

diagrams pt. 2

Coefficient Graphs

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recall that $G = (O, L, h, \tau)$

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m -electron operators

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what about $\langle \Phi_{ij}^{ab} | H_c \Omega | \Phi \rangle$?

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$a_{ab} \sim ij$

Coefficient Graphs

recall that $G = (O, L, h, \tau)$



m -electron operators

what about $\langle \Phi_{ij}^{ab} | H_c \Omega | \Phi \rangle$?



\tilde{a}_{ab}^{ij}
(bare excitation operator)

Coefficient Graphs

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a neat trick:

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$$\frac{\tilde{a}_i}{a_a}$$

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$$\tilde{a}_a^i = \bar{\delta}_{i'}^{a'} \tilde{a}_{a'}^{i'}$$

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$$\tilde{a}_{ab}^{ij}$$

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interaction tensor

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interaction tensor

Try it out!

Coefficient Graphs

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$$\tilde{a}_a^i = \bar{\delta}_{i'}^{a'} \tilde{a}_{a'}^{i'}$$

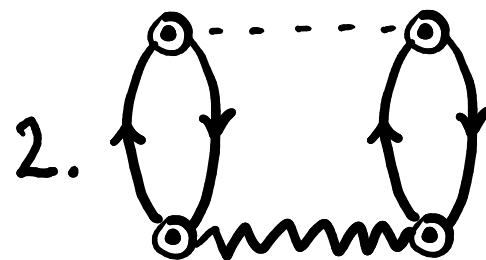
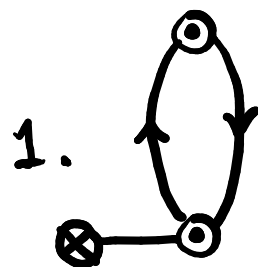
$$\bar{\delta}_{i'}^{a'} \equiv \delta_a^{a'} \delta_{i'}^i$$

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interaction tensor

Try it out!



Coefficient Graphs

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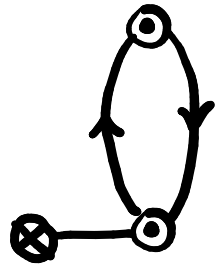
notation

Coefficient Graphs

notation

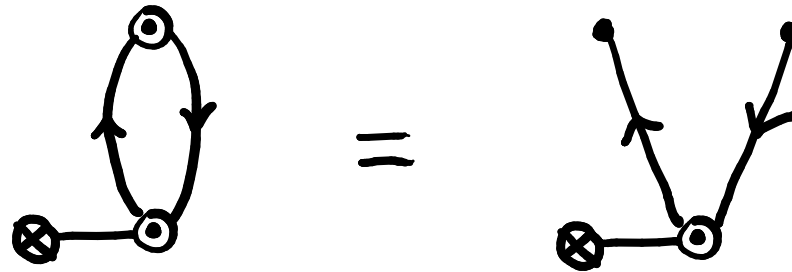
Coefficient Graphs

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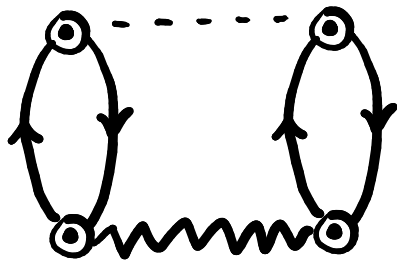
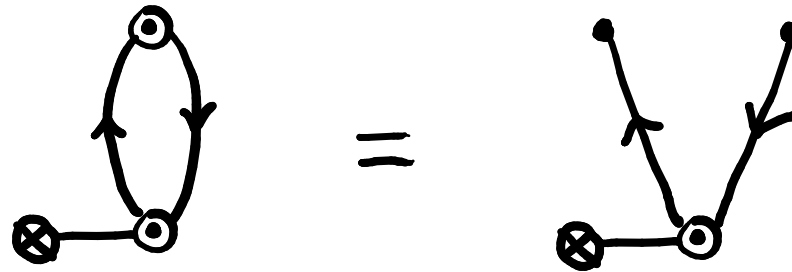
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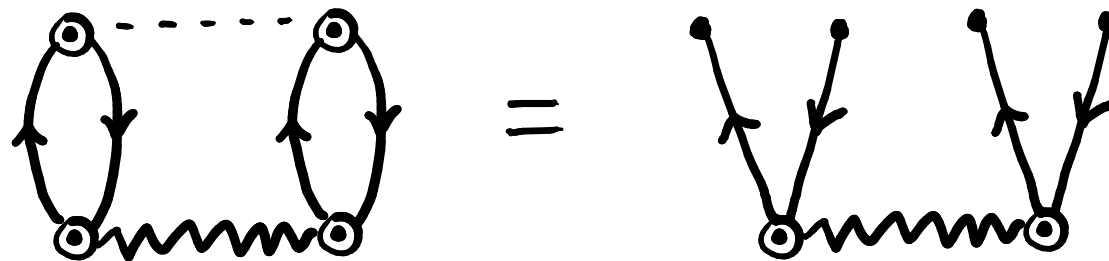
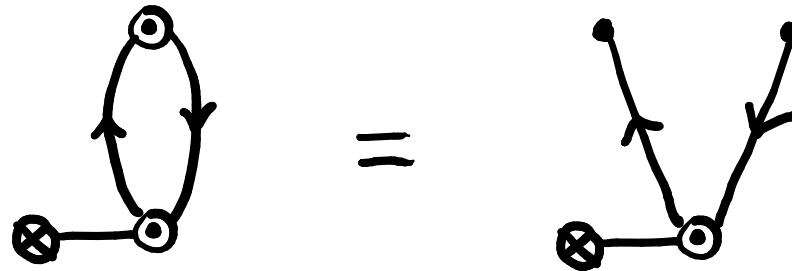
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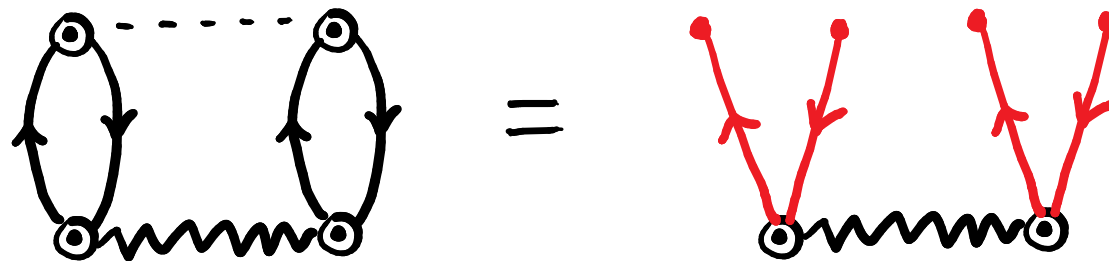
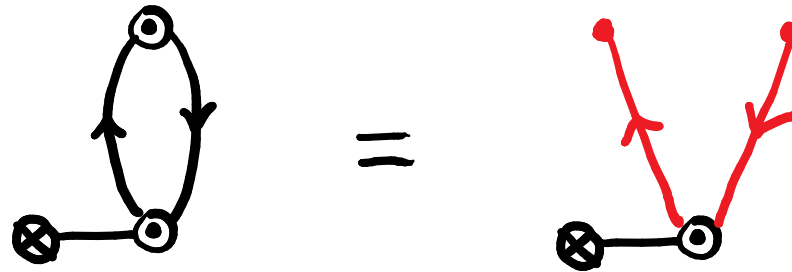
Coefficient Graphs

notation



Coefficient Graphs

notation



coefficient lines

Coefficient Graphs

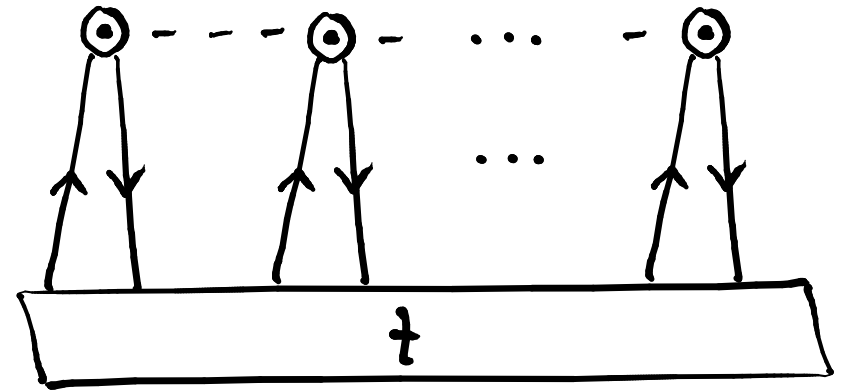
Coefficient Graphs

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useful result:

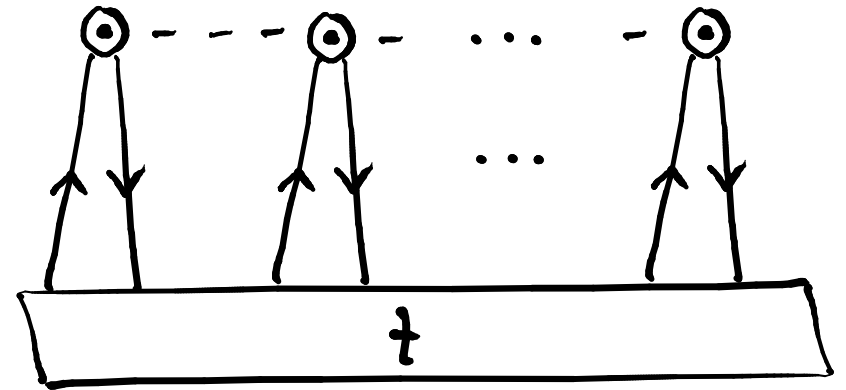
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Coefficient Graphs

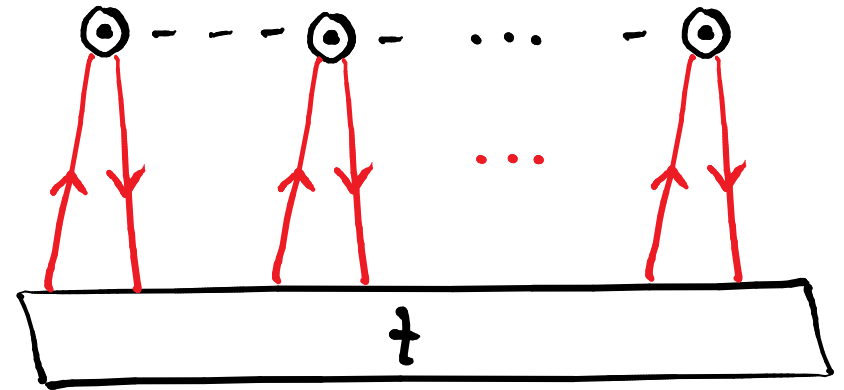
useful result:



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

Coefficient Graphs

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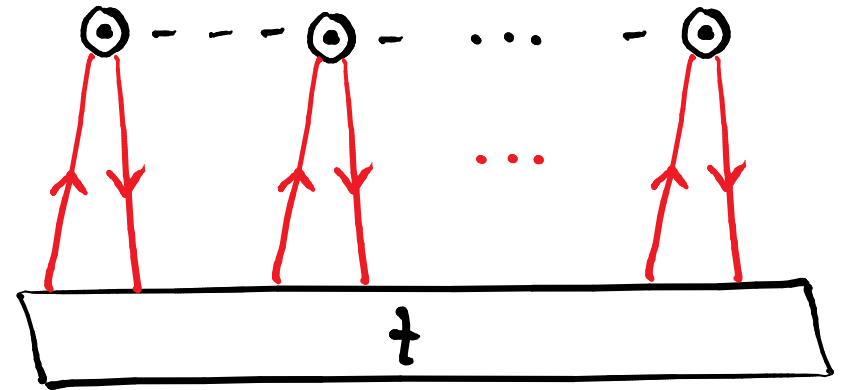


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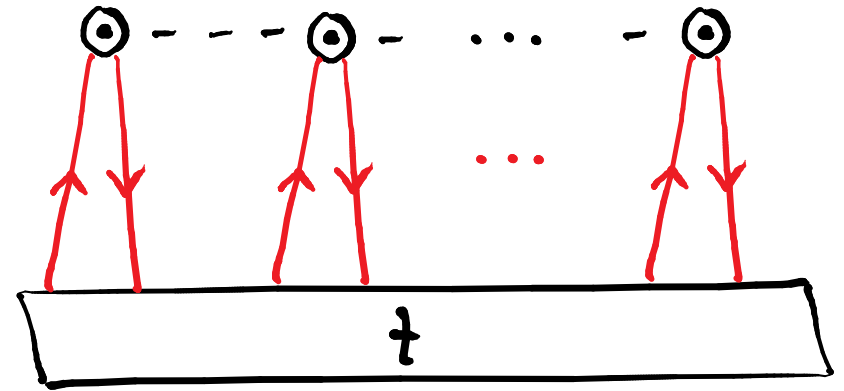
coeff lines

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

↓
equiv. coeff lines
factor

Coefficient Graphs

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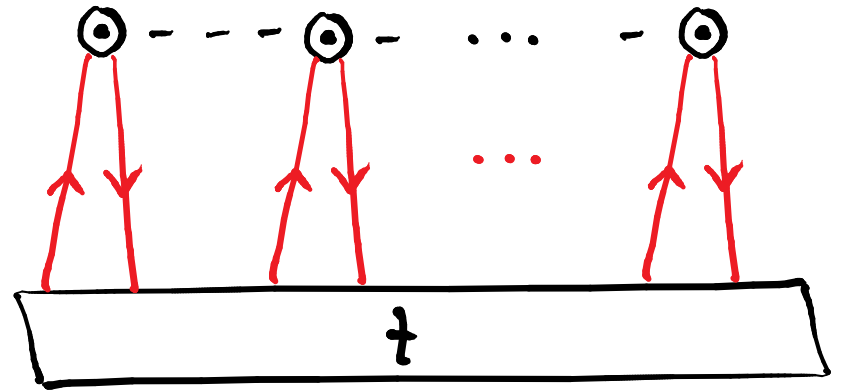
coeff lines

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

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Coefficient Graphs

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coeff lines

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↓
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factor

↓
antisymmetrize
inequiv. coeff lines

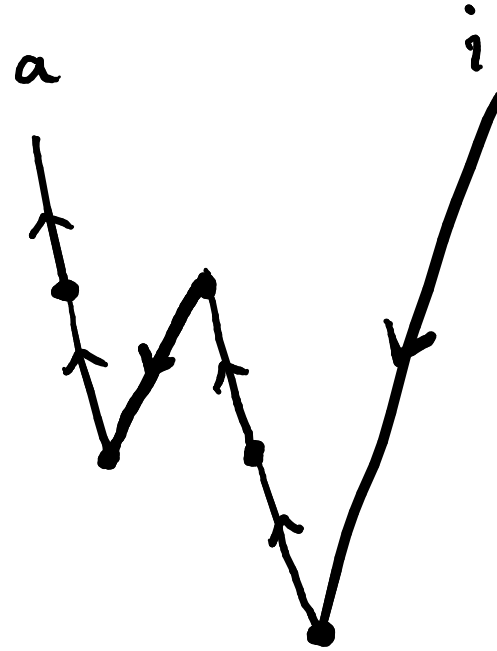
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$$1. \text{ open cycle} = (-)^n a_q^p$$

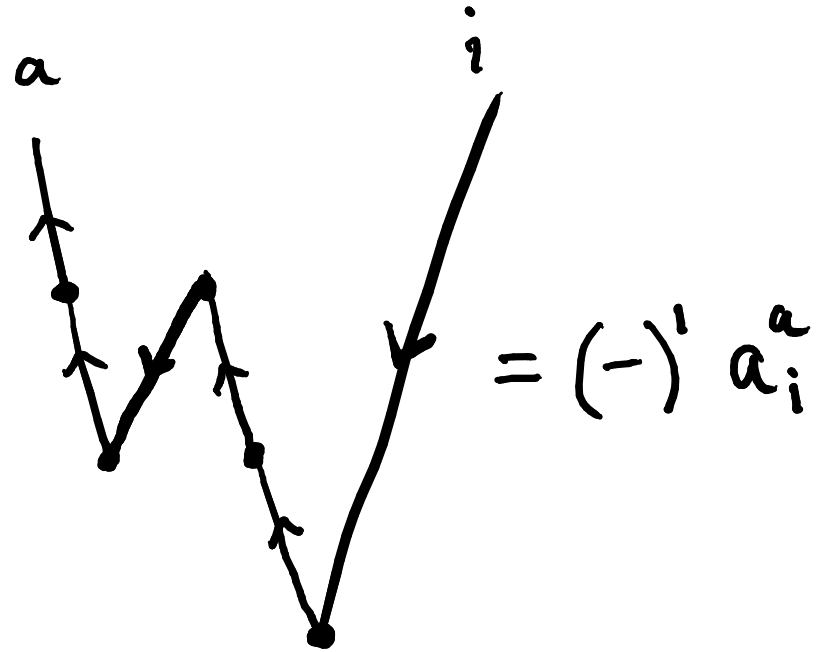
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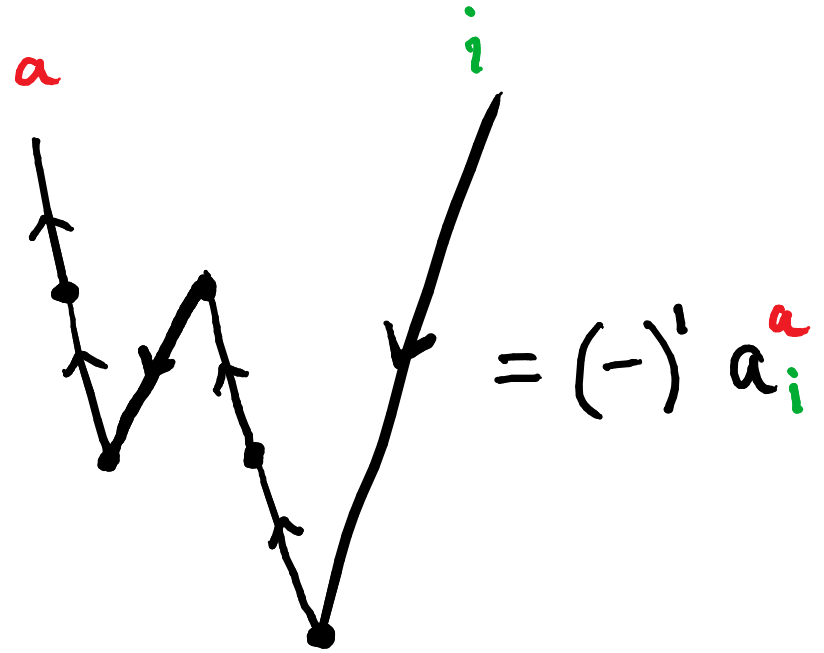
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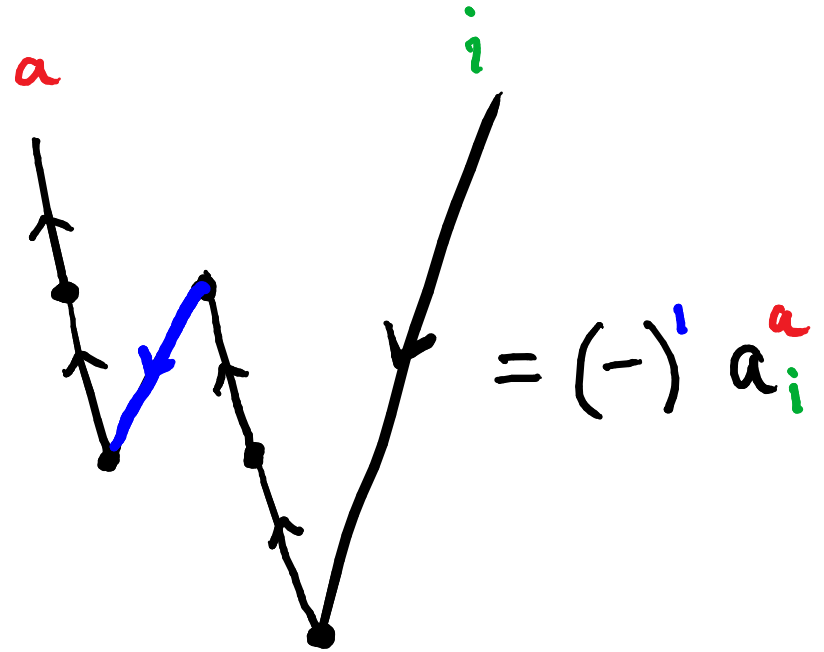
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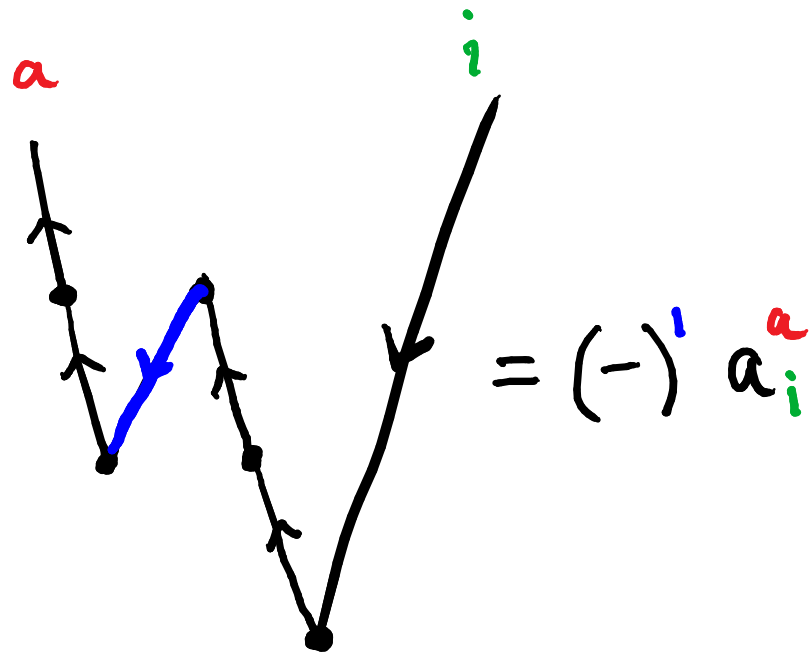
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$$1. \text{ open cycle} = (-)^n a_q^p$$

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



Wick's Thm for Graphs:

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

CID/CCD

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energy:

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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

$$E_c = \langle \Phi | H_c (1 + C_2) | \Phi \rangle$$

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 method. The numerator represents the expectation value of the cluster operator C_2 with the cluster Hamiltonian H_c and the reference state Φ . The denominator represents the norm of the wavefunction $(1 + C_2)|\Phi\rangle$. The diagrams are Feynman diagrams representing the terms in the expansion of the wavefunction and the energy.

Diagram 1 (top left): A diagram with two vertices. The left vertex has an incoming line from the left and an outgoing line to the right. The right vertex has an incoming line from the left and an outgoing line to the right. There is a horizontal line connecting the two vertices, with a wavy line above it.

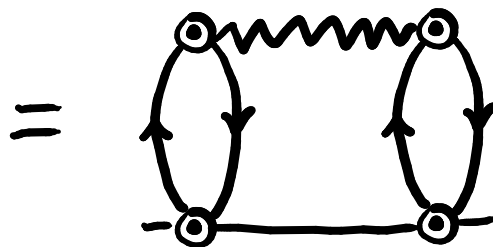
Diagram 2 (top right): A diagram with two vertices. The left vertex has an incoming line from the left and an outgoing line to the right. The right vertex has an incoming line from the left and an outgoing line to the right. There is a horizontal line connecting the two vertices, with a wavy line above it.

Diagram 3 (bottom): A diagram with two vertices. The left vertex has an incoming line from the left and an outgoing line to the right. The right vertex has an incoming line from the left and an outgoing line to the right. There is a horizontal line connecting the two vertices, with a wavy line above it.

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.

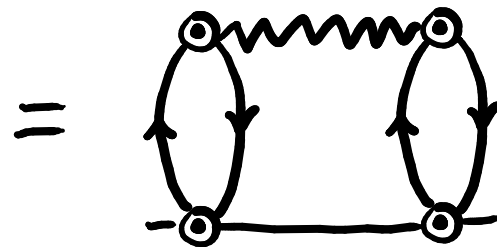


CID/CCD energy

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

The diagrams in the fraction are:

- Diagram 1:** A circle with a cross inside, connected by a horizontal line to a circle with an upward arrow. The upward arrow has a small upward tick mark above it.
- Diagram 2:** A circle with a cross inside, connected by a wavy line to a circle with an upward arrow. The upward arrow has a small upward tick mark above it. To the right of this is another circle with an upward arrow, also with a small upward tick mark above it.
- Diagram 3:** A horizontal line connecting two circles, each with a downward arrow. Each downward arrow has a small downward tick mark 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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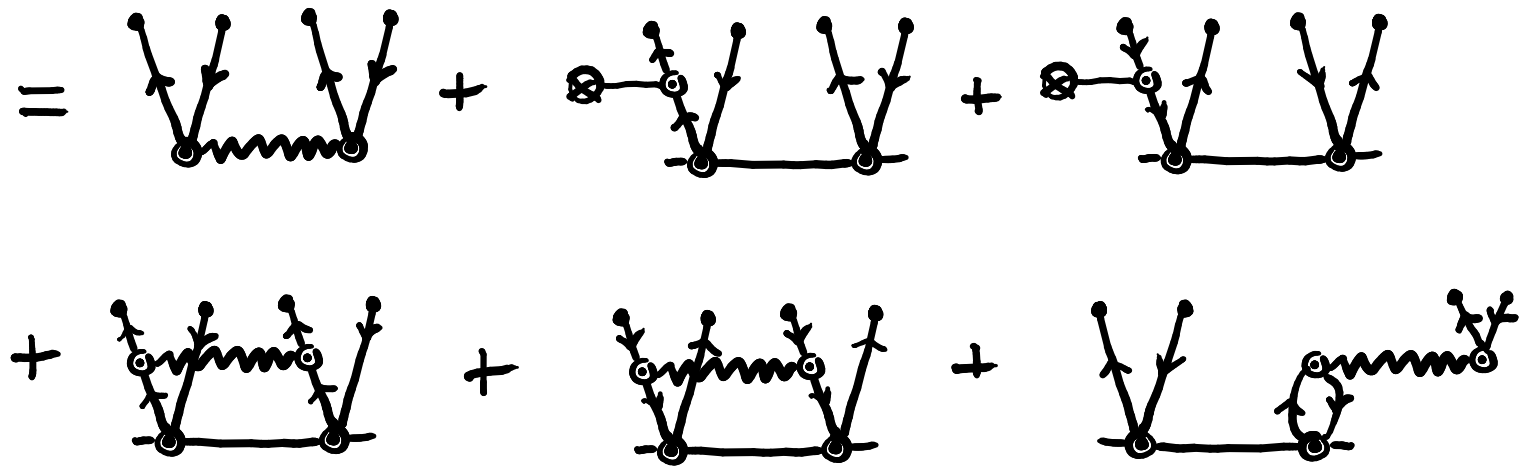
$$E_c c_{ab}^{ij} = \langle \Phi_{ij}^{ab} | H_c (1 + C_2) | \Phi \rangle$$

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

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 incoming lines. The second term is a diagram with a wavy line connecting two vertices, each with two incoming lines. The denominator is a diagram with a solid line connecting two vertices, each with two incoming lines, preceded by a plus sign and the number 1. The entire expression is enclosed in a double-lined box.

CID coeff equations

$$E_c c_{ab}^{ij} = \langle \Phi_{ij}^{ab} | H_c (1 + C_2) | \Phi \rangle$$



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

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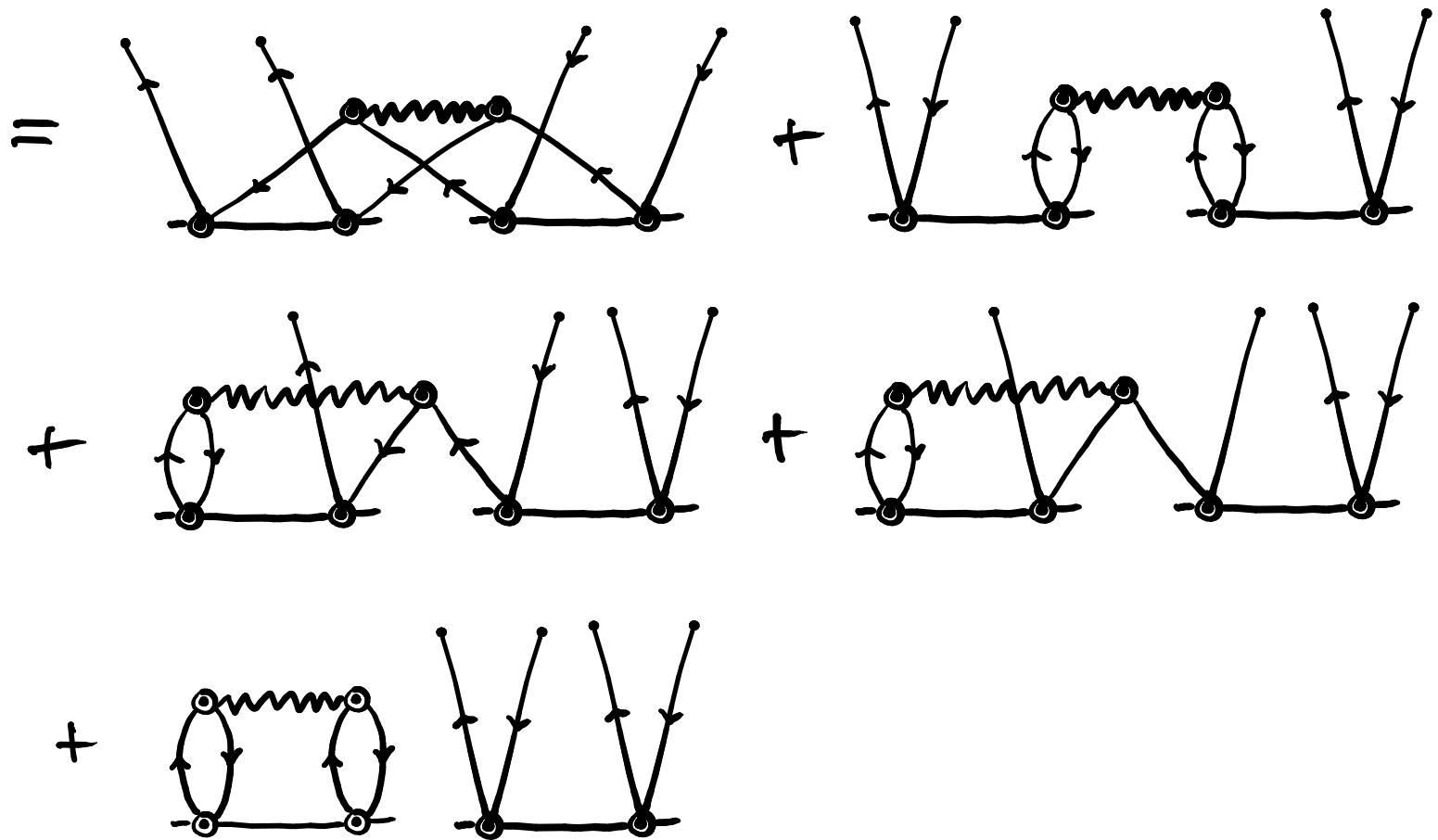
$$= \left(\begin{array}{c} \text{diagram 1} + \text{diagram 2} \end{array} \right)$$

The diagram 1 consists of a horizontal line with four vertices. The first and third vertices are connected by a dashed line. Each vertex has two external lines (one incoming, one outgoing) and a vertical line with an arrow pointing up.

The diagram 2 consists of a horizontal line with four vertices. The first and second vertices are connected by a wavy line. Each vertex has two external lines (one incoming, one outgoing) and a vertical line with an arrow pointing up.

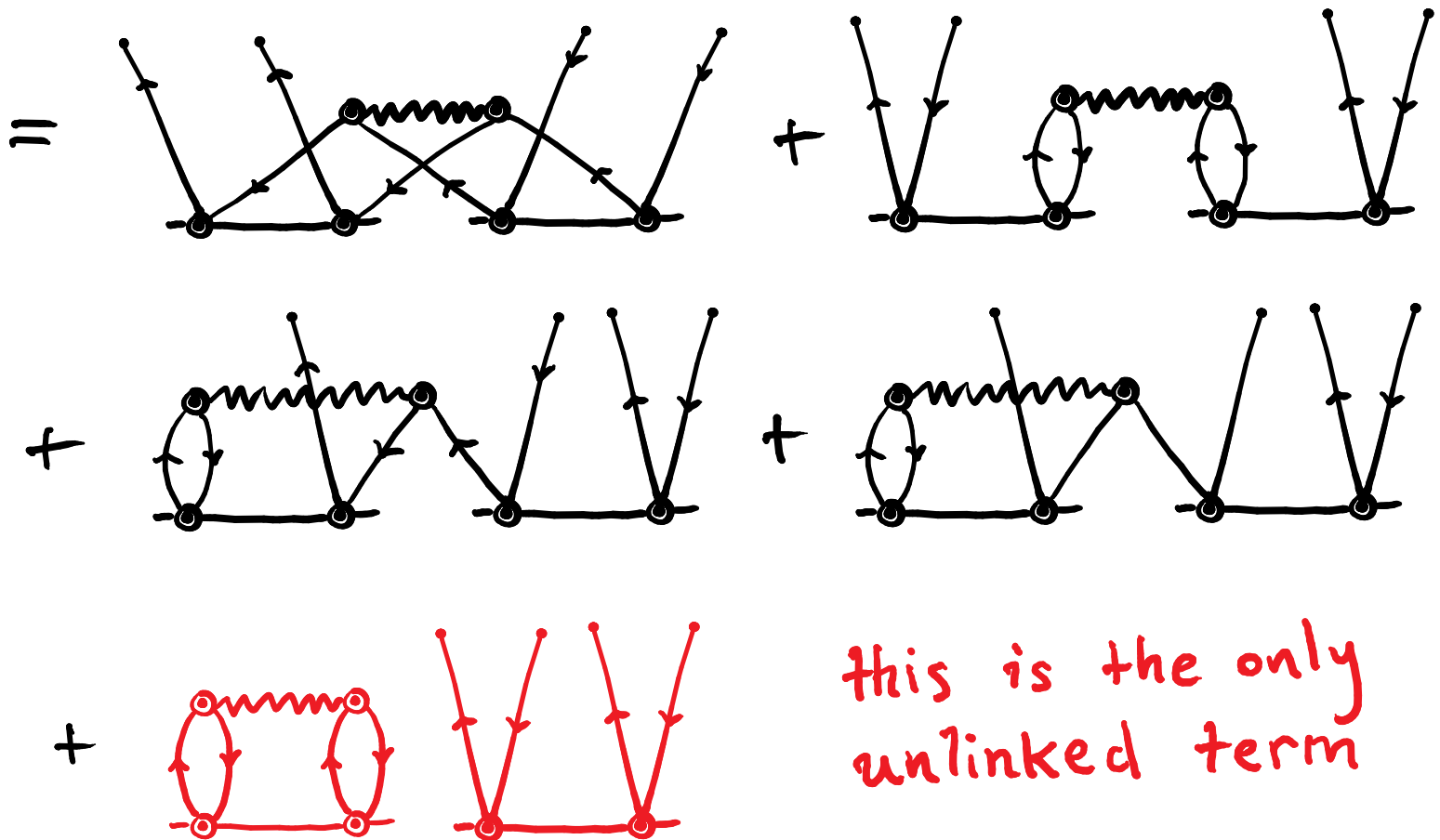
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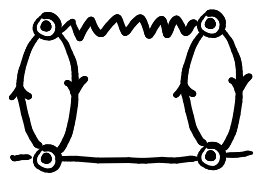


a closer look at the CCD equations:

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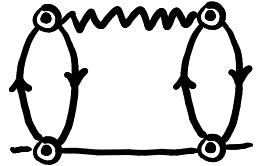
$$E_c = \langle \Phi | H_c \exp(C_2) | \Phi \rangle$$

a closer look at the CCD equations:

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


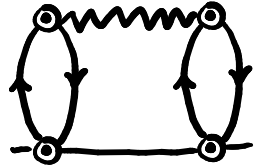
The diagram is a Feynman diagram representing a closed loop. It consists of two vertices, each represented by a small circle. These vertices are connected by two lines: a straight line at the bottom and a wavy line at the top. Arrows on the lines indicate a clockwise flow around the loop.

a closer look at the CCD equations:

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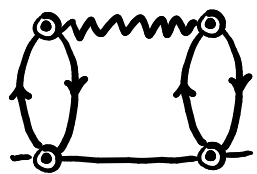
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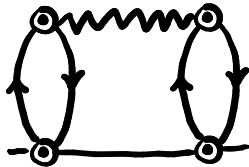
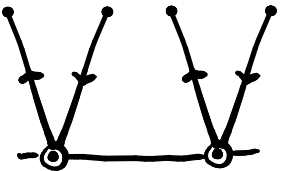
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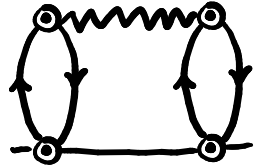
$$E_c c_{ab}^{ij} = \langle \Phi_{ij}^{ab} | H_c \exp(C_2) | \Phi \rangle_L$$

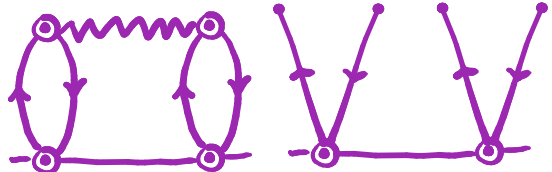
a closer look at the CCD equations:

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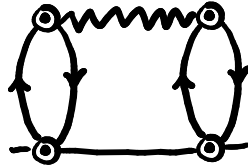
$$E_c c_{ab}^{ij} = \langle \Phi_{ij}^{ab} | H_c \exp(C_2) | \Phi \rangle_L +$$



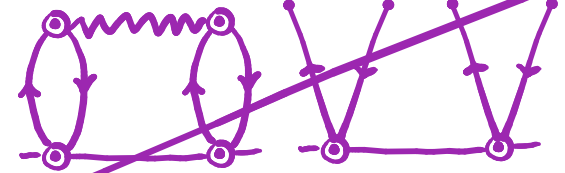
a closer look at the CCD equations:

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


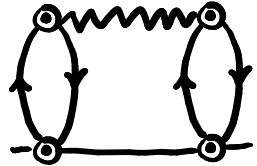
$$E_c c_{ab}^{ij} = \langle \Phi_{ij}^{ab} | H_c \exp(C_2) | \Phi \rangle_L +$$


a closer look at the CCD equations:

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


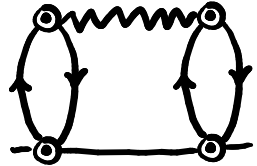
~~$$E_c C_{ab}^{ij} = \langle \Phi_{ij}^{ab} | H_c \exp(C_2) | \Phi \rangle_L +$$
~~

a closer look at the CCD equations:

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


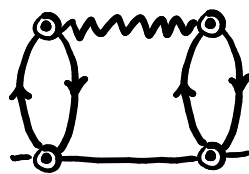
$$0 = \langle \Phi_{ij}^{ab} | H_c \exp(c_2) | \Phi \rangle_L$$

a closer look at the CCD equations:

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


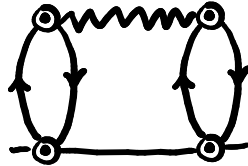
$$0 = \langle \Phi_{ij}^{ab} | F_c \exp(C_2) | \Phi \rangle_L$$

a closer look at the CCD equations:

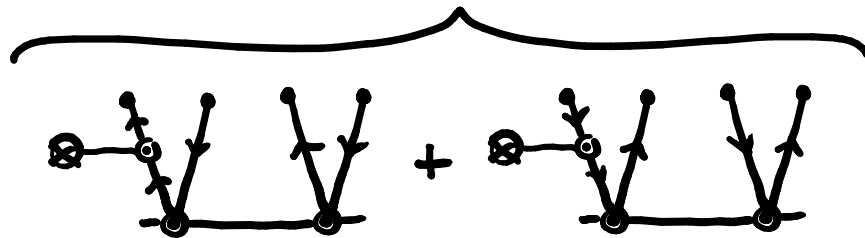
$$E_c = \langle \Phi | H_c \exp(c_2) | \Phi \rangle =$$


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

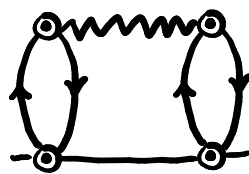
a closer look at the CCD equations:

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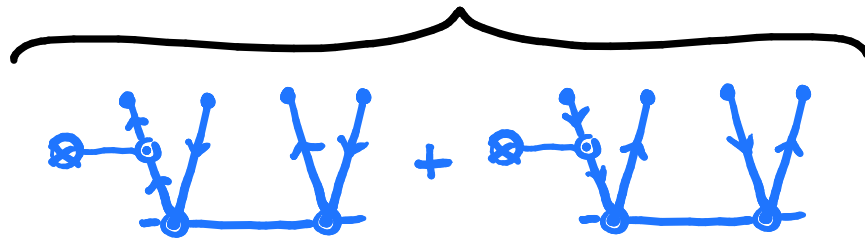
$$0 = \langle \Phi_{ij}^{ab} | F_c \exp(c_2) | \Phi \rangle_L + \langle \Phi_{ij}^{ab} | V_c \exp(c_2) | \Phi \rangle_L$$



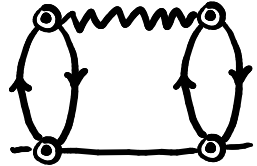
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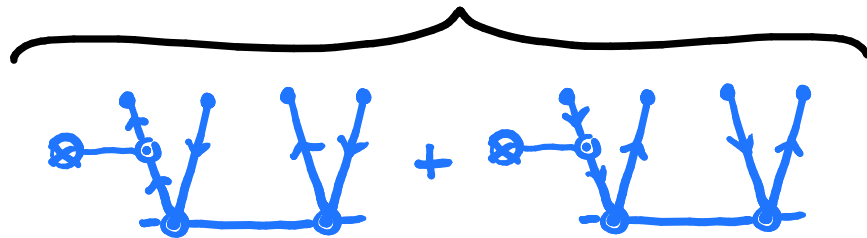
$$0 = \langle \Phi_{ij}^{ab} | F_c \exp(c_2) | \Phi \rangle_L + \langle \Phi_{ij}^{ab} | V_c \exp(c_2) | \Phi \rangle_L$$

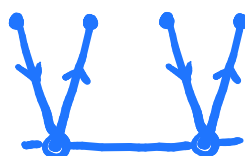


a closer look at the CCD equations:

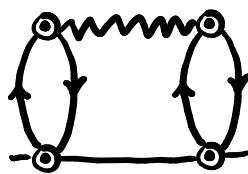
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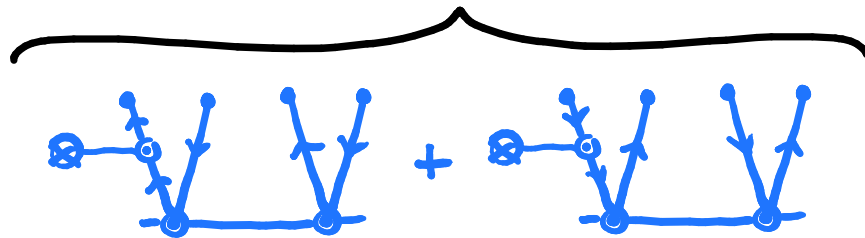


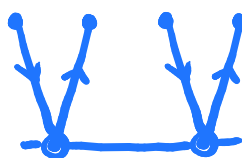
$$= -(\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b)$$


a closer look at the CCD equations:

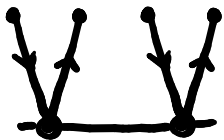
$$E_c = \langle \Phi | H_c \exp(C_2) | \Phi \rangle =$$


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


(assumes
Brillouin's
Thm. holds)



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

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

CCD:

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

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

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

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

CEPA₀:

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

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

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

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

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

$$\text{CEPA}_0: \Psi \rightarrow (1 + C_2) \Phi$$

$$\text{MP2:}$$

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

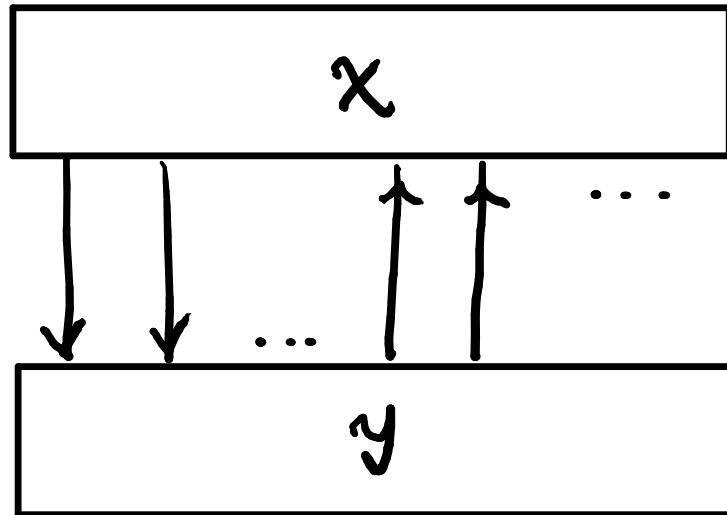
$$\text{CCD: } \Psi \rightarrow (1 + c_2 + \frac{1}{2} c_2^2 + \dots) \Phi$$

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

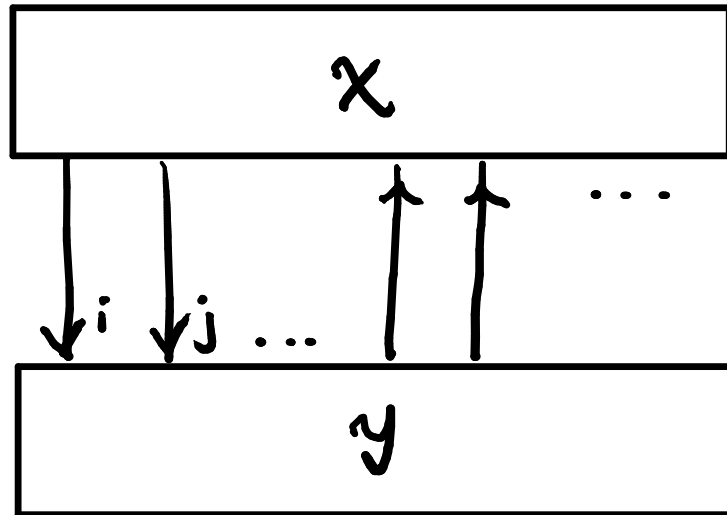
$$\text{MP2: } \Psi \rightarrow \Phi$$

resolvent line:

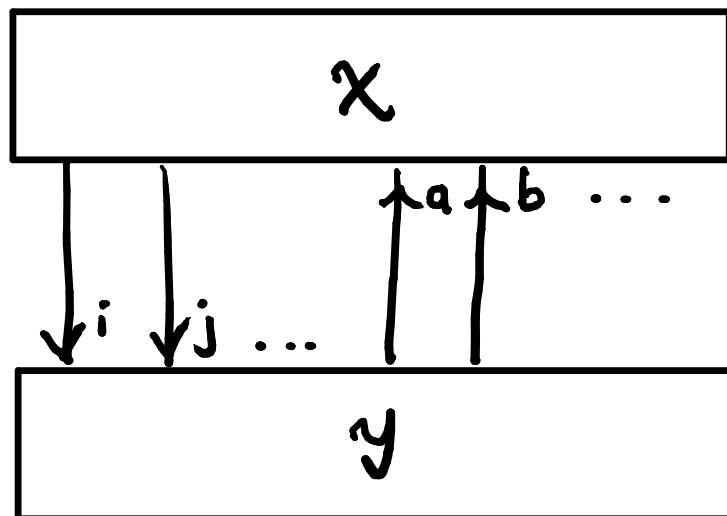
resolvent line:



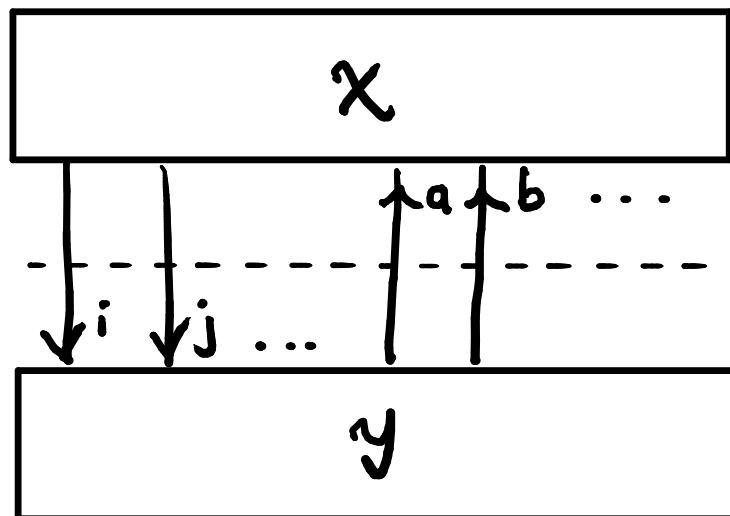
resolvent line:



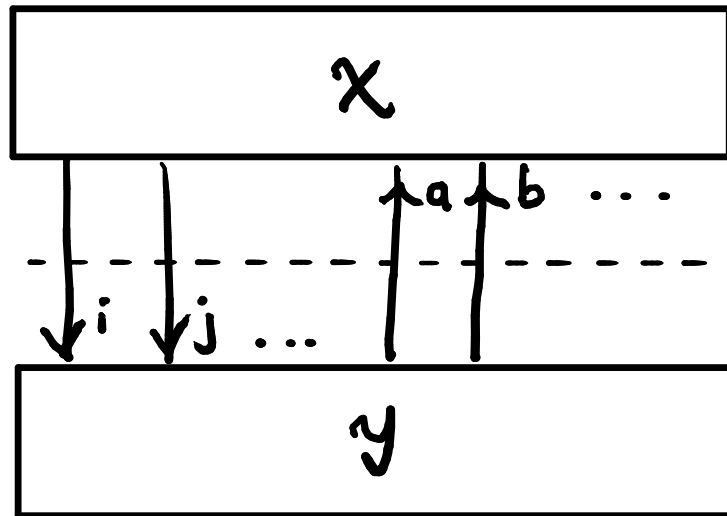
resolvent line:



resolvent line:

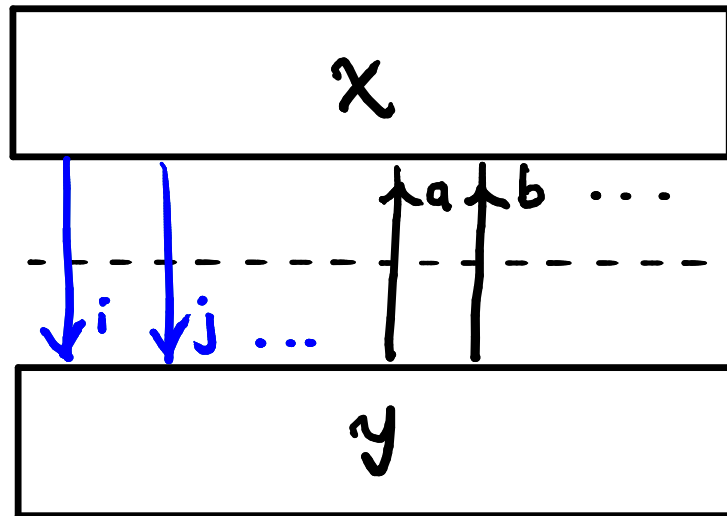


resolvent line:



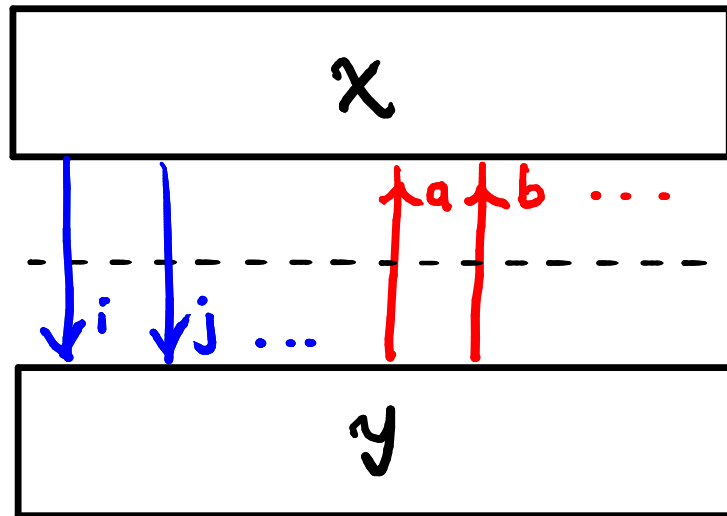
$$= \frac{x_{ij\dots}^{ab\dots} y_{ab\dots}^{ij\dots}}{\epsilon_i + \epsilon_j + \dots - \epsilon_a - \epsilon_b - \dots}$$

resolvent line:

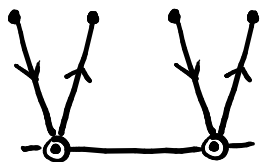


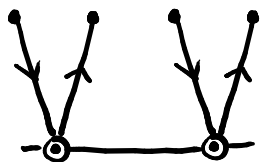
$$= \frac{X_{ij\dots}^{ab\dots} Y_{ab\dots}^{ij\dots}}{\epsilon_i + \epsilon_j + \dots - \epsilon_a - \epsilon_b - \dots}$$

resolvent line:



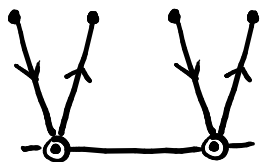
$$= \frac{X_{ij\dots}^{ab\dots} Y_{ab\dots}^{ij\dots}}{\epsilon_i + \epsilon_j + \dots - \epsilon_a - \epsilon_b - \dots}$$





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

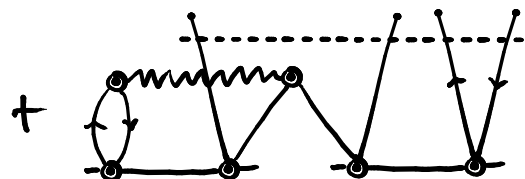
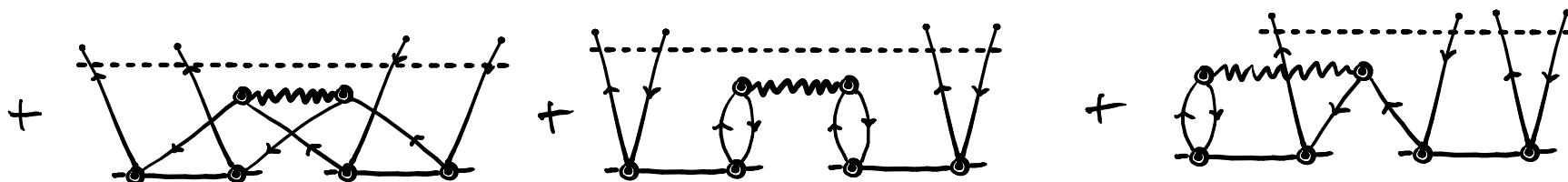
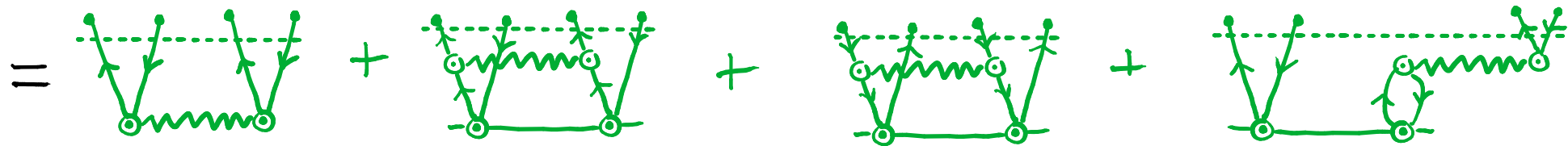
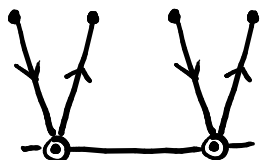
The equation shows the expansion of the initial diagram into a sum of eight more complex Feynman diagrams. Each diagram includes a horizontal line with vertices, wavy internal lines, and various loop structures. Some diagrams feature dashed horizontal lines at the top, and others include self-energy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



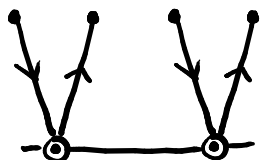
$$\begin{aligned}
 &= \text{Diagram 1} + \text{Diagram 2} + \text{Diagram 3} + \text{Diagram 4} \\
 &+ \text{Diagram 5} + \text{Diagram 6} + \text{Diagram 7} \\
 &+ \text{Diagram 8}
 \end{aligned}$$

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 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
CEPA₀



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

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 external legs.

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

The second row shows three black diagrams. The first has a wavy internal line and a dashed line. The second and third show diagrams with wavy internal lines and self-energy loops on the external legs.

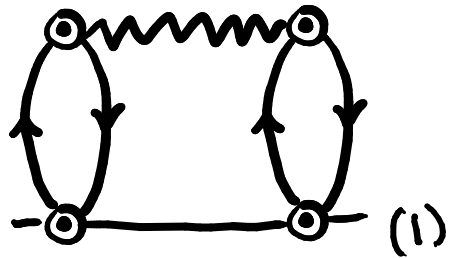
$$+ \text{[Black diagram 4]}$$

The third row shows a single black diagram with a wavy internal line, a dashed line, and a self-energy loop on one of the external legs.

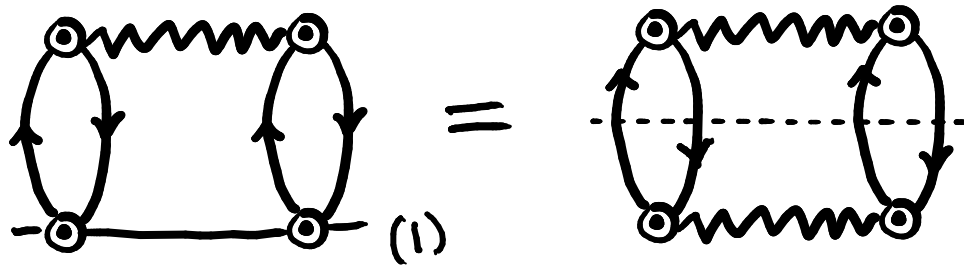
CCD
CEPA₀
MP2

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 upwards. A horizontal dashed line connects the two vertical edges in the middle.

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.