FYS4480/9480 lecture November, 7, 2024

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$$H = \underbrace{\sum_{i=1}^{2} a_i^\dagger a_i \varepsilon_i}_{H_0} + \underbrace{\lambda \sum_{i \neq j = 1,2} a_i^\dagger a_j}_{H_I}$$

$$H_0 |\phi_1\rangle = \varepsilon_1 |\phi_1\rangle \qquad |\phi_1\rangle = a_1^\dagger |0\rangle$$

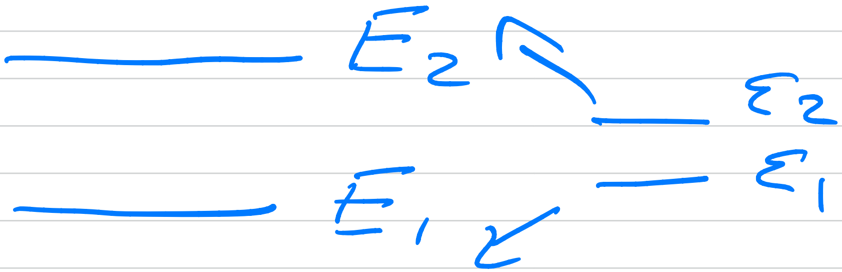
$$H_0 |\phi_2\rangle = \varepsilon_2 |\phi_2\rangle$$

$$|\phi_2\rangle = a_2^\dagger |0\rangle$$

$$\langle \Phi_1 | H | \phi_1 \rangle = \varepsilon_1 \quad \langle \phi_2 | H | \phi_2 \rangle = \varepsilon_2$$

$$\langle \Phi_1 | H | \phi_2 \rangle = \lambda$$

$$\det\begin{bmatrix} \varepsilon_1 - E_1 & \lambda \\ \lambda & \varepsilon_2 - E_1 \end{bmatrix} = 0$$



BW - pert-theory

$$\Delta E_1 = E_1 - \varepsilon_1 = \frac{\lambda^2}{E_1 - \varepsilon_2} \Rightarrow$$

$$\Delta E_1 \rightarrow (E_1 - \varepsilon_1)(E_1 - \varepsilon_2) - \lambda^2 = 0$$

RS - pert theory (3-order)

$E_1 \to \varepsilon_1 \quad (E_2 \to \varepsilon_2)$

$$\Delta E_1 (RSPT) = \underbrace{\langle \Phi_1 | H_1 | \Phi_1 \rangle}_{=0}$$

$$+ \frac{\langle \Phi_1 | H_1 | \Phi_2 \rangle \langle \Phi_2 | H_1 | \Phi_1 \rangle}{\varepsilon_1 - \varepsilon_2}$$

$$+ \frac{\langle \Phi_1 | H_1 | \Phi_2 \rangle \langle \Phi_2 | H_1 | \Phi_2 \rangle \langle \Phi_2 | H_1 | \Phi_1 \rangle}{(\varepsilon_1 - \varepsilon_2)^2}$$

$$- \frac{\langle \Phi_1 | H_1 | \Phi_1 \rangle \langle \Phi_1 | H_1 | \Phi_2 \rangle \langle \Phi_2 | H_1 | \Phi_1 \rangle}{(\varepsilon_1 - \varepsilon_2)^2}$$

$$= \frac{\lambda^2}{\varepsilon_1 - \varepsilon_2} \neq \Delta E_1 (BWPT) = \frac{\lambda^2}{E_1 - \varepsilon_2}$$

Diagonalize the Eigenvalue problem

$$E_1 = \frac{1}{2}\left(\varepsilon_1 + \varepsilon_2 - (\varepsilon_2 - \varepsilon_1)\sqrt{1 + 4\frac{\lambda^2}{(\varepsilon_2 - \varepsilon_1)^2}}\right)$$

$$\varepsilon_2 - \varepsilon_1 \neq 0 \qquad \left|\frac{\lambda}{\varepsilon_2 - \varepsilon_1}\right| < 1$$

$$E_1 - \varepsilon_1 = \Delta E_1 = \frac{\lambda^2}{\varepsilon_1 - \varepsilon_2} - \frac{\lambda^4}{(\varepsilon_1 - \varepsilon_2)^3} + \cdots$$

$$\Delta E_1 (BWPT) = \frac{\lambda^2}{\varepsilon_1 - \varepsilon_2} = \frac{\lambda^2}{\varepsilon_1 - \varepsilon_2 + \Delta E_1}$$

$$= \frac{\lambda^2}{\varepsilon_1 - \varepsilon_2}\left[1 - \left(\frac{\Delta E_1}{\varepsilon_1 - \varepsilon_2}\right) + \left(\frac{\Delta E_1}{\varepsilon_1 - \varepsilon_2}\right)^2 + \cdots\right]$$

$$= \frac{\lambda^2}{\varepsilon_1 - \varepsilon_2}\left[1 - \frac{\lambda^2}{(\varepsilon_1 - \varepsilon_2)^2} + \cdots\right]$$

$$\Delta E_1^{(4)} (\text{RSPT}) =$$

$$\left\{ \begin{array}{l} \left(\langle \hat{H}_1 \rangle = \langle \Phi_1 | \hat{H}_1 | \Phi_1 \rangle \right) \\ \langle \hat{H}_1 \frac{\hat{Q}}{\hat{e}_0} \hat{H}_1 \rangle = \langle \Phi_1 | \hat{H}_1 \frac{\hat{Q}}{\hat{e}_0} \hat{H}_1 | \Phi_1 \rangle \\ \qquad \hat{Q} = |\Phi_2\rangle\langle\Phi_2| \\ \qquad \hat{e}_0 = \varepsilon_1 - \hat{H}_0 \end{array} \right.$$

$$= \langle \hat{H}_1 \frac{\hat{Q}}{\hat{e}_0} \underbrace{\hat{H}_1 \frac{\hat{Q}}{\hat{e}_0} \hat{H}_1}^{\approx 0} \frac{\hat{Q}}{\hat{e}_0} \hat{H}_1 \rangle$$

$$- \langle \hat{H}_1 \frac{\hat{Q}}{\hat{e}_0} \underbrace{\langle \hat{H}_1 \rangle}_{\approx 0} \frac{\hat{Q}}{\hat{e}_0} H_1 \frac{\hat{Q}}{\hat{e}_0} H_1 \rangle$$

$$-\langle \hat{H}_1 \frac{\hat{Q}}{\hat{e}_0} \hat{H}_1 \frac{\hat{Q}}{\hat{e}_0} \underbrace{\langle \hat{H}_1 \rangle}_{=0} \frac{\hat{Q}}{\hat{e}_0} \hat{H}_1 \rangle$$

$$+\langle \hat{H}_1 \frac{\hat{Q}}{\hat{e}_0} \underbrace{\langle \hat{H}_1 \rangle}_{=0} \frac{\hat{Q}}{\hat{e}_0} \overset{=0}{\langle \hat{H}_1 \rangle} \frac{\hat{Q}}{\hat{e}_0} \hat{H}_1 \rangle$$

$$-\langle \hat{H}_1 \frac{\hat{Q}}{\hat{e}_0} \underbrace{\langle \hat{H}_1 \frac{\hat{Q}}{\hat{e}_0} \hat{H}_1 \rangle}_{\frac{\lambda^2}{\varepsilon_1-\varepsilon_2}} \frac{\hat{Q}}{\hat{e}_0} \hat{H}_1 \rangle$$

2

$$\boxed{-\frac{\lambda^4}{(\varepsilon_1-\varepsilon_2)^3}}$$

$$\frac{Q^2}{e_0^2} = \frac{Q}{e_0^2} = \frac{|\phi_2\rangle\langle\phi_2|}{(\varepsilon_1-\hat{H}_0)^2}$$

$$\frac{1}{(\varepsilon_1-\varepsilon_2)^2}$$

Diagrams and Diagrammer

$$\Delta E_0^{(2)} = \langle \Phi_0 | H_1 \frac{\hat{Q}}{e_0} H_1 | \Phi_0 \rangle$$

$$\hat{Q} = \sum_{i>0} |\Phi_i\rangle\langle\Phi_i|$$

$$e_0 = \mathcal{E}_0 - \hat{H}_0$$

$$\hat{H}_0 |\Phi_i\rangle = \mathcal{E}_i |\Phi_i\rangle$$

$ijkl \ldots \leq F \qquad abcd \ldots > F$

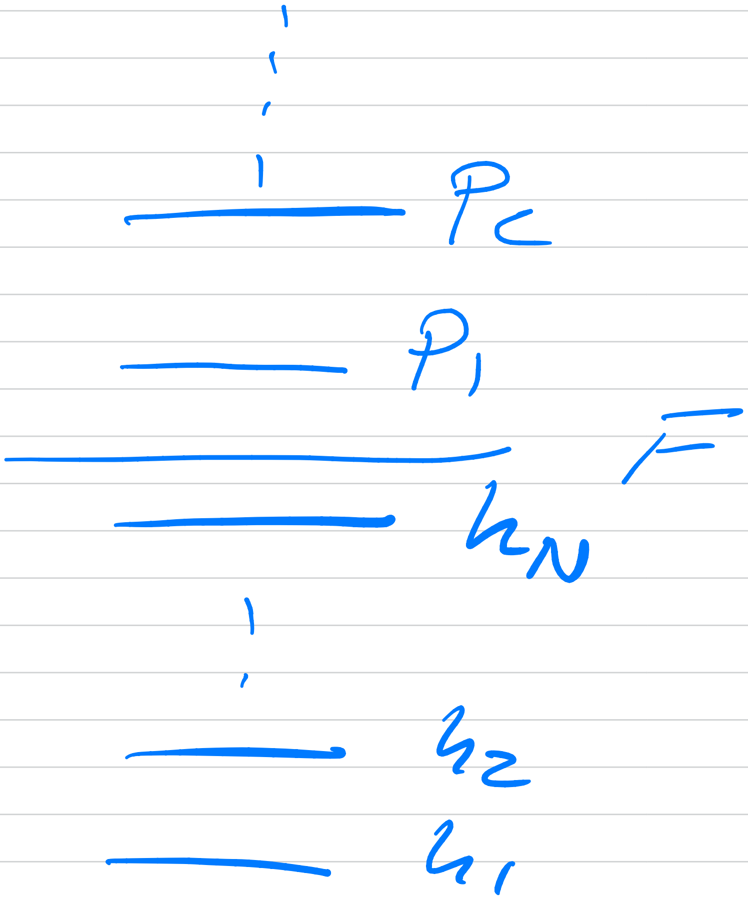
$$|\Phi_1\rangle = a^{+}_{p_1} a^{+}_{h_2} a^{+}_{h_3} \cdots a^{+}_{h_n} |0\rangle$$

$$= a^{+}_{p_1} a_{h_1} |\Phi_0\rangle$$

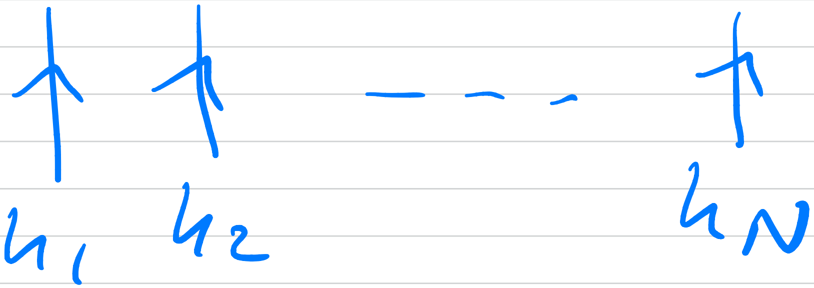
$$|\Phi_0\rangle = \prod_{h_i < F} a^{+}_{h_i} |0\rangle$$

$$|\Phi_2\rangle = a^{+}_{h_1} a^{+}_{p_2} a^{+}_{h_3} \cdots a^{+}_{h_N} |0\rangle$$

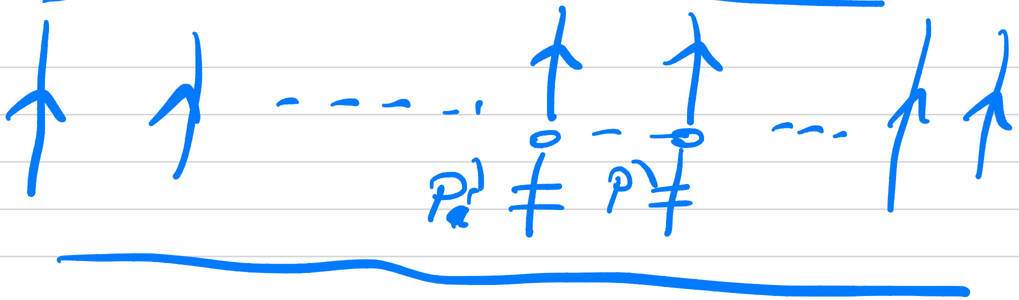
$$= a^{+}_{p_2} a_{h_2} |\Phi_0\rangle$$



$|\Phi_c\rangle$



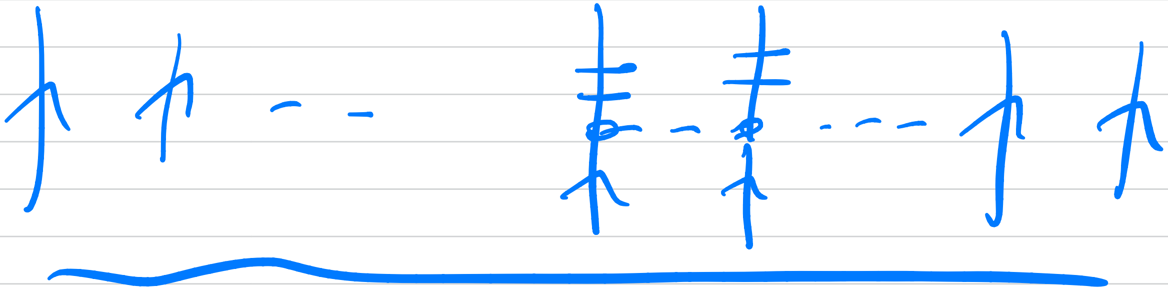
$$\sum_{i>0} \langle \Phi_0 |$$



$$\times \frac{1}{E_0 - E_i}$$

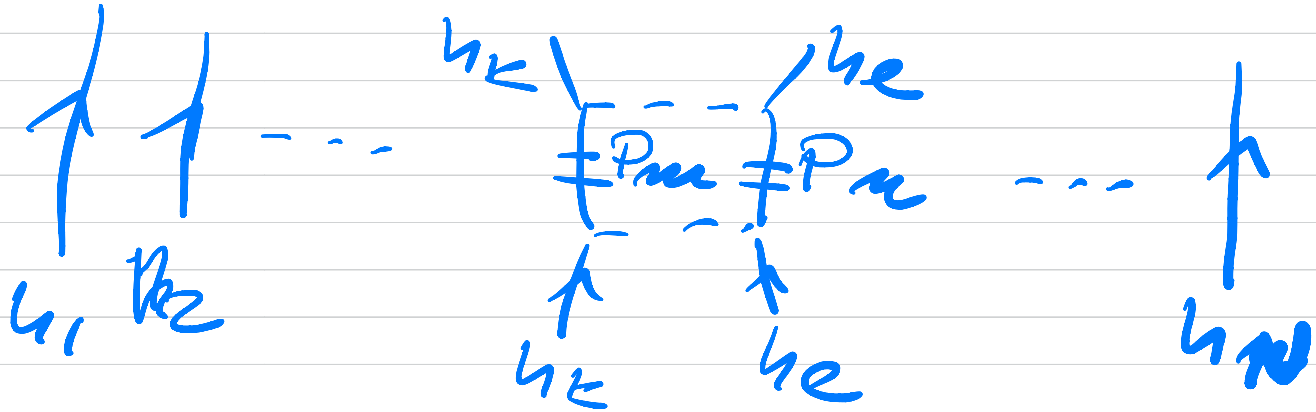
$$| \Phi_i \rangle$$

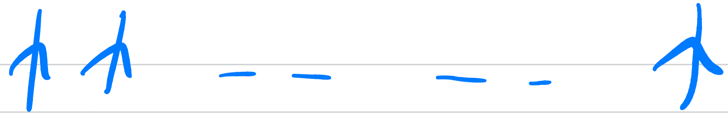
$$\times \quad \langle \Phi_i |$$

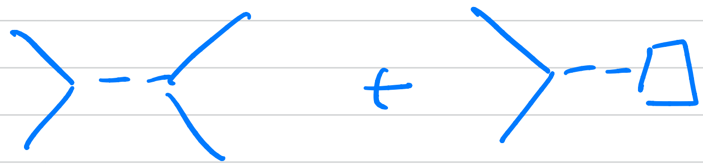


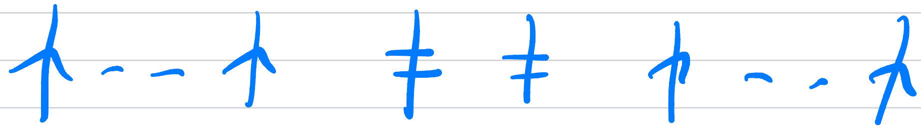
$$| \Phi_0 \rangle$$

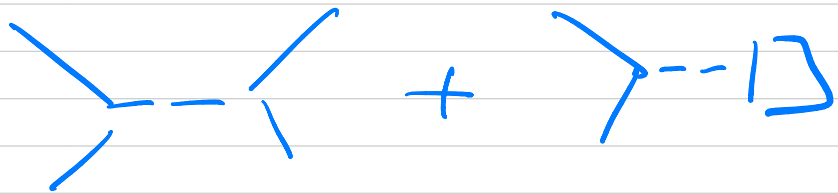
$$= \sum_{p_m p_n}$$

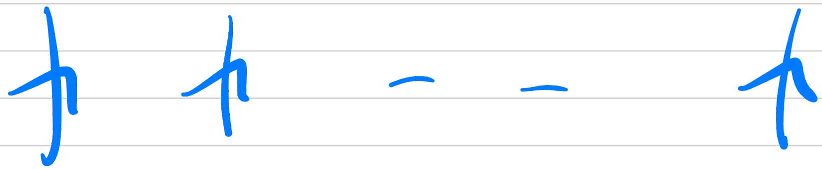


$\langle \Phi_0 | \rightarrow$ 

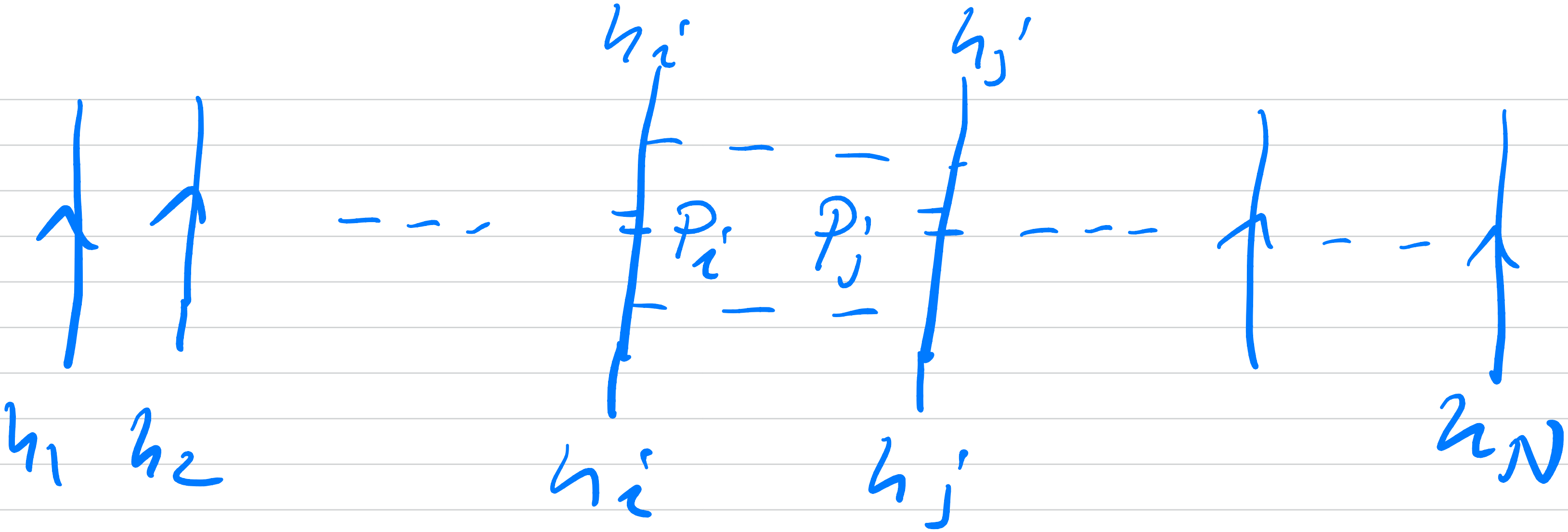
$H_1 \rightarrow$ 

$\dfrac{|\Phi_i\rangle\langle\Phi_i|}{\varepsilon_0 - \varepsilon_i} \rightarrow$ 

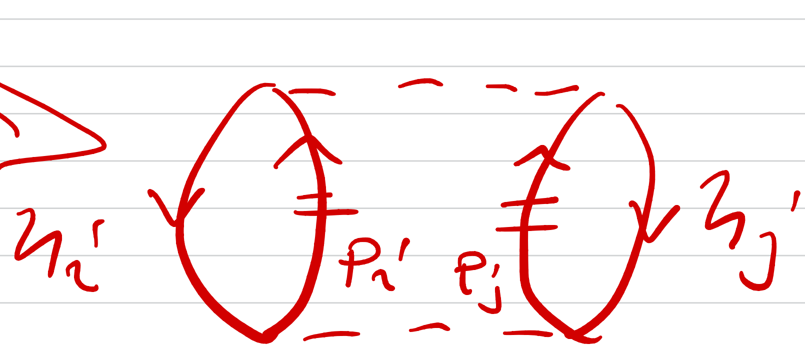
$H_1 \rightarrow$ 

$|\Phi_0\rangle \rightarrow$ 

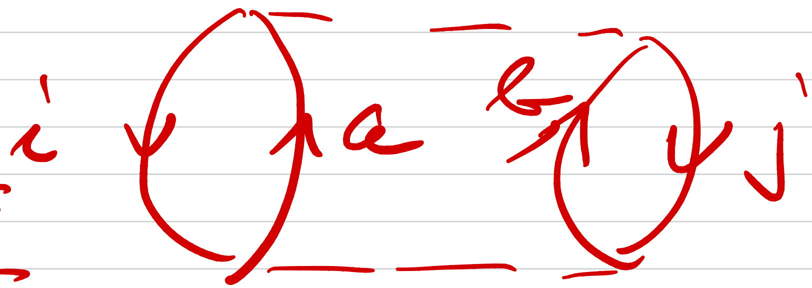
have to be contracted

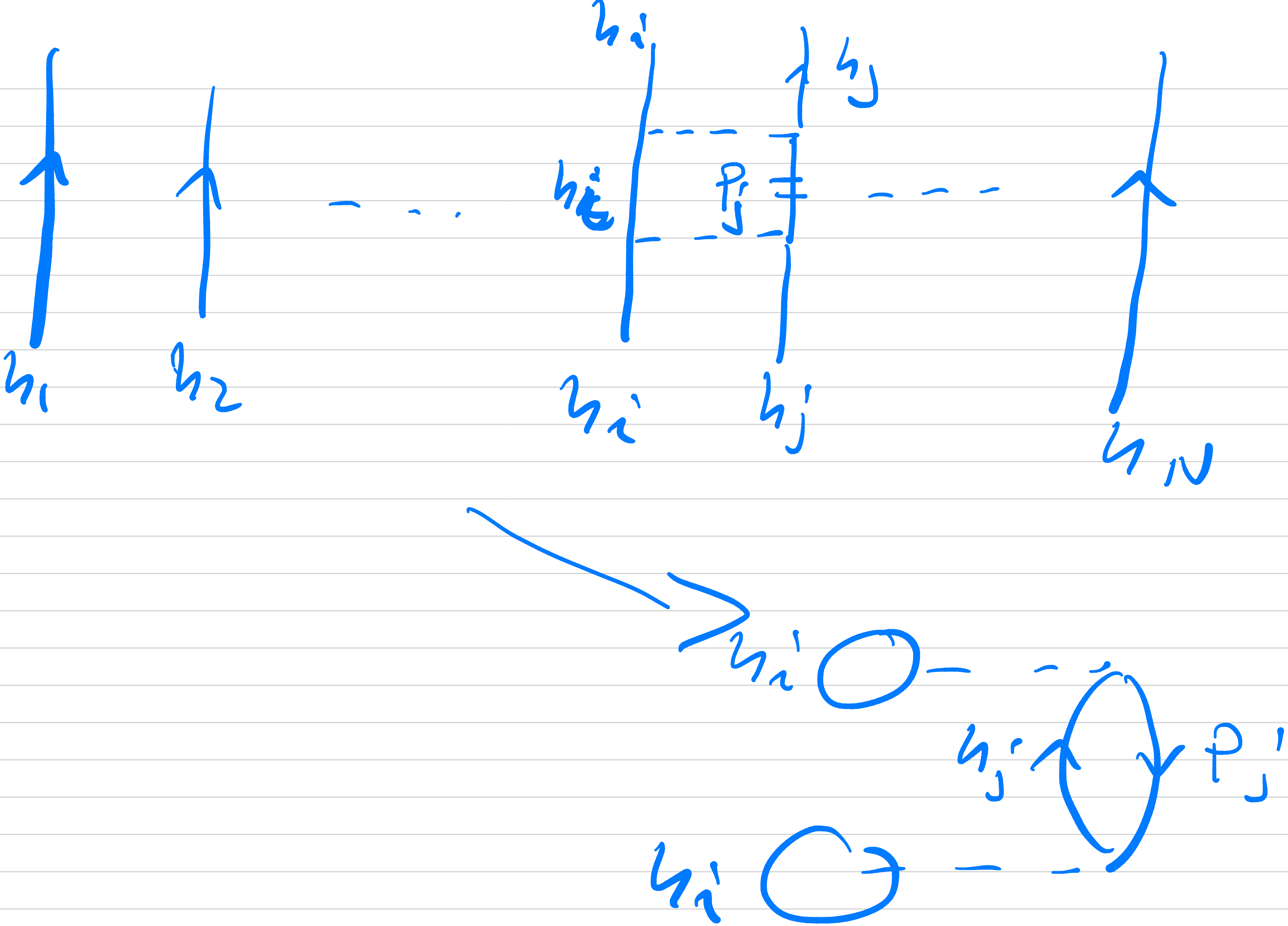


$$\sum_{\substack{h_i\, h_j' \\ p_i'\, p_j'}}$$

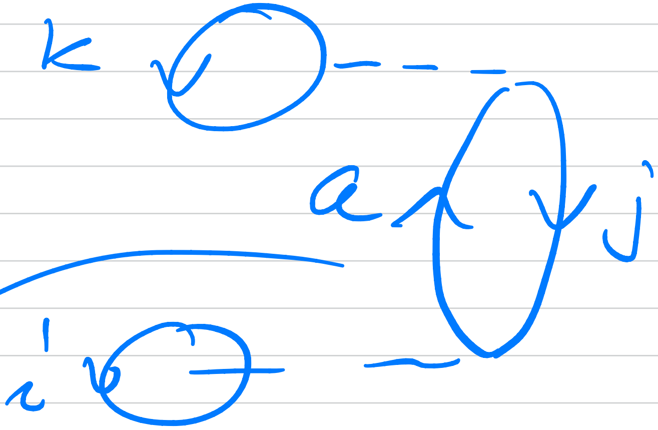


$$\sum_{\substack{ab > F \\ ij \le F}}$$





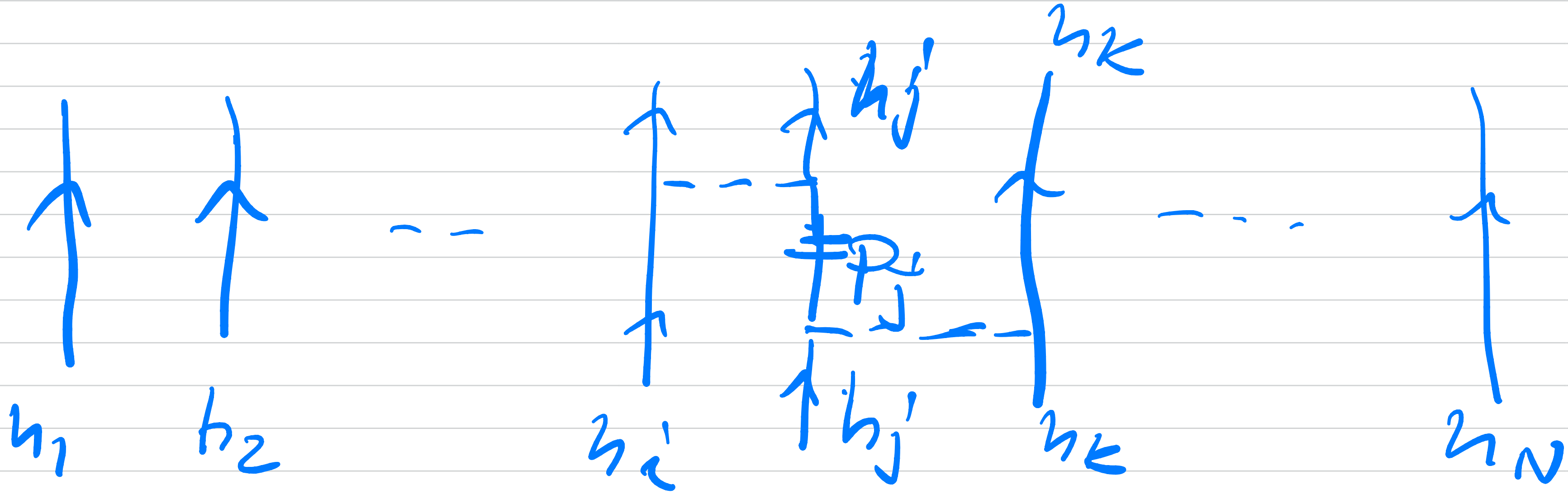
n_i'
n_j
n_i
P_j
n_1
n_2
n_i'
n_j'
n_N
n_i'
n_j'
P_j'
n_i'

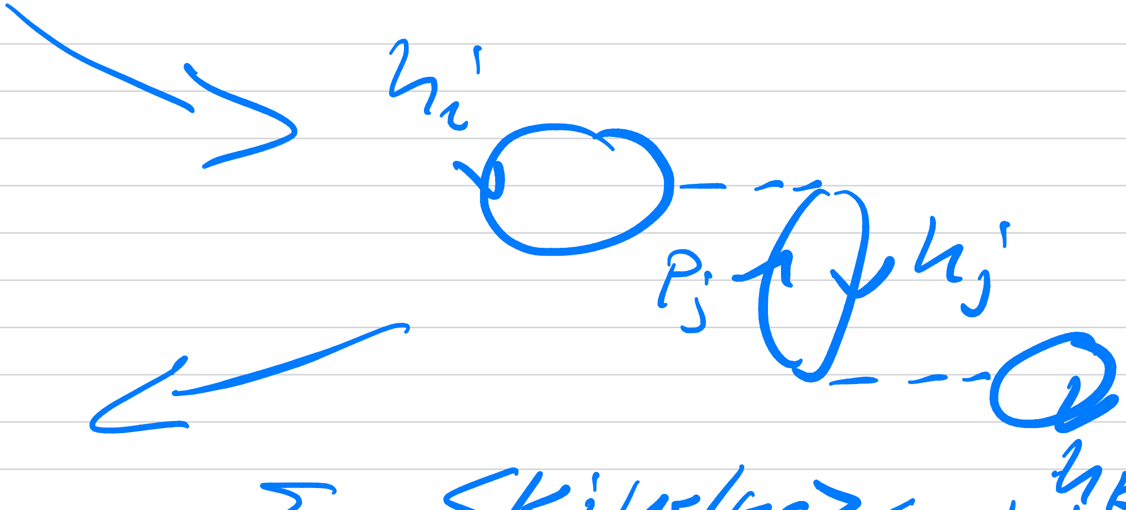


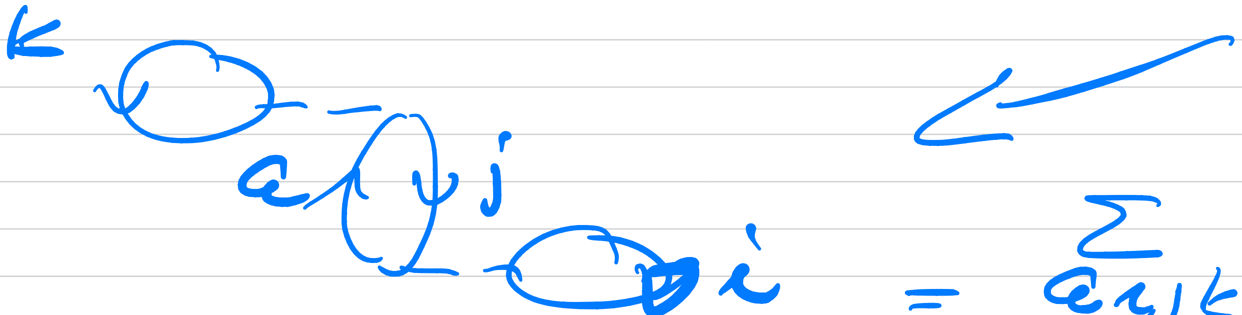
$$\varepsilon_a - \varepsilon_j + \varepsilon_0$$

$$= \sum_{aijk} \frac{\langle kj|v|ka\rangle\langle ia|v|ij\rangle}{\varepsilon_j - \varepsilon_a}$$

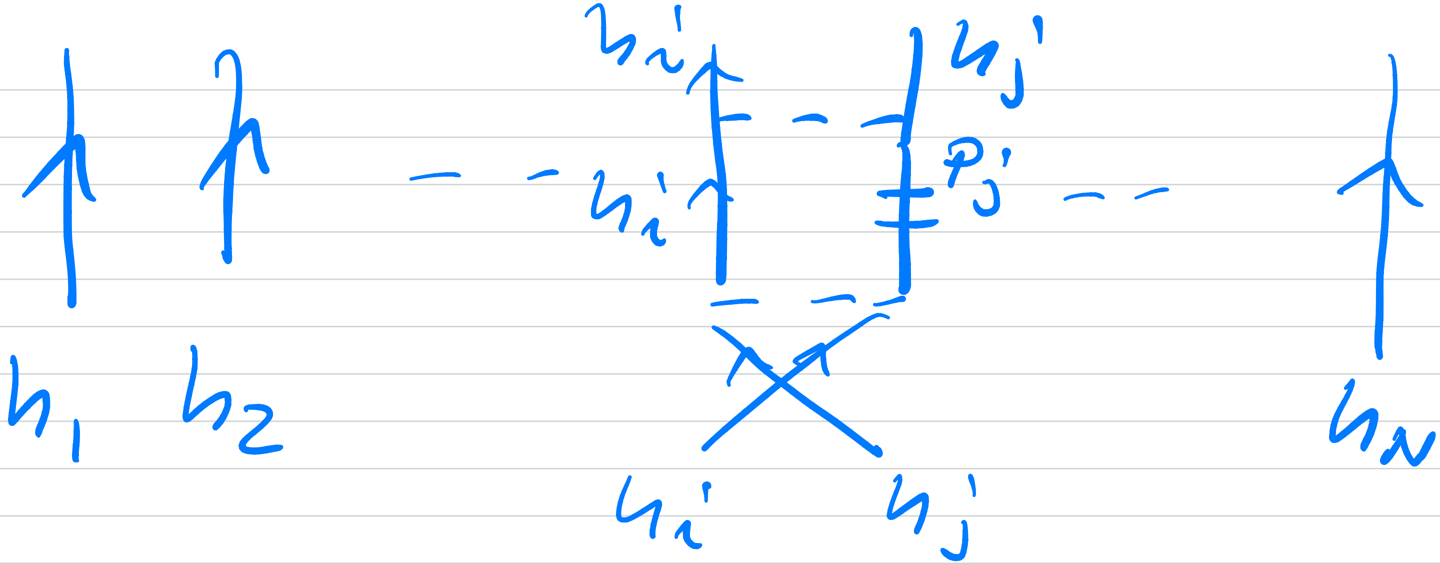
$$\frac{1}{\varepsilon_0 - (\varepsilon_a - \varepsilon_j) - \varepsilon_0} = \frac{1}{\varepsilon_j - \varepsilon_a}$$

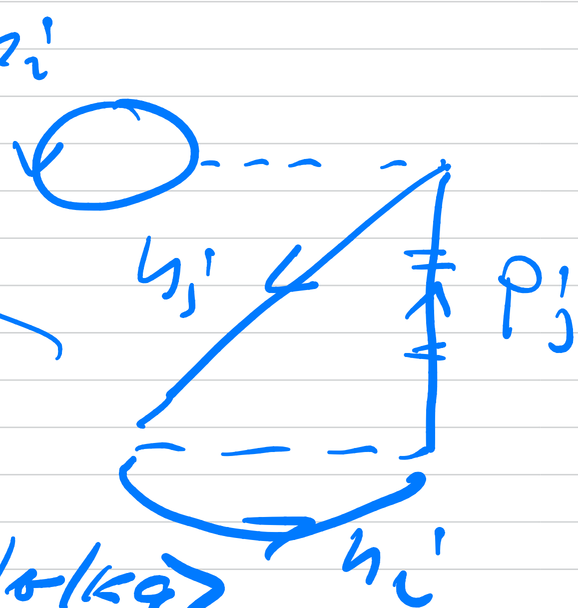


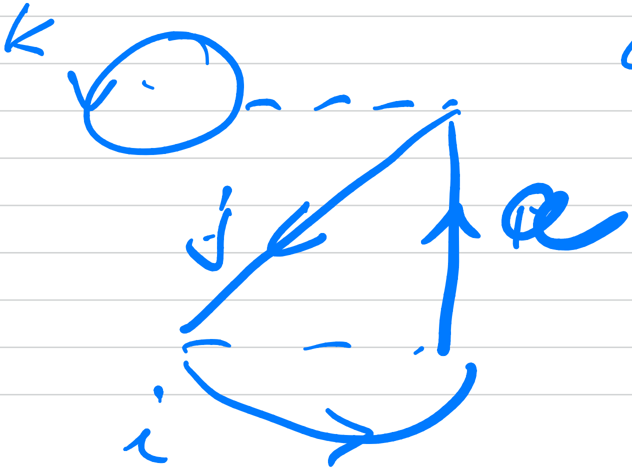




$$= \sum_{a,j,k} \frac{\langle kj|v|ka\rangle\langle ai|v|ji\rangle}{\varepsilon_i - \varepsilon_a}$$

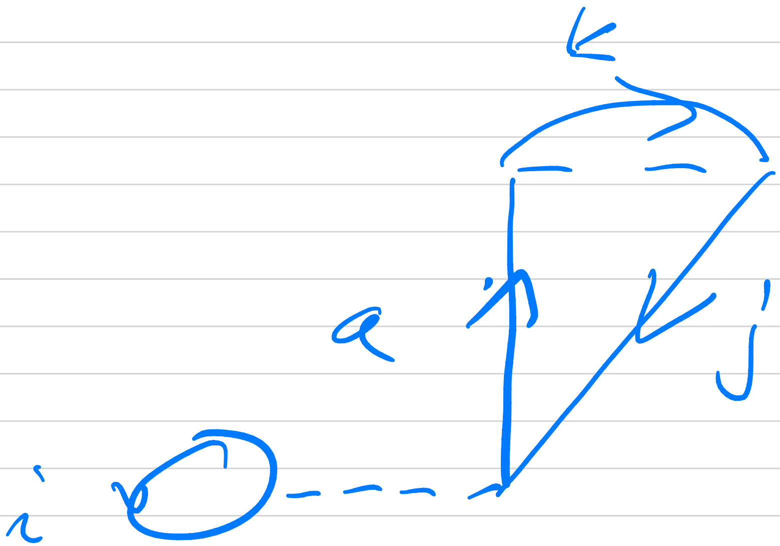




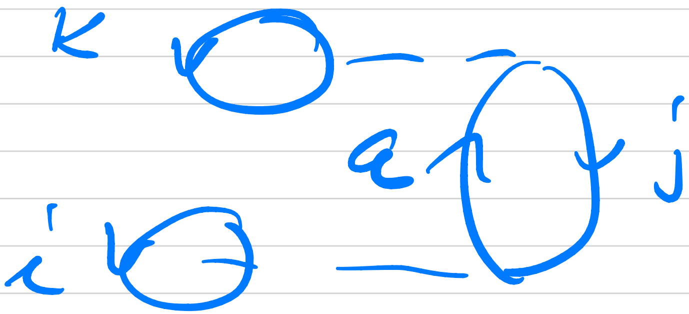


$$\propto \sum_{aijk} \frac{\langle kj|v|ka\rangle\langle ia|v|ji\rangle}{\varepsilon_i - \varepsilon_a}$$

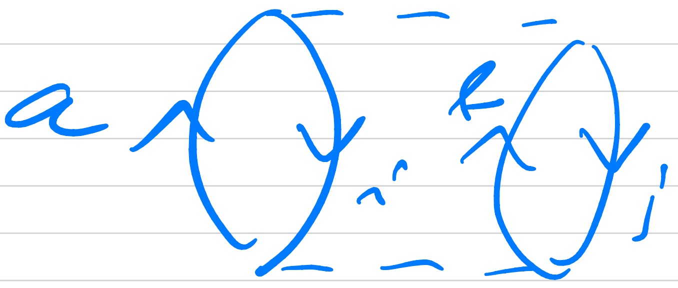
$$\langle ia \| v \| ji \rangle_{AS} = - \langle ia \| v \| ij \rangle_{AS}$$



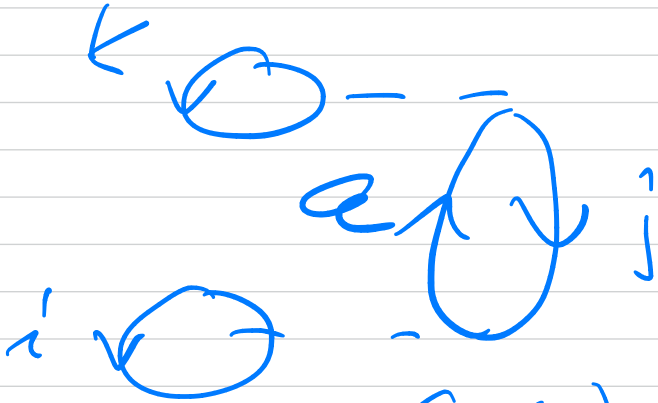
ip/h excitations to 2nd order



2nd-order



(4)



(16)

Diagram rules

(i) Draw all topologically distinct diagrams to a given order by linking up particle and hole lines with different interaction vertices, under the restriction that

a) the ordering of the interaction vertices is not altered

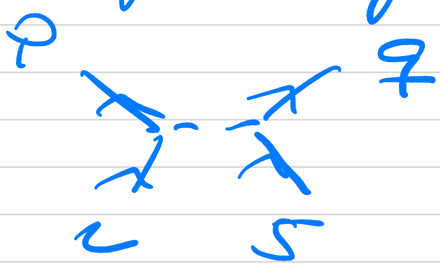
b) particle states remain as such. Idem for hole states

c) ordering of interactions at the beginning and at the end is unchanged.

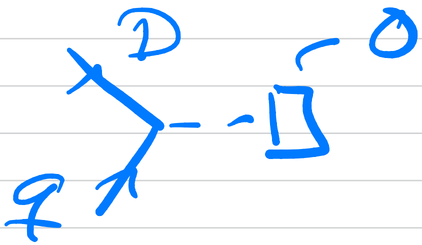
(ii) For each topologically distinct diagram

a) set up interaction vertices ()

b) each interaction gives a specific element



$\langle pq|v|rs\rangle$

or  $\langle p|O|q\rangle$

c) There is a factor $(-1)^{n_h + n_e}$

$n_e = \#$ closed loops

$n_h = \#$ hole lines

d) For each interval between two successive vertices

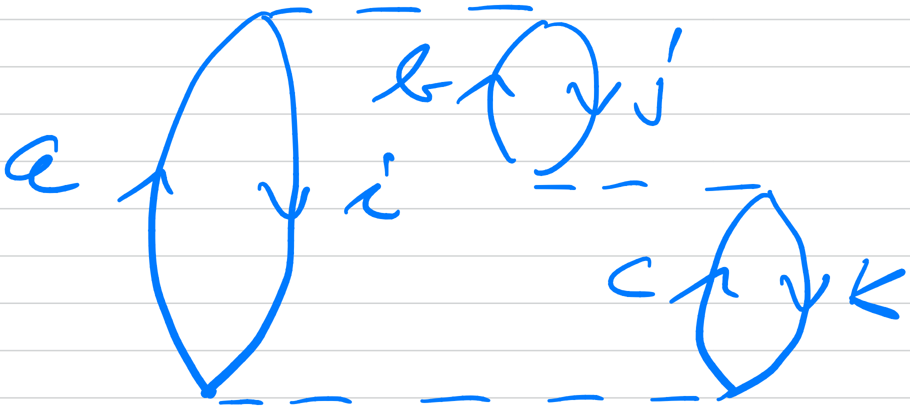
$$\frac{1}{\sum_i \varepsilon_i - \sum_a \varepsilon_a}$$

e) There is a factor
$\left(\frac{1}{2}\right)^{n_{ep}}$

n_{ep} = # equivalent pairs of lines which start and end at the same vertex

f) sum freely over freely over all intermediate states

Example



$$+ \sum_{\substack{abc \\ ijk}} \frac{\langle ij|v|ab\rangle \langle bk|v|jc\rangle \langle ac|v|ik\rangle}{(\varepsilon_i + \varepsilon_k - \varepsilon_a - \varepsilon_c)(\varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_b)}$$