

diagrams pt. 2

# Coefficient Graphs

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$\sim_{ij}$   
 $a_{ab}$

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(bare excitation operator)

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Try it out!

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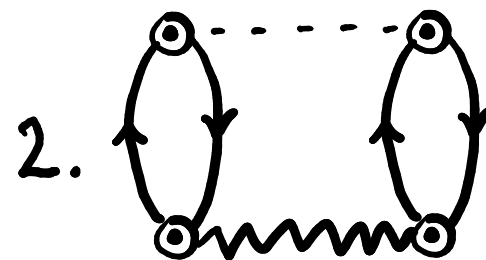
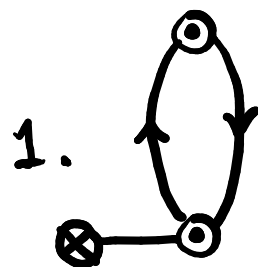
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interaction tensor

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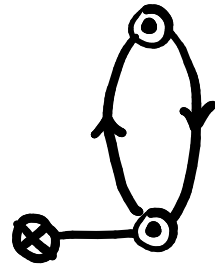
## notation

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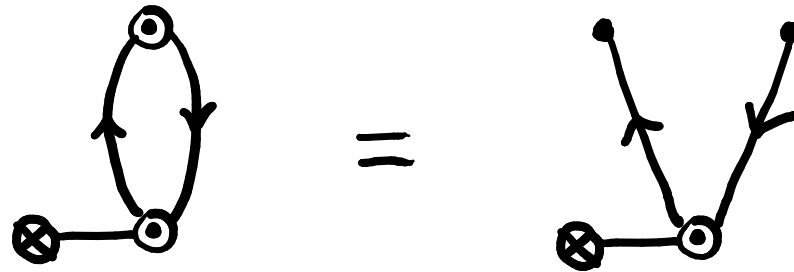
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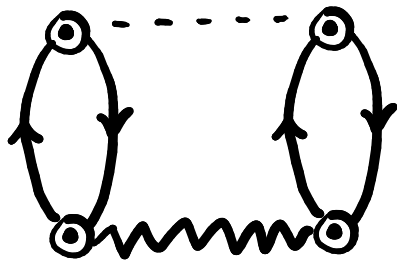
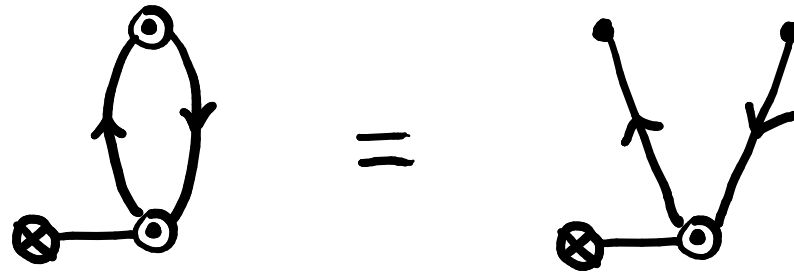
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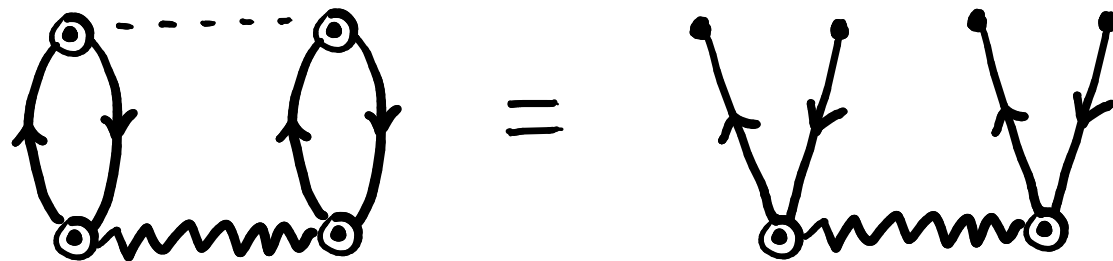
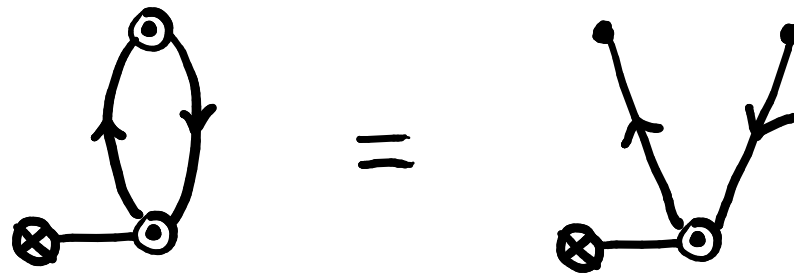
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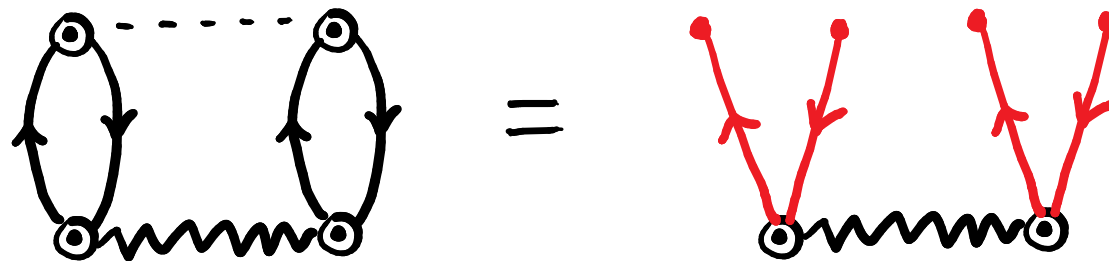
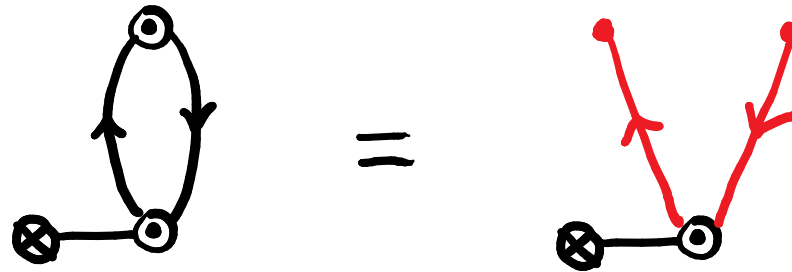
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notation



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coefficient lines

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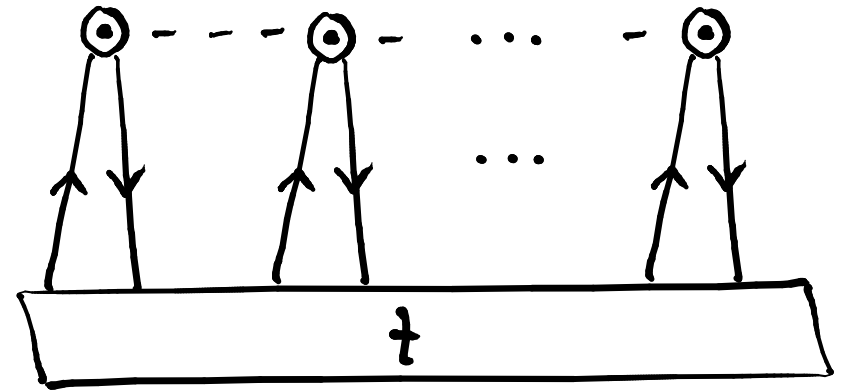
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useful result:

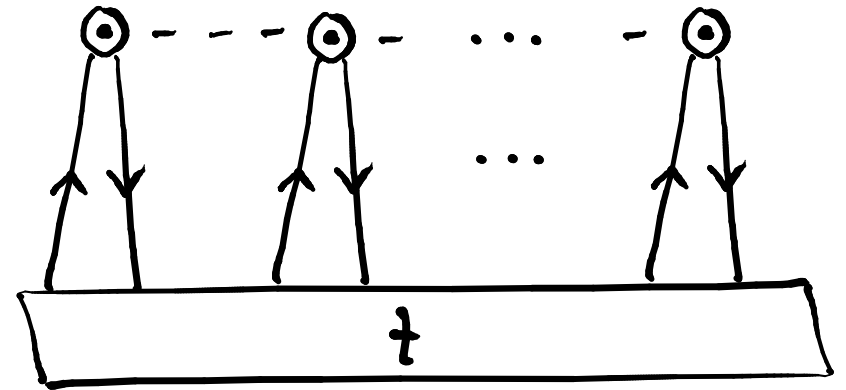
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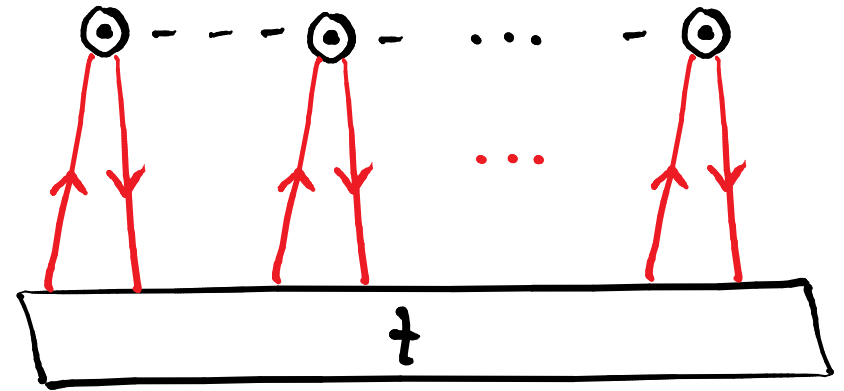
useful result:



$$\frac{1}{|P_1|! \cdots |P_h|! |Q_1|! \cdots |Q_k|!} \hat{P}^{(p_1/\cdots/p_m)}_{(q_1/\cdots/q_m)} t^{p_1 \cdots p_m}_{q_1 \cdots q_m}$$

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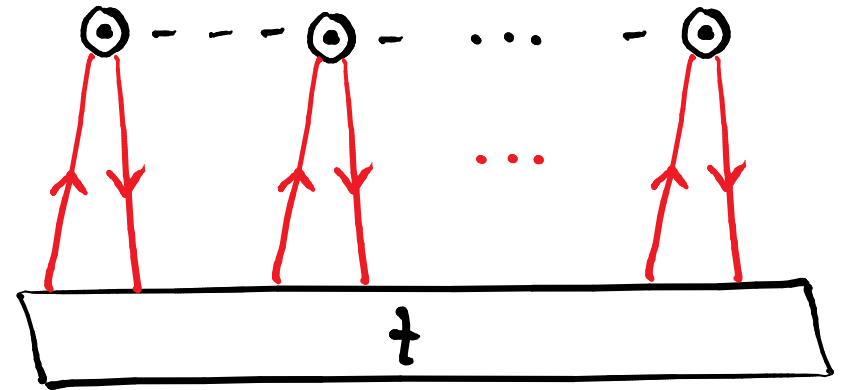
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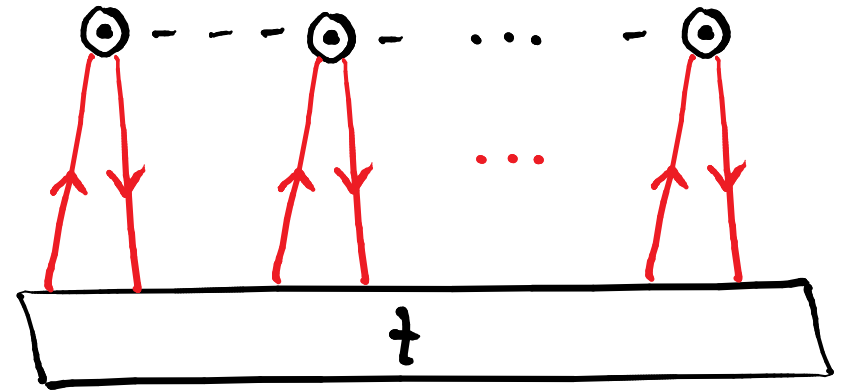
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↓  
equiv. coeff lines  
factor

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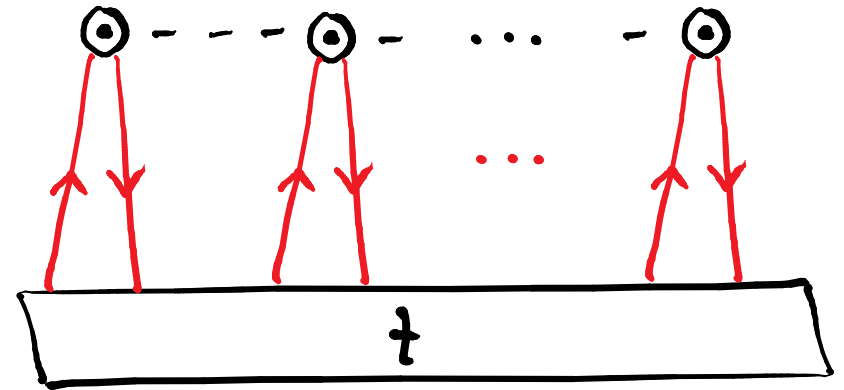
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$$\frac{1}{|P_1|! \cdots |P_n|! |Q_1|! \cdots |Q_k|!} \hat{P}_{(p_1/\cdots/p_m)}^{(q_1/\cdots/q_m)} t_{q_1 \cdots q_m}^{p_1 \cdots p_m} = \hat{P}_{(Q_1/\cdots/Q_k)}^{(P_1/\cdots/P_n)} t_{q_1 \cdots q_m}^{p_1 \cdots p_m}$$

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↓  
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factor

↓  
antisymmetrize  
inequiv. coeff lines

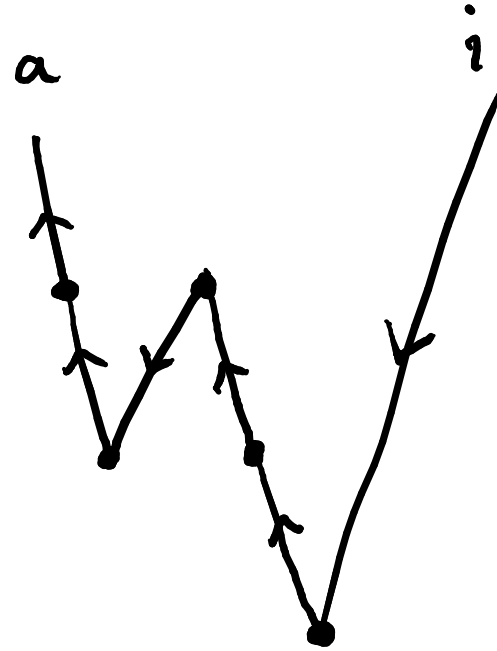
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$$1. \text{ open cycle} = (-)^n a_q^p$$

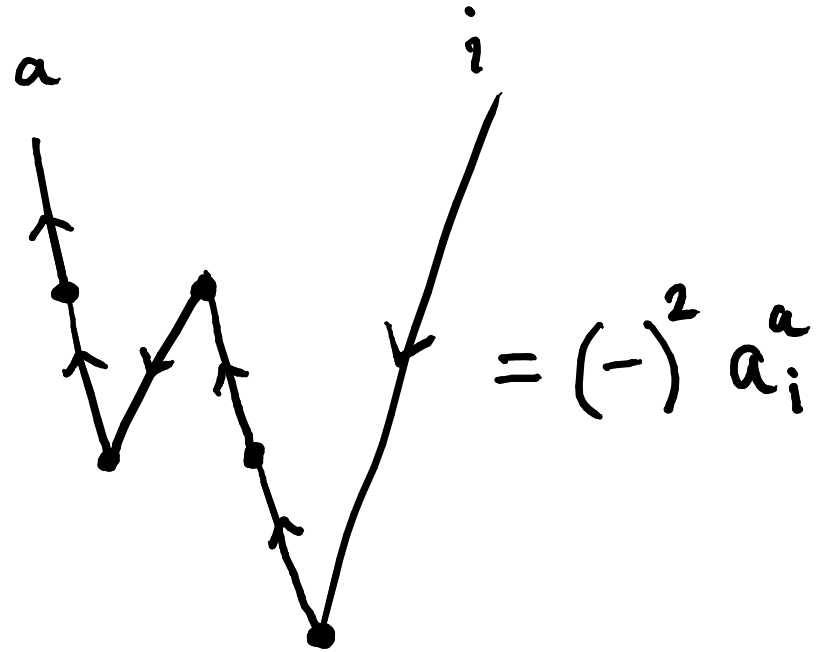
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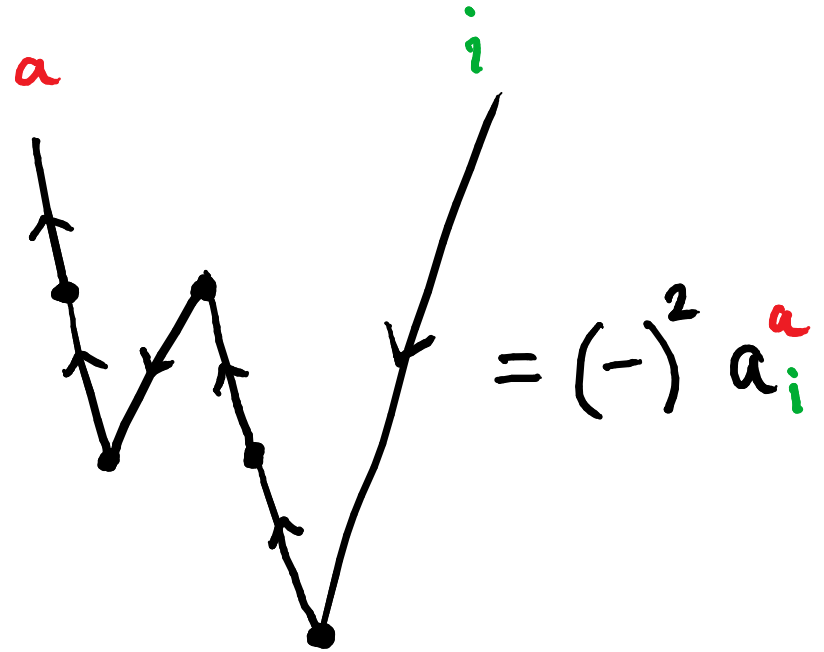
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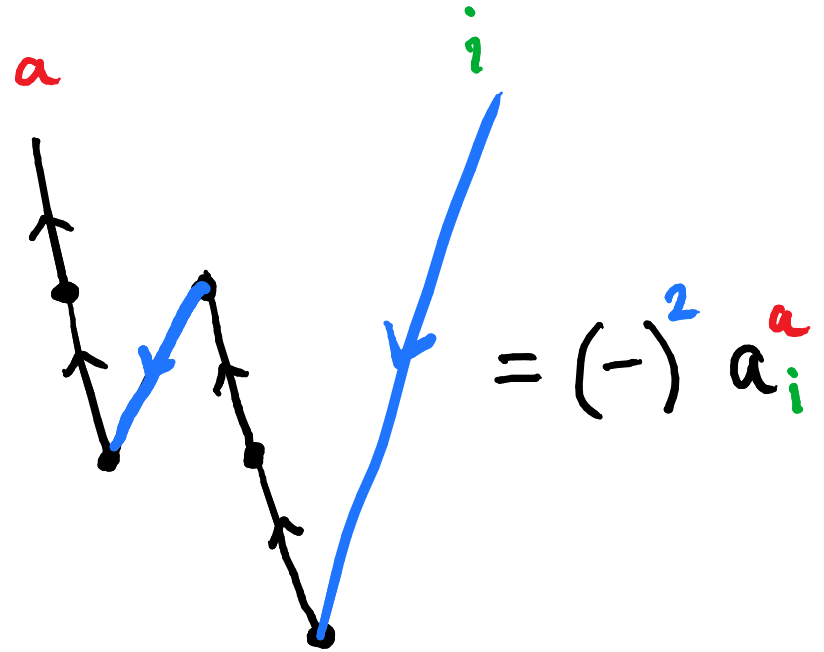
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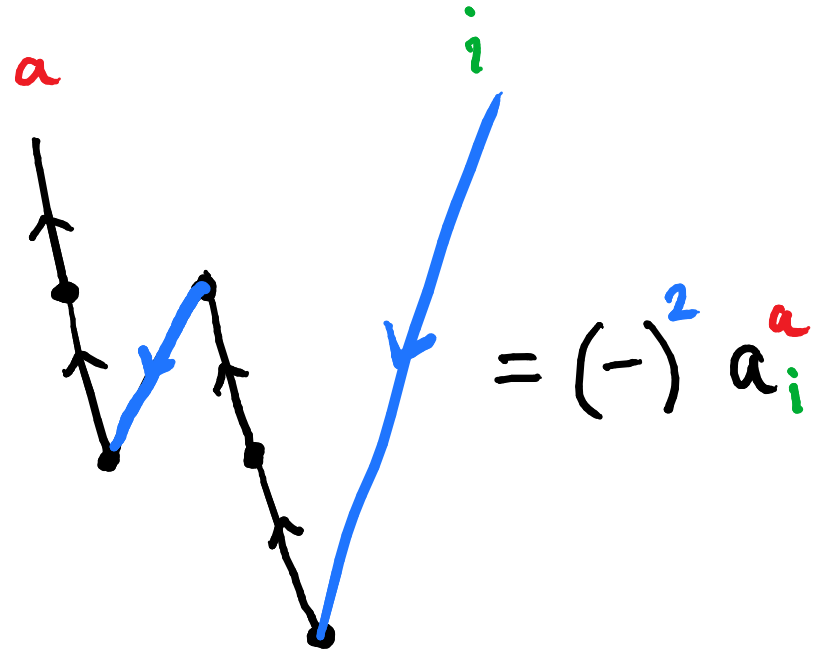
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2. loop =  $(-)^{h+1}$

Wick's Thm for Graphs:

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# Wick's Thm for Graphs:

$$G = :G: + \underbrace{\sum_c^{ctr(G)} :c(G):}_{\text{unique graph contractions}}$$

CID/CCD

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 $+ \frac{1}{2} \langle \Phi_{ij}^{ab} | H_c c_2^2 | \Phi \rangle$

CID / CCD energy

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$E_c$



CID / CCD energy

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CID / CCD energy

$$E_c = \langle \Phi | H_c (1 + C_2) | \Phi \rangle = \frac{\left( \begin{array}{c} \text{diagram 1} + \text{diagram 2} \end{array} \right)}{\left( 1 + \text{diagram 3} \right)}$$

The equation shows the calculation of the correlation energy  $E_c$  using the Coupled Cluster Doubles (CCD) method. The numerator represents the expectation value of the cluster operator  $C_2$  with the Hamiltonian  $H_c$  and the reference state  $\Phi$ . The denominator represents the norm of the wavefunction  $(1 + C_2)|\Phi\rangle$ .

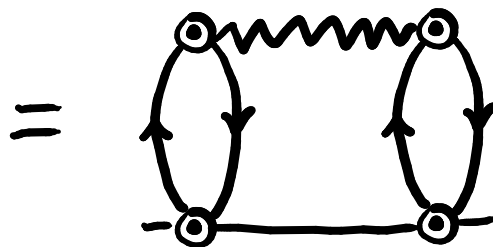
The diagrams are as follows:

- Diagram 1:** A diagram representing the first term in the numerator, showing a double excitation from the reference state  $\Phi$  to a virtual state. It consists of a circle with a cross (representing a virtual orbital) and a circle with a dot (representing an occupied orbital), connected by a horizontal line. Above the circle with a dot are two upward arrows, and below it are two downward arrows.
- Diagram 2:** A diagram representing the second term in the numerator, showing a double excitation from the reference state  $\Phi$  to a virtual state. It consists of a circle with a cross and a circle with a dot, connected by a horizontal line. Above the circle with a dot are two upward arrows, and below it are two downward arrows. A wavy line connects the two circles.
- Diagram 3:** A diagram representing the third term in the denominator, showing a double excitation from the reference state  $\Phi$  to a virtual state. It consists of a circle with a cross and a circle with a dot, connected by a horizontal line. Above the circle with a dot are two upward arrows, and below it are two downward arrows. A wavy line connects the two circles.

CID / CCD energy

$$E_c = \langle \Phi | H_c (1 + C_2) | \Phi \rangle = \frac{\left( \begin{array}{c} \text{diagram 1} + \text{diagram 2} \end{array} \right)}{\left( 1 + \text{diagram 3} \right)}$$

The equation shows the correlation energy  $E_c$  as a ratio of two terms. The numerator contains two diagrams: the first is a self-energy diagram on a single orbital with one electron, and the second is a diagram with two orbitals and two electrons connected by a wavy line. The denominator contains a constant term '1' plus a diagram of two orbitals with two electrons connected by a horizontal line.

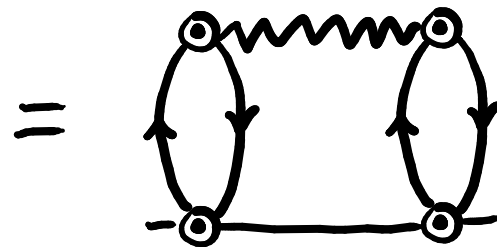


CID / CCD energy

$$E_c = \langle \Phi | H_c (1 + C_2) | \Phi \rangle = \frac{\left( \text{diagram 1} + \text{diagram 2} \right)}{\left( 1 + \text{diagram 3} \right)}$$

The diagrams are:

- Diagram 1: A circle with a cross, connected by a horizontal line to a circle with an upward arrow. The circle with the upward arrow has another upward arrow below it.
- Diagram 2: A circle with an upward arrow, connected by a wavy line to a circle with an upward arrow. The circle with the upward arrow has another upward arrow below it.
- Diagram 3: A circle with a downward arrow, connected by a horizontal line to a circle with a downward arrow. The circle with the downward arrow has another downward arrow below it.



$$= \frac{1}{2 \cdot 2} \bar{g}_{ij}^{ab} c_{ab}^{ij}$$

CID coeff equations

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$$E_c c_{ab}^{ij}$$

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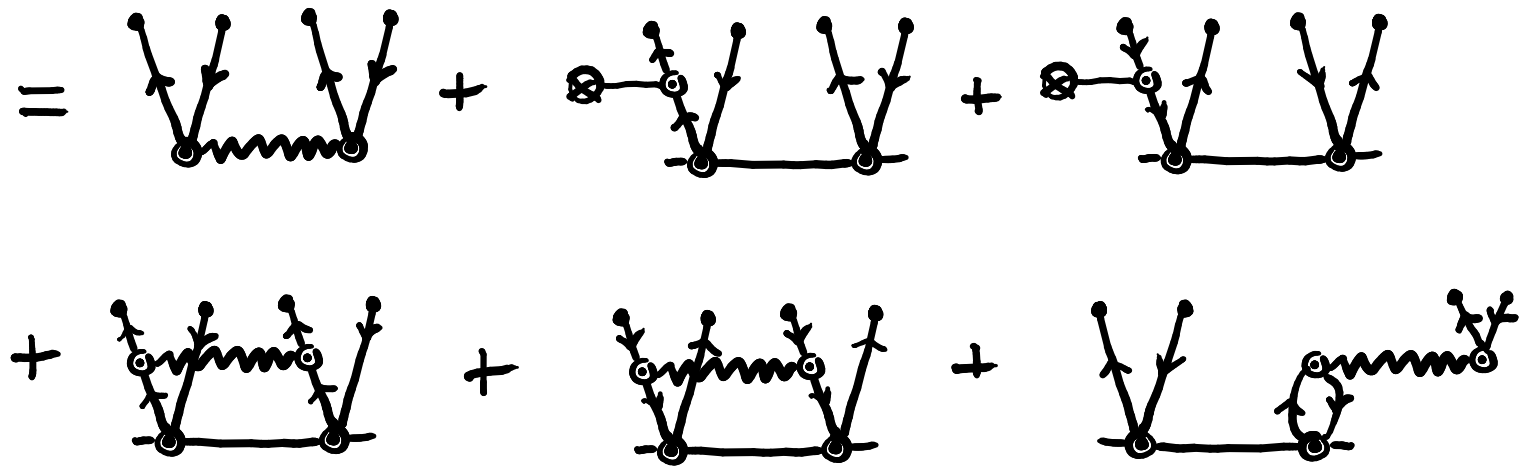
$$= \frac{\left( \begin{array}{c} \text{diagram 1} \\ \text{diagram 2} + \text{diagram 3} \end{array} \right)}{\left( 1 + \text{diagram 4} \right)}$$

The diagrammatic equation represents the CID coefficient equation. The numerator consists of two terms in parentheses. The first term is a diagram with a solid line connecting two vertices, each with two external lines. The second term is a diagram with a wavy line connecting two vertices, each with two external lines. The denominator is a diagram with a solid line connecting two vertices, each with two external lines, preceded by a plus sign and a constant term 1. The entire expression is enclosed in a double-lined box.



CID coeff equations

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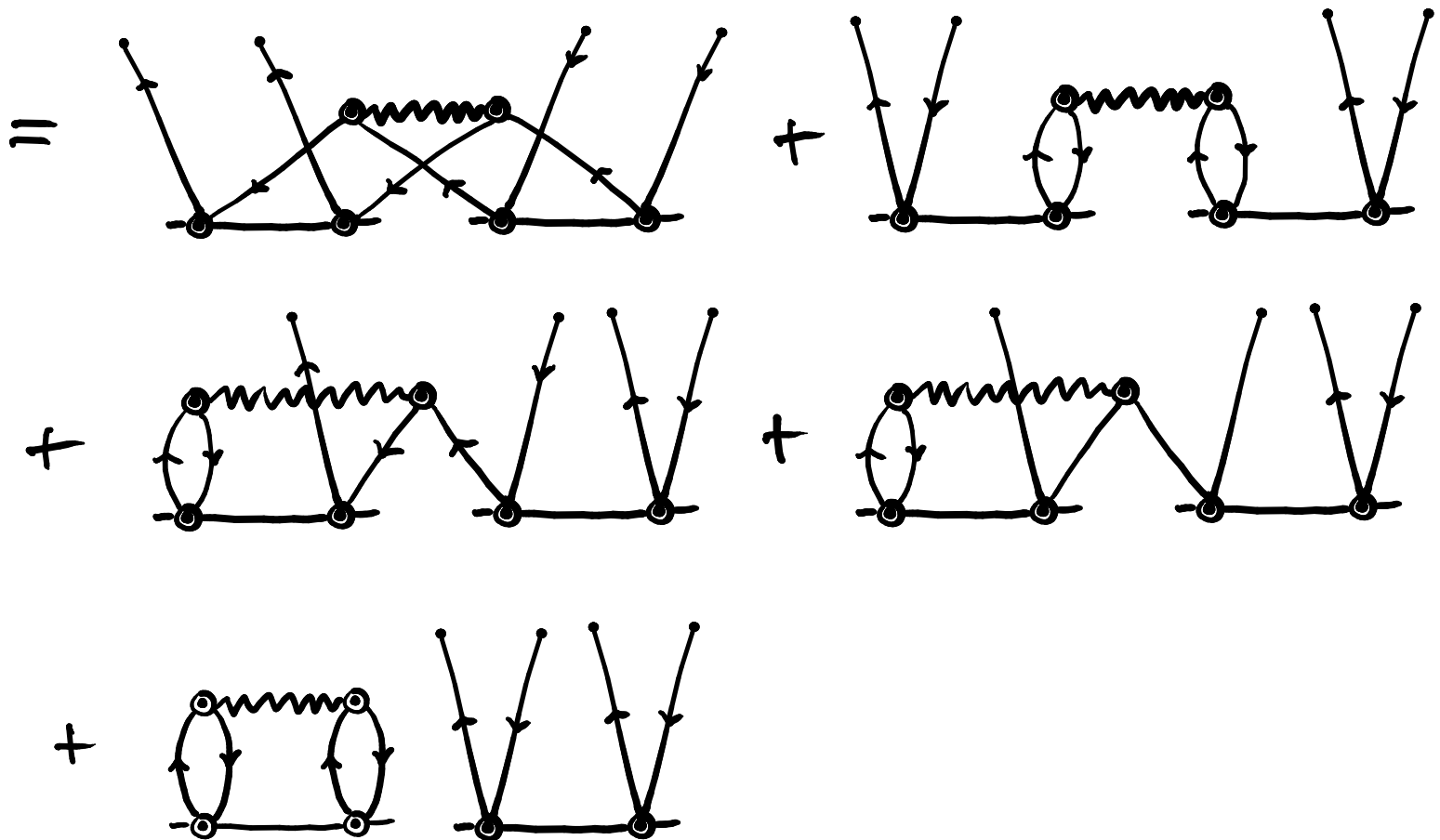
$$\frac{1}{2} \langle \Phi_{ij}^{ab} | H_c C_2^2 | \Phi \rangle$$

$$= \left( \begin{array}{c} \text{diagram 1} + \text{diagram 2} \end{array} \right)$$

The diagram shows two terms in parentheses, each representing a Feynman diagram. The first term shows a horizontal line with four vertices, each having two external lines. The second term shows a horizontal line with four vertices, each having two external lines, with a wavy line connecting the second and third vertices. The entire expression is enclosed in a large set of parentheses.

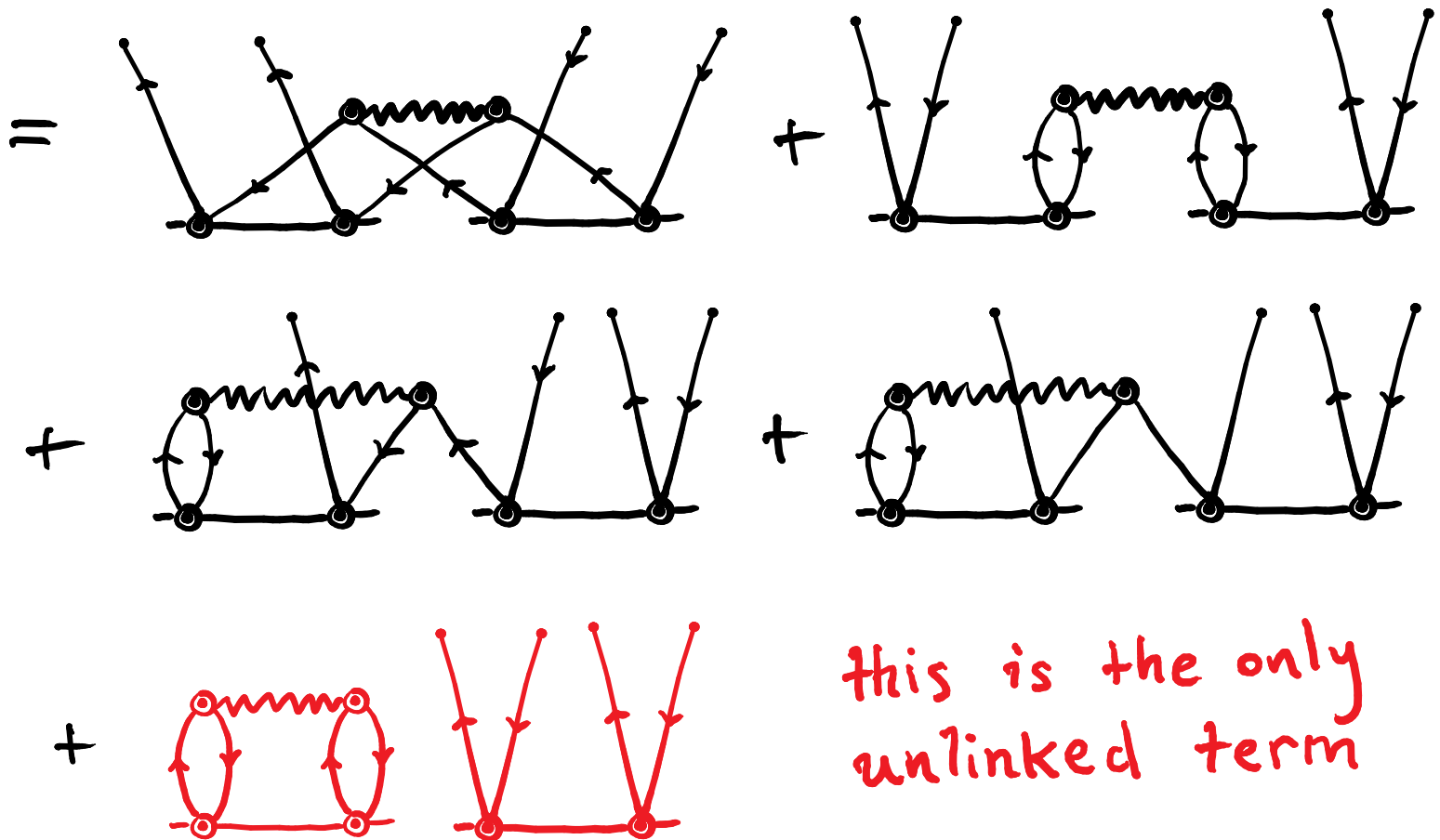
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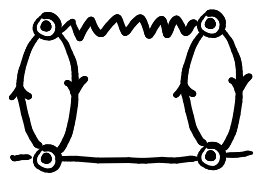
a closer look at the CCD equations:

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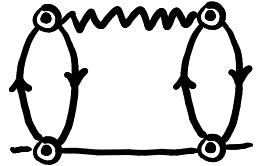
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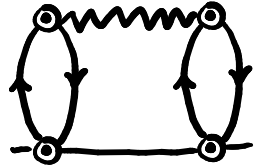
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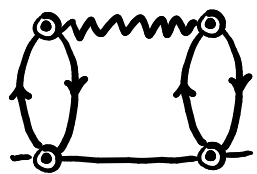
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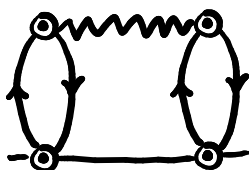
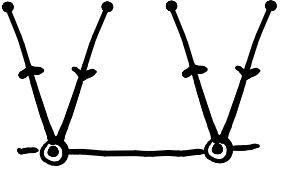
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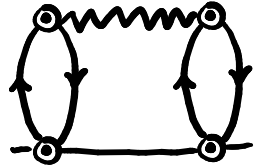
$$E_c c_{ab}^{ij} = \langle \Phi_{ij}^{ab} | H_c \exp(c_2) | \Phi \rangle_L$$

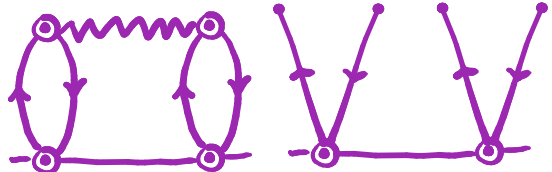
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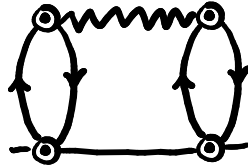
$$E_c c_{ab}^{ij} = \langle \Phi_{ij}^{ab} | H_c \exp(C_2) | \Phi \rangle_L +$$



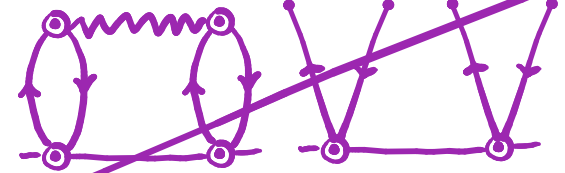
a closer look at the CCD equations:

$$E_c = \langle \Phi | H_c \exp(C_2) | \Phi \rangle =$$


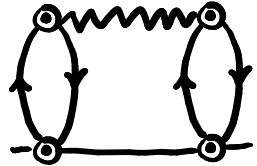
$$E_c c_{ab}^{ij} = \langle \Phi_{ij}^{ab} | H_c \exp(C_2) | \Phi \rangle_L +$$


a closer look at the CCD equations:

$$E_c = \langle \Phi | H_c \exp(C_2) | \Phi \rangle =$$


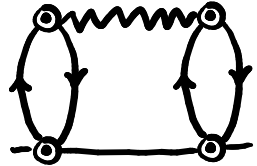
~~$$E_c C_{ab}^{ij} = \langle \Phi_{ij}^{ab} | H_c \exp(C_2) | \Phi \rangle_L +$$
~~

a closer look at the CCD equations:

$$E_c = \langle \Phi | H_c \exp(c_2) | \Phi \rangle =$$


$$0 = \langle \Phi_{ij}^{ab} | H_c \exp(c_2) | \Phi \rangle_L$$

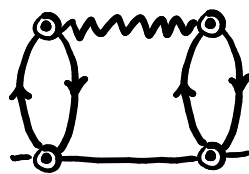
a closer look at the CCD equations:

$$E_c = \langle \Phi | H_c \exp(C_2) | \Phi \rangle =$$


$$0 = \langle \Phi_{ij}^{ab} | F_c \exp(C_2) | \Phi \rangle_L$$

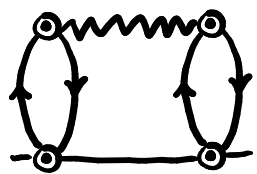


a closer look at the CCD equations:

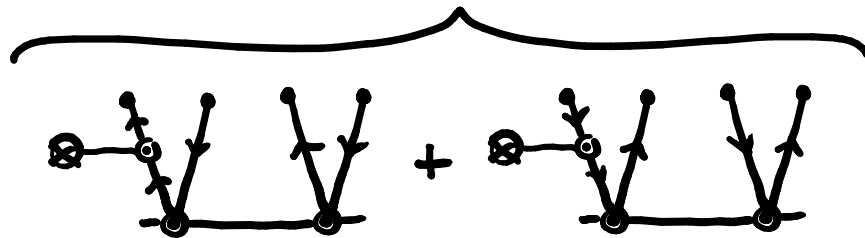
$$E_c = \langle \Phi | H_c \exp(c_2) | \Phi \rangle =$$


$$0 = \langle \Phi_{ij}^{ab} | F_c \exp(c_2) | \Phi \rangle_L + \langle \Phi_{ij}^{ab} | V_c \exp(c_2) | \Phi \rangle_L$$

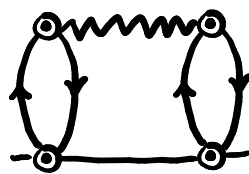
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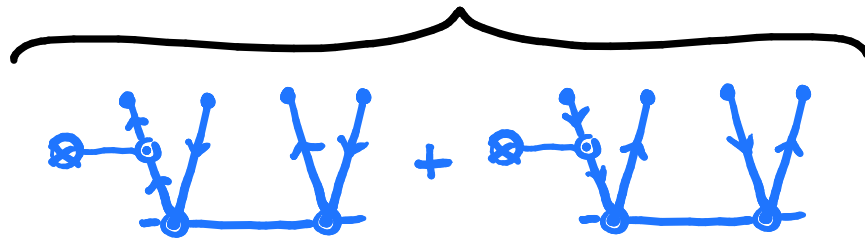
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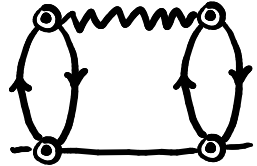
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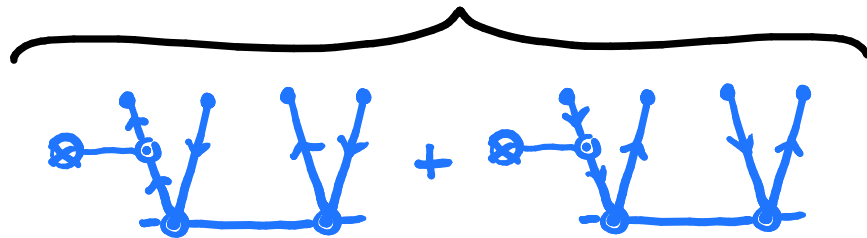
$$0 = \langle \Phi_{ij}^{ab} | F_c \exp(c_2) | \Phi \rangle_L + \langle \Phi_{ij}^{ab} | V_c \exp(c_2) | \Phi \rangle_L$$

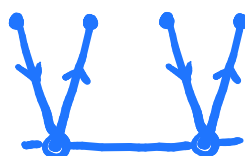


a closer look at the CCD equations:

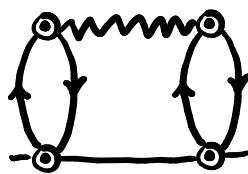
$$E_c = \langle \Phi | H_c \exp(c_2) | \Phi \rangle =$$


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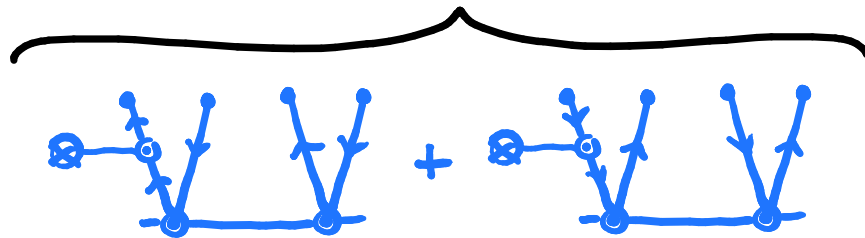


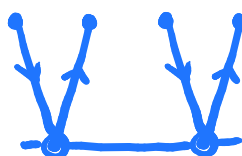
$$= -(\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b)$$


a closer look at the CCD equations:

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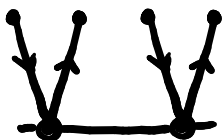
$$0 = \langle \Phi_{ij}^{ab} | F_c \exp(C_2) | \Phi \rangle_L + \langle \Phi_{ij}^{ab} | V_c \exp(C_2) | \Phi \rangle_L$$



$$= -(\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b)$$


(assumes  
Brillouin's  
Thm. holds)





$$\begin{array}{c} \bullet \\ \downarrow \\ \bullet \end{array} \begin{array}{c} \bullet \\ \downarrow \\ \bullet \end{array} = (\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b)^{-1} \langle \Phi_{ij}^{ab} | V_c | \Psi \rangle_L$$



$$\text{Diagram} = (\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b)^{-1} \langle \Phi_{ij}^{ab} | V_c | \Psi \rangle_L$$

CCD:

$$\text{Diagram} = (\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b)^{-1} \langle \Phi_{ij}^{ab} | V_c | \Psi \rangle_L$$

$$\text{CCD: } \Psi \rightarrow (1 + C_2 + \frac{1}{2} C_2^2 + \dots) \Phi$$

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$$\text{CCD: } \Psi \rightarrow (1 + C_2 + \frac{1}{2} C_2^2 + \dots) \Phi$$

CEPA<sub>0</sub>:

$$\text{Diagram} = (\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b)^{-1} \langle \Phi_{ij}^{ab} | V_c | \Psi \rangle_L$$

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$$\text{MP2:}$$

$$\text{Diagram} = (\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b)^{-1} \langle \Phi_{ij}^{ab} | V_c | \Psi \rangle_L$$

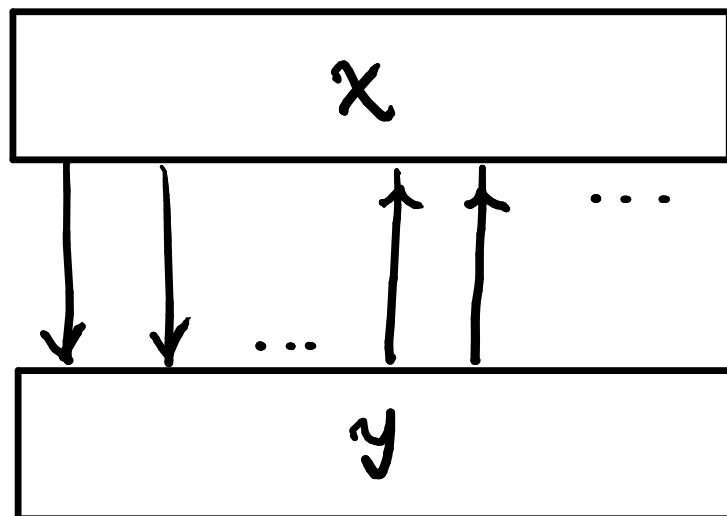
$$\text{CCD: } \Psi \rightarrow (1 + c_2 + \frac{1}{2} c_2^2 + \dots) \Phi$$

$$\text{CEPA}_0: \Psi \rightarrow (1 + c_2) \Phi$$

$$\text{MP2: } \Psi \rightarrow \Phi$$

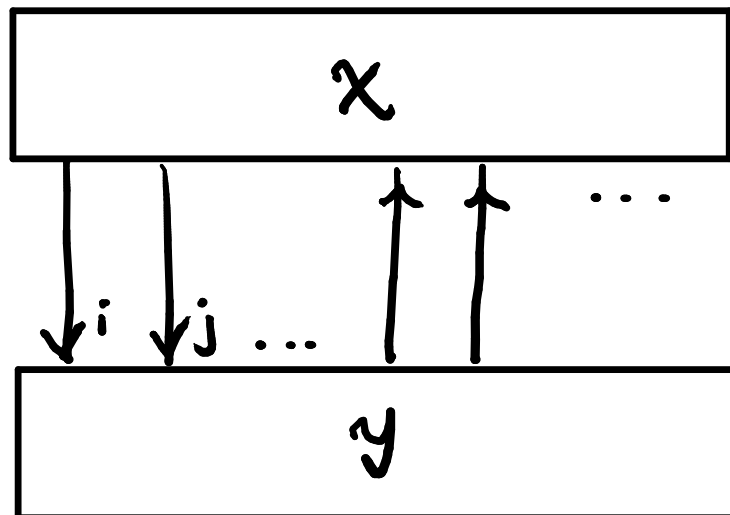
resolvent line:

resolvent line:

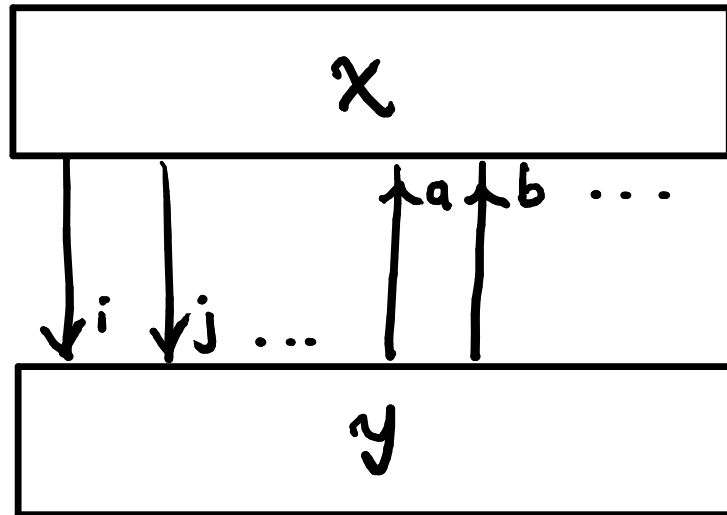




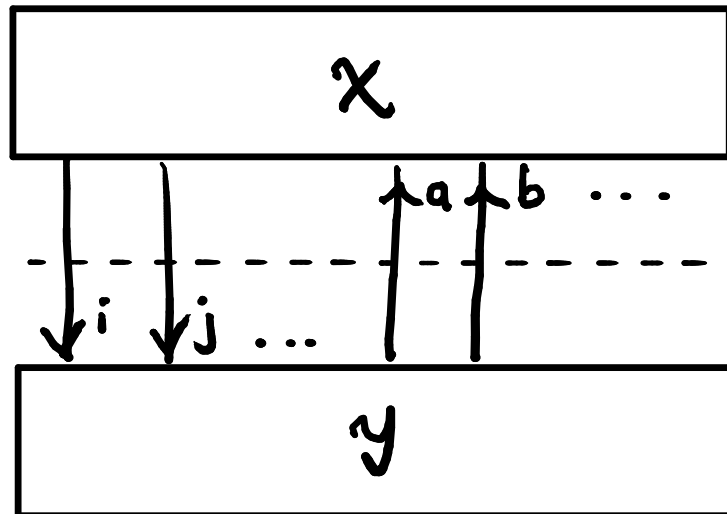
resolvent line:



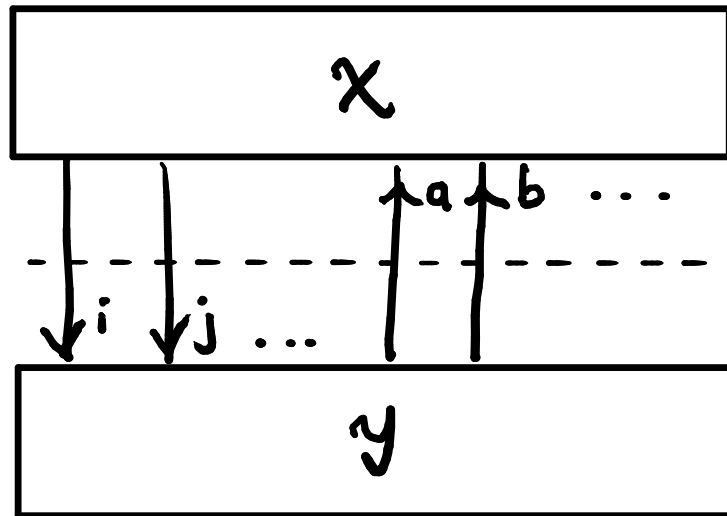
resolvent line:



resolvent line:

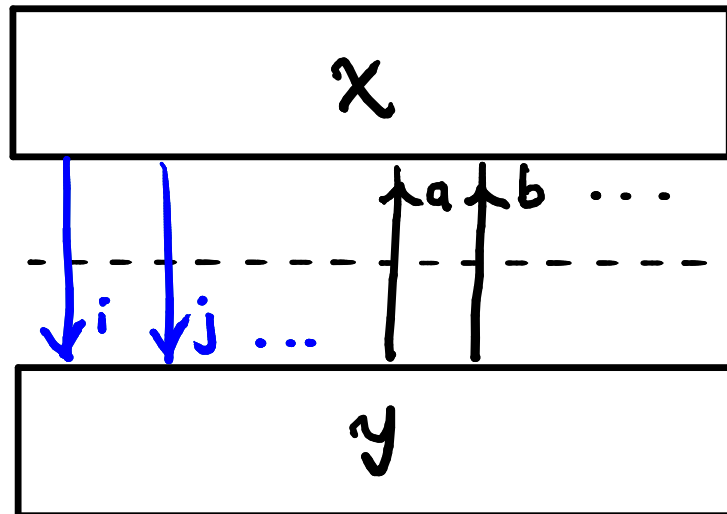


resolvent line:



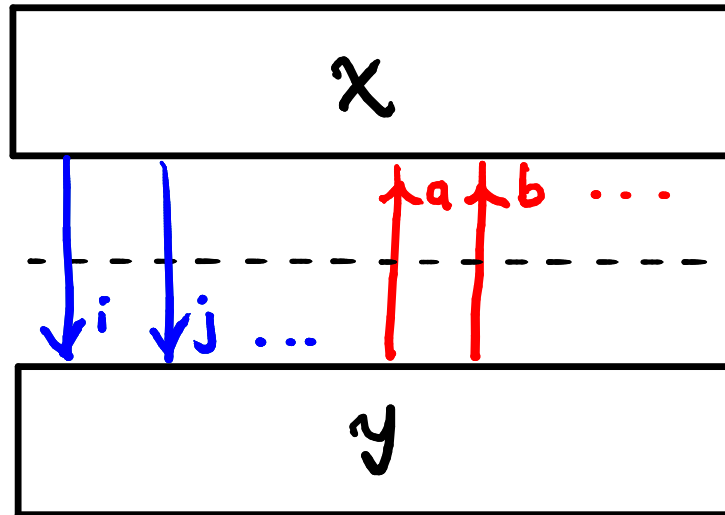
$$= \frac{x_{ij\dots}^{ab\dots} y_{ab\dots}^{ij\dots}}{\epsilon_i + \epsilon_j + \dots - \epsilon_a - \epsilon_b - \dots}$$

resolvent line:



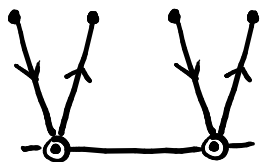
$$= \frac{X_{ij\dots}^{ab\dots} Y_{ab\dots}^{ij\dots}}{\epsilon_i + \epsilon_j + \dots - \epsilon_a - \epsilon_b - \dots}$$

resolvent line:

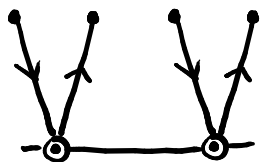


$$= \frac{X_{ij\dots}^{ab\dots} Y_{ab\dots}^{ij\dots}}{\epsilon_i + \epsilon_j + \dots - \epsilon_a - \epsilon_b - \dots}$$



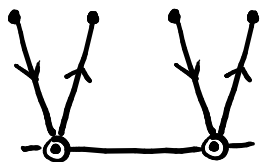






$$\begin{aligned}
 &= \text{Diagram 1} + \text{Diagram 2} + \text{Diagram 3} + \text{Diagram 4} \\
 &+ \text{Diagram 5} + \text{Diagram 6} + \text{Diagram 7} \\
 &+ \text{Diagram 8}
 \end{aligned}$$

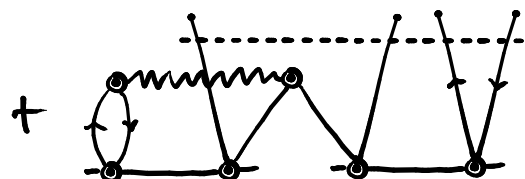
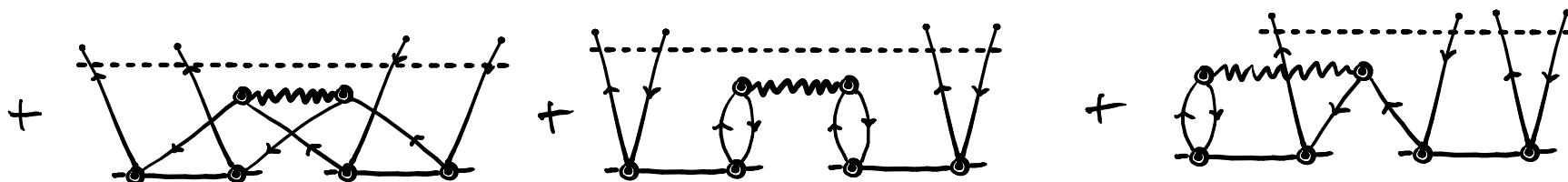
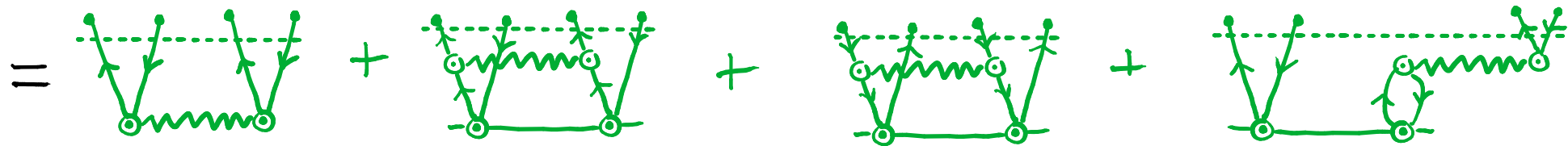
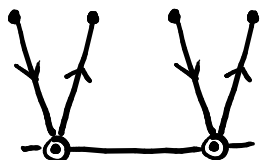
The equation shows the expansion of the initial diagram into a sum of eight more complex Feynman diagrams. Each diagram includes a horizontal line with vertices, wavy internal lines, and various loop structures. Some diagrams feature dashed horizontal lines at the top, and others include self-energy loops on the vertices or internal lines.



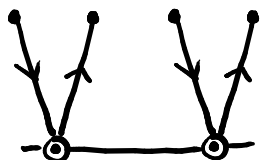
$$\begin{aligned}
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 &+ \text{Diagram 5} + \text{Diagram 6} + \text{Diagram 7} \\
 &+ \text{Diagram 8}
 \end{aligned}$$

The equation shows the expansion of the initial diagram into a sum of eight more complex Feynman diagrams. Each diagram includes a horizontal line with vertices, wavy internal lines, and various loop structures. Some diagrams have dashed horizontal lines above them. The diagrams are separated by plus signs, and the entire sum is preceded by an equals sign.

CCD



CCD  
CEPA<sub>0</sub>



$$= \text{[Purple diagram]} + \text{[Green diagram 1]} + \text{[Green diagram 2]} + \text{[Green diagram 3]}$$

The first row of the expansion shows four diagrams. The first is purple, with a wavy internal line and a dashed line above. The next three are green, showing various topologies with wavy internal lines and dashed lines, including self-energy loops on the vertices.

$$+ \text{[Black diagram 1]} + \text{[Black diagram 2]} + \text{[Black diagram 3]}$$

The second row shows three black diagrams. The first has a more complex internal structure with multiple vertices and a wavy line. The second and third show diagrams with self-energy loops on the vertices and a wavy internal line.

$$+ \text{[Black diagram 4]}$$

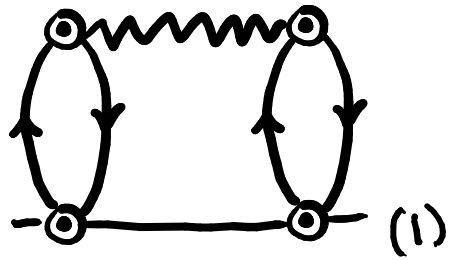
The third row shows a single black diagram, which is a variation of the first diagram in the second row, featuring a wavy internal line and a dashed line above.

CCD  
CEPA<sub>0</sub>  
MP2

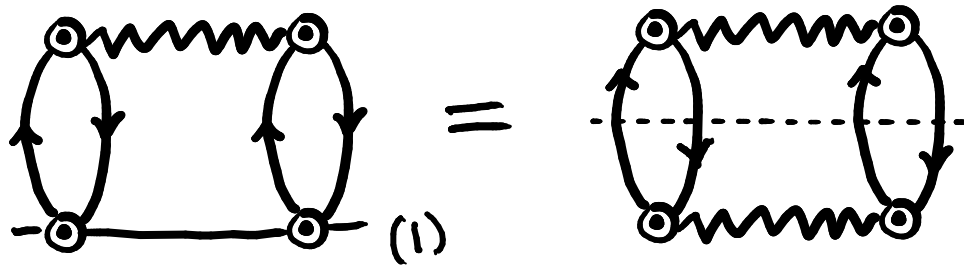


MP2 energy:

MP2 energy:



MP2 energy:





MP2 energy:

$$\begin{array}{c} \text{diagram 1} \end{array} = \begin{array}{c} \text{diagram 2} \end{array} = \frac{1}{4} \frac{\bar{g}_{ij}^{ab} \bar{g}_{ab}^{ij}}{\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b}$$

The first diagram is a rectangular loop with four vertices. The top and bottom edges are wavy lines, and the left and right edges are straight lines with arrows pointing upwards. It is labeled (1) at the bottom right.

The second diagram is a rectangular loop with four vertices. The top and bottom edges are wavy lines, and the left and right edges are straight lines with arrows pointing downwards. A horizontal dashed line connects the two vertical edges.

MP2 energy:

$$\begin{array}{c} \text{diagram 1} \end{array} = \begin{array}{c} \text{diagram 2} \end{array} = \frac{1}{4} \frac{\bar{g}_{ij}^{ab} \bar{g}_{ab}^{ij}}{\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b}$$

The first diagram is a rectangular loop with four vertices. The top and bottom edges are horizontal lines, and the left and right edges are vertical lines. The top edge is a wavy line, and the bottom edge is a straight line. The left and right edges are also wavy lines. The vertices are marked with small circles. The diagram is labeled (1) at the bottom right.

The second diagram is a rectangular loop with four vertices. The top and bottom edges are horizontal lines, and the left and right edges are vertical lines. The top and bottom edges are wavy lines, and the left and right edges are straight lines. The vertices are marked with small circles. A dashed horizontal line connects the two vertical edges.

(sloppy Einstein summation over  $i, j, a, b$ )

end.