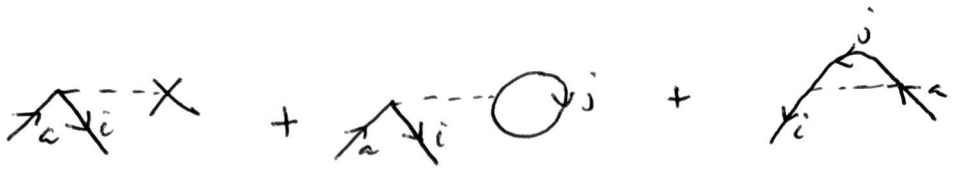
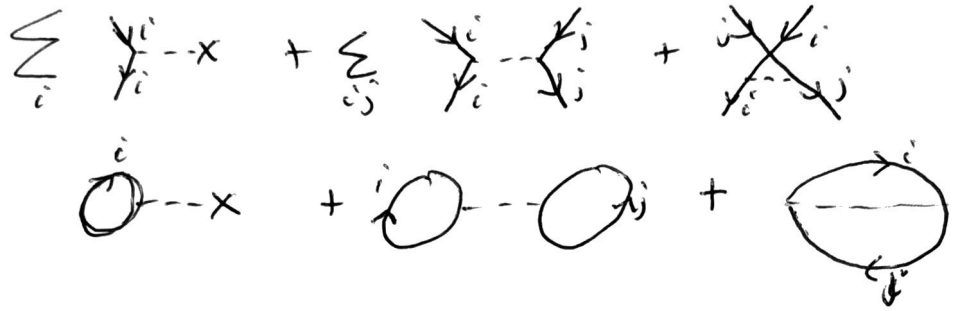
1.) $\langle \Phi | \hat{H} | \Phi_i^a \rangle = \langle i | f | a \rangle$

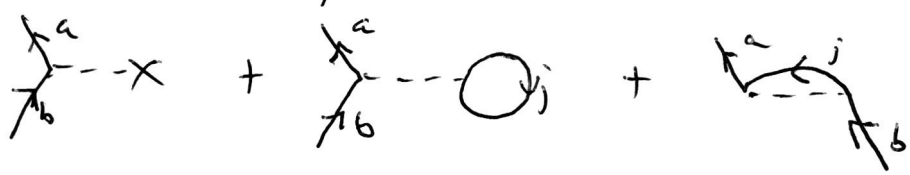


2.) $\langle \Phi_i^a | H | \Phi_j^b \rangle = \delta_{ij}\delta_{ab}\,\varepsilon_0^{ref} + \langle a|f|b\rangle \delta_{ij} - \langle i|f|j\rangle \delta_{ab} + \langle aj||vi||b\rangle_{AS}$

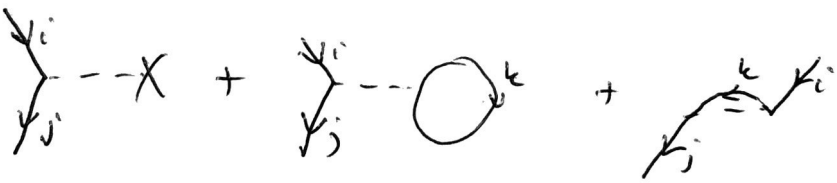
ε_0^{ref}: $\sum_i \langle i|h_0|i\rangle + \sum_{ij} \langle ij|v|ij\rangle_{AS}$



$\langle a|f|b\rangle$: $\langle a|h_0|b\rangle + \sum_j \langle aj|v|bj\rangle_{AS}$



$\langle j|f|i\rangle$: $\langle j|\hat{h}_0|i\rangle + \sum_k \langle jk|v|ik\rangle_{AS}$



$\langle aj||vi||b\rangle_{AS}$:

Hartree - Fock operator

$$\langle i | h^{HF} | i \rangle = \langle i | h_0 | i \rangle + \sum_j \langle ij | V | ij \rangle_{A-S}$$

$$\langle a | h^{HF} | a \rangle = \langle a | h_0 | a \rangle + \sum_j \langle aj | V | aj \rangle$$