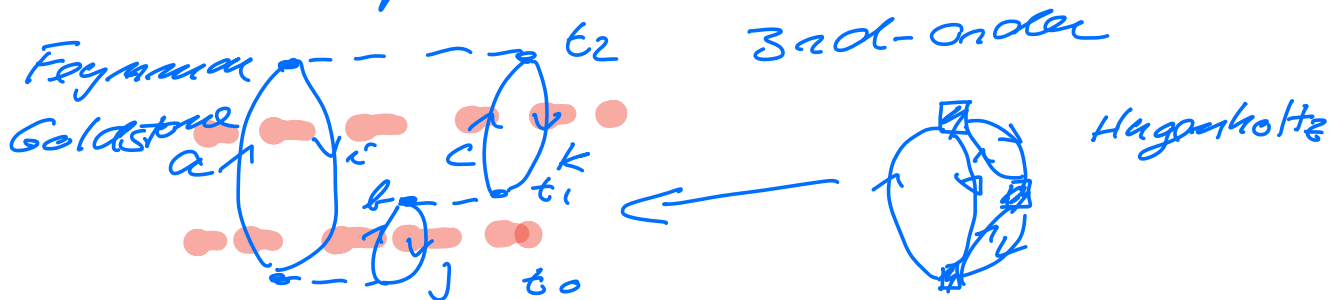


FYS 4480, NCU 4, 2022

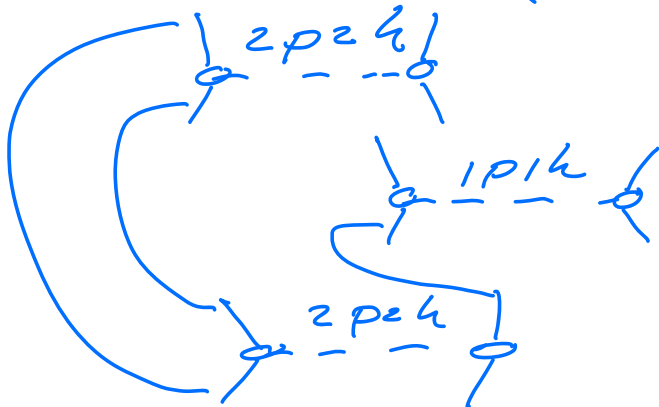
Examples

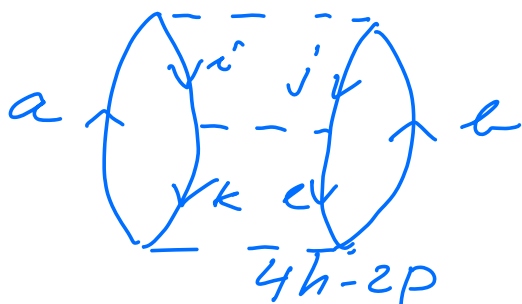


$$\begin{aligned}
 & + \sum_{\substack{abc \\ ijk}} \langle ik | v | ac \rangle_{2p2h} \langle jc | v | bk \rangle_{1p1h} \\
 & \times \langle ab | v | ij \rangle_{2p2h} \\
 & \times \frac{1}{(\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_c)(\epsilon_i + \epsilon_k - \epsilon_b - \epsilon_d)} \\
 & \times \frac{1}{(\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_c)(\epsilon_i + \epsilon_k - \epsilon_b - \epsilon_d)} \\
 & \times \frac{1}{(\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_c)(\epsilon_i + \epsilon_k - \epsilon_b - \epsilon_d)}
 \end{aligned}$$

$n_h = 3 \quad n_e = 3$

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



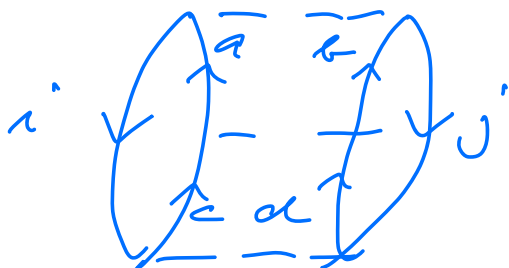


$$n_{ep} = 3 \quad \left(\frac{1}{2}\right)^3 = \frac{1}{8}$$

$$n_e = 2$$

$$n_h = 4$$

$$+ \frac{1}{8} \sum_{\substack{ab \\ ijkl}} \frac{\langle ij | v | ab \rangle \langle kl | v | ij \rangle \langle ab | v | kl \rangle}{(\epsilon_k + \epsilon_l - \epsilon_a - \epsilon_b)(\epsilon_i + \epsilon_j - \epsilon_c - \epsilon_d)}$$



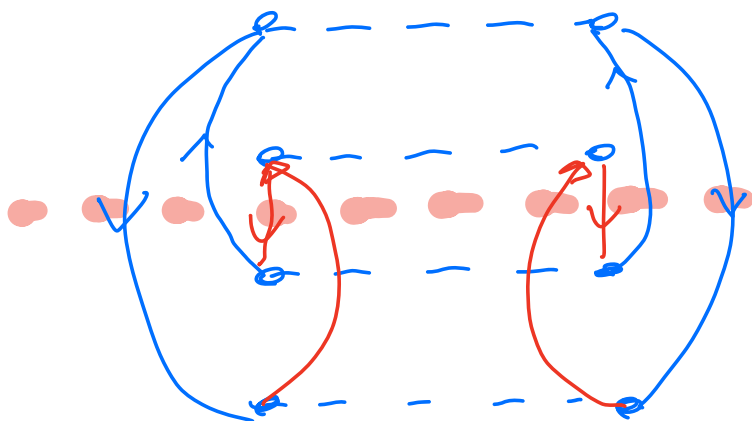
$$n_{ep} = 3 \rightarrow \frac{1}{8}$$

$$n_h = 2 \quad n_e = 2$$

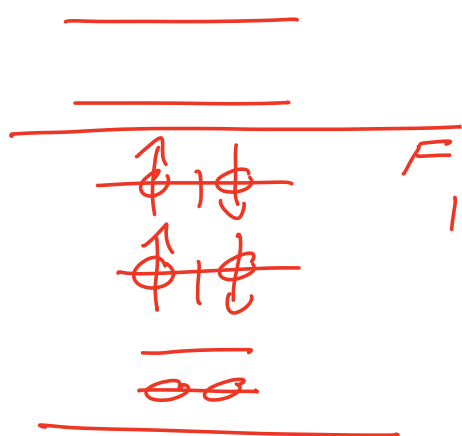
$$+ \frac{1}{8} \sum_{\substack{ij \\ ab \\ cd}} \frac{\langle ij | v | ab \rangle \langle ab | v | cd \rangle \langle cd | v | ij \rangle}{(\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b)(\epsilon_c + \epsilon_d - \epsilon_i - \epsilon_j)}$$

$2h-4p$

4th-order



4h-4p
excitation



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

$1\Phi_0$

$\phi\phi$

$\phi\phi$

4p4h

$1\Phi_1$

$\phi\phi$

$\phi\phi$

$\phi\phi$

Model for exercise week 45
simple two level-model

$$\begin{array}{c}
 \varepsilon_2 \text{ --- } |\Phi_2\rangle \\
 \varepsilon_1 \text{ --- } |\Phi_1\rangle
 \end{array}
 \quad \varepsilon_1 < \varepsilon_2$$

$$\begin{aligned}
 &= a_1^\dagger |0\rangle \\
 |\Phi_2\rangle &= a_2^\dagger |0\rangle \\
 &= (a_2^\dagger a_1) |\Phi_1\rangle \\
 &= |\Phi_1^2\rangle
 \end{aligned}$$

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

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

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

$$\hat{H}_I = g \sum_{p,q} a_p^\dagger a_q$$

$$\langle \Phi_1 | \hat{H}_0 | \Phi_1 \rangle = \varepsilon_1$$

$$\begin{aligned}
 \langle 0 | a_1 g \sum_{p,q} a_p^\dagger a_q a_1^\dagger | 0 \rangle &= g \\
 \overbrace{a_1 a_p^\dagger a_q}^{\delta_p, \delta_{q,1}} a_1^\dagger &
 \end{aligned}$$

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

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

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

$$\langle \Phi_2 | H | \Phi_2 \rangle = \epsilon_2 + g$$

Hamiltonian ;
matrix

$$\begin{bmatrix} \epsilon_1 + g & g \\ g & \epsilon_2 + g \end{bmatrix}$$

MBPT (KS)

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

$$\Delta E = E - W_0$$

$$\Delta E^{FCI} = E - E_0^{ref} = E - \epsilon_1 - g$$

$$\begin{aligned}
 \Delta E^{MBPT} &= E - W_0 - \langle \Phi_1 | H_1 | \Phi_1 \rangle \\
 &= E - W_0 - \Delta E^{(1)} \\
 &\equiv \Delta E^{FCI}
 \end{aligned}$$

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

$$W_0 = \epsilon_1, \quad m = 2$$

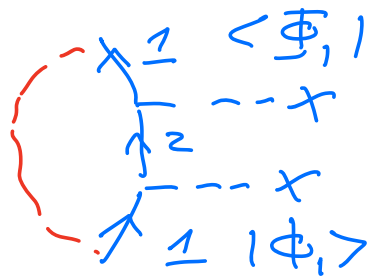
$$\begin{aligned}
 \Delta E^{(2)} &= \frac{|\langle \Phi_1 | H_1 | \Phi_2 \rangle|^2}{\epsilon_1 - \epsilon_2} \\
 &= \frac{g^2}{\epsilon_1 - \epsilon_2}
 \end{aligned}$$

$$H_1 = g \sum_{p,q} a_p^\dagger a_q$$

as operator

$$\begin{array}{c} \hline \diagup \text{---} x \\ \diagdown \text{---} x \\ \hline \end{array} \begin{array}{c} \Phi_1 \\ \Phi_1 \end{array} = \begin{array}{c} p \\ \diagdown \text{---} x \\ q \\ \diagup \text{---} x \end{array}$$

without Fermi vacuum



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