FYS4480/9480
September 19

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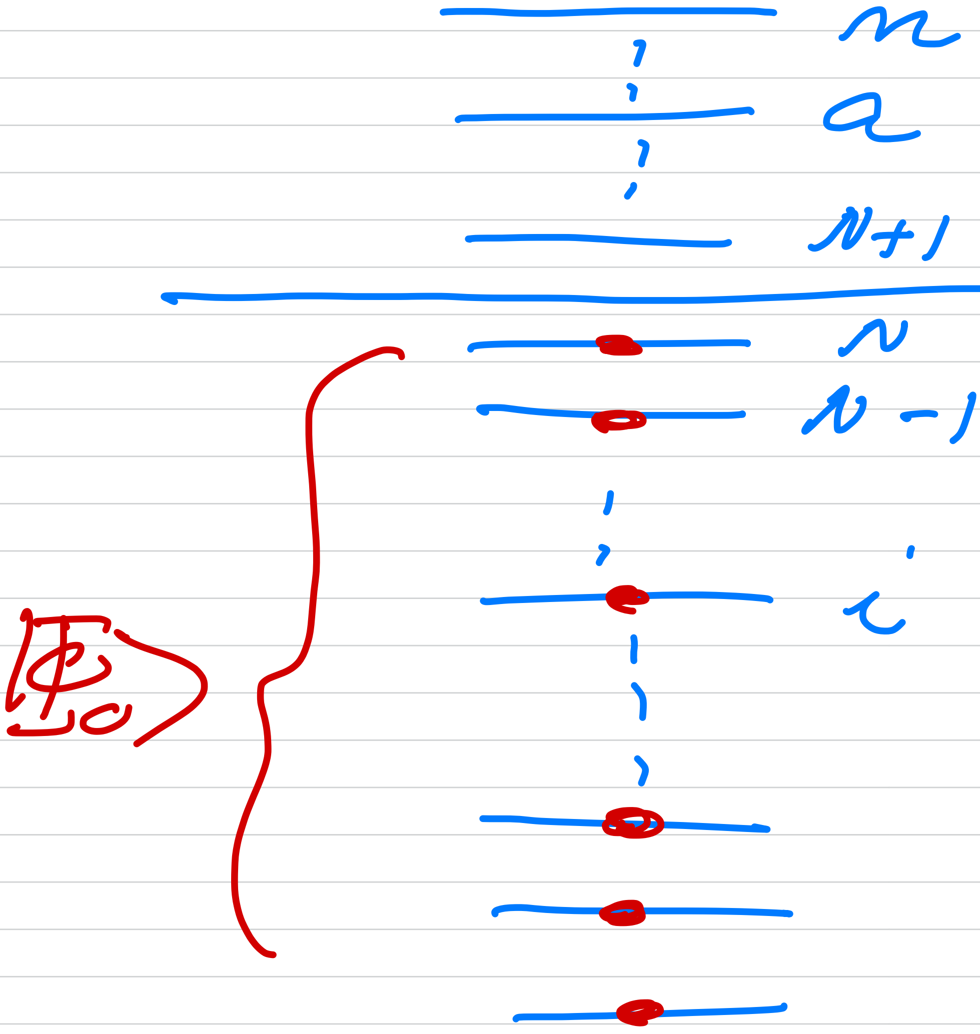


F

$\{abc\ldots\} > F$

$N \ll n$

$\{ijkl\ldots\} \leq F$

generic sp-state $\{pqrs\ldots\}$

total configurations

$$\binom{n}{N} = \frac{n!}{(n-N!)\,N!}$$

$$n \geq N$$

ONB

$$\hat{H}_c |\Phi_i\rangle = \varepsilon_i |\Phi_i\rangle$$

PH = 0p0h, 1p1h, 2p2h, ... NpNh

$|\Phi_0\rangle$

$$|\Phi_i^a\rangle = a_a^{+} a_i |\Phi_0\rangle$$

1p1h

$i \in |\Phi_0\rangle$

$a \notin$ — " —

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

$$= C_0|\Phi_0\rangle + \sum_{ai} C_i^a \underbrace{|\Phi_i^a\rangle}_{\underbrace{a_a^+ a_i}_{A_i^a} |\Phi_0\rangle}$$

$$+ \sum_{\substack{ab\\ij}} C_{ij}^{ab} \underbrace{|\Phi_{ij}^{ab}\rangle}_{a_a^+ a_b^+ a_j a_i |\Phi_0\rangle} + \cdots + NPNH$$

$$\overbrace{a_p a_q^{+}} = \delta_{pq} \quad \text{if} \quad p \wedge q > F$$

$$\overbrace{a_p^{+} a_q} = \delta_{pq} \quad \text{if} \quad p \wedge q \leq F$$

$$\langle \Phi_c | a_p^{+} a_q | \Phi_c \rangle = \delta_{pq}$$

$$q, p \in |\Phi_0\rangle$$

$$\overbrace{a_p a_q} = \overbrace{a_q^{+} a_p^{+}} = 0$$

$$\hat{H}_0 = \sum_{pq} \langle p | \hat{h}_0 | q \rangle \{ a_p^{+} a_q \} +$$

normal-ordered wrt $|\Phi_c\rangle$

$$+\underbrace{E_0^{\mathrm{Ref}}}_{\sum_{i\in F}\langle i|\hat{h}_0|i\rangle}$$

$$\langle pq|v|rs\rangle$$

$$\left(-\langle qp|v|rs\rangle\right.$$

$$\mathcal{H}_I=\frac{1}{4}\sum_{pqrs}\langle pq|v|rs\rangle_{AS}$$

$$\times\ \underbrace{a_p^{\dagger}a_q^{\dagger}a_s a_r}_{\text{normal-ordered wrt } |0\rangle}$$

$$a_p^\dagger a_q^\dagger a_s a_r = \{a_p^\dagger a_q^\dagger a_s a_r\}$$

normal-ordered wrt $|\Phi_C\rangle$

$$+ \{a_p^\dagger a_q^\dagger a_s a_r\}$$

$$\delta_{qs} \quad qs \le F$$

$$+ \{a_p^\dagger a_q^\dagger a_s a_r\}$$

$$-\delta_{qr} \quad qr \le F$$

$$+ \{a_p^\dagger a_q^\dagger a_s a_r\} + \{a_p^\dagger a_q^\dagger a_s a_r\}$$

$$-\delta_{qr} \qquad\qquad \delta_{pr}$$

$$+ \left\{ a_p^\dagger a_q^\dagger a_s a_r \right\} + \left\{ a_p^\dagger a_q^\dagger a_s a_r \right\}$$

$$\underbrace{\delta_{qs}}_{\leq F} \underbrace{\delta_{pr}}_{\leq F} \qquad - \delta_{qr} \delta_{ps} \leq F$$

$$\Longrightarrow$$

$$\mathcal{H}_I = \frac{1}{4} \sum_{pqrs} \langle pq | v | rs \rangle_{AS} \times \left\{ a_p^\dagger a_q^\dagger a_s a_r \right\}$$

$$+ \sum_{pqi} \langle pi | v | qi \rangle_{AS} \left\{ a_p^\dagger a_q \right\}$$

$$+ \frac{1}{2} \sum_{ij} \langle ij | v | ij \rangle$$

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

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

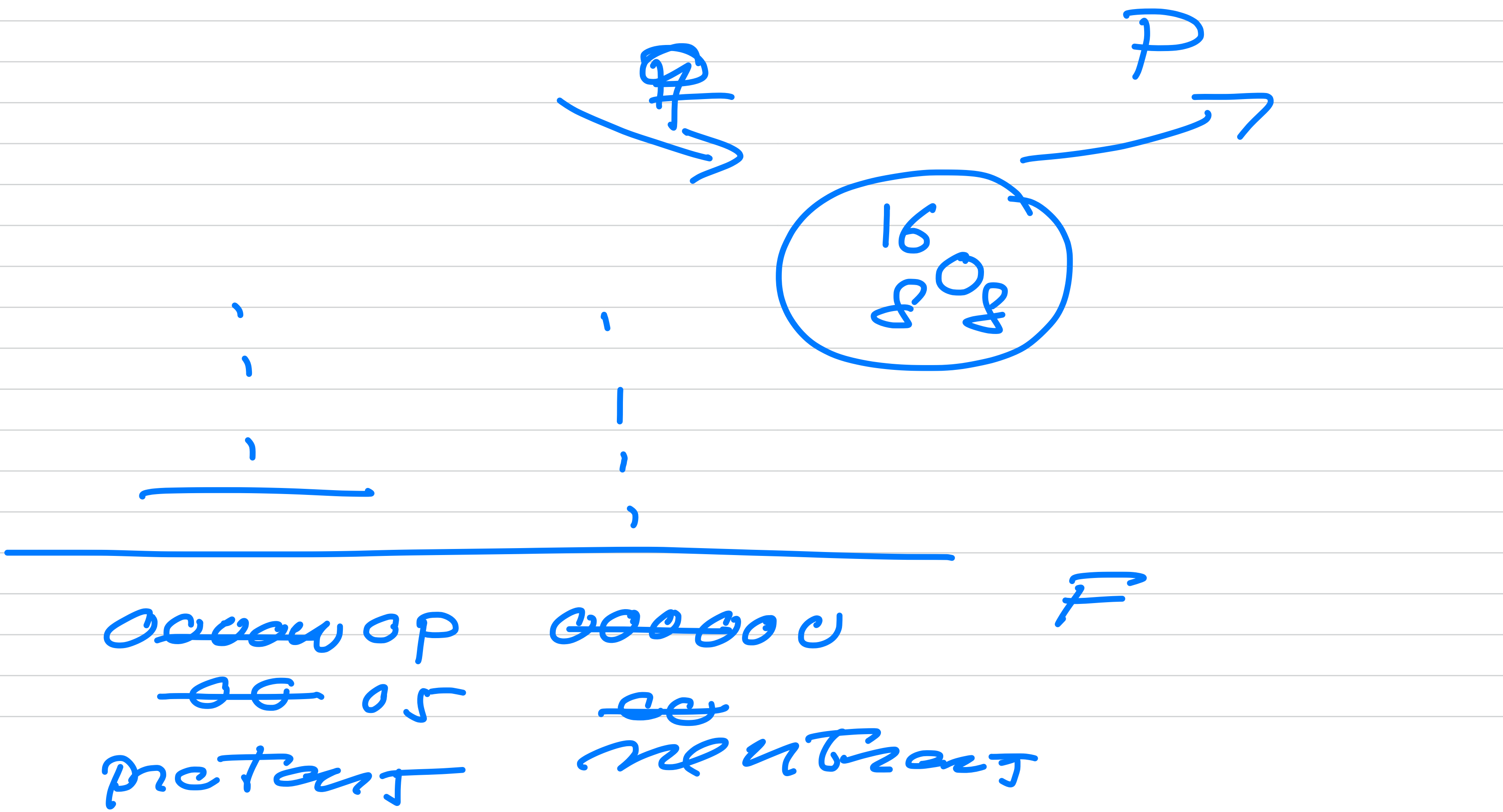
$$= \underbrace{E_0^{Ref}}_{\sum_{i \leq F} \langle i | h_0 | i \rangle + \frac{1}{2} \sum_{ij} \langle ij || ij \rangle_{AS}} +$$

$$\hat{V}_N = \frac{1}{4} \sum_{pqrs} \langle pq | v | rs \rangle_{AS} \{ a_p^\dagger a_q^\dagger a_s a_r \}$$

$$\hat{F}_N = \sum_{pq} \langle p | f | q \rangle \{ a_p^\dagger a_q \}$$

$$\langle p|\hat{f}|q\rangle = \langle p|\hat{h}_0|q\rangle + \sum_{i \leq F} \langle pi|v|qi\rangle_{AS}$$

Mean-Field



$$\langle \Phi_0 | \mathcal{H} | \underbrace{\Phi_i^a}_{1p1h} \rangle :$$

(i) $$\langle \Phi_0 | \underbrace{E_0^{Ref}}_{\text{constant}} | \Phi_i^a \rangle = 0$$

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

$$a_p^\dagger a_q \; a_a^\dagger a_i \implies$$

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

(iii) $$\langle \Phi_c | \hat{V}_N | \Phi_i^a \rangle = 0$$

$$\underbrace{\langle \Phi_c | a_p^\dagger a_q^\dagger a_s a_r}\, a_a^\dagger a_i | \Phi_0 \rangle$$

$$\hat{V}_N | \Phi_c \rangle = \begin{cases} \alpha | \Phi_0 \rangle \\ \alpha | \Phi_{ij}^{ab} \rangle \end{cases}$$

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

Example 2

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

(i) $\langle \Phi_0 | E_0^{Ref} | \Phi_{ij}^{ab} \rangle = 0$

$$= E_0^{Ref} \langle \Phi_0 | \Phi_{ij}^{ab} \rangle$$

$$= 0$$

(ii) $\langle \Phi_0 | \hat{F}_N | \Phi_{ij}^{ab} \rangle$

$$\underset{a_p^{\dagger} a_q}{F_N} | \Phi_0 \rangle = \text{const} \begin{cases} | \Phi_0 \rangle \\ | \Phi_i^a \rangle \end{cases}$$

$$\text{Const}\,\langle \Phi_h^{a} | \Phi_{kl}^{ca} \rangle = 0$$

1p1h 2p2h

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

$$= 0$$

(iii)

$$\frac{1}{4}\sum_{pqrs} \langle pq|v|rs\rangle_{AS}$$

$$\times \langle \Phi_0 | a_p^\dagger a_q^\dagger a_s a_r a_a^\dagger a_b^\dagger a_j a_i | \Phi_0\rangle$$

$$a_c^\dagger \quad a_k$$

$$a_p^\dagger a_q^\dagger a_s a_r \; a_a^\dagger a_b^\dagger a_j a_i \quad a$$

(i)

$$\delta_{sb}\,\delta_{ra}$$

$$\delta_{ip}\,\delta_{qj}$$

$$\langle ij|v|ab\rangle_{AS}$$

(ii)

$$-\langle ij|v|ba\rangle_{AS}$$

$$= \langle ij|v|ab\rangle_{AS}$$

(iii) $\quad \langle ji \| v \| ba \rangle_{AS} = \langle ij \| v \| ab \rangle_{AS}$

(iv) $\quad -\langle ji \| v \| ab \rangle_{AS} = \langle ij \| v \| ab \rangle_{AS}$

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

Example 3

$$\langle \Phi_0 | \mathcal{H} | \Phi_{ijk}^{abc} \rangle = 0$$

at most a two-body operator

Intermediate step before FCI

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

$$\mathcal{H}|\Psi_0\rangle = E_0|\Psi_0\rangle$$

$$= \sum_{PH} \mathcal{H}\, C_H^P |\Phi_H^P\rangle$$

$$= E_0 \sum_{PH} C_H^P |\Phi_H^P\rangle$$

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

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

$\langle \Phi_0 | \mathcal{H} | \Psi_0 \rangle$ in terms of Blocks

	$\langle \Phi_c \vert \mathcal{H} \vert \Phi_c \rangle$	1p1h $\langle \Phi_c \vert \mathcal{H} \vert \Phi_i^a \rangle$	2p2h $\langle \Phi_0 \vert \mathcal{H} \vert \Phi_{ij}^{ab} \rangle$
$\langle \Phi_c \vert$	E_0^{Ref}	$\langle i \vert f \vert a \rangle$	$\langle ij \vert\vert ab \rangle_{AS}$
$\langle \Phi_i^a \vert$	$\langle a \vert f \vert i \rangle$	$\langle \Phi_j^b \vert \mathcal{H} \vert \Phi_i^a \rangle$	×
2p2h	×	× ×	×
3p3h			
⋮			
NpNh			

$\langle\Phi_0\lvert \hat{H} \rvert\Phi_{ijk}^{abc}\rangle$	3p3h	— — —	4p4h		NpNh
1p1h	O		O	O	O
2p2h	X		X	O	O
3p3h	X		X	X	O
4p4h	X		X	X	X - -

	0p0h	1p1h	2p2h	3p3h	4p4h	- - .	NpNh
0p0h	X	X	X	0	0		0
1p1h	X	X	X	X	0	- -	0
2p2h	X	X	X	X	X	0 —	0
3p3h	0	X	X	X	X	X - -	0
4p4h	0	0	X				
⋮	0	0	0				
NpNh	0	0					

Sparse matrix

$$\langle \Phi_\lambda | \mathcal{H} | \Phi_\delta \rangle$$

eigenvalue problem

$$A\vec{x} = \lambda \vec{x}$$

$$U^T A U = D \qquad\qquad U U^T = U^T U$$

$$= U A U^T \qquad\qquad = \mathbb{1}$$

$$U A \vec{x} = \lambda U \vec{x} \qquad\qquad U^{-1} = U^T$$

$$\uparrow$$

$$\mathbb{1} = U^T U$$

$$(U A U^T) \underbrace{U \vec{x}}_{\vec{y}} = \lambda \underbrace{U \vec{x}}_{\vec{y}}$$

$$D \vec{y} = \lambda \vec{y}$$

$$u_M u_{M-1} \cdots u_1 A u_1^T u_2 \cdots u_{M-1} u_M$$

HF theory is equv. to setting $\langle i | f | a \rangle$

$$= \langle \Phi_0 | H | \Phi_i^a \rangle = 0$$

which means that there is a U which does this.