Lecture Fys4480, October 6, 2023

Hartree-Fock theory

$$|\delta\Phi_{HF}\rangle = \eta a_a^\dagger a_i |\Phi_{HF}\rangle$$

$$\langle \delta\Phi_{HF}|\hat{H}|\Phi_{HF}\rangle = 0 \quad \Rightarrow$$

$$\langle a|\hat{f}|i\rangle = \langle a|\hat{h}_0|i\rangle + \sum_j \langle aj|\hat{v}|ij\rangle_{AS} = 0$$

$$\langle p|\hat{f}|q\rangle = \varepsilon_p \delta_{pq}$$

$$\langle i|\hat{f}|i\rangle = \varepsilon_i$$

$$\langle a|\hat{f}|a\rangle = \varepsilon_a$$

$$\hat{h}^{HF}|p\rangle = \varepsilon_p|p\rangle \quad \text{one-body Hamiltonian}$$

assume our Hilbert space is given by only open and 1p1h configurations

$$\left(\hat{H} \right)$$

	open	1p1h
open	$\times$	$\times$
1p1h	$\times$	$\times$

$$U_{HF} H U_{HF}^{+} \longrightarrow$$

	$\tilde{\times}$	0
	0	$\tilde{\times}$

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

$$= \langle \Phi_{HF} | H | \Phi_i^a \rangle = 0$$

$$\begin{pmatrix} \tilde{X} & 0 \\ 0 & \tilde{X} \end{pmatrix}$$

$$E_0^{ref(HF)} = \sum_i \langle i | \hat{h}_0 | i \rangle + \frac{1}{2} \sum_{ij} \langle ij | v | ij \rangle_{AS}$$

$$= \sum_i \varepsilon_i^{HF} - \frac{1}{2} \sum_{ij} \langle ij | v | ij \rangle_{AS}$$

without HF : $\hat{h}_0 | \mu \rangle = \varepsilon_\mu | \mu \rangle$

$$E_0^{ref} = \sum_{\mu \leq F} \langle \mu | \hat{h}_0 | \mu \rangle + \frac{1}{2} \sum_{\mu\nu} \langle \mu\nu | \hat{v} | \mu\nu \rangle_{AS}$$

$$E_0 \le E_0^{Ref(HF)} \le E_0^{Ref}$$

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

$$\begin{pmatrix} \tilde{X} & 0 \\ 0 & \tilde{X} \end{pmatrix}$$

$$\langle \Phi_i^a | \hat{H} | \Phi_i^a \rangle = \varepsilon_a^{HF} - \varepsilon_i^{HF} + E_0^{Ref} + \sum_j \langle aj|v|ij\rangle_{AS}$$

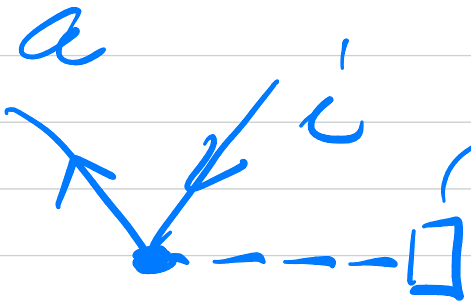
non-diag

$$\langle \Phi_i^a | H | \Phi_j^b \rangle = \langle aj|v|ib\rangle_{AS}$$

HF in diagrammatic form

$$\langle a|\hat{f}|i\rangle = \langle a|\hat{h}^{HF}|i\rangle = 0$$

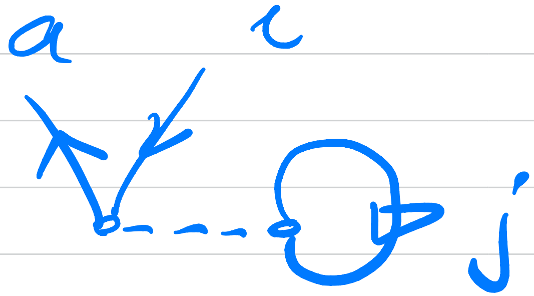
$$= \langle a|\hat{t} + \hat{u}_{ext}|i\rangle + \sum_{j \le F} \langle aj|\hat{v}|ij\rangle_{AS}$$



$(\hat{t} + \hat{u}_{ext})$

$+$

$\sum_j \langle aj|v|ij\rangle$



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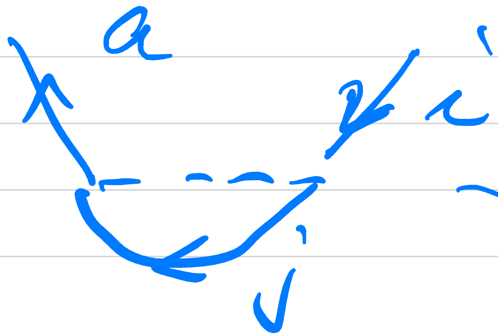
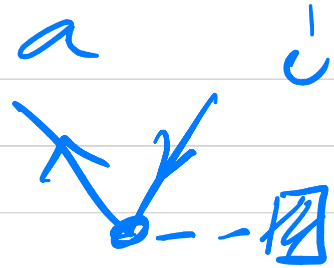


$\sim -\sum_j \langle aj|v|ji\rangle$



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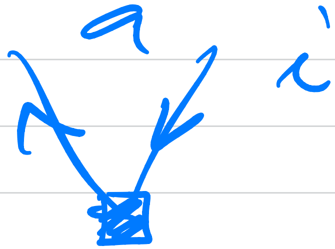

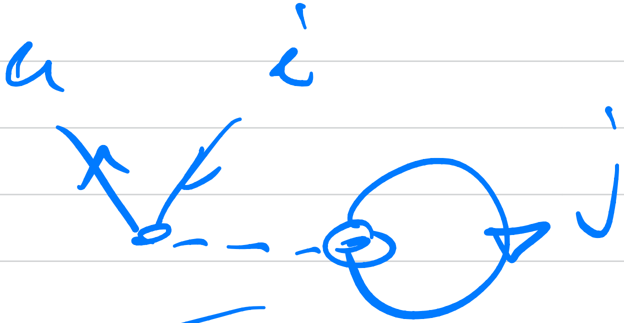

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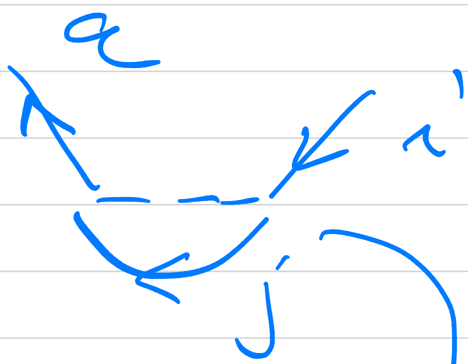


1 n_h

0 n_e

=

$\underbrace{1 \text{ hole}}_{n_h}$ $\underbrace{1 \text{ loop}}_{n_e}$ $\rightarrow (-1)^{n_h+n_e} = (-1)^2 = +1$

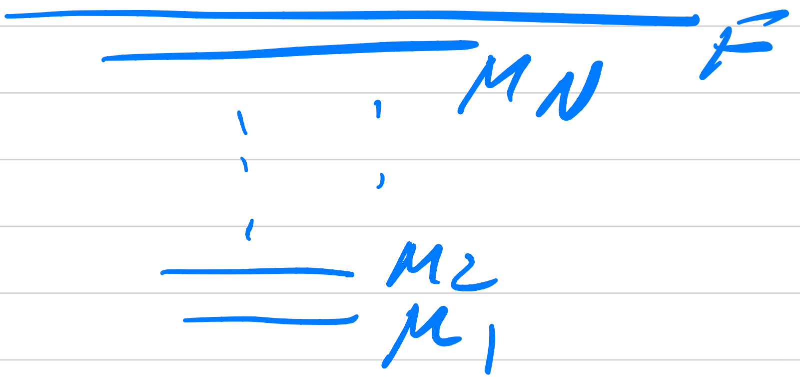
Third approach (Exercise week 40)

$$|a\rangle = \sum_{\mu} C_{a\mu} |\mu\rangle$$

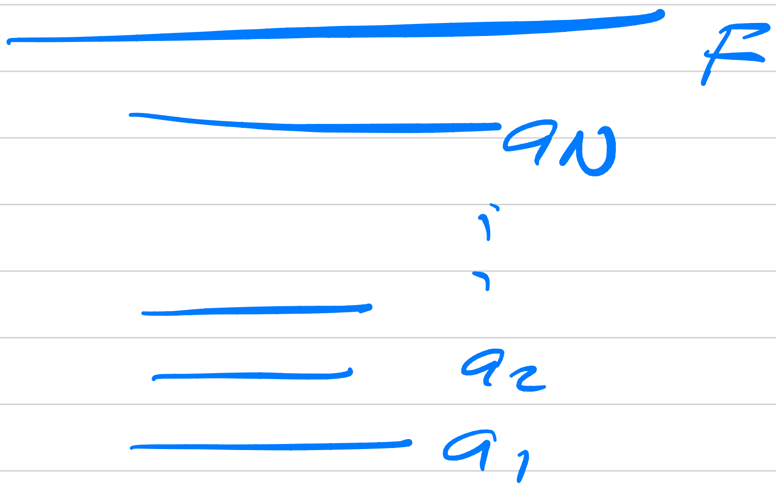
$$\hat{h}_0 |\mu\rangle = \varepsilon_\mu |\mu\rangle$$

$$\hat{h}^{HF} |a\rangle = \varepsilon_a^{HF} |a\rangle$$

$$\Phi_0 = \frac{1}{\sqrt{N!}} \begin{vmatrix} \varphi_{\mu_1}(x_1) & \cdots & \varphi_{\mu_1}(x_N) \\ \varphi_{\mu_2}(x_1) & & \vdots \\ \vdots & & \vdots \\ \varphi_{\mu_N}(x_1) & & \varphi_{\mu_N}(x_N) \end{vmatrix}$$



$$\Phi_0^{HF} = \frac{1}{\sqrt{N}} \begin{vmatrix} \varphi_{a_1}(x_1) & \cdots & \varphi_{a_1}(x_N) \\ \varphi_{a_2}(x_1) & & \vdots \\ \vdots & & \vdots \\ \varphi_{a_N}(x_1) & & \varphi_{a_N}(x_N) \end{vmatrix}$$



$$\langle \Phi_0 | \hat{H} | \Phi_0 \rangle = \sum_{\mu \le F} \langle \mu | \hat{h}_0 | \mu \rangle + \frac{1}{2} \sum_{\mu\nu} \langle \mu\nu | \hat{v} | \mu\nu \rangle_{AS}$$

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

$$= \sum_{i \le F} \langle i | \hat{h}_0 | i \rangle + \frac{1}{2} \sum_{ij} \langle ij | \hat{v} | ij \rangle_A$$

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

λ not restricted to be below F

$$\hat{h}_0 |\lambda\rangle = \varepsilon_\lambda |\lambda\rangle$$

$$= \sum_{i \le F} \sum_{\mu\nu} c_{i\mu}^* c_{i\nu} \boxed{\langle \mu | \hat{h}_0 | \nu \rangle}$$

precalculable

$+$

$$+ \frac{1}{2} \sum_{ij \le F} \underbrace{\sum_{\substack{\alpha\beta \\ \mu\nu}}}_{\text{not restricted to be below } F} C^{*}_{i\alpha} C^{*}_{j\beta} C_{i\mu} C_{j\nu}$$

$$\times \boxed{\langle \alpha\beta | \hat{v} | \mu\nu \rangle_{AS}}$$

often be "easily" calculated and tabulated ?

Variational calculus

$$\langle \Phi_0^{HF} | \Phi_0^{HF} \rangle = 1$$

$$\langle i | j \rangle = \sum_{\alpha\beta} c_{i\alpha}^* c_{j\beta} \underbrace{\langle \alpha | \beta \rangle}_{\delta_{\alpha\beta}}$$

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

$$\langle \Phi_0^{HF} | \Phi_0^{HF} \rangle = \sum_{i=1}^{N} \sum_{\alpha} c_{i\alpha}^* c_{i\alpha}$$

$$F[\Phi_0^{HF}] = E[\Phi_0^{HF}]$$

$$- \sum_{i=1}^{N} \sum_{\alpha} \varepsilon_{i\alpha} c_{i\alpha}^* c_{i\alpha}$$

Lagrange multiplier

$$\frac{\delta F[\Phi_0^{HF}]}{\delta c_{i'\alpha}^*} = 0$$

$$\frac{\delta}{\delta c_{i'\alpha}^*}\Big[c_{i'\alpha}^* c_{i'\alpha} \varepsilon_\alpha + \frac{1}{2}\sum_{j} \sum_{\beta\gamma\delta} c_{i'\alpha}^* c_{j\beta}^* c_{i\gamma} c_{j\delta} \langle\alpha\beta|v|\gamma\delta\rangle_{AS}$$

$$\langle\alpha|h_0|\alpha\rangle$$

$$- \varepsilon_{i'} c_{i'\alpha}^* c_{i'\alpha} \Big] = 0$$

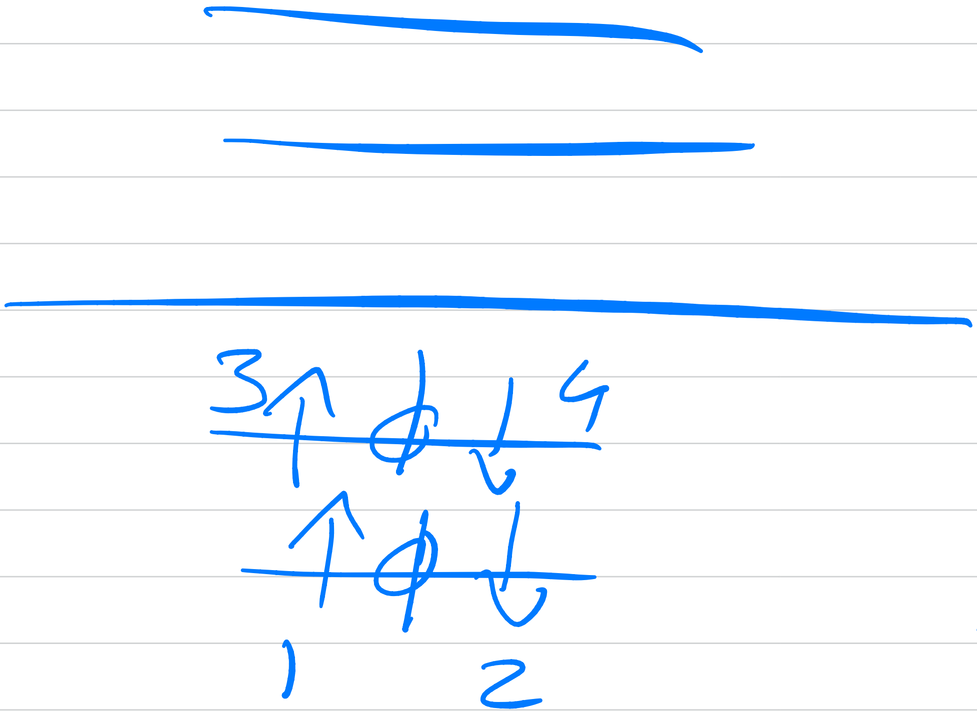
$$\left[C_{i\alpha}\, \varepsilon_\alpha + \sum_{j=1}^{N} \sum_{\beta\gamma\delta} C_{j\beta}^{*}\, C_{i\gamma}\, C_{j\delta} \times \langle \alpha\beta | v | \gamma\delta \rangle - \varepsilon_i\, C_{i\alpha} \right]$$

$$= 0$$

$$\hat{h}^{HF}_{\alpha\beta} = \langle \alpha | \hat{h}_0 | \beta \rangle + \sum_{j=1}^{N} \sum_{\gamma\delta} C_{j\gamma}^{*}\, C_{j\delta} \langle \alpha\gamma | \hat{v} | \beta\delta \rangle$$

$$\sum_{\beta} h^{HF}_{\alpha\beta}\, C_{i\beta} = \varepsilon_i^{HF}\, C_{i\alpha}$$

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



$$\begin{bmatrix} \langle 1|h^{HF}|1\rangle & \langle 1|h^{HF}|3\rangle \\ \langle & \langle 3|h^{HF}|3\rangle \end{bmatrix}$$

$$\langle 1|h^{HF}|4\rangle = 0$$

$$\langle 1|h^{HF}|1\rangle$$

$$\langle 1|h^{HF}|3\rangle$$

$$\langle 3|h^{HF}|3\rangle$$

stability of HF solution.

Thouless theorem:

a general SD $|\Phi'\rangle$

which is not orthogonal to

$$|\Phi_0\rangle = \prod_{i=1}^{N} a_i^+ |0\rangle$$

$$\boxed{|\Phi'\rangle = \exp\left\{ \sum_{a>F} \sum_{i\leq F} c_i^a a_a^+ a_i \right\}} \times |\Phi_0\rangle$$

$$\delta\Phi^{HF} \propto a_a^+ a_i |\Phi_0\rangle$$