Lecture FYS4480/9480, September 26, 2024

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$$|\Psi_0\rangle = \sum_{PH} C_H^P |\Phi_H^P\rangle$$

$$\hat{H}_0 |\Phi_H^P\rangle = E_H^P |\Phi_H^P\rangle$$

C_H^P represent the overlap $\langle\Psi_0|\Phi_H^P\rangle$

$$H|\Psi_0\rangle = E_0|\Psi_0\rangle$$

$$E_0 \leq \min_{c_H^P} \frac{\sum\limits_{\substack{PH \\ P'H'}} c_H^{*P} c_{H'}^{P'} \langle \Phi_H^P | H | \Phi_{H'}^{P'} \rangle}{\sum\limits_{\substack{PH \\ P'H'}} c_H^{*P} c_{H'}^{P'} \underbrace{\langle \Phi_H^P | \Phi_{H'}^{P'} \rangle}_{ONB}}$$

$$\Rightarrow \det(H - \lambda I)$$

$$\sum_{PH} c_H^P |\Phi_H^P\rangle = \underbrace{\quad 1p1h \quad}$$

$$c_0 |\Phi_0\rangle + \sum_{ai} c_i^a \underbrace{|\Phi_i^a\rangle}_{a_a^\dagger a_i |\Phi_0\rangle} +$$

$$\sum_{\substack{ab\\ij}} c_{ij}^{ab} \underbrace{\underbrace{a_a^\dagger a_b^\dagger a_j a_i |\Phi_0\rangle}_{|\Phi_{ij}^{ab}\rangle}}_{2p2h}$$

$$+ \ldots + NpNh$$

$$\langle \Phi_0 | H | \Phi_i^a \rangle$$

$$\langle \Phi_0 | H | \Phi_{ij}^{ab} \rangle$$

$$\langle \Phi_i^a | H | \Phi_j^b \rangle$$

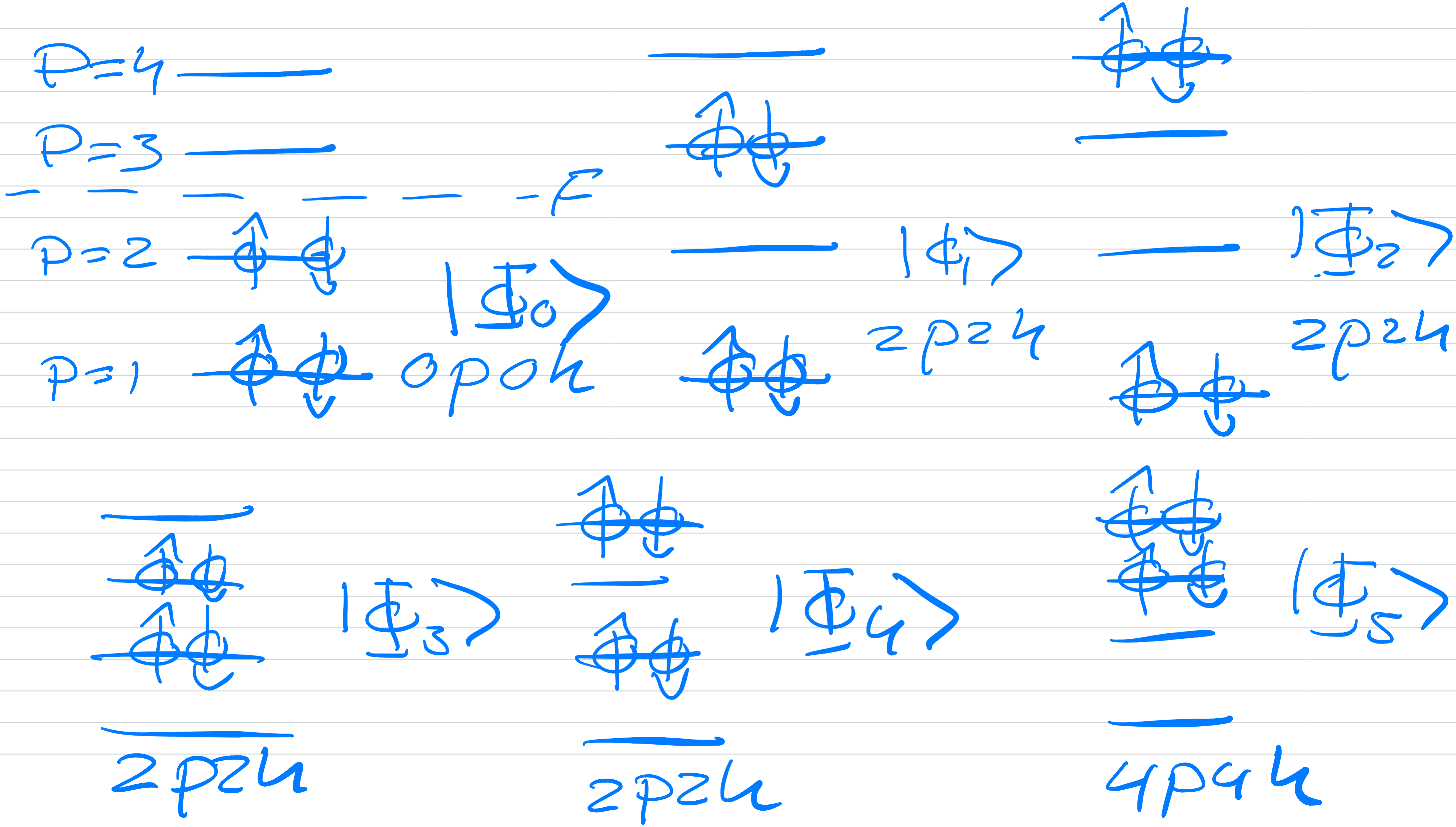
$$\langle \Phi_i^a | H | \Phi_{kl}^{cd} \rangle \ldots$$

Hamiltonian matrix

$$
\begin{array}{c|ccccccc}
 & 0p0h & 1p1h & 2p2h & 3p3h & & \cdots & NpNh \\
\hline
0p0h & \overset{E_0^{Ref}}{\langle \Phi_0 | H | \Phi_0 \rangle} & \langle \Phi_0 | H | 1p1h \rangle & \langle \Phi_0 | H | 2p2h \rangle & 0 & & \cdots & 0 \\
1p1h & \langle 1p1h | H | \Phi_0 \rangle & \langle 1p1h | H | 1p1h \rangle & \times & \times & 0 & - & 0 \\
2p2h & \langle 2p2h | H | \Phi_0 \rangle & \langle 2p2h | H | 1p1h \rangle & \times & \times & \times & 0 \cdots & 0 \\
3p3h & 0 & \times & \times & & & & \\
 & \vdots & 0 & \times & & & & \\
\vdots & \vdots & \vdots & 0 & & & & \\
\vdots & \vdots & \vdots & \vdots & & & & \\
NpNh & 0 & 0 & 0 & & & &
\end{array}
$$

$n = 8$ sp states

$N = 4$ particles



$$
\begin{bmatrix}
\langle \Phi_0 | H | \Phi_0 \rangle & \underbrace{\langle \Phi_0 | H | \Phi_1 \rangle \; - - \; \langle \Phi_0 | H | \Phi_4 \rangle}_{\langle \Phi_0 | H | 2p2h \rangle} & & \underbrace{\langle \Phi_0 | H | \Phi_5 \rangle}_{\langle \Phi_0 | H | 4p4h \rangle} \\
\langle \Phi_1 | H | \Phi_0 \rangle & & & \\
\langle \Phi_2 | H | \Phi_0 \rangle & x \quad x & x & x \\
\vdots & x & x & x \\
\langle \Phi_4 | H | \Phi_0 \rangle & x & \langle \Phi_4 | H | \Phi_4 \rangle & \\
0 & x & & \langle \Phi_5 | H | \Phi_5 \rangle
\end{bmatrix}
$$

$$\langle \Phi_0 | H | \Phi_{ij}^{ab} \rangle = \langle ab | v | ij \rangle_{AS}$$

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

$$\langle \Phi_0 | H | ph \rangle \Rightarrow$$

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

$$| \Phi_i^a \rangle = a_a^\dagger a_i | \Phi_0 \rangle$$

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

$$(H-E_0)|\Psi_0\rangle = 0$$

$$(H-E_0)\sum_{HP} C_H^P |\Phi_H^P\rangle = 0$$

$$\left(HC_i = E_i C_i \right)$$

First row of Hamiltonian matrix

$$\langle \Phi_0 | H - E_0 | \Psi_0 \rangle = 0$$

$$\langle \Phi_0 | H - E_0 | \Phi_0 \rangle + \sum_{ai} c_i^a \langle \Phi_0 | H - E_0 | \Phi_i^a \rangle$$

$$+ \sum_{\substack{ab\\ij}} c_{ij}^{ab} \langle \Phi_0 | H - E_0 | \Phi_{ij}^{ab} \rangle =$$

$$\underbrace{\langle \Phi_0 | H | \Phi_0 \rangle}_{E_0^{Ref}} - E_0$$

$$+ \sum_{ai} c_i^a \langle a | f | i \rangle$$

$$+ \sum_{\substack{ab\\ij}} c_{ij}^{ab} \langle ab | v | ij \rangle_{AS} = 0$$

$$\Delta E = E_0 - E_0^{Ref} = \sum_{ai} c_i^a \langle a | f | i \rangle + \sum_{\substack{ab\\ij}} c_{ij}^{ab} \langle ab | v | ij \rangle_{AS}$$

$$\langle \Phi_i^a | H - E_c | \Psi_c \rangle = 0$$

$$= \underbrace{\langle \Phi_i^a | H | \Phi_o \rangle} + \sum_{bj} c_j^b \langle \Phi_i^a | H - E_c | \Phi_j^b \rangle$$

$$+ \sum_{\substack{bc \\ jk}} c_{jk}^{bc} \langle \Phi_i^a | H | \Phi_{jk}^{bc} \rangle$$

$$+ \sum_{\substack{bcd \\ jke}} c_{jke}^{bcd} \langle \Phi_i^a | H | \Phi_{jke}^{bcd} \rangle$$

3p3h

$$= 0$$

$\Rightarrow$

$$\langle i | f | a \rangle + c_i^a \langle \Phi_i^a | H - E_0 | \Phi_i^a \rangle$$

$$+ \sum_{\substack{b \neq a \\ j \neq i}} \langle \Phi_i^a | H | \Phi_j^b \rangle c_j^b$$

$$+ \ldots = 0$$

$$\langle \Phi_i^a | H - E_0 | \Phi_i^a \rangle c_i^a =$$

$$\langle \Phi_i^a | H | \Phi_i^a \rangle - c_i^a E_0$$

$$\langle i|f|a\rangle + \Big[\langle a|f|a\rangle - \langle i|f|i\rangle + \langle ai\|ai\rangle_{AS}\Big] C_i^a$$

$$+ \sum_{\substack{b\neq a \\ j\neq i}} C_j^b \underbrace{\langle \Phi_i^a | H | \Phi_j^b\rangle}_{\langle aj\|bi\rangle_{AS}}$$

$$+ \ldots = E_0 C_i^a$$

Solve iteratively with a guess $C_i^a(0)$, $C_{ij}^{ab}(0)$, ...

in MBPT(2): $c_i^a(0) = \frac{\langle i|f|a\rangle}{\varepsilon_i - \varepsilon_a}$

$$c_{ij}^{ab}(0) = \frac{\langle ij|v|ab\rangle}{\varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_b}$$

guess: $c_{ijk}^{abc}(0) \ldots = 0$

Hartree-Fock theory Com first approximation

$$H \cdot C = E C$$

standard approach:

$$u^+ H u = D = \begin{bmatrix} \lambda_0 & & \\ & \ddots & \\ & & \lambda_{a-1} \end{bmatrix}$$

$$u^+ u = u u^+ = \mathbb{1} \qquad u^+ = u^{-1}$$

$$u_M^+ u_{M-1}^+ \cdots u_1^+ H u_1 u_2 \cdots u_M$$

$$= D$$

$$U_{2\times 2} = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}$$

$$U^{\dagger} H U = \begin{bmatrix} \lambda_1 & \\ & \lambda_2 \end{bmatrix}$$

choose θ so that the non-diagonal elements are zero

$$H = \begin{bmatrix} h_{11} & h_{12} \\ h_{21} & h_{22} \end{bmatrix}$$

$$U^{\dagger} H U = \begin{bmatrix} \tilde{h}_{11} & 0 \\ 0 & \tilde{h}_{22} \end{bmatrix}$$

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

Specific u which zero out $\langle 1p1h|H|\Phi_0\rangle$

$$
u^{\dagger} H u = \begin{array}{c|ccccc}
 & 0p0h & 1p1h & 2p2h & 3p3h \cdots & NpNh \\
 & \tilde{x} & 0 & \tilde{x} & 0 & \cdots 0 \\
 & 0 & \tilde{x} & \tilde{x} & & \\
2p2h & \tilde{x} & \tilde{x} & \tilde{x} & & \\
3p3h & 0 & \tilde{x} & \tilde{x} & & \\
 & \vdots & 0 & \tilde{x} & & \\
 & 0 & \vdots & 0 & & \\
 & & & \vdots & &
\end{array}
$$

new $E_0^{Ref} \leq$ old E_0^{Ref}

$\langle \Phi_0|H|1p1h\rangle = \langle \Phi_0|H|\Phi_i^a\rangle$

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

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

$$= 0$$

Standard Hartree-Fock

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

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

$$\langle i | f | a \rangle = 0 \Rightarrow h^{HF} | p \rangle = \varepsilon_p^{HF} | p \rangle$$

$$\hat{h}^{HF} = \underbrace{\hat{h}_0}_{(\hat{t} + \hat{u}_{ext})} + \hat{u}^{HF}$$

$$\langle p | \hat{u}^{HF} | q \rangle = \sum_{i \leq F} \langle pi | v | qi \rangle$$

The new basis $|p\rangle$ defines a new Ref state

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

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

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

$$\langle \Phi_0 | H | \Phi_0 \rangle$$

How do we find $|P\rangle$?

Variational calculus

(i) coordinate space variation

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

$\to$ coupled integro-differ. equations.

(ii) variation of coefficients

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

(iii) HF in 2nd quantization