Lecture FYS4480/9480, September 27, 2024

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1st quantization

$$\Phi_0(x_1, x_2 \ldots x_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \varphi_1(x_1) & \varphi_1(x_2) & \cdots & \varphi_1(x_N) \\ \varphi_2(x_1) & & & \vdots \\ \vdots & & & \vdots \\ \varphi_N(x_1) & & & \varphi_N(x_N) \end{vmatrix}$$

ONB:

$$\int dx\, \varphi_i^*(x)\, \varphi_j(x) = \delta_{ij}$$

variational calculus

$$\varphi_i(x) \longrightarrow N_i\left(\varphi_i(x) + \delta\varphi_i(x)\right)$$

$$i \leq F(N)$$

$$\delta\varphi_i = \eta\, \varphi_a(x) \qquad a > F$$

$$N_i^{-2} = \int dx \left(\varphi_i^* + \eta^* \varphi_a^*\right)\left(\varphi_i + \eta\varphi_a\right)$$

$$= 1 + |\eta|^2 \qquad |\eta| \ll 1$$

$N_i \simeq 1$ at linear order in η

$$\Phi_0 \to \Phi_0^{HF} + \eta\, \delta\Phi_0^{HF}$$

$$E_0^{HF} = \langle \Phi_0^{HF} | H | \Phi_0^{HF} \rangle \qquad \frac{\delta E_0^{HF}}{\delta \eta^*}$$

$$+ \left[\eta^* \langle \delta \Phi_0^{HF} | H | \Phi_0^{HF} \rangle \right. \qquad \frac{\delta E_0^{HF}}{\delta \eta}$$

$$\left. + \eta \langle \Phi_0^{HF} | H | \delta \Phi_0^{HF} \rangle \right]$$

$$+ |\eta|^2 \langle \delta \Phi_0^{HF} | H | \delta \Phi_0^{HF} \rangle$$

$|\eta| \ll 1$, leave out the quadratic term

$$\delta E_0^{HF} = \eta^* \langle \delta \Phi_0^{HF} | H | \Phi_0^{HF} \rangle$$

$$+ \eta \langle \Phi_0^{HF} | H | \delta \Phi_0^{HF} \rangle$$

in optimization

$$\delta E_0^{HF} = 0 \qquad \delta E_0^{HF}$$

(i) $\eta = \mathrm{Re}\,\eta + i\,\mathrm{Im}\,\eta$

(ii) H is Hermitian.

$$\langle \delta \Phi_0^{HF} | H | \Phi_0^{HF} \rangle = 0$$

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

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

we have a variation

$$|\delta\Phi_0^{HF}\rangle = \eta\, a_a^\dagger a_i |\Phi_0^{HF}\rangle$$

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

$$= \eta^* \langle \Phi_0^{HF} | a_i^\dagger a_a H | \Phi_0^{HF}\rangle = 0$$

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

$$\langle \Phi_0^{HF} | a_i^\dagger a_a \sum_{pq} \langle p|f|q\rangle a_p^\dagger a_q | \Phi_0^{HF}\rangle$$

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

$$= 0$$

$$\eta \ \langle \Phi_0^{HF} | H | \delta\Phi_0^{HF}\rangle = 0 = \langle i|f|a\rangle$$

Back to FCI

$$\langle \Phi_0 | H | 1p1h \rangle = 0$$

original Hamiltonian matrix

$$
\begin{array}{c|cccccc}
 & |\Phi_0\rangle & |1p1h\rangle & |2p2h\rangle & |3p3h\rangle & \cdots & |NpNh\rangle \\
\hline
\langle \Phi_0| & \times & \times & \times & 0 & \cdots & 0 \\
\langle 1p1h| & \times & \times & \times & \times & \cdots & 0 \\
\langle 2p2h| & \times & \times & \times & \ddots & & \\
\vdots & 0 & \times & \times & & \ddots & \\
\vdots & \vdots & 0 & \times & & & \\
 & \vdots & \vdots & 0 & & & \ddots \\
\langle NpNh| & 0 & \vdots & \vdots & & &
\end{array}
$$

$$U_{HF}^{\dagger} \hat{H} U_{HF} =$$

$$\begin{bmatrix} \tilde{x} & 0 & \tilde{x} & 0 & \cdots & 0 \\ 0 & \tilde{x} & \tilde{x} & \tilde{x} & 0 & \cdots \\ \tilde{x} & \vdots & \ddots & & & \\ 0 & \vdots & & & \ddots & \\ \vdots & & & & & \end{bmatrix}$$

HF - choice

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

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

$$\langle i | f | i \rangle = \varepsilon_i^{HF} \wedge \langle a | f | a \rangle = \varepsilon_a^{HF}$$

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

$$f \rightarrow h^{HF} \qquad \hat{t} + \hat{u}_{ext}$$

$$\langle q|h^{HF}|p\rangle = \langle q|\hat{h}_0|p\rangle + \langle q|u^{HF}|p\rangle$$

$$\sum_j \langle qj|v|pj\rangle_{AS}$$

$$H = \begin{bmatrix} H_{00} & H_{01} \\ H_{01} & H_{11} \end{bmatrix}$$

Jacobi's method

$$\begin{bmatrix} \cos & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix} \begin{bmatrix} H_{00} & H_{01} \\ H_{01} & H_{11} \end{bmatrix} \begin{bmatrix} \cos & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}$$

$$= \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix}$$

$$H_{01} \cdot (c^2 - s^2) + (H_{00} - H_{11}) cs = 0$$

$$\tau = \frac{H_{11} - H_{00}}{2 H_{10}}$$

$$t = \tan\theta = -\tau \pm \sqrt{1 + \tau^2}$$

Interpretation:

$$E[\Phi_0(N)] = \sum_{i \le F} \langle i | h_0 | i \rangle + \frac{1}{2} \sum_{ij} \langle ij | v | ij \rangle$$

$$E[\Phi_0(N-1)] = \sum_{\substack{i \le F \\ i \neq k}} \langle i | h_0 | i \rangle + \frac{1}{2} \sum_{\substack{ij \\ i \neq k \\ j \neq k}} \langle ij | v | ij \rangle$$

remove electron in state k

$$E[\Phi_0(N)] - E[\Phi_0(N-1)] =$$

$$\langle k | h_0 | k \rangle + \sum_{j \leq F} \langle kj | v | kj \rangle$$

$$= \varepsilon_k^{HF}$$

Na : $11 e^-$

Na^+ : $10 e^-$

ionization energy :

$$E(Na) - E(Na^+)$$

$$E[\Phi_0(N+1)] - E[\Phi_0(N)] = \varepsilon_a^{HF}$$

Nuclear physics

$$BE(A) \simeq E[\Phi_0^{HF}(A)]$$

$A = N + Z$

Example ^{16}O

$BE(A-1)$

$\simeq E[\Phi_0^{H}(A-1)]$

$BE(A+1)$

$1s0d$

	protons		neutrons	
$0p$	6	$0p_{1/2}$	6	$0p_{1/2}$ F
$0s$	2		2	

protons neutrons

$$BE(^{16}O) - BE(^{15}N)$$

$$E[\Phi_0^{HF}(^{16}O)] - E[\Phi_0^{H}(^{15}N)]$$

$$= \varepsilon^{HF}_{0p_{1/2}^{\pi}}$$

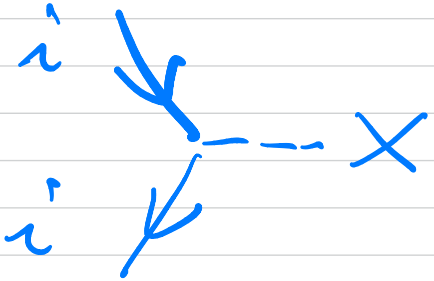
$$BE(^{17}O) - BE(^{16}O) \simeq \varepsilon^{HF}_{0d_{5/2}^{\nu}}$$

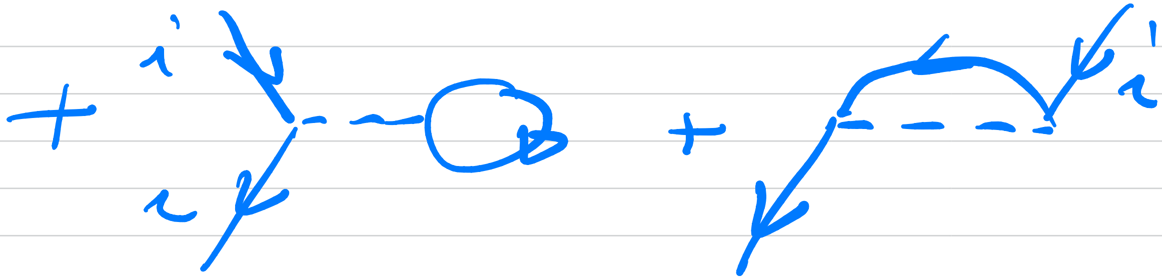
Diagrammatic representation of HF

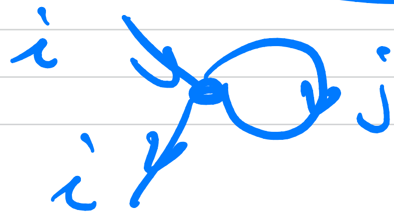
$$\langle i | f | i \rangle = \langle i | h^{HF} | i \rangle$$

$$= \langle i | h_0 | i \rangle + \sum_j \langle ij | v | ij \rangle_{As}$$

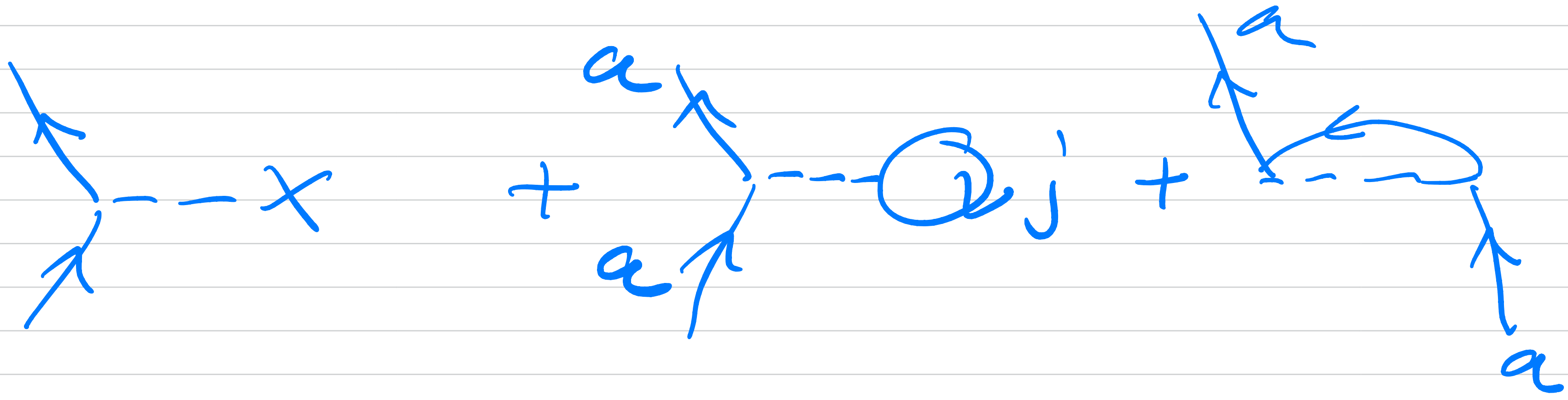
$$\langle ij | v | ij \rangle - \langle ij | v | ji \rangle$$



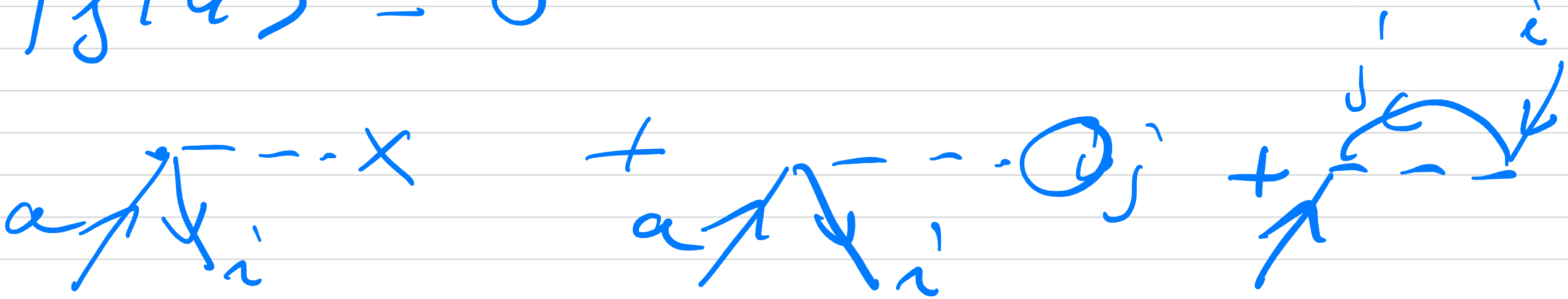




$\langle a | f | a \rangle$



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



$= 0$

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