FYS4480/9480, lecture October 3, 2025

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coordinate up of SD.

$$\frac{\Phi_0^{HF}}{\det} = \frac{\det(C)\,\Phi_0}{\det}$$

$$\left(|p\rangle = \sum_{\lambda} C_{p\lambda} |\lambda\rangle \right)$$

Stability of HF equations
(Thouless' Theorem)

$$|\Phi_0^{HF}\rangle = |c\rangle = \prod_{i\le F}^{N} a_i^{+}|0\rangle$$

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

$$|\delta c\rangle = \eta\, a_a^{+} a_i |c\rangle$$

HF - requirements

$$\langle \delta c | \mathcal{H} | c\rangle = \langle c | \mathcal{H} | \delta c\rangle = 0$$

$$\langle a | f | i\rangle = 0 \quad \wedge \quad \langle i | f | a\rangle = 0$$

$$\langle oph | \mathcal{H} | ph\rangle = 0$$

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

$$= e^{\hat{T}_1} |c\rangle$$

$$\hat{T}_1 = \sum_{ai} c_i^a a_a^\dagger a_i$$

(i) $\exp(a+b) = \exp(a)\exp(b)$

(ii) $e^{\sum_i x_i}$

$$\sum_{i=1}^{n} x_i = x_1 + x_2 - - + x_n$$

$$e^{\sum_i x_i} = e^{x_1} e^{x_2} e^{x_3} - - e^{x_n}$$

$$= \prod_{i=1}^{n} e^{x_i}$$

$$\sum_{a r'} = \sum_{i \le F} \sum_{a > F}^{\infty}$$

$$|C'\rangle = \prod_{i \le F} \Big(1 + \sum_{a > F} c_r^a a_a^\dagger a_r$$

$$+ \frac{1}{2} \underbrace{\Big(\sum_{a > F} c_r^a a_a^\dagger a_{r'} \Big)^2}_{} + \cdots \Big) |C\rangle$$

$$\Big(\sum_{a > F} c_r^a a_a^\dagger a_{r'} \Big) \Big(\sum_{b > F} c_r^b a_b^\dagger a_{r'} \Big)$$

$$\sum_{ab > F} c_r^a c_r^b \, a_a^\dagger a_{r'} a_b^\dagger a_{r'} \quad |C\rangle$$

$$|c'\rangle = \prod_{i \subseteq F} \left(1 + \sum_{a > F} c_i^a a_a^\dagger a_i\right)|c\rangle$$

$$|c\rangle = a_{i_1}^\dagger a_{i_2}^\dagger \cdots a_{i_N}^\dagger |0\rangle$$

$$|c'\rangle = \,?$$

$$\{ i \in \{ i_1, i_2, i_3, \ldots, i_N \} \}$$

$$|c'\rangle = \Big\{ \Big[\Big(1 + \sum_a c_{i_1}^a a_a^\dagger a_{i_1} \Big) a_{i_1}^\dagger \Big]$$

$$\times \Big[\Big(1 + \sum_a c_{i_2}^a a_a^\dagger a_{i_2} \Big) a_{i_2}^\dagger \Big]$$

$$\vdots$$

$$\times \Big[\Big(1 + \sum_a c_{i_N}^a a_a^\dagger a_{i_N} \Big) a_{i_N}^\dagger \Big]$$

$$\times |0\rangle \Big\}$$

$$= \prod_{i \le F} \underbrace{\Big(a_i^\dagger + \sum_{a>F} c_i^a a_a^\dagger \Big)}_{b_i^\dagger} |0\rangle$$

Define $b_n^{+} = a_n^{+} + \underbrace{\sum_{a>F} c_n^{a}}_{\text{constant}} a_a^{+}$

$$|c'\rangle = \prod_{i \le F}^{N} b_n^{+} |0\rangle$$

$$|\lambda\rangle = a_\lambda^{+} |0\rangle$$

$$|p\rangle = a_p^{+} |0\rangle$$

$$a_p^{+} = \sum_{\lambda} \underbrace{c_{p\lambda}}_{\text{no restrictions}} a_\lambda^{+}$$

Define

$$\tilde{b}_i^{+} = \underbrace{\sum_p g_{ip}\, a_p^{+}}_{\text{unconstrained}}$$

$$|\tilde{c}\rangle = \prod_{i \le F} \tilde{b}_i^{+} |0\rangle$$

we want to show that $|\tilde{c}\rangle = |c\rangle$

assume $\langle c|\tilde{c}\rangle = \underline{1}$

$\langle c|\tilde{c}\rangle =$ $\qquad |\tilde{c}\rangle = \prod_{r\le F} \tilde{f}_r^+ |0\rangle$

$$\langle c| a_{i'_N} \cdots a_{i'_2} \underline{a_{i'_1}} \underbrace{\left(\sum_{p=1}^{i_N} g_{i_1 p}\, a_p^+\right)}_{\underline{\tilde{b}^+_{1}}}$$

$$\times \left(\sum_{q=1}^{i_N} g_{i_2 q}\, a_q^+\right) \cdots$$

$$\times \left(\sum_{t=1}^{i_N} g_{i_N t}\, a_t^+\right) |0\rangle$$

2 states : $\underline{i'_1} = \underline{1}$ $\quad i'_2 = 2$

$$\langle 0 | a_2 a_1 (g_{11} a_1^\dagger + g_{12} a_2^\dagger)$$

$$\times (g_{21} a_1^\dagger + g_{22} a_2^\dagger) | 0 \rangle$$

$$= \langle 0 | a_2 a_1 (g_{11} a_1^\dagger \cancel{g_{21} a_1^\dagger}$$

$$+ g_{11} a_1^\dagger g_{22} a_2^\dagger$$

$$+ g_{12} a_2^\dagger g_{21} a_1^\dagger$$

$$+ g_{12} a_2^\dagger \cancel{g_{22} a_2^\dagger}) | 0 \rangle$$

$$= \langle 0 | a_2 a_1 (\underbrace{g_{11} g_{22} - g_{12} g_{21}}) a_1^\dagger a_2^\dagger | 0 \rangle$$

$$= \det g = \begin{vmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{vmatrix}$$

$$\langle c | \xi \rangle = \underline{1} = \det g$$

$$\sum_k g_{ik} g^{-1}_{kj} = \delta_{ij}$$

$$\sum_j g^{-1}_{ij} g_{jk} = \delta_{ik}$$

$$\sum_i g^{-1}_{ki} \tilde{b}^{+}_{i} = \sum_i g^{-1}_{ki} \sum_{p=\underline{i_1}}^{\infty} g_{ip} q^{+}_{p}$$

$$= a_k^+ + \sum_i \sum_{p=i_{N+1}}^{\ell} g^{-1}_{ki} g_{i'p}\, a_p^+$$

$$C_{kp} = \sum_{i \leq F} g^{-1}_{ki} g_{i'p}$$

can rewrite the first line above as

$$a_k^+ + \sum_{p=i_{N+1}}^{\ell} C_{kp}\, a_p^+ \qquad k \leq F$$

$$a_{\cancel{k}i}^+ + \sum_{a>F} C_i^a a_a^+ = b_i^+$$

$$|\tilde{c}\rangle = \prod_{i \le F} \tilde{b}_i^{+} |0\rangle = \prod_{i \le F} b_i^{+} |0\rangle$$

$$b_i^{+} = a_i^{+} + \sum_{a > F} c_i^{a} a_a^{+}$$

$\Rightarrow$

$$|c'\rangle = \exp\left\{ \sum_{ai} c_i^{a} a_a^{+} a_i \right\} |0\rangle$$

Thouless' theorem.

$$\langle c | \mathcal{H} | c \rangle = \langle \Phi_0^{HF} | \mathcal{H} | \Phi_0^{HF} \rangle$$

$$= E_0^{HF} \quad (E_0^{Ref}(HF))$$

$$\langle c | \mathcal{H} | c \rangle \leq \langle \Phi_0 | \mathcal{H} | \Phi_0 \rangle$$

$$\langle \delta c | \mathcal{H} | c \rangle = 0$$

$$\langle 1p1h | \mathcal{H} | 0p0h \rangle = 0$$

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

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

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

$$\langle c'|c'\rangle = 1 + \left(\underbrace{\langle c|}_{0p0h} \underbrace{a_a^\dagger a_i\,|c\rangle}_{1p1h} \delta c_i^a \right) +$$

$$2$$

$$\sum_{\substack{ab\\ij}} \delta^* c_i^a \, \delta c_j^b \, \langle c| a_i^\dagger a_a a_b^\dagger a_j |c\rangle = \sum_{ai} |\delta c_i^a|^2 + \dots$$

$$= 1 + \sum_{a\,r'} |\delta c_r^a|^2 + O(\delta c^3)$$

$$\langle c' | \mathcal{H} | c' \rangle = \underbrace{\langle c | \mathcal{H} | c \rangle}_{E_0^{HF}}$$

$$+ \underbrace{\langle \delta c | \mathcal{H} | c \rangle}_{= 0} + \underbrace{\langle c | \mathcal{H} | \delta c \rangle}_{= 0}$$

$$+ \langle \delta c | \mathcal{H} | \delta c \rangle$$

$$\langle \delta c | \mathcal{H} | \delta c \rangle =$$

$$\sum_{\substack{a r' \\ b j'}} \delta^* c_r^a \, \delta c_j^b \langle c | a_r^\dagger a_a \mathcal{H} a_b^\dagger a_j | c \rangle$$

(i)

$$+ \frac{1}{2} \sum_{\substack{a r' \\ b j'}} \delta c_r^a \, \delta c_j^b \langle c | \mathcal{H} a_a^\dagger a_r a_b^\dagger a_j$$

(ii) $\times | c \rangle$

$$+ \frac{1}{2} \sum_{\substack{a r' \\ b j'}} \delta c_r^{*a} \, \delta c_j^{*b} \times$$

$$\langle c | a_j^\dagger a_b \, a_r^\dagger a_a \mathcal{H} | c \rangle$$

(iii)

$$\mathcal{H} = E_0^{HF} + \hat{F}_N + \hat{V}_N$$

(i) $\displaystyle\sum_{\substack{ab \\ i'j'}} \delta c_i^{*a} \, \delta c_j^{b}$

$$\times \langle \underset{\Phi_0^{HF}}{\underbrace{c}} | a_i^\dagger a_a \left(E_0^{HF} + \hat{F}_N + \hat{V}_N \right) a_{i'}^\dagger a_{j'} | c \rangle$$

$$E_0^{HF} \; a_i^\dagger a_a \, a_b^\dagger a_{j'} \qquad \delta_{i'j'},\ \delta_{ab}$$

$$\sum_{ai} |\delta c_i^a|^2 \, E_0^{HF}$$

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

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

$$\langle a|\hat f|b\rangle\, \delta_{ij} = \delta_{ab}\, \varepsilon_a^{HF} \times \delta_{ij}$$

$$\hat f|p\rangle = \varepsilon_p^{HF}|p\rangle$$

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

$$-\ \delta_{ab}\ \delta_{ij}\ \varepsilon_i^{HF}$$

$$\frac{1}{4}\sum_{pqrs} \langle pq|v|rs\rangle_{AS} \times$$

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

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

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

$$= \frac{1}{4} \langle aj|v|ib\rangle_{AS}$$

$$+\ 3\ \text{more} \Rightarrow \langle aj|v|ib\rangle_{AS}$$

The first term reads

$$\sum_{ai} |\delta c_i^a|^2 \left(E_c^{HF} + (\varepsilon_a^{HF} - \varepsilon_i^{HF}) \right)$$

$$+ \sum_{\substack{ab \\ ij}} \delta c_i^{a*} \delta c_j^b \langle aj|v|bi \rangle_{AS}$$

2nd term

$$\langle c| (E_c^{HF} + \hat{F}_N + \hat{V}_N) a_a^\dagger a_i a_b^\dagger a_j |c\rangle$$

$$\langle \text{op}\, \text{ch} | f | 2\text{p}2\text{h} \rangle \quad a_a^\dagger a_b^\dagger a_j a_i |c\rangle$$

$$2\text{p}2\text{h}$$

2nd Term

$$\sum_{pqrs} \langle c | a_p^\dagger a_q^\dagger a_s a_r a_a^\dagger a_b^\dagger a_j a_i | c \rangle \times \langle pq | v | rs \rangle$$

$$= \langle ij | v | ab \rangle_{AS}$$

2nd term :

$$\sum_{\substack{ab \\ ij}} \delta c_r^{a} \, \delta c_s^{b} \, \langle ij | v | ab \rangle_{AS}$$

3rd term

$$\sum_{\substack{ab \\ ij}} \delta \overset{*}{c}_r^{a} \, \delta \overset{*}{c}_s^{b} \, \langle ab | v | ij \rangle_{AS}$$

$$\langle c' | \mathcal{H} | c' \rangle = E_0^{HF} \left(1 + \sum_{an'} |\delta c_n^a|^2\right)$$

$$+ \Delta E + O(\delta c^3)$$

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

$$+ \frac{\Delta E^{(1st,\, 2nd,\, 3rd)}}{1 + \sum_{an'} |\delta c_n^a|^2}$$

For E_0^{HF} to be minimum

we need $\Delta E \geq 0$

Diagonal elements

$$\varepsilon_a^{HF} - \varepsilon_r^{HF} + \langle af \| ri \rangle_{AS}$$