THIRD-ORDER MBPT CORRECTION TO ENERGY

$$K_0^{(3)} = \langle \Phi_0 | W R^{(0)} W R^{(0)} W | \Phi_0 \rangle$$

$$W = W_1 + W_2 = Q_N + V_N$$

$$K_0^{(3)} = K_0^{(3)}(A) + K_0^{(3)}(B) + K_0^{(3)}(C) + K_0^{(3)}(D)$$

$$K_0^{(3)}(A) = \langle \Phi_0 | V_N R^{(0)} V_N R^{(0)} V_N | \Phi_0 \rangle$$

$$K_0^{(3)}(B) = \langle \Phi_0 | V_N R^{(0)} V_N R^{(0)} Q_N | \Phi_0 \rangle$$

$$+ \langle \Phi_0 | V_N R^{(0)} Q_N R^{(0)} V_N | \Phi_0 \rangle$$

$$+ \langle \Phi_0 | Q_N R^{(0)} V_N R^{(0)} V_N | \Phi_0 \rangle$$

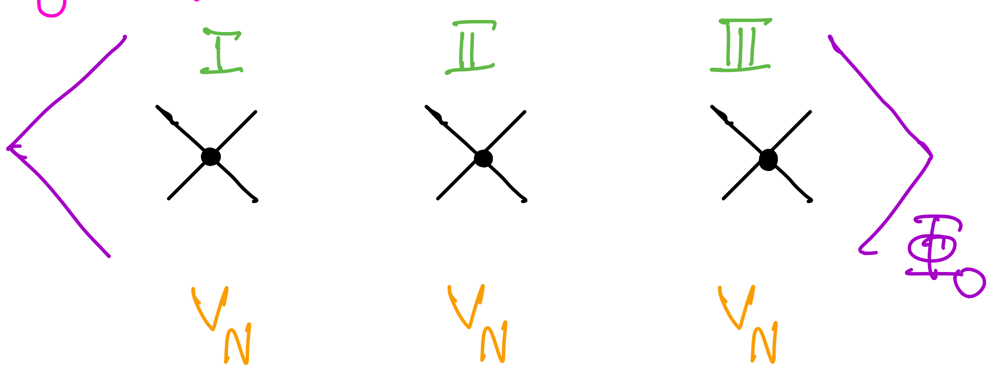
$$K_0^{(3)}(C) = \langle \Phi_0 | Q_N R^{(0)} Q_N R^{(0)} V_N | \Phi_0 \rangle$$

$$+ \langle \Phi_0 | Q_N R^{(0)} V_N R^{(0)} Q_N | \Phi_0 \rangle$$

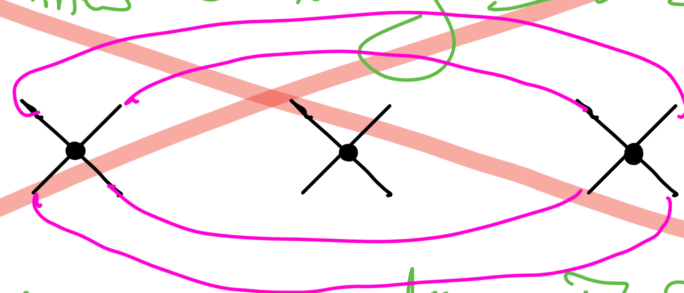
$$+ \langle \Phi_0 | V_N R^{(0)} Q_N R^{(0)} Q_N | \Phi_0 \rangle$$

$$K_0^{(3)}(D) = \langle \Phi_0 | Q_N R^{(0)} Q_N R^{(0)} Q_N | \Phi_0 \rangle$$

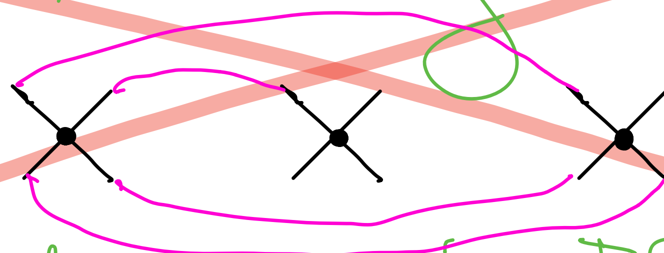
$K_0^{(3)}(A)$:



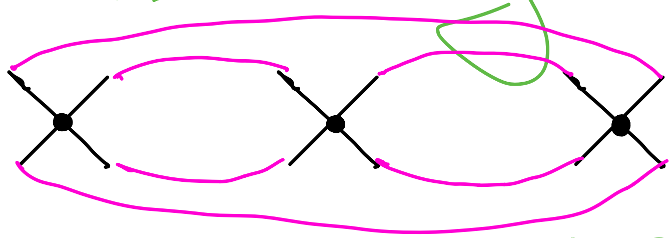
~~No lines connecting I & II:~~



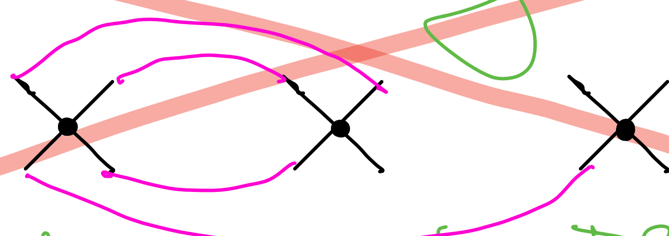
~~1 line connecting I & II:~~



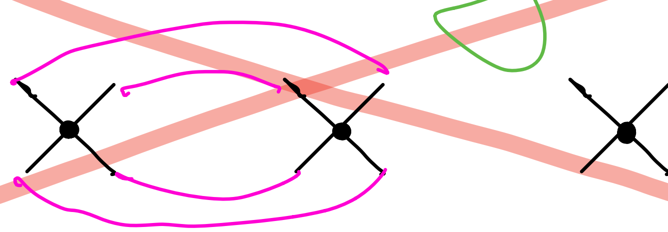
2 lines connecting I & II:

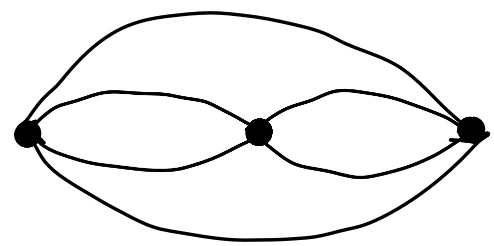


~~3 lines connecting I & II:~~

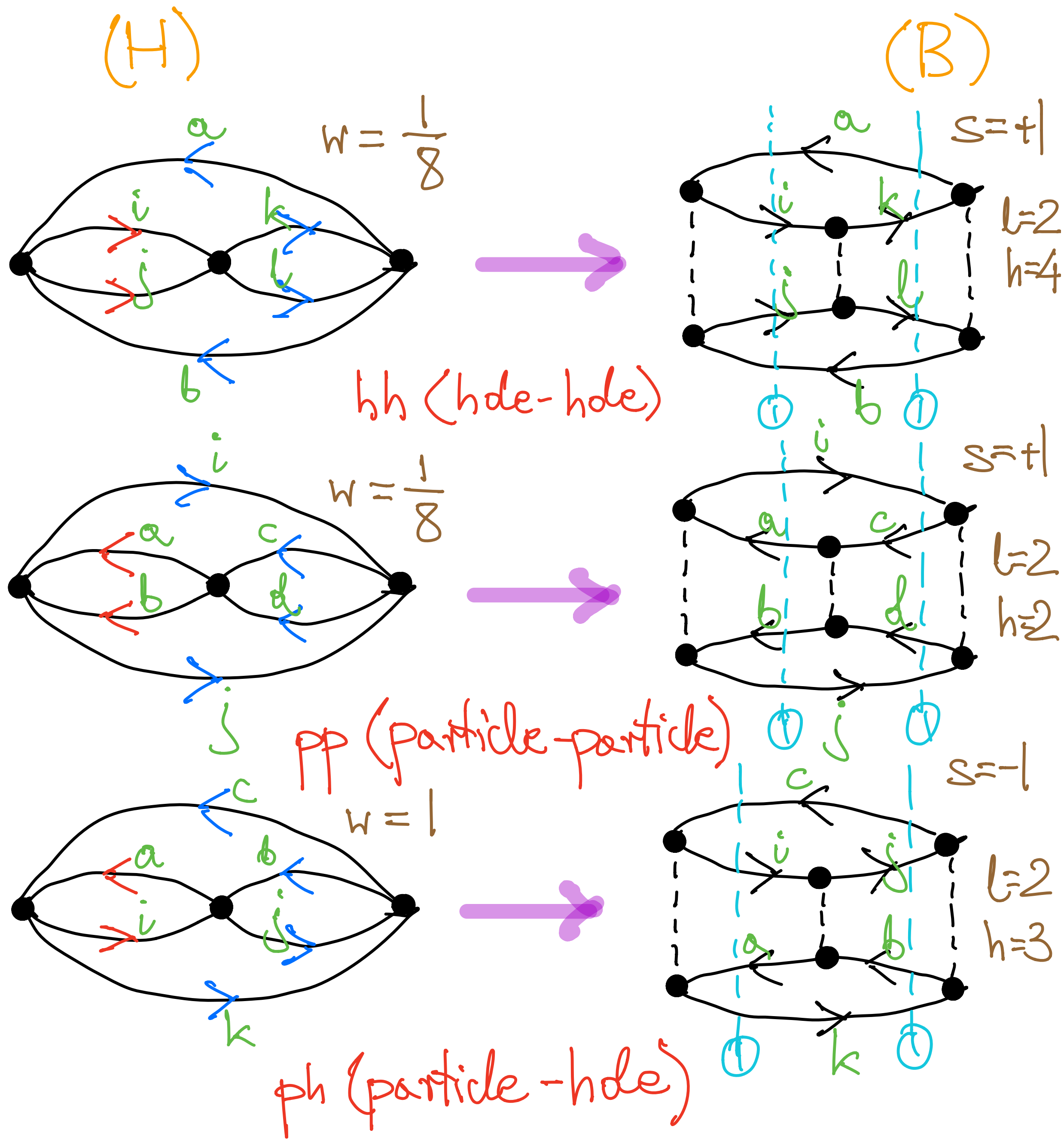


~~4 lines connecting I & II:~~





Nonoriented resulting Hugenholtz skeleton



$$k_0^{(3)}(A) = k_0^{(3)}(hh) + k_0^{(3)}(pp) + k_0^{(3)}(ph)$$

$$k_0^{(3)}(hh) = \frac{1}{8}\sum_{abijkl} \langle ab|\hat{v}|kl\rangle_A \langle kl|\hat{v}|ij\rangle_A \times \langle ij|\hat{v}|ab\rangle_A \, \Delta^{(1)}(i,j;a,b)\, \Delta^{(1)}(k,l;a,b)$$

(bra ⟷ ket ; i ⟺ a, j ⟺ b, ...)

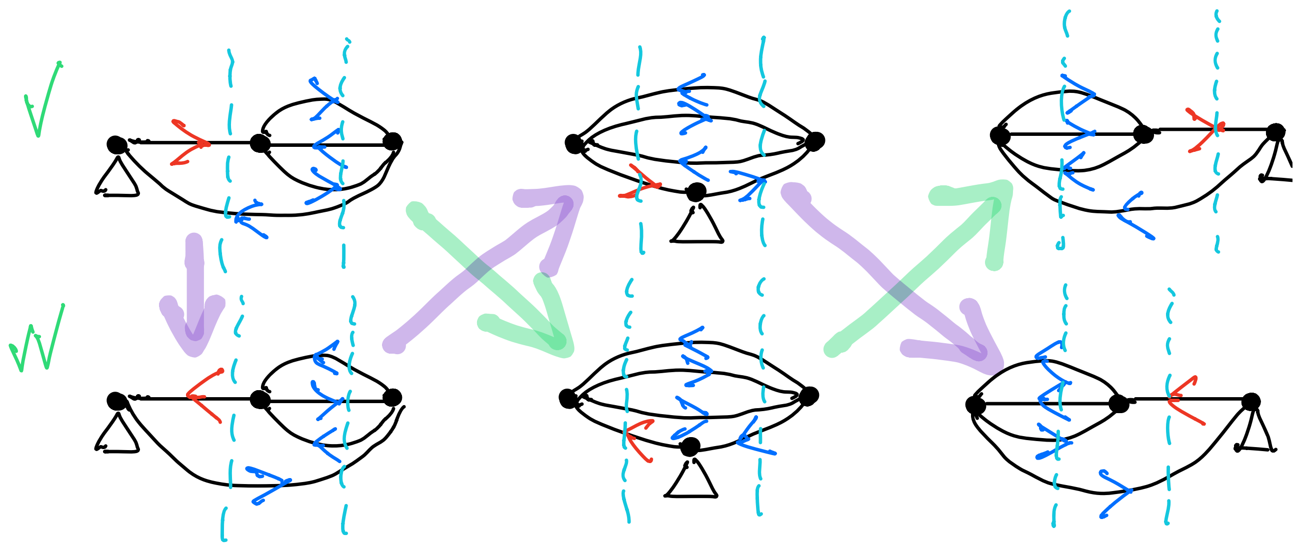
$$k_0^{(3)}(pp) = \frac{1}{8}\sum_{abcdij} \langle ij|\hat{v}|ab\rangle_A \langle ab|\hat{v}|cd\rangle_A \times \langle cd|\hat{v}|ij\rangle_A \, \Delta^{(1)}(i,j;a,b)\, \Delta^{(1)}(i,j;c,d)$$

$$k_0^{(3)}(ph) = -\sum_{abcijk} \langle bc|\hat{v}|kj\rangle_A \langle ja|\hat{v}|ib\rangle_A \times \langle ik|\hat{v}|ca\rangle_A \, \Delta^{(1)}(i,k;a,c)\, \Delta^{(1)}(j,k;b,c)$$

(!) hh is adjoint to pp; ph is self-adjoint (bra ⟷ ket; i ⟷ a, j ⟷ b, ...)

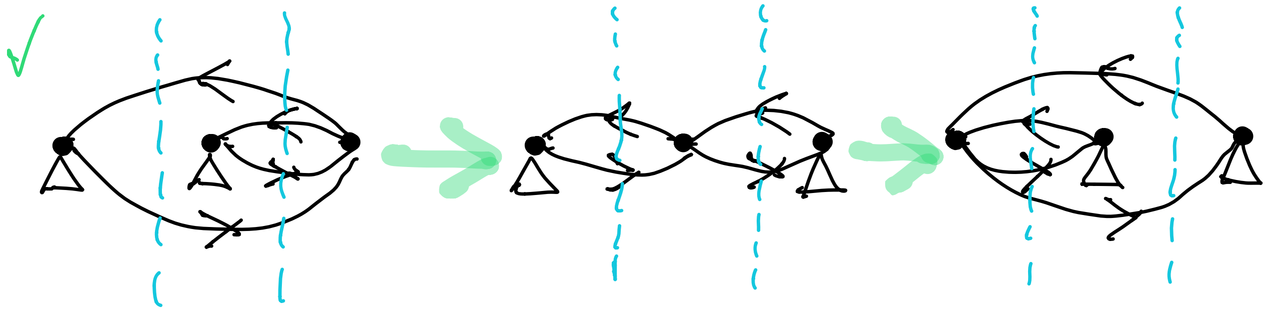
$$k_0^{(3)}(ph) = -\sum_{ijkabc} \langle cb|\hat v|jk\rangle_A \langle aj|\hat v|bi\rangle_A \times \langle ki|\hat v|ac\rangle_A \, \Delta^{(1)}(i,k;a,c)\, \Delta^{(1)}(j,k;b,c)$$

$k_0^{(3)}(B)$:

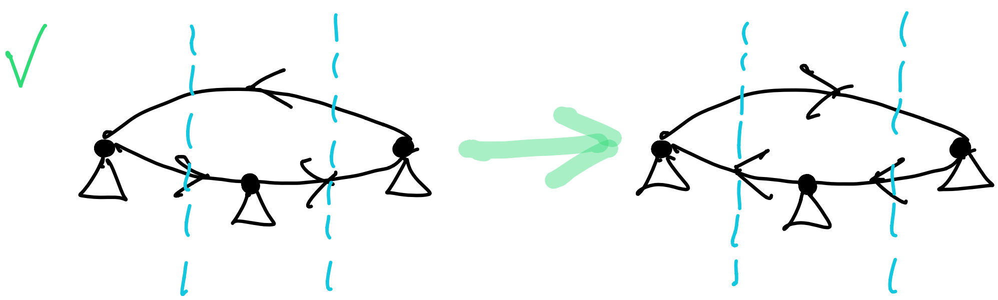


(arrows indicate time versions of the 2nd kind)

$K_0^{(3)}(C)$:



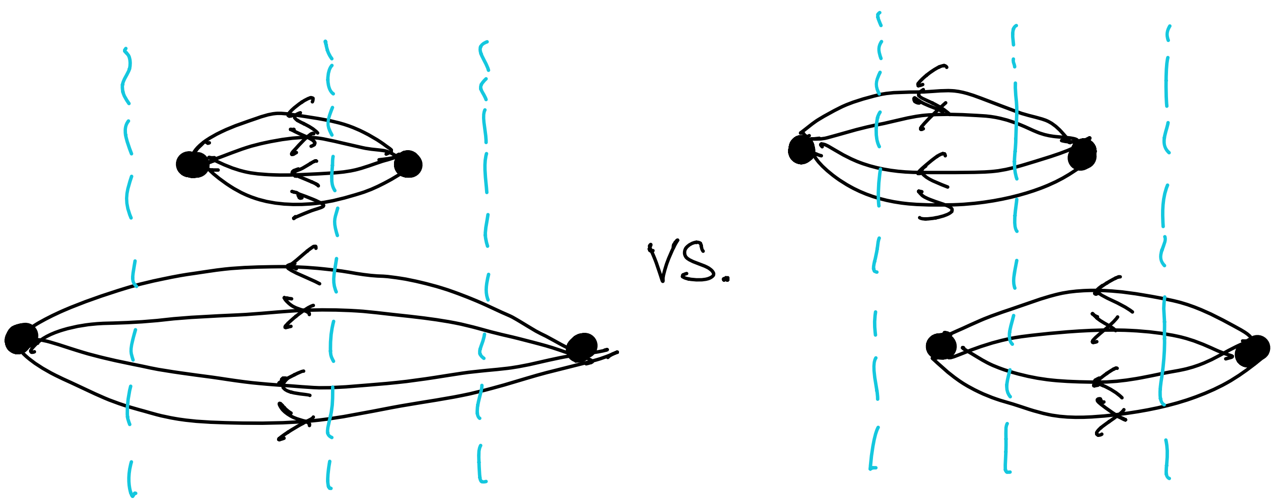
$K_0^{(3)}(D)$:

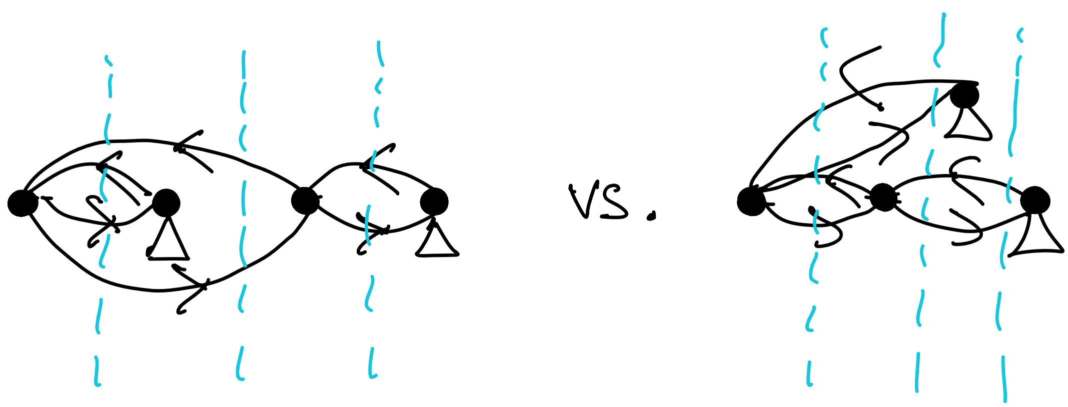


IN GENERAL,

we distinguish between TIME VERSIONS of the first and second kind.

Time versions of the 1st kind:
permute vertices along the time axis without changing the p-h character of any fermion line.





Time versions of the 2nd kind: vertices are permuted along the time axis and at least one line changes its p-h character.

Examples: $K_0^{(3)}(X)$, $X = B, C, D$

MBPT(3) correction $K_0^{(3)}$ does not bring higher-than-doubly excited contributions.

$$\langle \Phi_0 | W \underbrace{R^{(0)}}_{1,2} W \underbrace{R^{(0)}}_{1,2} W | \Phi_0 \rangle$$

$(Q_N + V_N)$

To bring <u>new physics</u>, we must go

to MBPT(n) with $n > 3$ in energy.
Also, no d-m cancellations in MBPT(3) in energy.

4-TH ORDER CORRECTION TO ENERGY

principal term

$$E_0^{(4)} = \langle \Phi_0 | W R^{(0)} W R^{(0)} W R^{(0)} W | \Phi_0 \rangle$$

$$- \underbrace{\langle \Phi_0 | W R^{(0)} W | \Phi_0 \rangle}_{E_0^{(2)}} \langle \Phi_0 | W R^{(0)2} W | \Phi_0 \rangle$$

renormaliza-tion term

$$W = Q_N + V_N$$

Focus on $W \rightarrow V_N$ terms (present independent of the choice of orbitals; in H-F case, $Q_N = 0$).

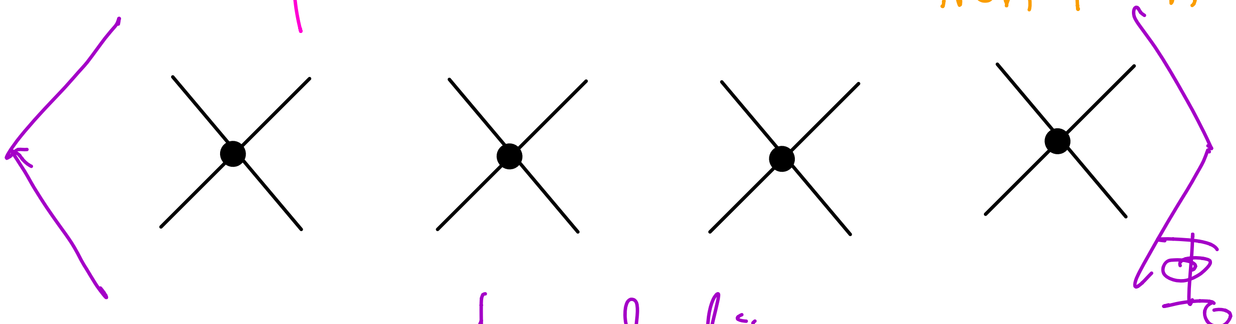
$$\langle \Phi_0 | V_N R^{(0)} V_N R^{(0)} V_N R^{(0)} V_N | \Phi_0 \rangle$$

principal term

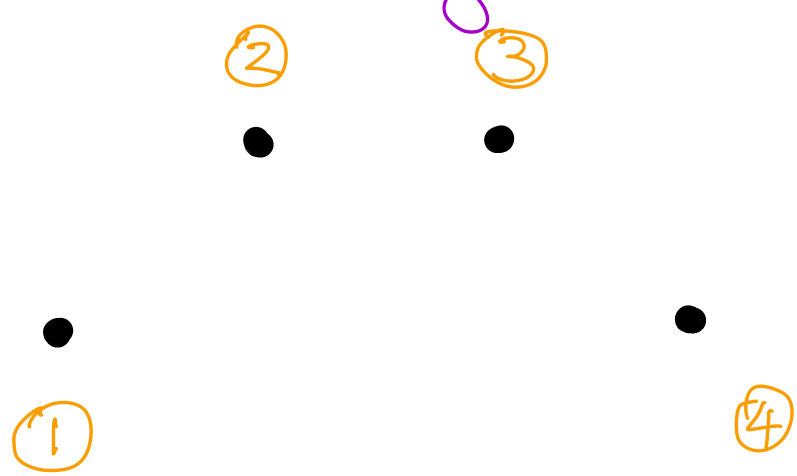
$$- \langle \Phi_0 | V_N R^{(0)} V_N | \Phi_0 \rangle \langle \Phi_0 | V_N R^{(0)2} V_N | \Phi_0 \rangle$$

renormalization term

Principal term:



no external lines,
avoid dangerous denominators

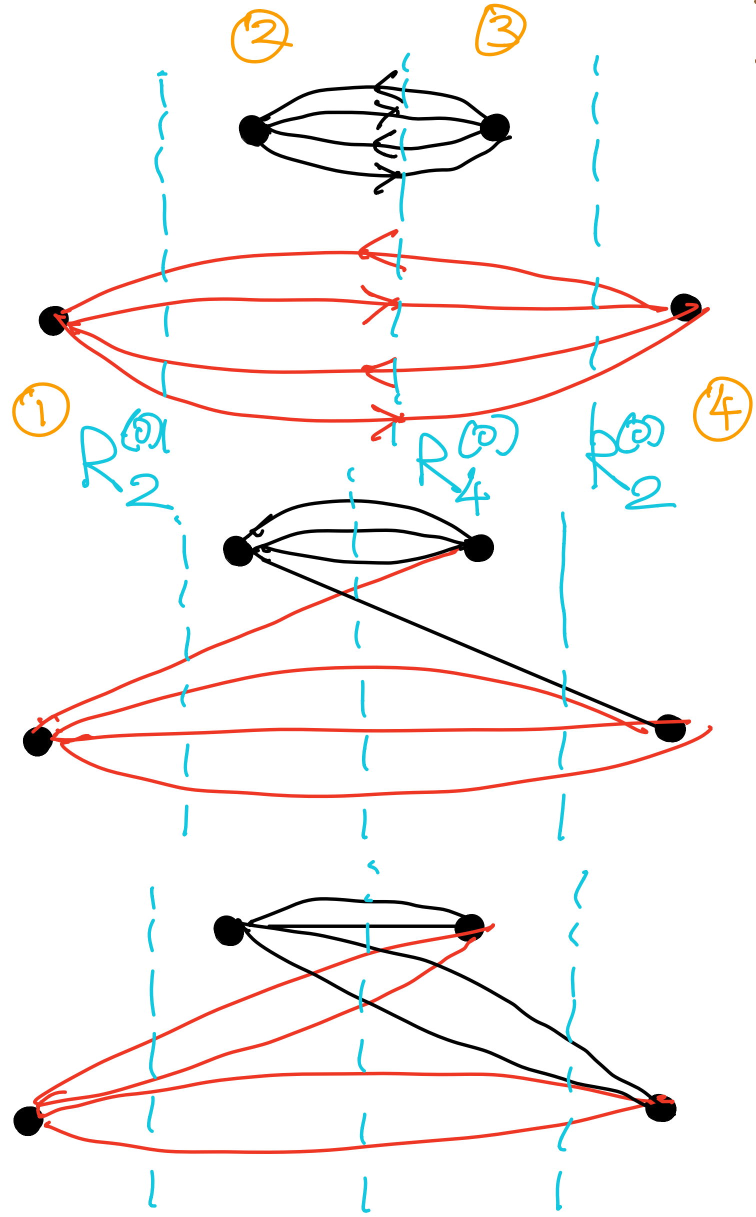


We will organize our work according to the # of lines connecting ① & ②.

Within each group, we will consider d-ms according to the # of lines between ① & ④.

NO LINES BETWEEN ① & ②:

\# of lines between ① & ④



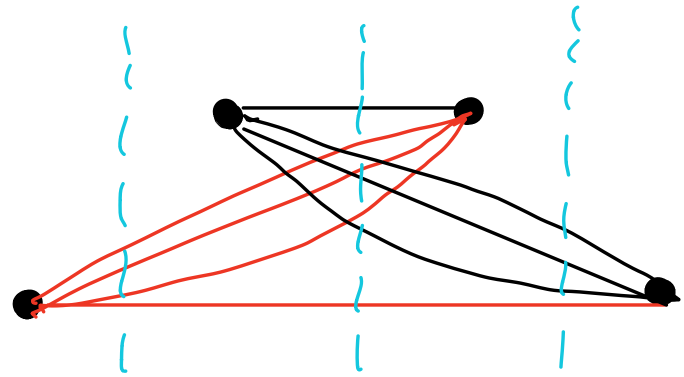
(I) $4+0$

\# of lines between ① & ③

(II) $3+1$

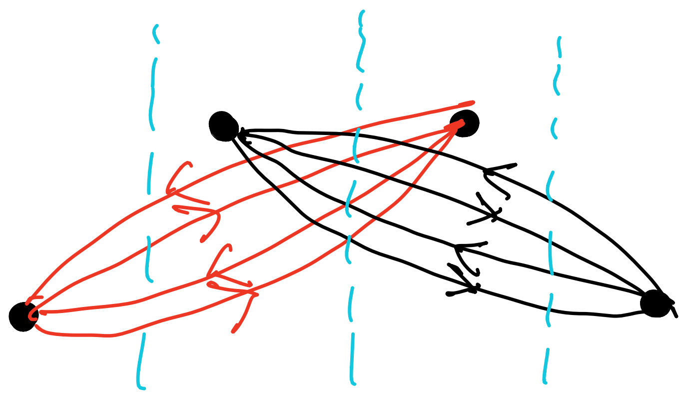
(III) $2+2$

(IV)



1+3

(V)

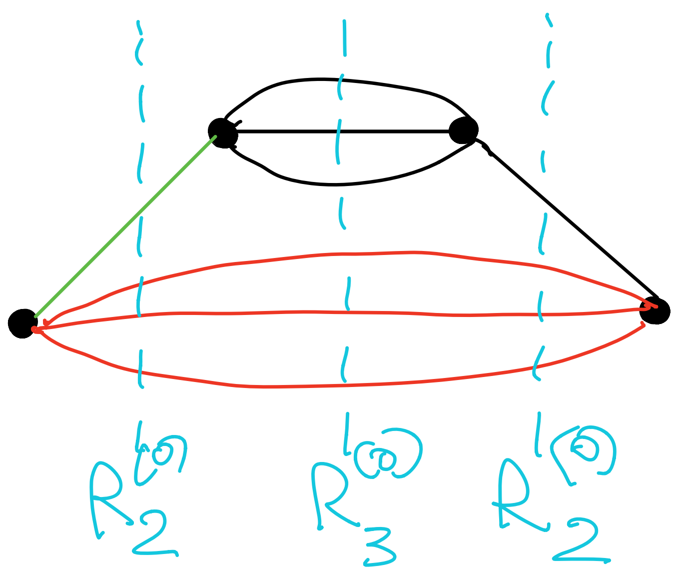


0+4

---

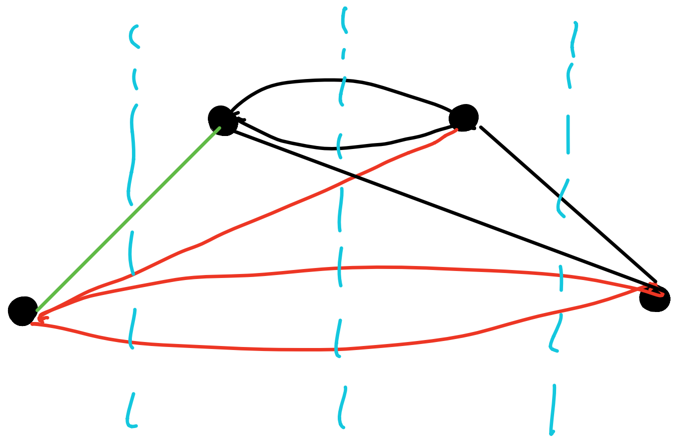
1 LINE BETWEEN ① & ②:

(VI)



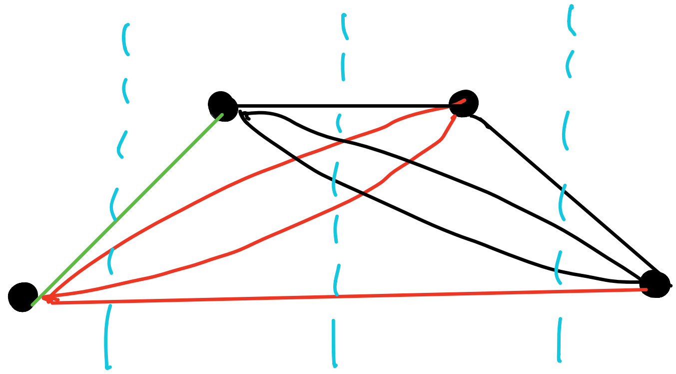
3+0

(VII)



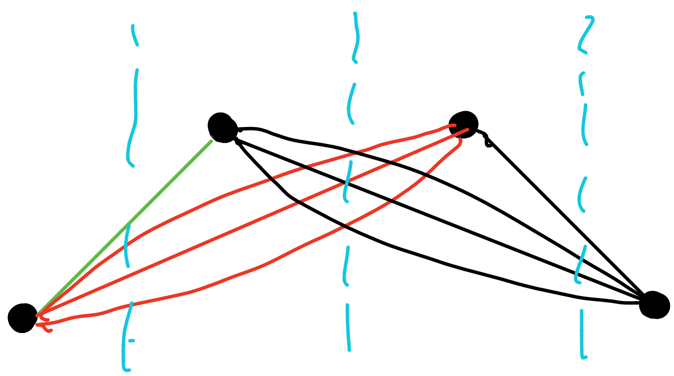
2+1

(VIII)



1+2

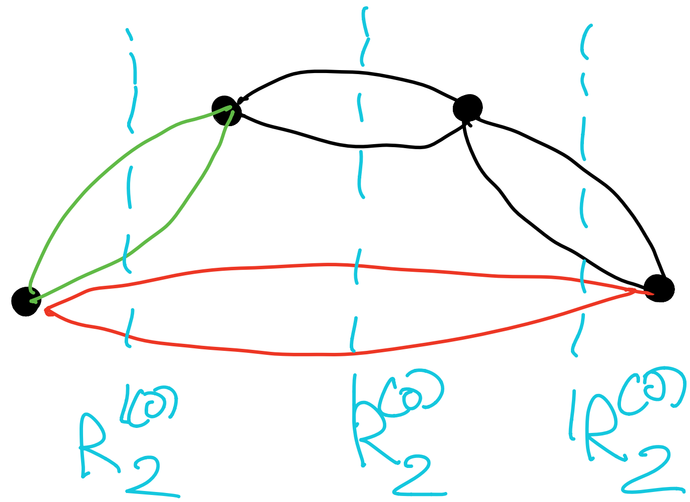
(IX)



0+3

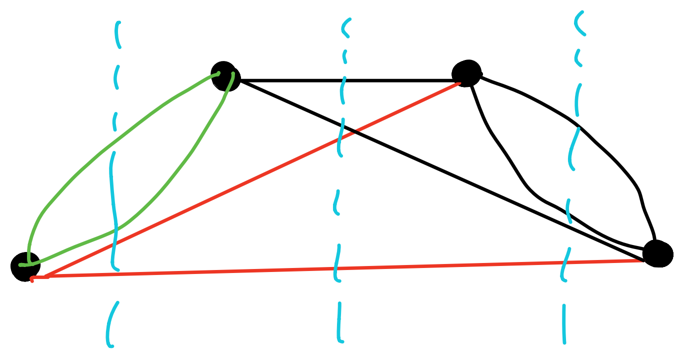
2 LINES BETWEEN 1 & 2:

(X)



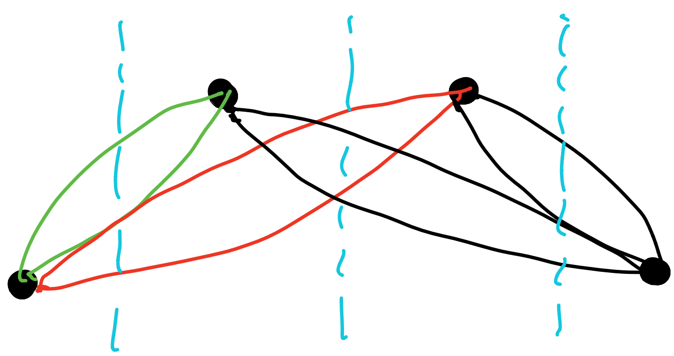
2+0

(XI)



1+1

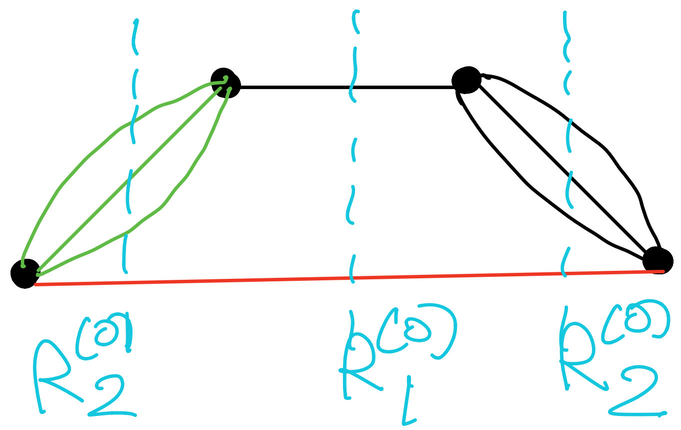
(XII)



0+2

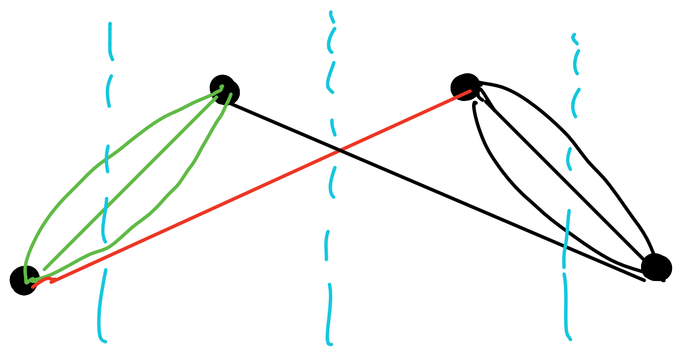
3 LINES BETWEEN 1 & 2:

(XIII)



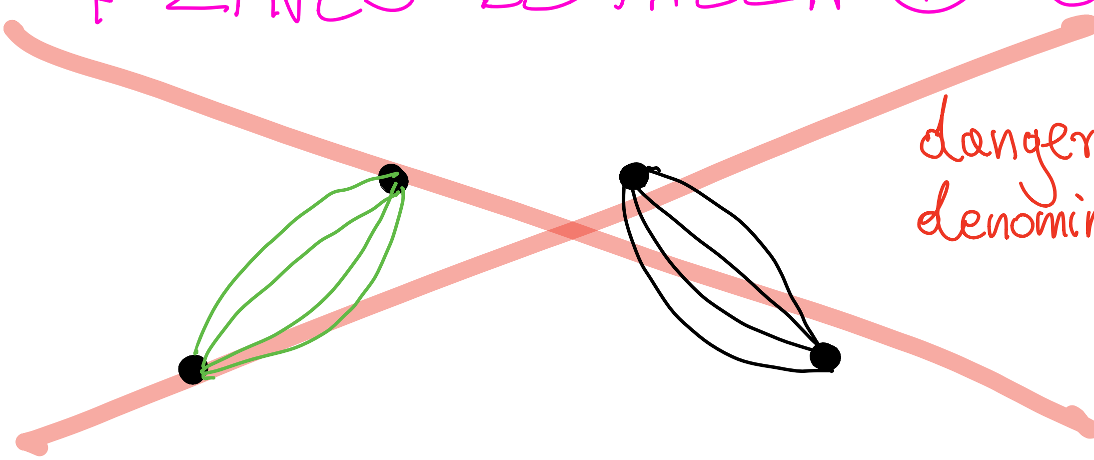
1+0

(XIV)



0+1

4 LINES BETWEEN 1 & 2:



dangerous denominator

Let us focus on the CONNECTED diagrams: (II)–(IV), (VI)–(XIV)

By examining the reduced resolvents in the middle:

(II) – (IV) use $R_4^{(\infty)}$ (quadruples)

(VI) – (IX) use $R_3^{(\infty)}$ (triples)

(X) – (XII) use $R_2^{(\infty)}$ (doubles)

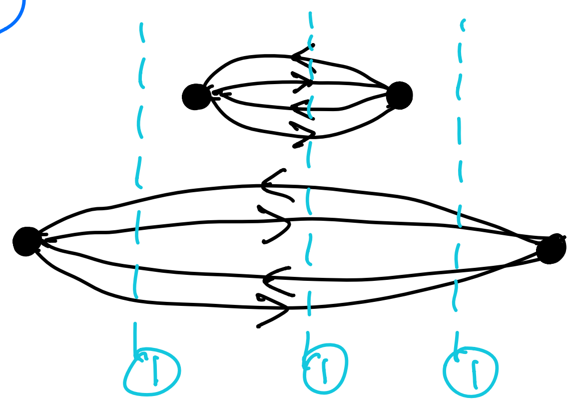
(XIII), (XIV) use $R_1^{(\infty)}$ (singles)

$$k_0^{(4)} \rightarrow k_0^{(4)}(S) + k_0^{(4)}(D) + k_0^{(4)}(T) + k_0^{(4)}(Q)$$

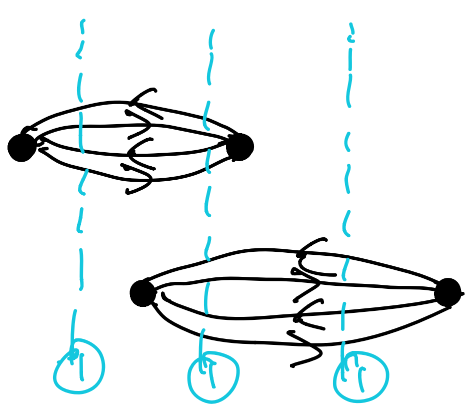
MBPT(4) in energy: MBPT(4)[SDTQ]

DISCONNECTED DIAGRAMS FROM THE PRINCIPAL TERM:

(I)

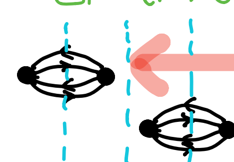


(V)



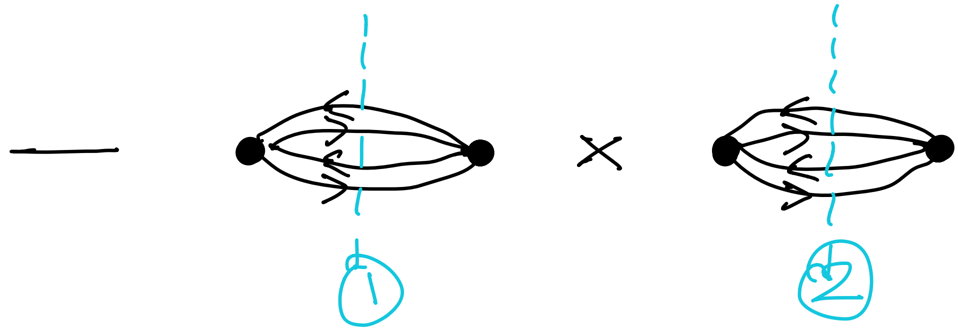
Note that (I) and (V) are the only allowed time versions of the 1st kind.

The third time version of the 1st kind



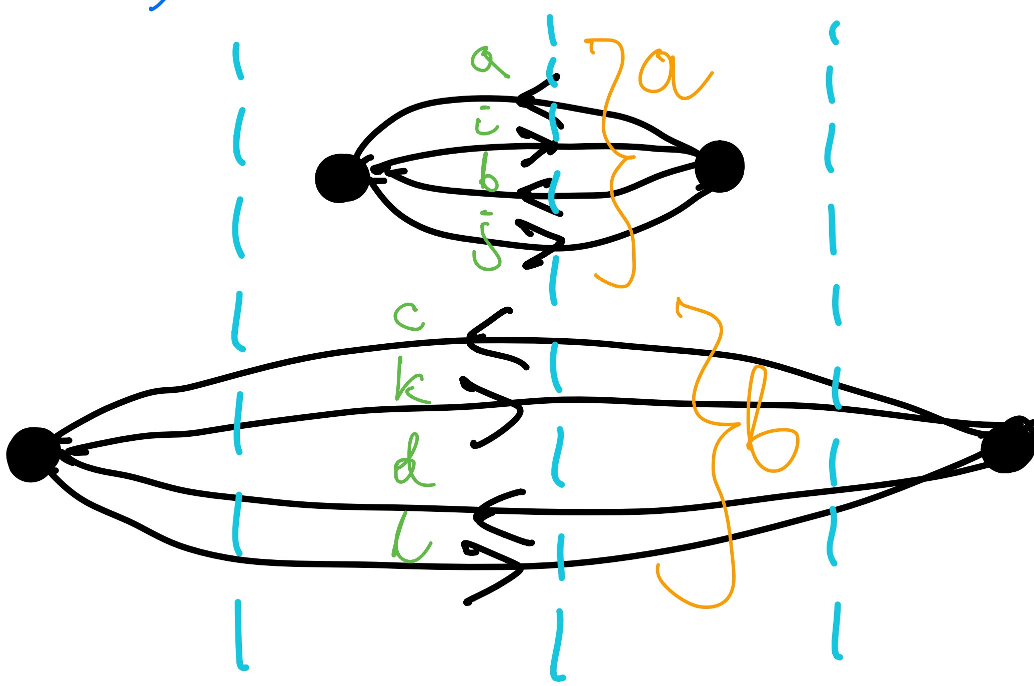
is not allowed (dangerous denominator)

RENORMALIZATION TERM:



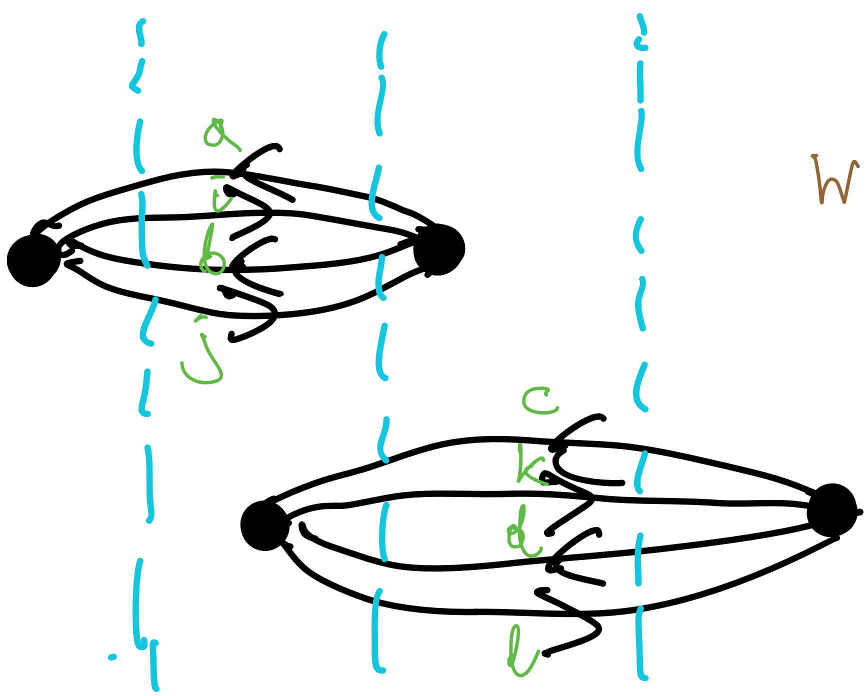
LET US NOW FOCUS ON THE DISCONNECTED DIAGRAMS (I) AND (V).

(I)



$W = \frac{1}{16}$

(V)



$W = \frac{1}{16}$

Weights and signs for (I) & (V) are the same. Numerators for (I) & (V) are the same. The only difference between (I) & (V) is in the denominators.

Let us define:

$$a = \varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_b$$

$$b = \varepsilon_k + \varepsilon_l - \varepsilon_c - \varepsilon_d$$

$$(\mathrm{I}): \quad \frac{N}{b(a+b)b}$$

$$(\mathrm{V}): \quad \frac{N}{a(a+b)b}$$

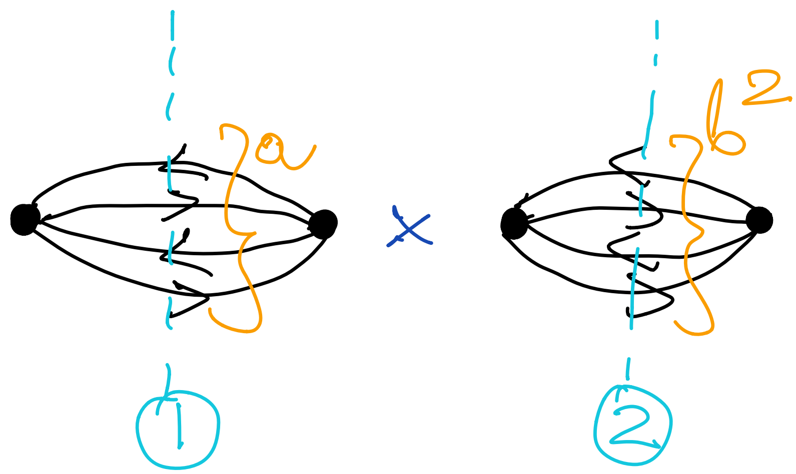
$$(\mathrm{I}) + (\mathrm{V}) = \frac{N}{(a+b)b} \times$$

$$\times \left(\frac{1}{a} + \frac{1}{b} \right)$$

$$= \frac{N}{\cancel{(a+b)}\,b} \cdot \frac{\cancel{(a+b)}}{ab}$$

$$\text{(I)} + \text{(V)} = \frac{N}{a\,b^2}$$

$=$



$$= \langle \Phi_0 | V_N R^{(0)} V_N | \Phi_0 \rangle$$

$$\times \langle \Phi_0 | V_N R^{(0)2} V_N | \Phi_0 \rangle$$

The disconnected diagrams from the principal term add up to

$$\langle \Phi_0 | W R^{(0)} W | \Phi_0 \rangle$$

$$\times \langle \Phi_0 | W R^{(0)2} W | \Phi_0 \rangle \quad \checkmark$$

$$K_0^{(4)} = \langle \Phi_0 | W (R^{(0)} W)^3 | \Phi_0 \rangle$$

$$- \langle \Phi_0 | W R^{(0)} W | \Phi_0 \rangle \langle \Phi_0 | W R^{(0)2} W | \Phi_0 \rangle$$

$$= \langle \Phi_0 | \{ W (R^{(0)} W)^3 \}_C | \Phi_0 \rangle$$

connected

$\underline{\text{II}} - \underline{\text{IV}},$
$\underline{\text{VI}} - \underline{\text{XIV}}$

$$\cancel{+\langle\Phi_0|\{W(R^{(0)}W)^3\}_{DC}|\Phi_0\rangle}$$

I, V

disconnected

$$\cancel{-\langle\Phi_0|WR^{(0)}W|\Phi_0\rangle\langle\Phi_0|WR^{(0)2}W|\Phi_0\rangle},$$

because

$$\langle\Phi_0|\{W(R^{(0)}W)^3\}_{DC}|\Phi_0\rangle$$

$$=\langle\Phi_0|WR^{(0)}W|\Phi_0\rangle\langle\Phi_0|WR^{(0)2}W|\Phi_0\rangle$$

$$K_0^{(4)} = \langle \Phi_0 | \{ W (R^0 W)^3 \}_c | \Phi_0 \rangle$$

This cancellation of disconnected diagrams in the principal term with renormalization terms happens in EVERY MBPT order in energy, i.e.,

$$\boxed{k_0^{(n+1)} = \langle \Phi_0 | \{ W (R^{(0)} W)^n \}_C | \Phi_0 \rangle}$$

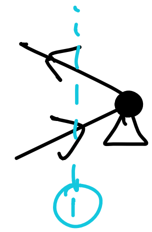
THIS IS THE FAMOUS LINKED CLUSTER THEOREM FOR ENERGY CORRECTIONS.

WHAT ABOUT WAVE FUNCTION CORRECTIONS?

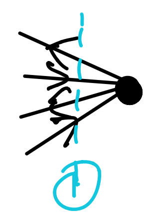
We already studied the 1st order correction $|\Psi_0^{(1)}\rangle$.

$$|\Psi_0^{(1)}\rangle = |\Psi_0^{(1)}(S)\rangle + |\Psi_0^{(1)}(D)\rangle$$

$$= R_1^{(0)} Q_N |\Phi_0\rangle$$



$$+ R_2^{(0)} V_N |\Phi_0\rangle .$$



Let us look at $|\Psi_0^{(2)}\rangle$:

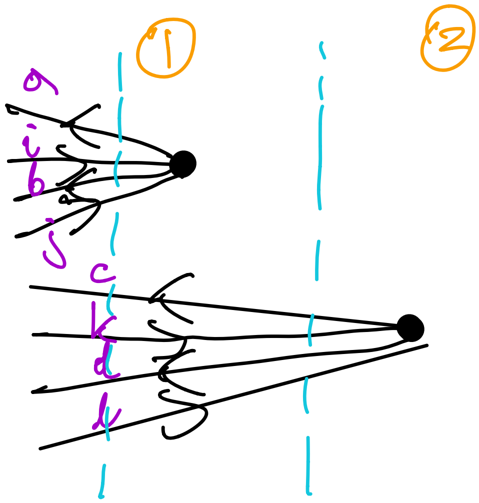
$$|\Psi_0^{(2)}\rangle = R^{(0)} W R^{(0)} W |\Phi_0\rangle,$$

$W = Q_N + V_N$. We will focus on V_N part:

$$R^{(0)} V_N R^{(0)} V_N |\Phi_0\rangle$$

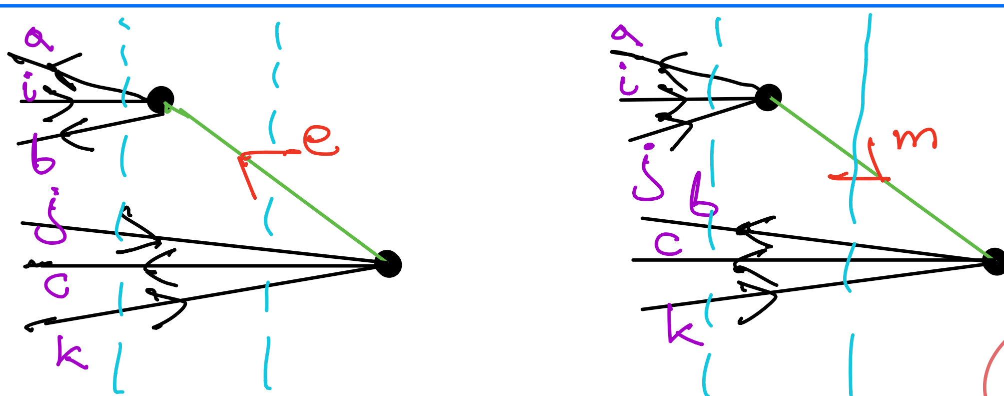
 $|\Phi_0\rangle$

resulting d-ms with external lines extending to the left, avoiding dangerous denominators



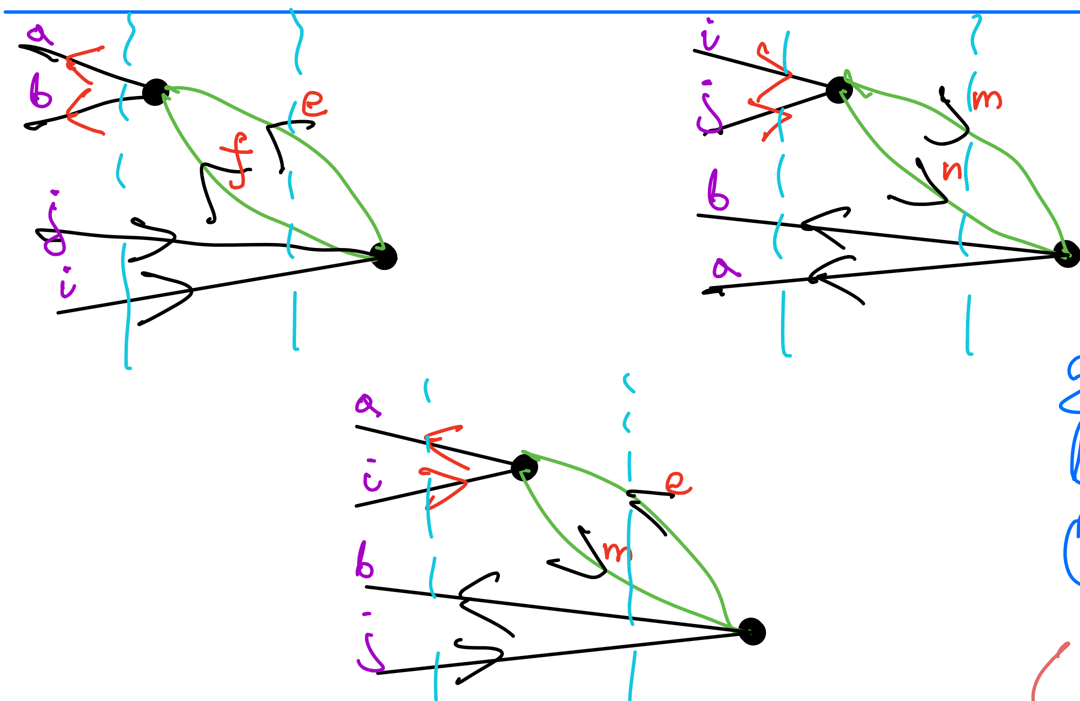
0 lines between 1 & 2

(Q)



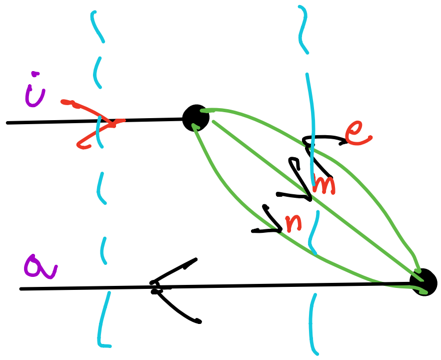
1 line between 1 & 2

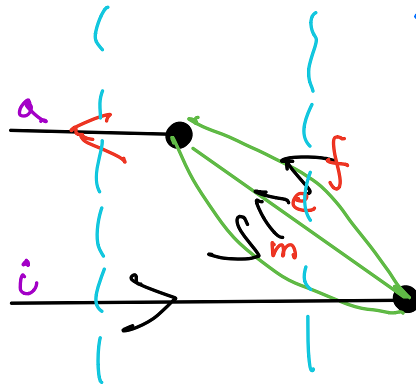
(1)



2 lines between 1 & 2

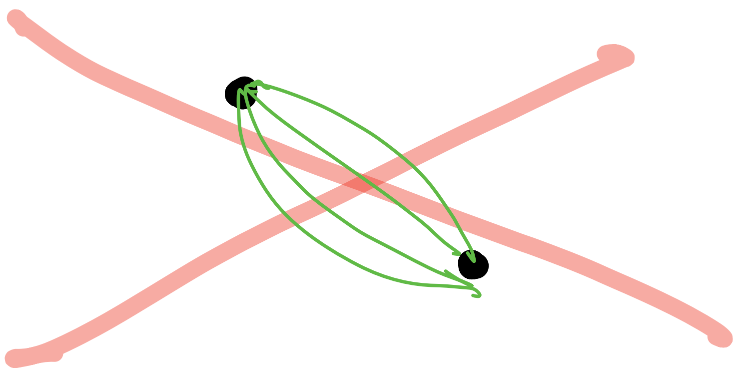
(D)





3 lines between ① & ②

(S)



dangerous denominator

4 lines between ① & ②

$|\Phi_i^a\rangle$

$|\Phi_{ijk}^{abc}\rangle$

$$|\Psi_0^{(2)}\rangle = |\Psi_0^{(2)}(S)\rangle + |\Psi_0^{(2)}(D)\rangle + |\Psi_0^{(2)}(T)\rangle + |\Psi_0^{(2)}(Q)\rangle$$

$|\Phi_{ij}^{ab}\rangle$

$|\Phi_{ijkl}^{abcd}\rangle$

$|\Psi_0^{(2)}\rangle$ contains a disconnected contribution that does not cancel out.

Thus, if there are some cancellations in wave function corrections, they must involve more than just disconnected diagrams.