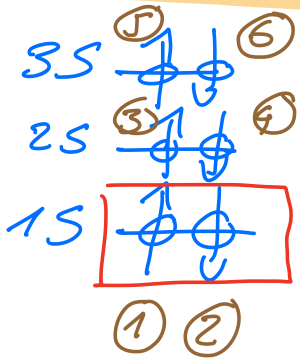
FYS4480, oct 20, 2022



Midterm 1

$l = 0$

$\Phi_0(He)$

$\langle pq|\hat{v}|1s\rangle$: $\langle 12|\hat{v}|12\rangle_{AS}$

$\langle 13|\hat{v}|13\rangle_{AS}$

$\vdots$

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stability of HF equations (need Thouless' theorem)

$$|\Phi_c\rangle = |c\rangle = \prod_{i=1}^{N} a_i^{+} |0\rangle$$

(SD in 2nd quantisation)

Thouless' theorem

$$|c'\rangle = |c\rangle + |\delta c\rangle$$

$$= \left(1 + \sum_{ai} \delta c_{ai}\, a_a^{+} a_i\right)|c\rangle$$

$$\langle c|H|c\rangle = E_0^{HF}$$

$$\frac{\langle c'|H|c'\rangle}{\langle c'|c'\rangle} \geq E_0^{HF}$$

$$|\delta c\rangle = \sum_{ai} \delta c_{ai}\, a_a^{\dagger} a_i |c\rangle$$

$$\langle \delta c | H | c\rangle = 0$$

$$= \sum_{ai} \delta c_{ai}^{*} \langle c| a_i^{\dagger} a_a \hat{H} |c\rangle = 0$$

$$\hat{H} = \sum_{pq} \langle p|\hat{f}|q\rangle a_p^{\dagger} a_q$$

$$+ \frac{1}{4} \sum_{pqrs} \langle pq|v|rs\rangle_{AS}\, a_p^{\dagger} a_q^{\dagger} a_s a_r$$

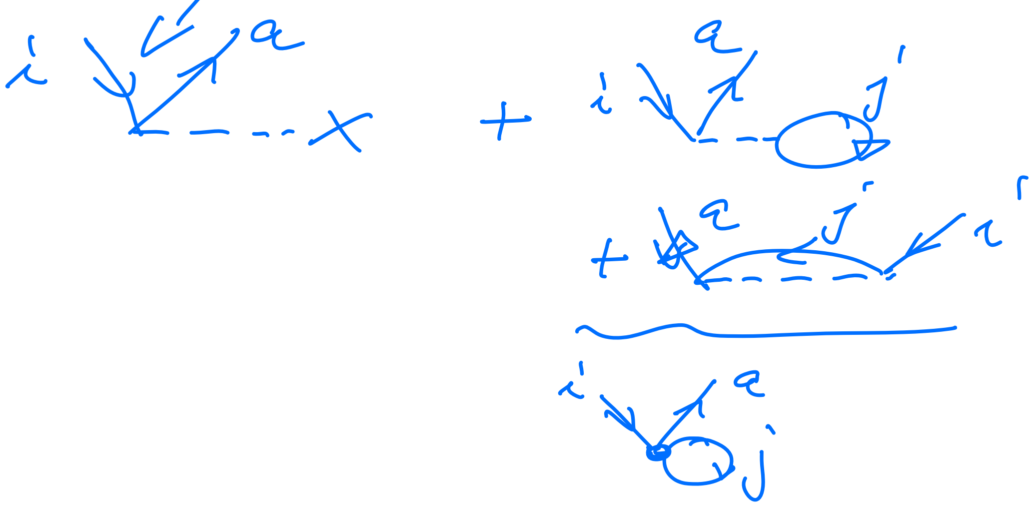
$$\sum_{ai}\sum_{pq} \langle c| a_i^{\dagger} a_a a_p^{\dagger} a_q |c\rangle$$

$$\delta_{ap}\delta_{iq} \qquad \langle p|f|q\rangle$$

$$\sum_{ai}\sum_{pqrs} \langle c|\{a_i^{\dagger} a_a\}\{a_p^{\dagger} a_q^{\dagger} a_s a_r\}|c\rangle$$

$$\Rightarrow \sum_{ai} \delta c_{ai} \overbrace{\langle a | f | i \rangle}^{=0} = 0$$

$$\langle a | f | i \rangle = \langle a | h_0 | i \rangle + \sum_{j \leq F} \langle aj | \hat{v} | ij \rangle_{AS}$$



Stability of HF equations

$$\frac{\langle c' | H | c' \rangle}{\langle c' | c' \rangle} \geq \langle c | H | c \rangle$$

$$|c'\rangle = \exp\left\{ \sum_{ai} \delta c_{ai} a_a^\dagger a_i \right\} |c\rangle$$

$$= \Big(1 + \sum_{ai} \delta c_{ai} a_a^\dagger a_i + \frac{1}{2} \sum_{ai} \sum_{bj} \delta c_{ai} \delta c_{bj} \ldots$$

$$\langle c'|c'\rangle \hat{=} 1 + \sum_{ai} |\delta c_{ai}|^2$$

$$\langle c'|c'\rangle \neq \underline{1}$$

intermediate normalization

$$\langle c'|c\rangle = \underline{1}$$

$$\langle c'|H|c'\rangle =$$

$$\langle c|H|c\rangle + \sum_{ai}\sum_{bj} \delta c_{ai}^{*} \delta c_{bj}$$

$$\times \langle c| a_i^{+} a_a H a_b^{+} a_j |c\rangle$$

$$+ \frac{1}{2} \sum_{ai}\sum_{bj} \delta c_{ai} \delta c_{bj}$$

$$\times \langle c| H a_a^{+} a_i a_b^{+} a_j |c\rangle$$

$$+ \frac{1}{2} \sum_{\substack{ai\\bj}} \delta c_{ai}^{*} \delta c_{bj}^{*}$$

$$\times \langle c| a_j^{+} a_b a_i^{+} a_a H |c\rangle$$

$$\exp\left(\sum_{ai} \delta a_i\, a_a^{+} a_i\right)|c\rangle$$

$$\simeq |c\rangle + \Big(\sum_{ai} \delta c_{ai}\, a_a^\dagger a_i\Big)|c\rangle + \frac{1}{2}\Big(\sum_{ai} \delta c_{ai}\, a_a^\dagger a_i\Big)^2 |c\rangle$$

$$\langle c' | H | c' \rangle = \langle c | H | c \rangle + \underbrace{\langle c | H | \delta c \rangle}_{=0} + \underbrace{\langle \delta c | H | c \rangle}_{=0} + \langle \delta c | H | \delta c \rangle + \langle c | H | \delta^2 c \rangle + \langle \delta^2 c | H | c \rangle$$

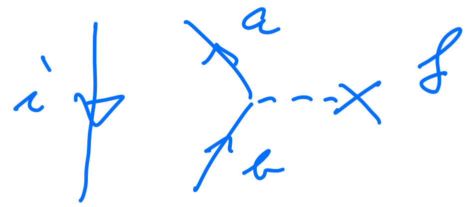
$$\langle c | a_i^\dagger a_a H a_b^\dagger a_j | c \rangle$$

$$\langle c | a_i^\dagger a_a \, a_p^\dagger a_q \, a_b^\dagger a_j | c \rangle$$

$$\delta_{ij}\, \delta_{ap}\, \delta_{qb}$$

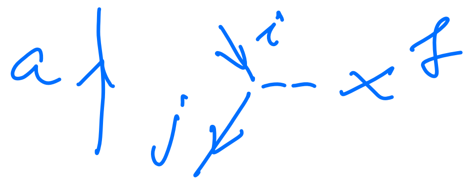
$$\underbrace{\langle a | f | b \rangle}_{\varepsilon_a^{HF} \delta_{ab}} \delta_{ij}$$

$$\varepsilon_a^{HF} \delta_{ab} \delta_{ij}$$



$\langle c | a_r^\dagger a_a \; a_p^\dagger a_q \; a_b^\dagger a_j | c \rangle$ $\quad a_r^\dagger a_p^\dagger a_q a_j$

$- \langle j | f | i \rangle \delta_{ab}$



$\langle c | a_r^\dagger a_a \; a_p^\dagger a_q^\dagger a_s a_r \; a_b^\dagger a_j | c \rangle$

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

$- \langle aj | v | bi \rangle_{AS} \frac{1}{4}$

in total (3 more)

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

$\langle \delta c | H | \delta c \rangle$

$$- \sum_{\substack{ai \\ bj}} \left(\langle a | f | b \rangle \delta_{ij} - \langle j | f | i \rangle \delta_{ab} - \langle aj | v | bi \rangle_{AS} \right) \delta c_{ai}^* \delta c_{bj}$$

$$\langle c | H | (\delta c)^2 \rangle \propto$$

$$\langle c | H \, a_a^\dagger a_i a_b^\dagger a_j | c \rangle$$

(i) $\langle c | a_p^\dagger a_q \, a_a^\dagger a_i \, a_b^\dagger a_j | c \rangle$

$$= 0$$

(ii) $\langle c | a_p^\dagger a_q^\dagger a_s a_r \, a_a^\dagger a_i \, a_b^\dagger a_j | c \rangle$

$$- \langle j i | \hat{v} | a b \rangle_{AS}$$

$$= + \langle i j | \hat{v} | a b \rangle_{AS} \frac{1}{4}$$

$$\Rightarrow \langle i j | \hat{v} | a b \rangle_{AS}$$

$$\langle (\delta c)^2 | H | c \rangle = \langle a b | \hat{v} | i j \rangle_{AS}$$