Lecture Fys4480, September 28, 2023

FCI

$$H|\Psi_i\rangle = E_i|\Psi_i\rangle$$

$$|\Psi_i\rangle = \sum_{j=0}^{D} c_{ij}|\Phi_j\rangle$$

$$\langle\Phi_i|\Phi_j\rangle = \delta_{ij}$$

Ground state

$$|\Psi_0\rangle = (c_0 + \hat{C})|\Phi_0\rangle$$

$\hat{C}$ = correlation operator

$$\langle\Psi_0|\Phi_0\rangle = c_0 = 1$$

$$c_0 + \hat{C} = \sum_{PH} c_H^P A_H^P$$

PH = 0p0h, 1p1h, 2p2h etc

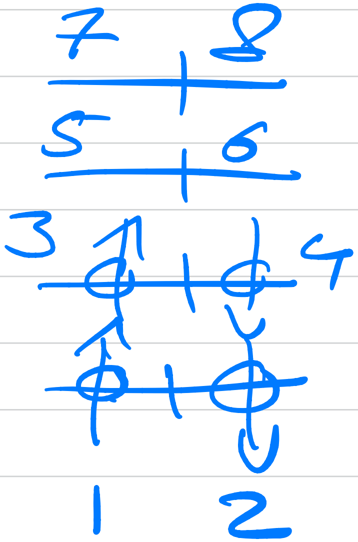
$$\hat{C} = \sum_{ai} c_i^a a_a^\dagger a_i + \sum_{\substack{ab\\ij}} c_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i$$

$$+ \ldots + NpNh$$

(not limited to $|\Psi_0\rangle$)

Example (pairing, 2nd midterm)

$n = 8$, $N = 4$, no-broken pairs

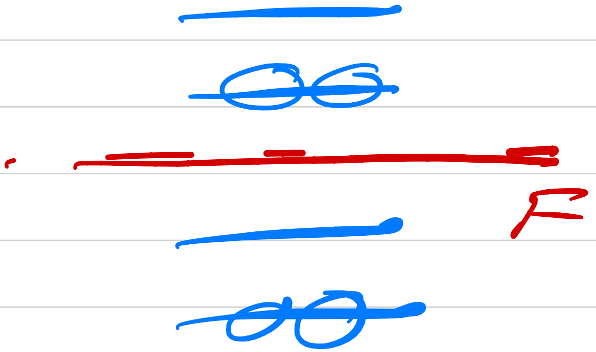


$p = 2$

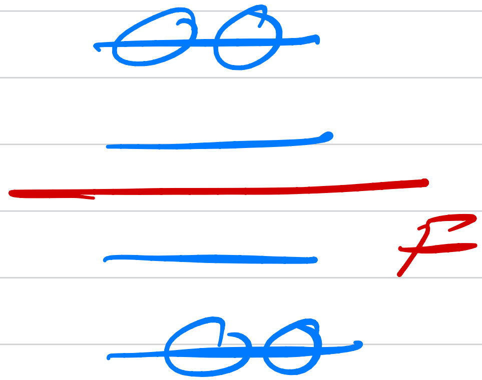
$p = 1$

$|\Phi_0\rangle$

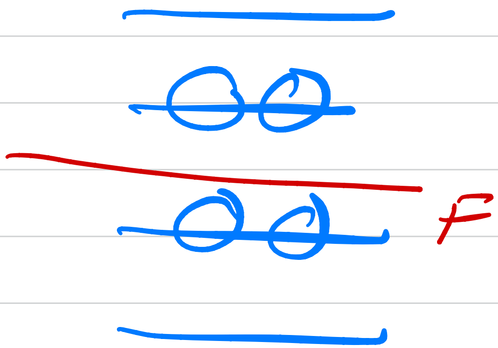
$$\binom{4}{2} = \frac{4!}{2!\,2!} = 6$$



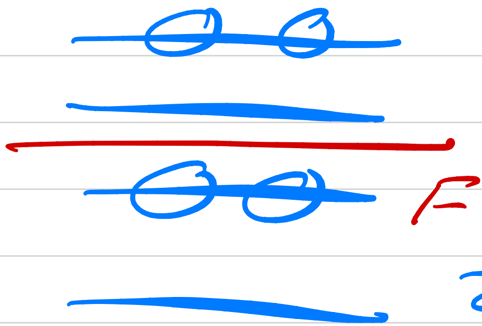
$|\phi_1\rangle$ 2p2h , no 1p1h



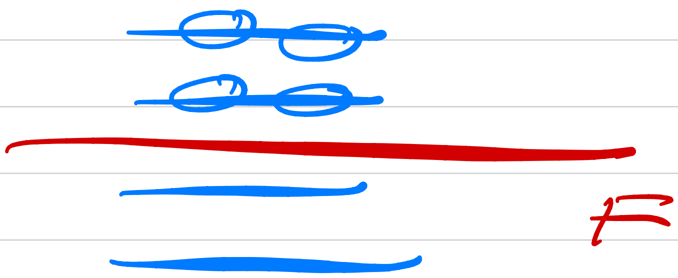
$|\phi_2\rangle$ 2p2h



$|\Phi_3\rangle$ 2p2h



$|\phi_4\rangle$ 2p2h



4p4h $|\Phi_5\rangle$

$$|\Psi_0\rangle = c_0|\Phi_0\rangle + c_1|\Phi_1\rangle + \dots$$
$$c_5|\Phi_5\rangle$$

$$|\Psi_0\rangle = |\Phi_0\rangle + \sum_{\substack{ab\\ij}} c_{ij}^{ab}|\Phi_{ij}^{ab}\rangle$$

$c_0 = 1$

$$+ \sum_{\substack{abcd\\ijkl}} c_{ijkl}^{abcd} \underbrace{|\Phi_{ijkl}^{abcd}\rangle}_{|\Phi_5\rangle}$$

$$H|\Psi_i\rangle = E_i|\Psi_i\rangle \qquad \langle \Phi_i|\Phi_j\rangle = \delta_{ij}$$

$$|\Psi_i\rangle \to |\Psi_0\rangle \qquad E_i \to E_0$$

$$\sum_{\substack{pH\\ p'H'}} (C_H^p)^* (C_{H'}^{p'}) \langle \Phi_H^p | H - E_0 | \Phi_{H'}^{p'} \rangle = 0$$

$$\left\{ \langle \Psi_0 | H | \Psi_0 \rangle = \sum_{\substack{pH\\ p'H'}} (C_H^p)^* (C_{H'}^{p'}) \langle \Phi_H^p | H | \Phi_{H'}^{p'} \rangle \right\}$$

$$\mathcal{L} = \langle \Psi_0 | H - E_0 | \Psi_0 \rangle$$

constraint $\langle \Psi_0 | \Psi_0 \rangle = 1$

$$\frac{\partial \mathcal{L}}{\partial (C_H^P)^*} = 0$$

$$\sum_{P'H'} \Big[\langle \Phi_H^P | H | \Phi_{H'}^{P'} \rangle C_{H'}^{P'} - E_0 C_{H'}^{P'} \langle \Phi_H^P | \Phi_{H'}^{P'} \rangle \Big]$$

$P'H' \to j \qquad PH \to i$

$$\sum_j \Big[\underbrace{\langle \Phi_i | H | \Phi_j \rangle}_{H_{ij}} - E c_j \delta_{ij} \Big]$$

$$\sum_j H_{ij} c_j = E_0 c_i$$

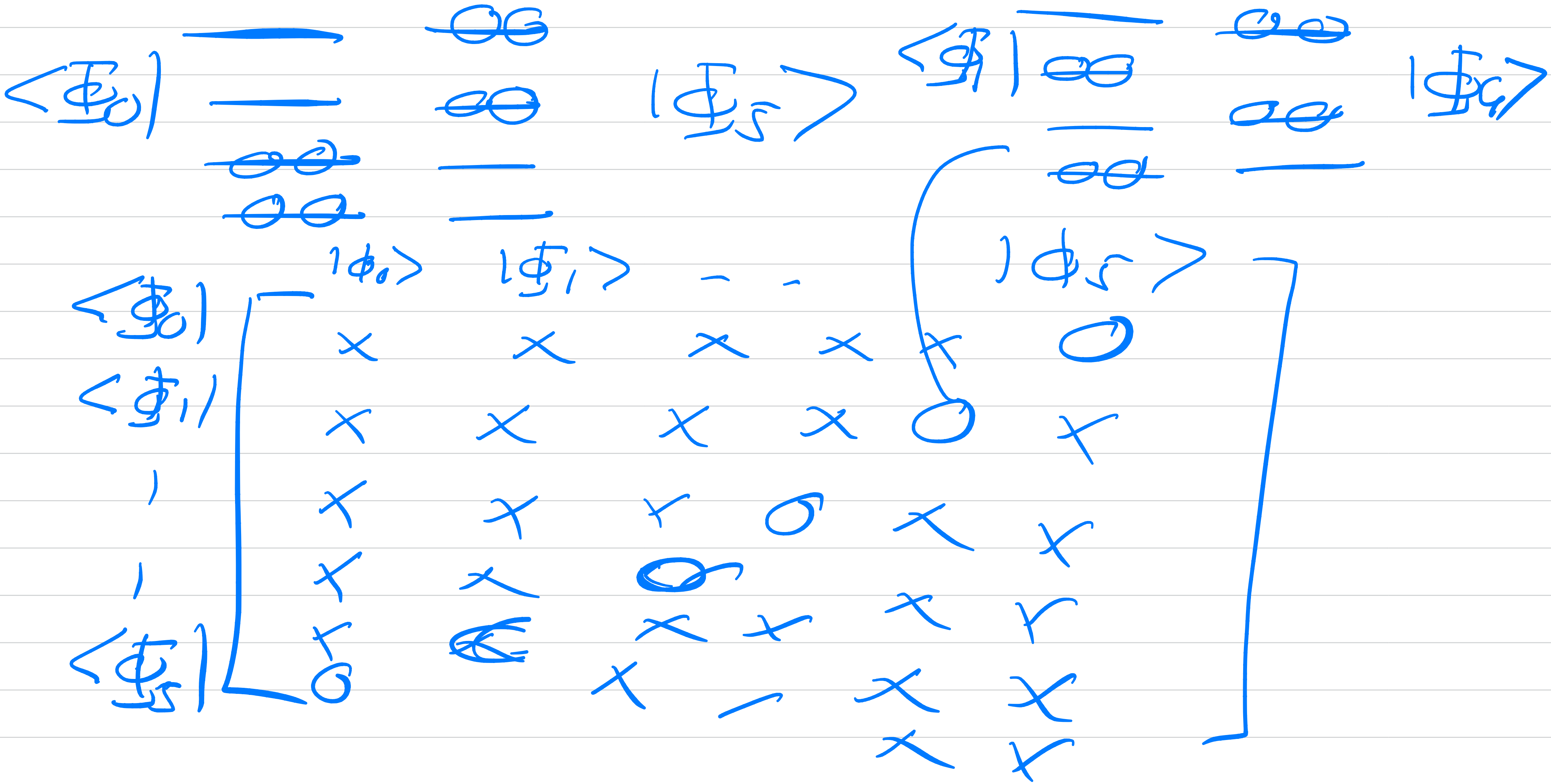
$$\Rightarrow \hat{H} \hat{C} = E \hat{C}$$

Pairing example

$$\hat{C} = \begin{bmatrix} c_0 \\ c_1 \\ c_2 \\ \vdots \\ c_5 \end{bmatrix}$$

$$\hat{H} = \begin{bmatrix} H_{00} & H_{01} & \cdots & H_{05} \\ H_{10} & & & \\ \vdots & & & \\ H_{50} & - & - & H_{55} \end{bmatrix}$$

$$H_{05} = \langle \underset{0p0h}{\Phi_0} | \hat{H} | \underset{4p4h}{\Phi_5} \rangle = 0$$



$\langle \Phi_0|$
$|\Phi_5\rangle$
$\langle \Phi|$
$|\Phi_6\rangle$
$|\phi_0\rangle$ $|\Phi_1\rangle$ - - $|\phi_5\rangle$
$\langle \Phi_0|$
$\langle \Phi_1|$
$\langle \Phi_5|$

E_0

$$\sum_j \langle \Phi_i | H | \Phi_j \rangle c_j - E_0 c_j \delta_{ij}$$

First row $\quad i = 0 \quad |\Phi_0\rangle$

$$\langle \Phi_0 | H | \Phi_0 \rangle c_0 - E_0 c_0 +$$

$$\langle \Phi_0 | H | \Phi_1 \rangle c_1 + \langle \Phi_0 | H | \Phi_2 \rangle c_2$$

$$+ \cdots + \langle \Phi_0 | H | \Phi_S \rangle c_S -$$

2nd row

$$\langle \Phi_1 | H - E_0 | \Phi_0 \rangle c_0 + \langle \Phi_1 | H - E_0 | \Phi_1 \rangle c_1$$

$$+ \langle \Phi_1 | H - E_0 | \Phi_2 \rangle c_2 + \cdots$$

$$+ \langle \Phi_1 | H - E_0 | \Phi_5 \rangle c_5$$

$$\hat{H} \cdot C = E_0 C$$

$$\sum_{(j=0)(j\neq 0)}^{5} \langle \Phi_0 | H | \Phi_j \rangle c_j = E_0 c_0$$

$$\sum_{j=0\,(j\neq 1)}^{5} \langle \Phi_1 | H | \Phi_j \rangle c_j = E_0 c_1$$

$$\vdots$$

$$\sum_{j=0}^{5} \langle \Phi_5 | H | \Phi_j \rangle = E_0 c_5$$

General case with ph excitations:

First row ($c_0 = 1$)

$$\langle \Phi_0 | H - E_0 | \Phi_0 \rangle +$$

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

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

$$+ + \cdots + \sum_{\substack{NP \\ NH}} \langle \Phi_0 | H - E_0 | \Phi_{NH}^{NP} \rangle c_{NH}^{NP}$$

with at most a two-body operator;

$$E_0^{Ref} = \sum_{j \le F} \langle j | \hat{h}_0 | j \rangle + \frac{1}{2} \sum_{ij} \langle ij | \hat{v} | ij \rangle_{AS}$$

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

$$+ \sum_{\substack{ab \\ ij}} c_{ij}^{ab} \langle \Phi_0 | H | \Phi_{ij}^{ab} \rangle = 0$$

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

$$= \langle i | \hat{h}_0 | a \rangle + \sum_{j \le F} \langle ij | \hat{v} | aj \rangle_{AS}$$

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

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

$$\underline{\Delta E} = E_0 - E_0^{Ref}$$

correlation energy

from diagonalization

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

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

and now, multiply with one possible 1p1h excitation $|\Phi_i^a\rangle$

$$\langle \Phi_i^a | H - E_0 | \Phi_0 \rangle$$

$$+ \sum_{bj} C_j^b \langle \Phi_i^a | H - E_0 | \Phi_j^b \rangle$$

$$+ \sum_{\substack{bc \\ jk}} C_{jk}^{bc} \langle \Phi_i^a | H - E_0 | \underset{2p2h}{\Phi_{jk}^{bc}} \rangle$$

$$+ \sum_{\substack{bcd \\ jkl}} C_{jkl}^{bcd} \langle \Phi_i^a | H - E_0 | \Phi_{jkl}^{bcd} \rangle$$

$$\langle \Phi_i^a | H | \Phi_0 \rangle - E_0 c_i^a + \sum_{\substack{b \\ j}} c_j^b \langle \Phi_i^a | H | \Phi_j^b \rangle + \sum_{\substack{bc \\ jk}} c_{jk}^{bc} \langle \Phi_i^a | H | \Phi_{jk}^{bc} \rangle + \sum_{\substack{bcd \\ jkl}} c_{jkl}^{bcd} \langle \Phi_i^a | H | \Phi_{jkl}^{bcd} \rangle$$

to solve non-linear eqs in the unknown coefficients C, we would solve the coupled equations iteratively;

$$(C_i^a)^{(0)}$$

$$\langle a|\hat{f}|i\rangle = E_0 \, (C_i^a)^{(0)}$$

$$E_0 = E_0^{Ref} + \cancel{\sum C_i^a \langle i|\hat{f}|a\rangle + \sum t_{ij}^{ab} \langle ij|v|ab\rangle}$$

$$E_0 \simeq E_0^{Ref} \simeq \sum_j \varepsilon_j$$

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

$$\hat{D} = U^T H U \qquad UU^T = U^T U = \mathbb{1}$$