Lecture Fys4480, September 29, 2023

Diagrammatic representation

Shavitt & Bartlett, chapters 3, 4

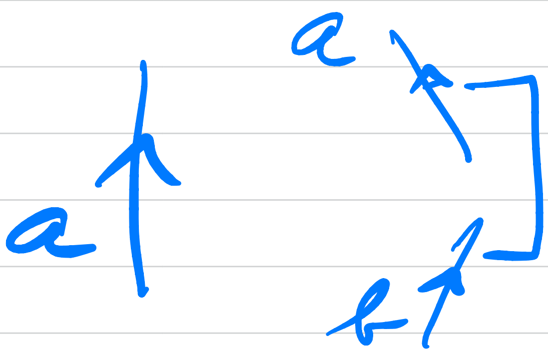
with new vacuum we have

(i) $\overbrace{a_a a_b^\dagger} = \langle \Phi_0 | a_a a_b^\dagger | \Phi_0 \rangle$

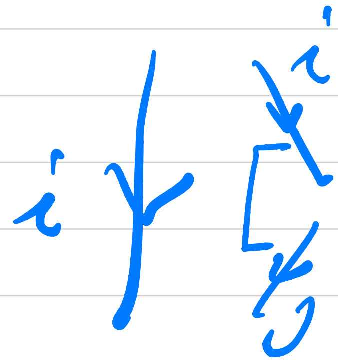
$= \delta_{ab} \qquad a, b > F$

(ii) $\overbrace{a_i^\dagger a_j} = \delta_{ij} \qquad ij \leq F$

$\overbrace{a_a a_b^\dagger}$



$\overbrace{a_i^\dagger a_j}$

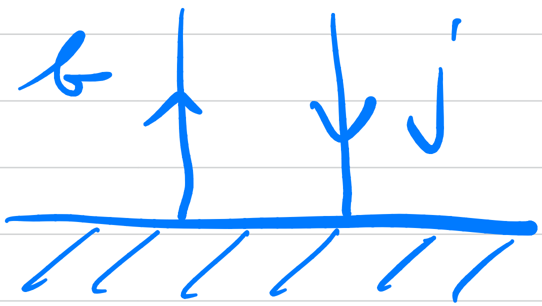


$$\langle \Phi_i^a | H | \Phi_j^b \rangle$$

hole-lines are down going arrows

particle-lines are up going arrows

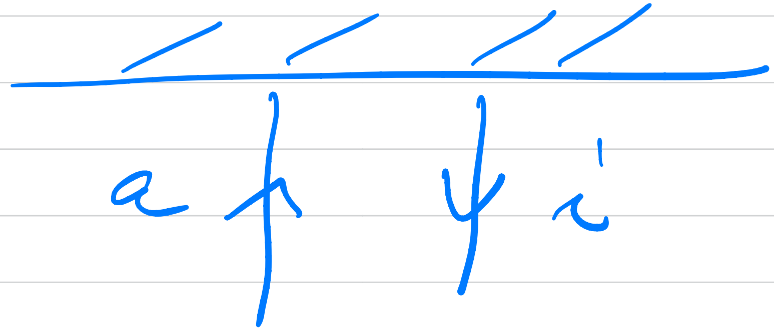
$$|\Phi_j^b\rangle = a_b^\dagger a_j |\Phi_0\rangle$$



$|\Phi_0\rangle$

$$\langle \Phi_i^a | = \langle \Phi_0 | a_i^\dagger a_a$$

$\langle \Phi_0 |$

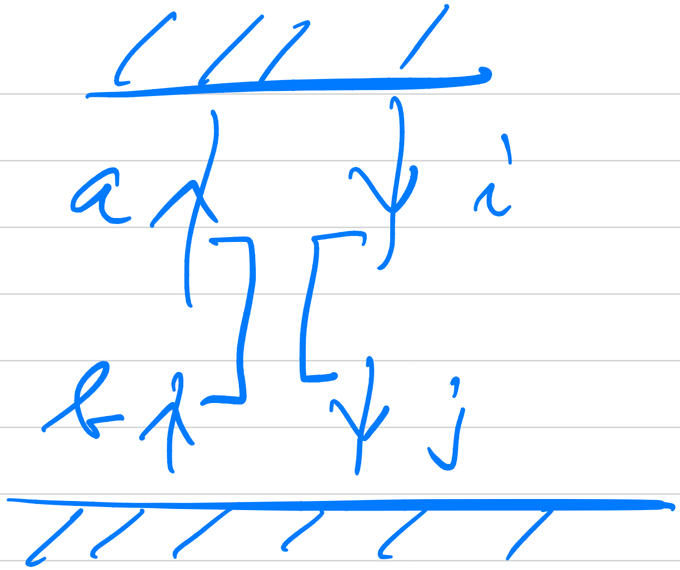


$$\langle \Phi_i^a | H | \Phi_j^b \rangle$$

$$= \langle \Phi_i^a | E_0^{Ref} + \hat{F}_N + \hat{V}_N | \Phi_j^b \rangle$$

$$= E_0^{Ref} \langle \Phi_i^a | \Phi_j^b \rangle$$

$$\langle \Phi_0 | a_a^\dagger a_a a_b^\dagger a_j | \Phi_0 \rangle$$



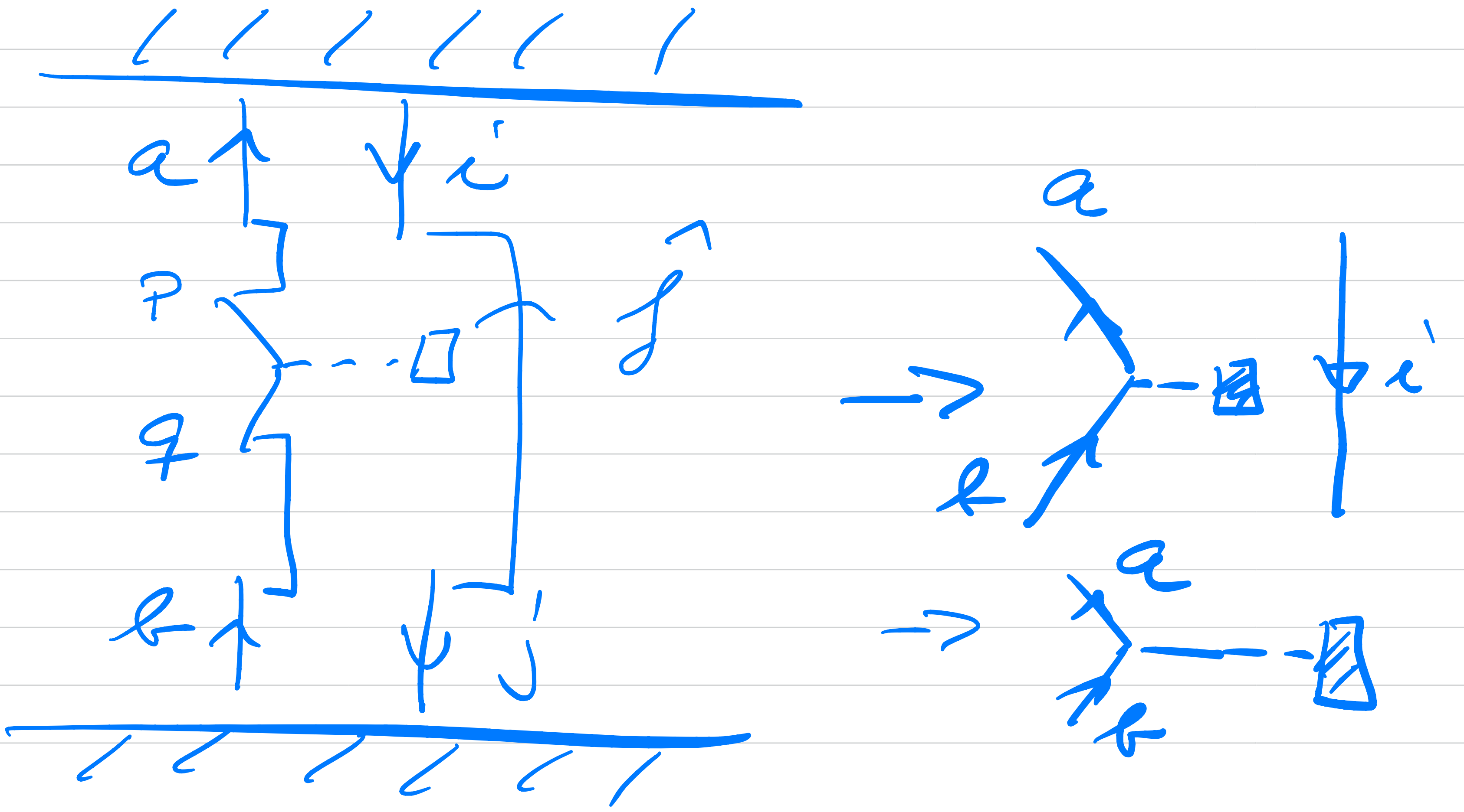
$$\delta_{ab}\,\delta_{ij}$$

$$+ \quad \langle \Phi_i^a | \hat{F}_N | \Phi_j^b \rangle \; ;$$

$$\sum_{pq} \langle \Phi_0 | a_i^\dagger a_a \, a_p^\dagger a_q \, a_b^\dagger a_j | \Phi_0 \rangle \times \langle p | f | q \rangle$$

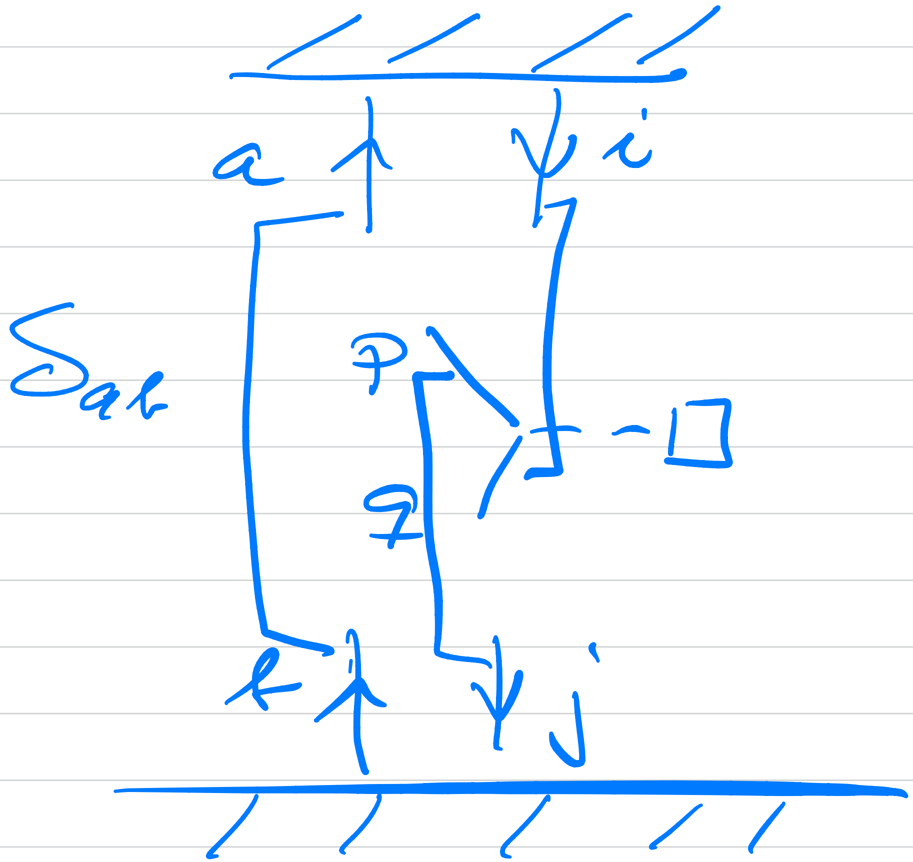
$$a_i^\dagger a_a \, a_p^\dagger a_q \, a_b^\dagger a_{j'}$$

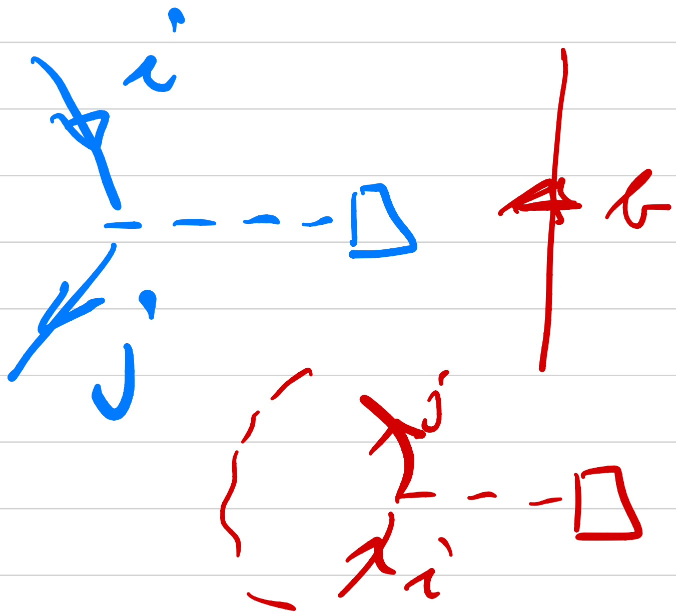
$$\delta_{ij'} \, \delta_{ap} \, \delta_{qb} \;\longrightarrow\; \langle a | g' | b \rangle$$



$$a_i^{\dagger} a_a \, a_p^{\dagger} a_q \, a_b^{\dagger} a_j$$

$$-\delta_{iq}\,\delta_{pj}\,\delta_{ab} \qquad -\langle j|f|i\rangle$$





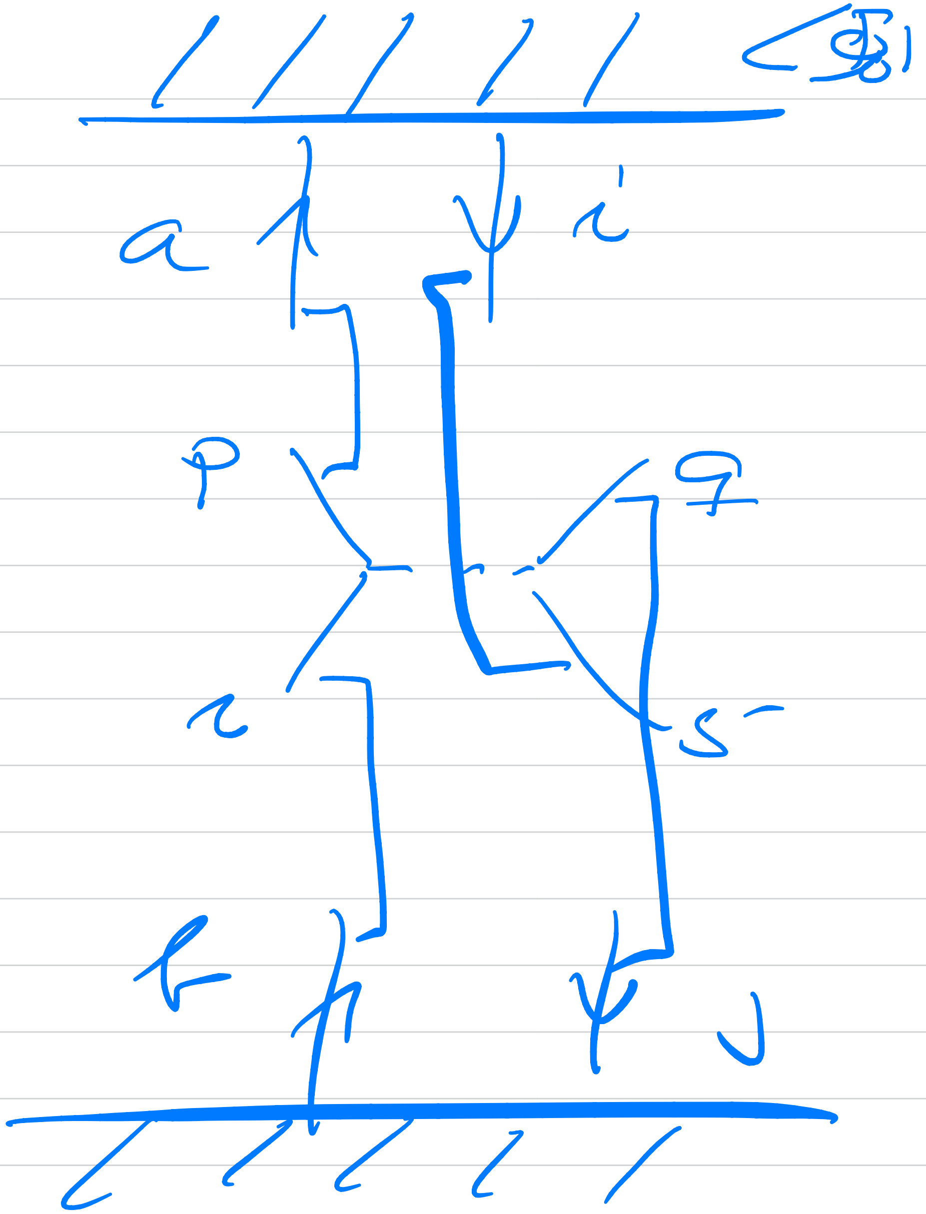
$$\langle \Phi_i^a | \hat{V}_N | \Phi_j^b \rangle \qquad \langle pq|v|rs\rangle$$

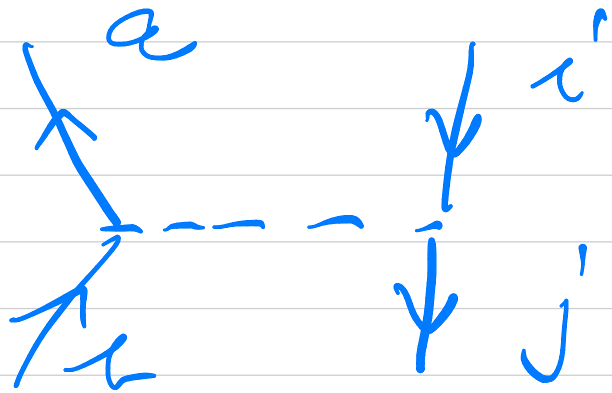
$$a_i^\dagger a_a \, a_p^\dagger a_q^\dagger a_s a_r \, a_b^\dagger a_j$$

$$-\delta_{is}\,\delta_{qj}\,\delta_{ap}\,\delta_{rb}$$

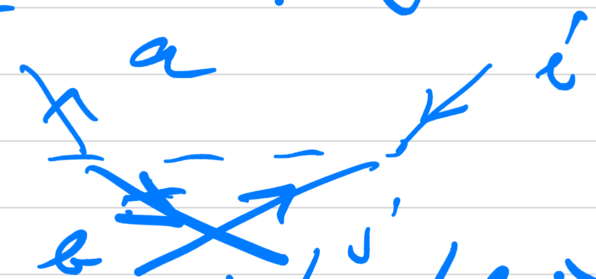
$$-\langle aj|\hat{v}|bi\rangle_{AS}$$

$$= +\langle aj|v|ib\rangle_{AS}$$

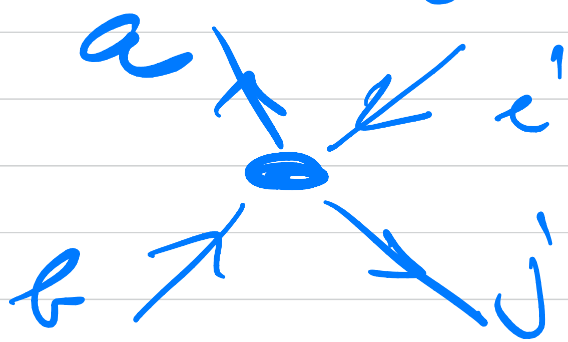




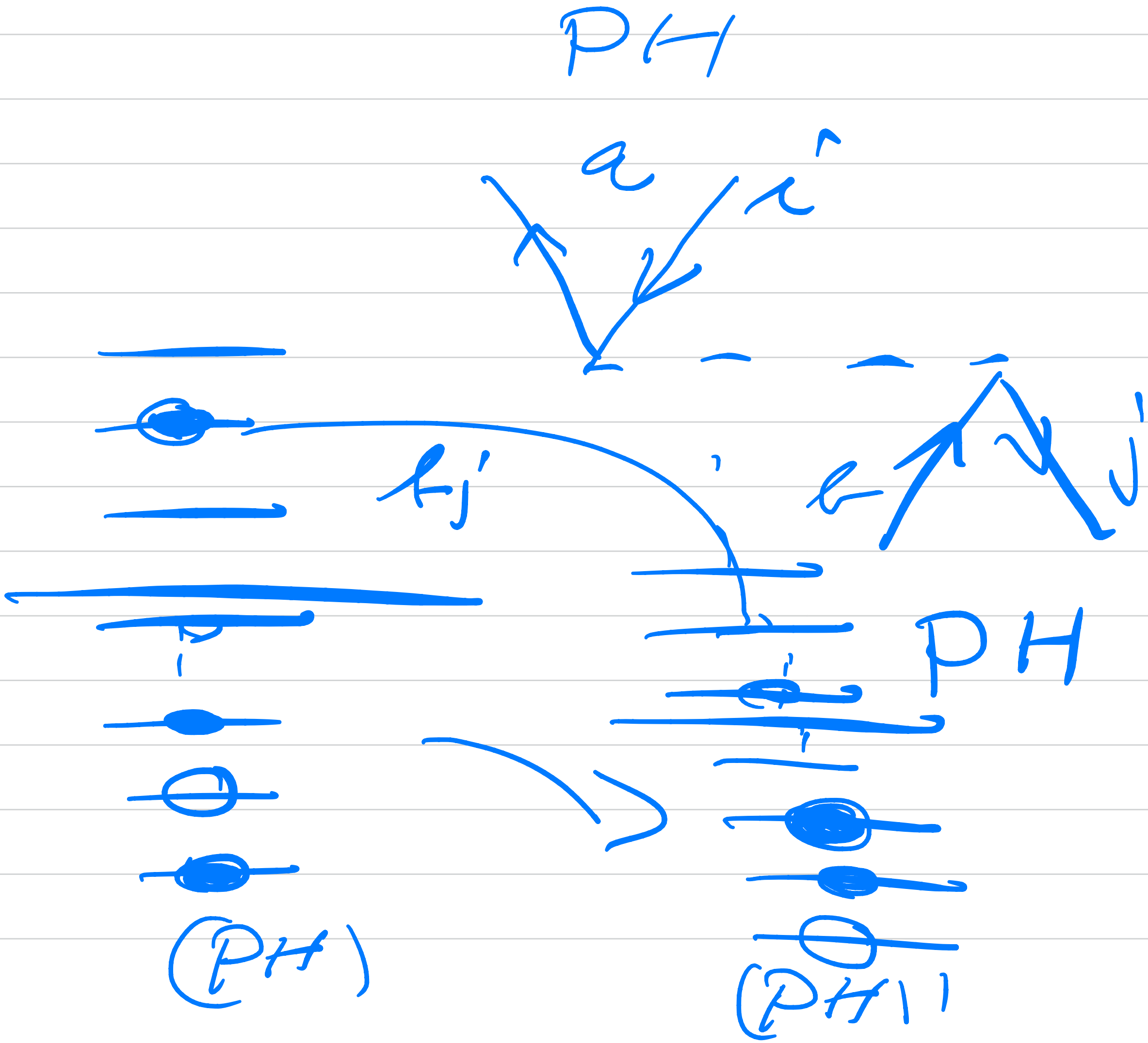
$+$



$$-\langle aj \,|\, v \,|\, bi \rangle_{AS}$$



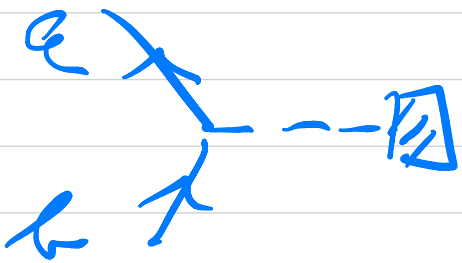
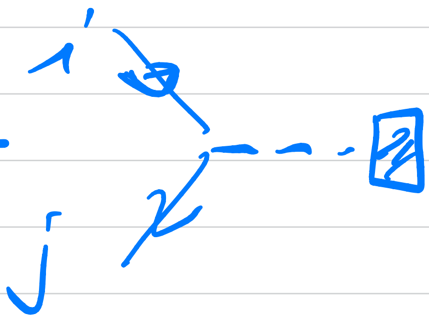
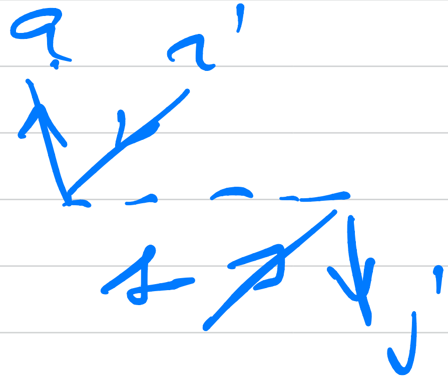
$$-\langle aj|v|bi\rangle = \langle aj|v|ib\rangle$$



1p1h diagram

$$\langle \Phi_i^a | \hat{H} | \Phi_j^b \rangle$$

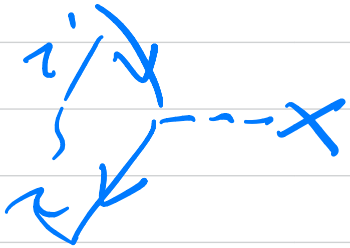
$$= \delta_{ij} \delta_{ab} E_0^{ref} \quad (i \downarrow a \uparrow)$$

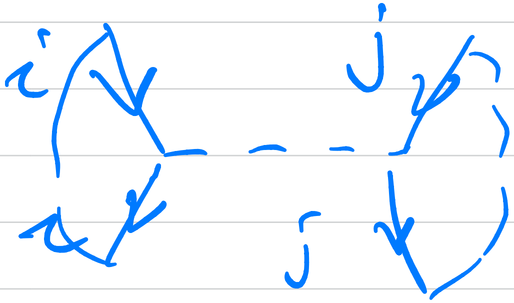
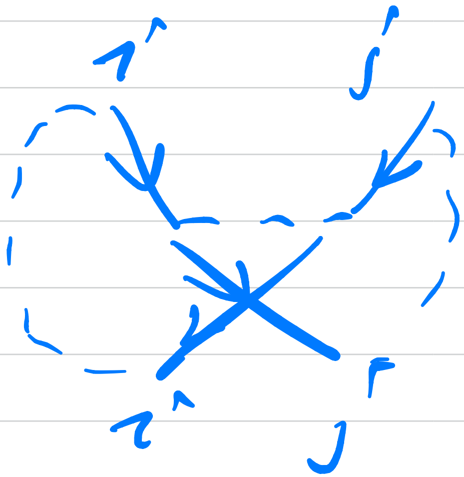
$+$  $+$  $+$ 

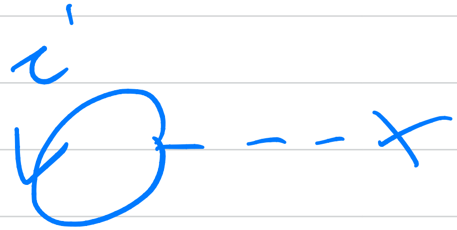
$$= E_0^{ref} \delta_{ij} \delta_{ab} + \langle a | \hat{f} | b \rangle \delta_{ij}$$

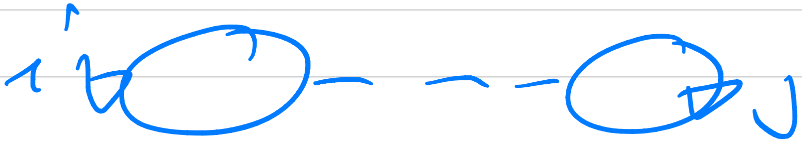
$$- \langle j | \hat{f} | i \rangle \delta_{ab} + \langle aj | v | ib \rangle$$

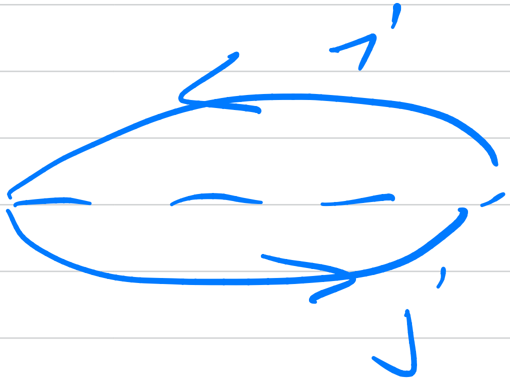
$$E_0^{ref} = \sum_{i \le F} \langle i | \hat{h}_0 | i \rangle + \frac{1}{2} \sum_{ij} \left\{ \langle ij | v | ij \rangle - \langle ij | v | ji \rangle \right\}$$

$$\sum_{i \le F}$$ 

$$+ \frac{1}{2} \sum_{ij} \Bigg\{$$  $+$  $\Bigg\}$

=  (a)

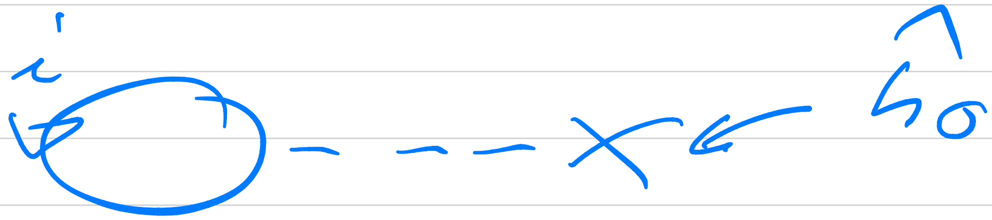
+  (b)

+  (c)

Additional rules

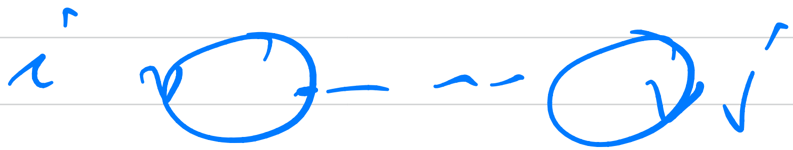
- count number of hole lines n_h
- count number of closed loops

- number of holes which go through the whole diagram.

(a) 

$$\left.\begin{array}{l} n_h = 1 \\ n_e = 1 \end{array}\right\} \quad (-1)^{n_h + n_e} = +1$$

$$+ \langle i | \hat{h}_0 | i \rangle$$

(b) 

$n_h = 2$

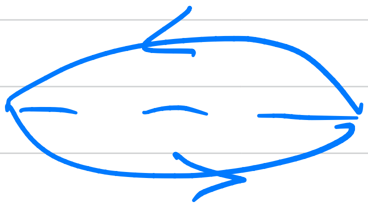
$n_e = 2$

additional rule: factor $\frac{1}{2}$ for every pair of lines which start at the same vertex and end at the same vertex.

— Each closed loop is a sum

$$+\frac{1}{2}\sum_{i'j'} \langle i'j'|v|i'j'\rangle$$

(c)



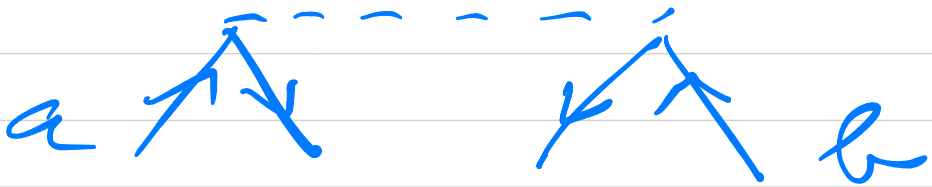
$n_e = 1$

$n_h = 2$

$$-\frac{1}{2}\sum_{ij} \langle ij|v|ji\rangle$$

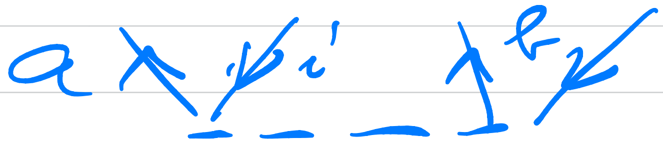
Example $\langle \Phi_0 | \hat{V}_N | \Phi_{ij}^{ab} \rangle$

$$= \langle ij | v | ab \rangle$$



2p2h

$\langle \Phi_{ij}^{ab} | \hat{V}_N | \Phi_0 \rangle$ $\langle ab | v | ij \rangle$



2p2h
excitation