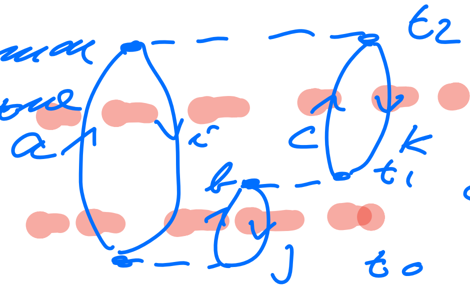
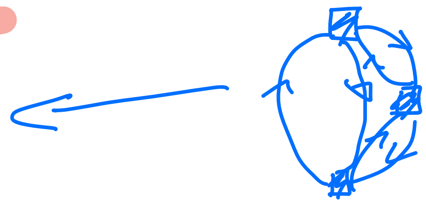
FYS 4480, Nov 4, 2022

Examples

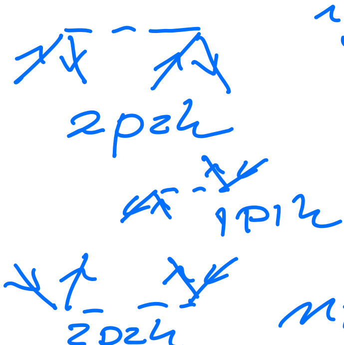
3rd-order





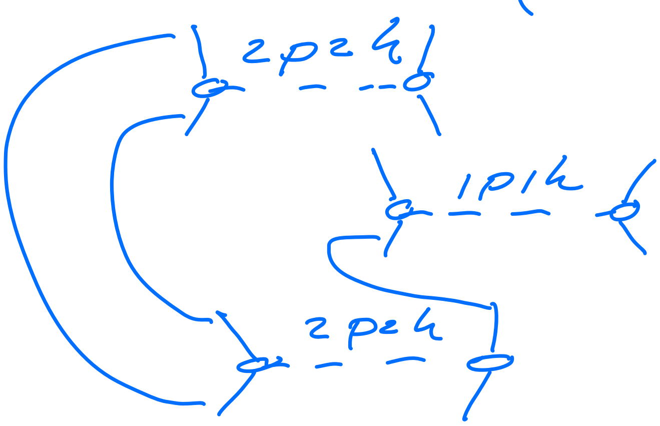
$$+\sum_{\substack{abc\\ijk}} \underbrace{\langle ik|v|ac\rangle}_{2p2h}\underbrace{\langle jc|v|bk\rangle}_{1p1h} \times \underbrace{\langle ab|v|ij\rangle}_{2p2h}$$

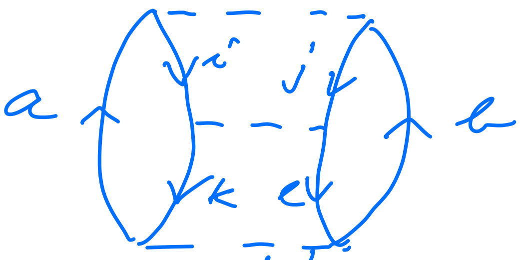
$$\times \frac{1}{(\epsilon_i+\epsilon_j-\epsilon_a-\epsilon_b)(\epsilon_i+\epsilon_k-\epsilon_a-\epsilon_c)}$$



$n_h = 3 \qquad n_p = 3$

$$\sum_{mn}\frac{\langle\Phi_0|H_1|\Phi_m\rangle\langle\Phi_m|H_1|\Phi_n\rangle\langle\Phi_n|H_1|\Phi_0\rangle}{(W_0-W_m)(W_0-W_n)}$$





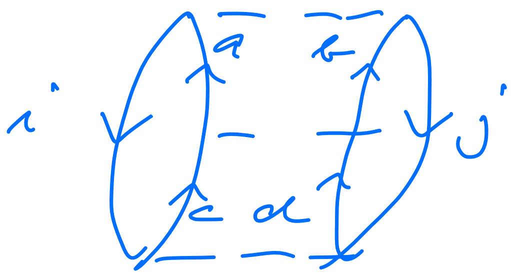
$n_{ep} = 3 \quad \left(\frac{1}{2}\right)^3 = \frac{1}{8}$

$n_e = 2$

$n_h = 4$

$4h - 2p$

$$+\frac{1}{8}\sum_{\substack{ab\\ijkl}} \frac{\langle ij|v|ab\rangle\langle kl|v|ij\rangle\langle ab|v|kl\rangle}{(\varepsilon_k+\varepsilon_l-\varepsilon_a-\varepsilon_b)(\varepsilon_i+\varepsilon_j-\varepsilon_a-\varepsilon_b)}$$



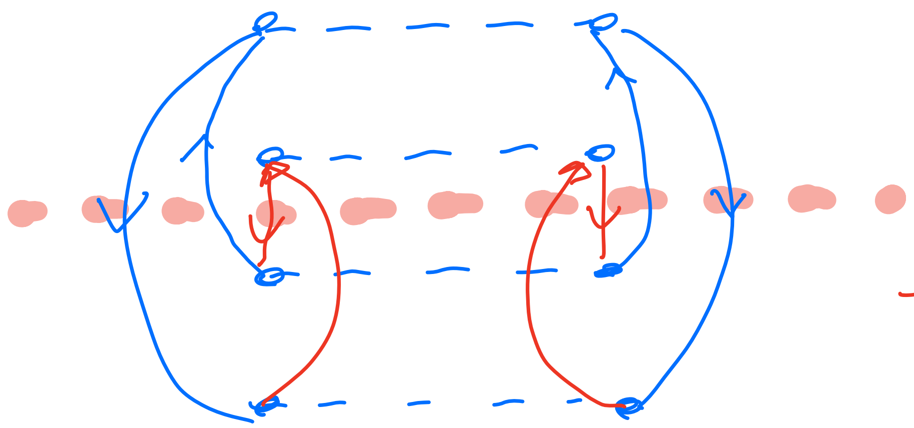
$n_{ep} = 3 \rightarrow 1/8$

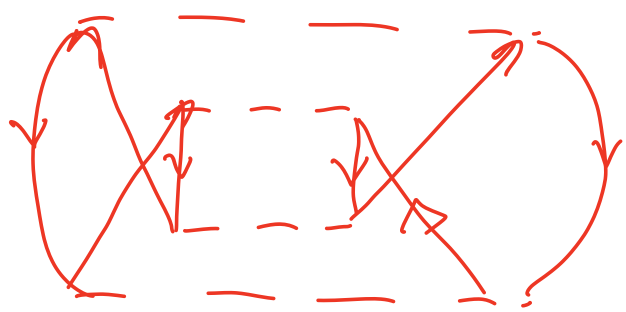
$n_h = 2 \qquad n_e = 2$

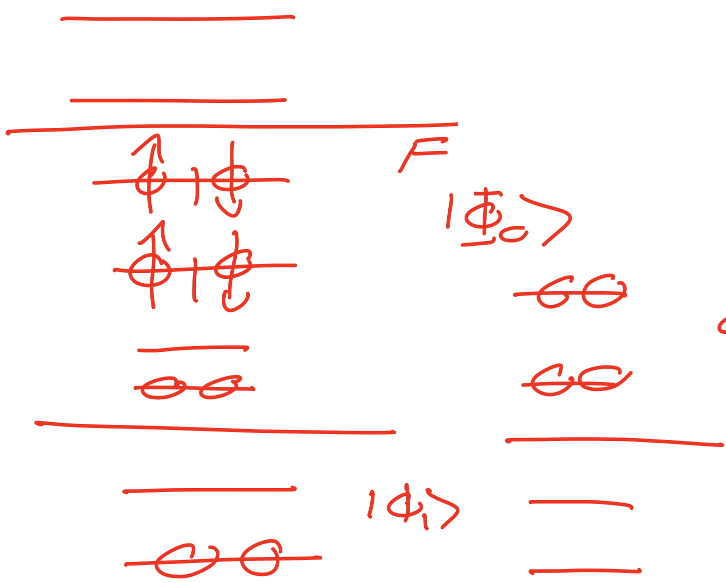
$$+\frac{1}{8}\sum_{\substack{ij\\ab\\cd}} \frac{\langle ij|v|ab\rangle\langle ab|v|cd\rangle\langle cd|v|ij\rangle}{(\varepsilon_i+\varepsilon_j-\varepsilon_a-\varepsilon_b)(\varepsilon_i+\varepsilon_j-\varepsilon_c-\varepsilon_d)}$$

$2h - 4p$

4th-order







$\binom{4}{2} = 6$

4p4ε

Model for exercise week 45

simple two level-model

ε_2 ——— $|\Phi_2\rangle$ $\quad \varepsilon_1 < \varepsilon_2$

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ε_1 ——— $|\Phi_1\rangle = a_1^\dagger |0\rangle$

$$|\Phi_2\rangle = a_2^\dagger |0\rangle$$

$$= (a_2^\dagger a_1)|\Phi_1\rangle$$

$$= |\Phi_1^2\rangle$$

$$\hat{H} = \hat{H}_0 + \hat{H}_I$$

$$\hat{H}_0 |\Phi_i\rangle = \varepsilon_i |\Phi_i\rangle$$

$$\hat{H}_0 = \sum_{p=1}^{2} \varepsilon_p a_p^\dagger a_p \qquad \langle p|h_0|q\rangle = \delta_{pq}\varepsilon_p$$

$$\hat{H}_1 = g \sum_{pq} a_p^\dagger a_q$$

$$\langle \Phi_1 | H_0 | \Phi_1 \rangle = \varepsilon_1$$

$$\langle 0| a_1 g \sum_{pq} a_p^\dagger a_q a_1^\dagger |0\rangle = g$$

$$\overbrace{a_1 \, a_p^\dagger} \, \overbrace{a_q \, a_1^\dagger} \qquad \delta_{p1}\delta_{q1}$$

$$\langle \Phi_1 | H | \Phi_2 \rangle =$$

$$\langle \Phi_1 | g \sum_{pq} a_p^\dagger a_q (a_2^\dagger a_1) | \Phi_1 \rangle$$

$$\left(\langle 0 | a_1 \, g \sum_{pq} a_p^\dagger a_q \, a_2^\dagger | 0 \rangle = g \right.$$

$$a_p^\dagger a_q \, a_2^\dagger a_1$$

$$\langle \Phi_2 | H | \Phi_2 \rangle = \varepsilon_2 + g$$

Hamiltonian matrix:

$$\begin{bmatrix} \varepsilon_1 + g & g \\ g & \varepsilon_2 + g \end{bmatrix}$$

MBPT (RS)

$$\Delta E^{(1)} = \langle \Phi_1 | H_1 | \Phi_1 \rangle = g$$

$$\Delta E = E - W_0$$

$$\Delta E^{FCI} = E - E_0^{Ref} = E - \varepsilon_1 - g$$

$$\Delta E^{MBPT} = E - W_0 - \langle \Phi_1 | H | \Phi_1 \rangle$$

$$= E - W_0 - \Delta E^{(1)}$$

$$\equiv \Delta E^{FCI}$$

$$\Delta E^{(2)} = \sum_m \frac{|\langle \Phi_1 | H_1 | \Phi_m \rangle|^2}{W_0 - W_m}$$

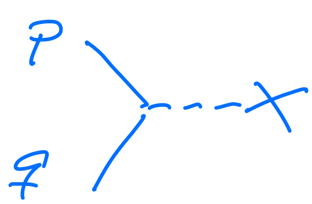
$W_0 = \varepsilon_1 \qquad m = 2$

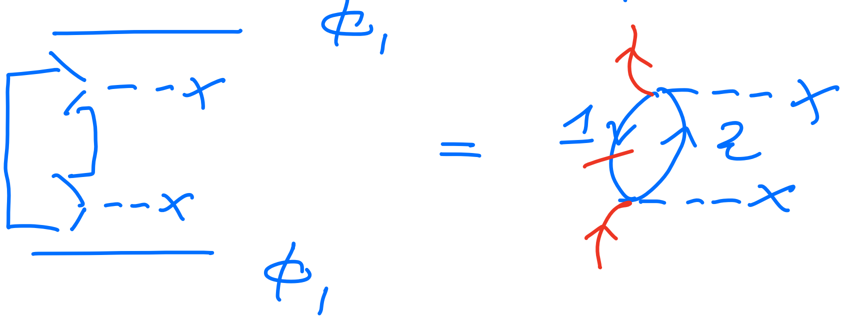
$$\Delta E^{(2)} = \frac{|\langle \Phi_1 | H_1 | \Phi_2 \rangle|^2}{\varepsilon_1 - \varepsilon_2}$$

$$= \frac{g^2}{\varepsilon_1 - \varepsilon_2}$$

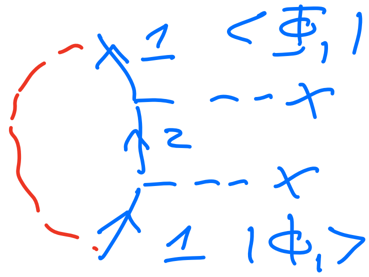
$$H_1 = g \sum_{pq} a_p^\dagger a_q$$

as operator





without Fermi vacuum



$$\langle \Phi_1 | H_1 | \Phi_2 \rangle \langle \Phi_2 | H_1 | \Phi_1 \rangle$$