Lecture FYS4480/9480, October 3, 2024

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Hartree-Fock algorithm;

variation $\quad |\Phi_0^{HF}\rangle = |\Phi_0\rangle + |\delta\Phi\rangle$

$$\langle \delta\Phi_0 | H | \Phi_0 \rangle = 0$$

$$\left(\langle \Phi_0 | H | \delta\Phi_0 \rangle = 0 \right)$$

$$\langle i | f | a \rangle = \langle \Phi_i^a | H | \Phi_0 \rangle = 0$$

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

$$|p\rangle = \sum_{\lambda} c_{p\lambda} |\lambda\rangle$$

$|\Phi_0^{HF}\rangle$ is defined by the SD composed by $|p\rangle$

$|\Phi_0\rangle$ is defined by the SD using $|\lambda\rangle$. Both $|p\rangle$ and $|\lambda\rangle$ are members of an ONB

$$\langle \Phi_0 | H | \Phi_0 \rangle = \sum_{\lambda \leq F} \langle \lambda | h_0 | \lambda \rangle$$

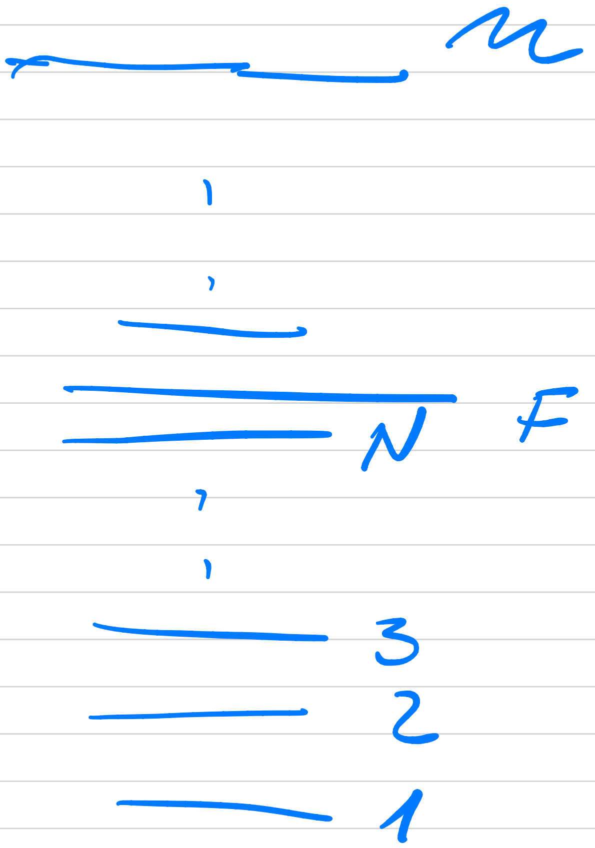
$$+ \frac{1}{2} \sum_{\gamma\delta \leq F} \langle \gamma\delta | v | \gamma\delta \rangle_{AS}$$

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

$$\sum_{i \leq F} \langle i | h_0 | i \rangle$$

$$+ \frac{1}{2} \sum_{ij} \langle ij | v | ij \rangle_{AS}$$

$$= \sum_{i \le N} \sum_{\alpha\beta} C^*_{i\alpha} C_{i\beta} \langle \alpha | h_0 | \beta \rangle$$



$$+ \frac{1}{2} \sum_{ij \le N} \sum_{\alpha\beta\gamma\delta} C^*_{i\alpha} C^*_{j\beta} C_{i\gamma} C_{j\delta}$$

$$\times \langle \alpha\beta | v | \gamma\delta \rangle_{AS}$$

$$= E_0[C]$$

$$(\alpha, \beta) \in \{1, 2, 3, \ldots, n\}$$

$$\langle p|q\rangle = \delta_{pq} = \sum_{\alpha\beta} c_{p\alpha}^* c_{q\beta} \langle\alpha|\beta\rangle$$

$$= \sum_{\alpha} |c_{p\alpha}|^2$$

Define a functional

$$F[c] = E_0[c] - \sum_{i=1}^{N} \lambda_i \sum_{\alpha} |c_{i\alpha}|^2$$

$$\frac{dF[c]}{dc^*} \quad \text{or} \quad \frac{dF[c]}{dc}$$

$$\frac{d F[c]}{d c_{i\alpha}^{*}} = 0$$

$$\Rightarrow \sum_{\beta} c_{i\beta} \langle \alpha | h_0 | \beta \rangle +$$

$$\sum_{j \leq N} \sum_{\beta\gamma\delta} c_{j\beta}^{*} c_{j\delta} c_{i\gamma} \langle \alpha\beta | v | \gamma\delta \rangle_{AS}$$

$$= \lambda_i c_{i\alpha} = \varepsilon_i^{HF} c_{i\alpha}$$

$$\langle \alpha\beta | v | \gamma\delta \rangle_{AS} = -\langle \beta\alpha | v | \gamma\delta \rangle \quad \text{etc}$$

Define a new operator h^{HF}

$$h^{HF}_{\alpha\beta} = \langle\alpha|h_0|\beta\rangle + \sum_{j\le N}\sum_{\gamma\delta} C^*_{j\gamma} C_{j\delta} \langle\alpha\gamma|v|\beta\delta\rangle$$

can then rewrite

$$\sum_{\beta} h^{HF}_{\alpha\beta} C_{i\beta} = \varepsilon^{HF}_i C_{i\alpha}$$

$$h^{HF} C = \lambda C = \varepsilon^{HF} C$$

Stability of HF eqs. & Thouless' theorem, in 1st quantization

$$\underset{\sim}{\Phi}_0^{HF} = \det(C)\, \underset{\sim}{\Phi}_0$$

$$\text{det} \qquad\qquad\qquad\qquad \text{det}$$

Can we find something similar in 2nd quantization.

Thouless' theorem, use this in the analysis of the stability of HF.

$$|\Phi_0^{HF}\rangle = |c\rangle = \prod_{i=1}^{N} a_i^{\dagger}|0\rangle$$

Express

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

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

$$\langle \delta c|H|c\rangle = 0 = \langle a|f|i\rangle = 0$$

$$\langle c|H|\delta c\rangle \quad \text{or} \quad \langle i|f|a\rangle = 0$$

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

$$|c'\rangle = \prod_{i \le F} \Big[1 + \sum_{a>F} c_i^a a_a^\dagger a_i + \frac{1}{2}\Big(\sum_{a>F} c_i^a a_a^\dagger a_i\Big)^2 + \dots \Big] |c\rangle$$

$$i \in \{1,2\}$$

A

$$|c'\rangle = \exp\Big\{ \sum_a c_1^a a_a^\dagger a_1 + \sum_a c_2^a a_a^\dagger a_2 \Big\} |c\rangle$$

B

$$= \exp\{A+B\} = \exp A \; \exp B$$

$$[A, B] = 0$$

$$[a_a^\dagger a_1 , a_b^\dagger a_2] =$$

$$a_a^\dagger a_1 a_b^\dagger a_2 - a_b^\dagger a_2 a_a^\dagger a_1$$

$$\text{— " —} \quad - a_b^\dagger (a_a^\dagger a_2) a_1$$

$$\text{— " —} \quad - a_a^\dagger a_b^\dagger a_2 a_1$$

$$\text{— " —} \quad - (a_a^\dagger a_1 a_b^\dagger a_2) = 0$$

$$\frac{1}{2}\Big(\sum_a c_i^a a_a^\dagger a_i\Big)^2 =$$

$$\frac{1}{2}\sum_{ab} c_i^b c_i^a \underbrace{a_a^\dagger a_i a_b^\dagger a_i}|c\rangle$$

$$- a_a^\dagger a_b^\dagger a_i a_i |c\rangle$$

when a_i^2 or higher powers,

then $a_i^n |c\rangle = 0$

$\Rightarrow$

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

$$|c\rangle = \prod_{i \leq F} a_i^\dagger |0\rangle$$

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

i_N

i_3

i_2

i_1

$$\times\, a_{i_1}^\dagger a_{i_2}^\dagger \cdots a_{i_N}^\dagger |0\rangle$$

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

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

$$\times$$

$$\left[\left(1 + \sum_a c_{i_2}^a \, a_a^\dagger a_{i_2} \right) a_{i_2}^\dagger \right]$$

$$\times$$

$$\vdots$$

$$\left[\left(1 + \sum_a c_{i_N}^a \, a_a^\dagger a_{i_N} \right) a_{i_N}^\dagger \right] \Big\} |0\rangle$$

$$= \prod_{i \leq F} \underbrace{\left(a_i^\dagger + \sum_a c_i^a a_a^\dagger \right)}_{b_i^\dagger} |0\rangle$$

$$\Rightarrow \quad |c'\rangle = \prod_{i \leq F} b_i^\dagger |0\rangle$$

$|\lambda\rangle \; : \; a^{\dagger}_{\lambda}|0\rangle$

$|p\rangle \; : \; a^{\dagger}_{p}|0\rangle$

$$|p\rangle = \sum_{\lambda} c_{p\lambda} |\lambda\rangle$$

$$a^{\dagger}_{p} = \sum_{\lambda} c_{p\lambda} a^{\dagger}_{\lambda}$$

λ — no restriction

can we construct a general

$$|\tilde{c}\rangle = \prod_{r \le F} \tilde{b}_r^{+} |0\rangle \quad ?$$

$$\tilde{b}_i^{+} = \sum_p g_{ip}\, a_p^{+}$$

we want to show that

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

$$\langle c|\tilde{c}\rangle =$$

$$\langle c|\, a_{i_N} a_{i_{N-1}} \cdots a_{i_2} a_{i_{\underline{1}}} \times$$

$$\left(\sum_{p=i_1}^{i_N} g_{i_{\underline{1}} p}\, a_p^{+}\right)\left(\sum_{q=i_1}^{i_N} g_{i_2 q}\, a_q^{+}\right)$$

$\cdots$

$$\times \cdots \left(\sum_{t=i_1}^{i_N} g_{i_N t}\, a_t^{+} \right) |0\rangle$$

2 states

$i_1 = 1 \quad i_2 = 2$

$$\langle 0 | a_2 a_1 \left[(g_{11} a_1^{+} + g_{12} a_2^{+}) \times (g_{21} a_1^{+} + g_{22} a_2^{+}) \right] |0\rangle$$

$$\Big(\cancel{g_{11} a_1^{+} g_{21} a_1^{+}} + g_{11} a_1^{+} g_{22} a_2^{+} + g_{12} a_2^{+} g_{21} a_1^{+} + \cancel{g_{12} a_2^{+} g_{22} a_2^{+}} \Big) |0\rangle$$

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

we have

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

$$= g_{11} g_{22} - g_{12} g_{21} = \det g$$

$$\langle 0 | \tilde{0} \rangle = 1 = \det g$$

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

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

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

$$= a^{+}_{k} + \sum_i \sum_{p=i_{N+1}}^{\infty} g^{-1}_{ki} g_{ip} a^{+}_{p} \sum_{p \le F} + \sum_{p > F}$$

Define $C_{kp} = \sum_{i \le F} g^{-1}_{ki}\, g_{ip}$

we can rewrite

$$a_k^\dagger + \sum_{p=N+1}^{\infty} c_{kp}\, a_p^\dagger \qquad k \le F$$

$$= a_k^\dagger + \sum_{a>F} c_r^a\, a_a^\dagger = b_k^\dagger$$

$$|\tilde{c}\rangle = \prod_{r \le F} \tilde{b}_r^\dagger |0\rangle = \prod_{r \le F} b_r^\dagger |0\rangle$$

$$\Rightarrow \quad |c'\rangle = \exp\left\{ \sum_{ar} c_r^a\, a_a^\dagger a_r \right\} |0\rangle$$