FYS4480/9480, lecture October 2, 2025

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Reference state $|\Phi_0\rangle \rightarrow$

$|\Phi_0^{HF}\rangle$

$$\langle \Phi_0^{HF} | \hat{H} | \Phi_0^{HF} \rangle \geq E_0 \text{ (exact)}$$

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

Variational calculus

(i) coordinate space variation

SP - state

$$|\varphi_\alpha(x)\rangle \to |\varphi_\alpha(x)\rangle + |\delta\varphi_\alpha(x)\rangle$$

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

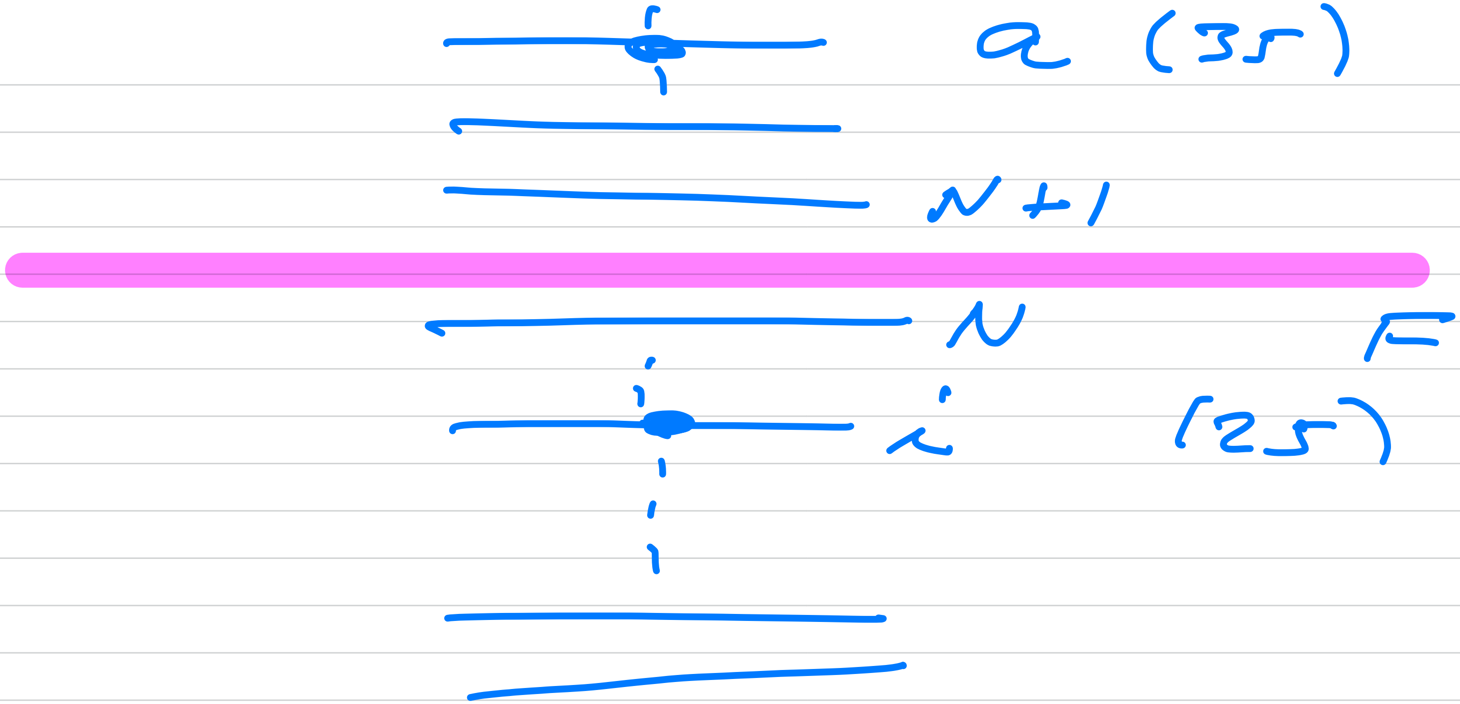
ONB

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

(ii) variation of coefficients

$$|p\rangle = \sum_\lambda c_{p\lambda} \underbrace{|\lambda\rangle}_{\text{ONB-basis}}$$

$$\langle \lambda | \sigma \rangle = \delta_{\lambda\sigma}$$



$$\varphi_i(x) \rightarrow \underbrace{N_i'}_{\text{Norm constant}} \left(\varphi_i(x) + \delta\varphi_i(x) \right)$$

$i \le F$

$$\delta\varphi_i(x) = \eta\, \varphi_a(x)$$

$|\eta| \ll 1 \qquad a > F$

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

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

$N_c \simeq 1$ at linear order in η

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

$$E_0^{HF} = \langle \Phi_0^{HF} | \mathcal{H} | \Phi_0^{HF} \rangle$$

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

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

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

$|\eta| \ll 1$, leave out quadratic terms in optimization

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

$$\eta^* \langle \delta \Phi_0^{HF} | \hat{\mathcal{H}} | \Phi_0^{HF} \rangle$$

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

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

(ii) $\hat{\mathcal{H}}$ is hermitian $\Rightarrow$

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

$\Rightarrow$ integro-differential eqs.

2nd quantization

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

Define a new variation

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

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

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

$$= 0$$

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

$$(i') \quad \langle \Phi_0^{HF} | a_i^{+} a_a \sum_{pq} \langle p | \hat{f} | q \rangle a_p^{+} a_q$$

$$\times | \Phi_0^{HF} \rangle$$

$$= \langle \Phi_0^{HF} | a_i^{+} a_a \hat{F}_N | \Phi_0^{HF} \rangle$$

$$\left\{ a_i^{+} a_a a_p^{+} a_q = \delta_{ap} \delta_{iq} \right\}$$

$$= \langle a | \hat{f} | i \rangle = \langle a | \hat{h}_0 | i \rangle$$

$$+$$

$$+ \sum_{j \leq F} \langle aj \| \hat{v} \| ij \rangle_{AS}$$

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

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

Back of FCI

$$
\begin{array}{c|cccccc}
 & 0p0h & 1p1h & 2p2h & 3p3h & \cdots & NpNh \\
\hline
0p0h & \times & \times & \times & 0 & \cdots & 0 \\
1p1h & \times & \times & \times & & & \\
2p2h & \times & \times & \times & & & \\
\vdots & 0 & \cancel{\times} & \times & \times & & \\
\vdots & \vdots & 0 & \times & & & \\
\vdots & \vdots & \vdots & 0 & & & \\
NpNh & 0 & \vdots & \vdots & & &
\end{array}
$$

The eqs $\langle i|\hat{f}|a\rangle = \langle a|\hat{f}|i\rangle$

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

$= H$

$$\mathcal{U}^{\dagger}_{HF}\, H\, \mathcal{U}_{HF} \rightarrow$$

$$
\begin{array}{c|c}
 & \begin{array}{cccccc} 0p0h & 1p1h & & & & \end{array} \\
\begin{array}{c} 0p0h \\ 1p1h \\ \\ \\ \\ \\ \\ \end{array} &
\begin{bmatrix}
\tilde{X} & 0 & \tilde{X} & 0 & 0 & \cdots & 0 \\
0 & \tilde{X} & & & & & 0 \\
\tilde{X} & \tilde{X} & & & \tilde{X} & & \\
0 & \tilde{X} & & & & & \\
0 & 0 & & & & & \\
\vdots & \vdots & & & & & \\
 & & 0 & & & &
\end{bmatrix}
\end{array}
$$

standard HF

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

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

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

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

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

$$\langle p|\hat{u}^{HF}|q\rangle = \sum_{j\le F}\langle pj|\hat{v}|qj\rangle_{AS}$$

our original sp-basis $|\alpha\rangle$

$$E_0^{Ref} = \langle \Phi_c | \mathcal{H} | \Phi_c \rangle$$

$$= \sum_{\alpha \le F} \underbrace{\langle \alpha | \hat{h}_0 | \alpha \rangle}_{\varepsilon_\alpha} + \frac{1}{2} \sum_{\substack{\alpha\beta \\ \le F}} \langle \alpha\beta | \hat{v} | \alpha\beta \rangle_{AS}$$

$$\left(\hat{h}_0 |\alpha\rangle = \varepsilon_\alpha |\alpha\rangle \right)$$

$$|\Phi_0\rangle = \prod_{\alpha \le F} a_\alpha^\dagger |0\rangle$$

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

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

Single SD

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

$$= \sum_{i \le F} \langle i | \hat{h}_0 | i \rangle +$$

$$\frac{1}{2} \sum_{i,j \le F} \langle ij | \hat{w} | ij \rangle_{AS}$$

$$= \sum_{i \le F} \sum_{\alpha\beta} C_{i\alpha}^{*} C_{i\beta} \underbrace{\langle \alpha | \hat{h}_0 | \beta \rangle}_{\delta_{\alpha\beta} \varepsilon_\alpha} +$$

$$\frac{1}{2} \sum_{ij \le F} \sum_{\alpha\beta\gamma\delta} C_{i\alpha}^* C_{j\beta}^* C_{i\gamma} C_{j\delta}$$

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

known and can be calculated,

$$\langle \alpha | \hat{h}_0 | \beta \rangle = \varepsilon_\alpha \delta_{\alpha\beta}$$

use variational calculus and vary $C_{i\alpha}$

$$\frac{\delta E_0^{HF}}{\delta C_{i\alpha}^*} = 0$$