▶ Two pairs of particle/hole external lines.
- ▶ Final excitation level: +2



Elements:  $\hat{H}_N$



Elements:  $\hat{T}$



# CCSD $\hat{T}_2$ amplitude equation

$$\begin{aligned}
 0 = & \text{diagram 1} + \text{diagram 2} + \text{diagram 3} + \text{diagram 4} \times + \times \text{diagram 5} + \text{diagram 6} \\
 & + \text{diagram 7} + \text{diagram 8} + \text{diagram 9} + \text{diagram 10} + \text{diagram 11} \\
 & + \text{diagram 12} + \text{diagram 13} + \text{diagram 14} + \text{diagram 15} + \text{diagram 16} \times \\
 & + \text{diagram 17} \times + \text{diagram 18} + \text{diagram 19} + \text{diagram 20} + \text{diagram 21} \\
 & + \text{diagram 22} + \text{diagram 23} + \text{diagram 24} + \text{diagram 25} + \text{diagram 26} \\
 & + \text{diagram 27} + \text{diagram 28} + \text{diagram 29} + \text{diagram 30} + \text{diagram 31}
 \end{aligned}$$

The diagrams represent various terms in the CCSD  $\hat{T}_2$  amplitude equation, showing different topologies of electron interactions (solid lines) and virtual excitations (dashed lines) between occupied and virtual orbitals. Some terms are marked with a cross (x) to indicate they are zero due to orbital orthogonality or other symmetry constraints.

# 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.  $(t_{\text{in}}^{\text{out}}, t_{\text{lin, rin}}^{\text{lout, rout}})$
- ▶ 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.

# CCSD $\hat{T}_2$ amplitude equation

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