Lecture FYS4480, September 22, 2023

Definitions

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

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

$$|\Phi_i\rangle = a_i |\Phi_c\rangle \quad i \in \{|\Phi_0\rangle\}$$

N-1 state

$$|\Phi^a\rangle = a_a^\dagger |\Phi_c\rangle \quad a \notin \{|\Phi_0\rangle\}$$

N+1 state

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

1p1h

$$a \notin \{|\Phi_c\rangle\} \quad i \in \{|\Phi_c\rangle\}$$

$$|\Phi_{ij}^{ab}\rangle_{2p2h} = a_a^\dagger a_b^\dagger a_j a_i |\Phi_c\rangle$$

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

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

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

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

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

$$= \sum_{i \leq F} \langle i | \hat{h}_0 | i \rangle + \frac{1}{2} \sum_{ij} \langle ij | | ij \rangle_{AS}$$

Examples

$$\langle \Phi_0 | \hat{H} | \Phi_i^a \rangle :$$

$$\langle \Phi_0 | \hat{V}_N | \Phi_i^a \rangle + \langle \Phi_0 | \hat{F}_N | \Phi_i^a \rangle$$

$$+ \underbrace{\langle \Phi_0 | \Phi_i^a \rangle}_{=0} E_0^{Ref}$$

$\hat{V}_N$

$$\langle \Phi_c | \{a_p^\dagger a_q^\dagger a_s a_r\} \underbrace{\{a_a^\dagger a_i\}}_{1p1h} | \Phi_c \rangle$$

$\hat{F}_N$

$$\langle \Phi_c | \hat{F}_N | \Phi_i^a \rangle$$

$$\langle \Phi_c | a_p^\dagger a_q a_a^\dagger a_i | \Phi_c \rangle \rightarrow$$

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

Relevant for HF theory

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

$$\langle \Phi_0 | \hat{F}_N | \Phi_{ij}^{ab} \rangle =$$

$$\sum_{pq} \langle p | \hat{f} | q \rangle \langle \Phi_0 | \underset{\substack{\diagup \\ 0p0h \\ 1p1h}}{a_p^\dagger a_q} \; \underbrace{a_a^\dagger a_i a_b^\dagger a_j | \Phi_0 \rangle}_{2p2h}$$

$$\langle \Phi_0 | \hat{V}_N | \Phi_{ij}^{ab} \rangle \propto$$

$$a_p^+ a_q^+ a_s a_r \; a_a^+ a_b^+ a_j a_i$$

(i)

$$\frac{1}{4}\langle ij|v|ab\rangle_{AS}$$

(ii)

$$-\frac{1}{4}\langle ij|v|ba\rangle_{AS} = \frac{1}{4}\langle ij|v|ab\rangle$$

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

$a \leftrightarrow b$

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

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

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

$$-\frac{1}{4}\langle ji|v|ab\rangle_{AS}$$

$$= \frac{1}{4}\langle ij|v|ab\rangle_{AS}$$

$$+\frac{1}{4}\langle ji|v|ba\rangle_{AS}$$

$$= \frac{1}{4}\langle ij|v|ab\rangle_{AS}$$

$\Rightarrow$

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

(Condon-Slater rule)

$$\langle \Phi_i^a | H | \Phi_j^b \rangle \qquad j \neq i$$

$$a \neq b$$

$$\langle \Phi_i^a | \Phi_j^b \rangle = \delta_{ij} \delta_{ab}$$

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

$$\langle \Phi_0 | a_i^\dagger a_a a_b^\dagger a_j | \Phi_0 \rangle$$

$= \delta_{ij} \delta_{ab}$

$$= \langle aj | v | ib \rangle_{AS}$$

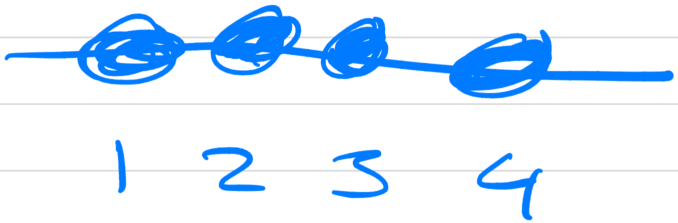
$$+ \delta_{ij} \langle a | f | b \rangle - \delta_{ab} \langle j | f | i \rangle$$

Lipkin model

$n = 8$ sp states

$N = 4$

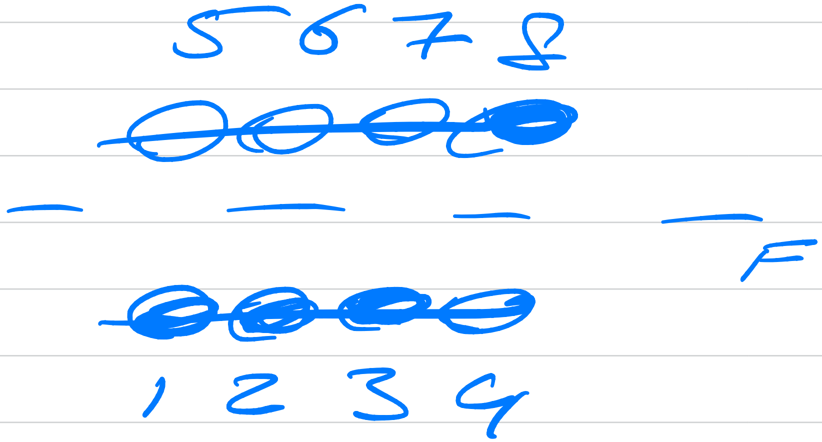
$$\left.\right\} \#SD = \binom{8}{4} = 70$$



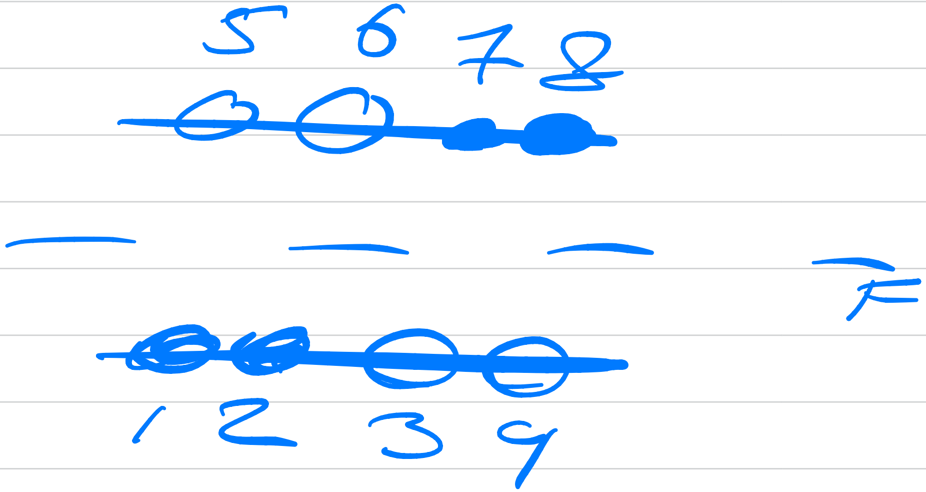
$|\Phi_0\rangle$

opok

4p4h



1p1h



2p2h

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

$$\langle \Phi_0 | H | \Phi_{ijkl}^{abcd} \rangle = 0$$

	0p0h	1p1h	2p2h	3p3h	4p4h
0p0h	X	X	X	0	0
1p1h	X	X	X	X	0
2p2h	X	X	X	X	X
3p3h	0	X	X	X	X
4p4h	0	0	X	X	X

FCI (Full configuration interaction) theory

Basis of SDs $|\Phi_\lambda\rangle$,

$$\langle \Phi_\lambda | \Phi_\delta \rangle = \delta_{\lambda\delta}$$

Expand a state

$$|\Psi_i\rangle = \sum_{\lambda=0}^{\infty} c_{i\lambda} |\Phi_\lambda\rangle$$

$$= \sum_{\lambda} c_{i\lambda} |\Phi_\lambda\rangle$$

$$= c_{i0} |\Phi_0\rangle + \sum_{\lambda=1}^{\infty} c_{i\lambda} |\Phi_\lambda\rangle$$

we will reorganize the sum

$\sum_\lambda c_{i\lambda} |\Phi_\lambda\rangle$ in terms of

PH excitations. $|\Psi_0\rangle =$

$$C_0 |\Phi_0\rangle + \sum_{ai} C_i^a \underbrace{|\Phi_i^a\rangle}_{1p1h}$$

$$+ \sum_{\substack{ab\\ij}} C_{ij}^{ab} \underbrace{|\Phi_{ij}^{ab}\rangle}_{2p2h} + \ldots + NPNH$$

$$= C_0 |\Phi_0\rangle + \sum_{ai} C_i^a a_a^\dagger a_i |\Phi_0\rangle$$

$$+ \sum_{\substack{ab\\ij}} C_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i |\Phi_0\rangle + \ldots$$

$$+ NPNH$$

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

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

$$+ \ldots + NPNH$$

$$\Rightarrow \quad |\Psi_c\rangle = \sum_{PH} c_H^P | \Phi_H^P \rangle$$

$$= \sum_{PH} \left(c_H^P \hat{A}_H^P \right) | \Phi_0 \rangle$$

$\hat{A}_H^P$ is 1p1h $A_H^D = a_a^\dagger a_i$

$$\sum_{PH} |C_H^P|^2 = 1$$

$$\langle \Psi_0 | \Psi_0 \rangle = \sum_{\substack{PH \\ P'H'}} (C_H^P)^* C_{H'}^{P'} \langle \Phi_H^P | \Phi_{H'}^{P'} \rangle$$

$$= \sum_{PH} |C_H^P|^2 = 1$$

intermediate normalization

$$\langle \Phi_0 | \Psi_0 \rangle = C_0 = 1$$

$$|\Psi_0\rangle = (1 + \hat{C}) |\Phi_0\rangle$$

$\hat{C}$ = correlation operator

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

$$\mathcal{L}(C_H^P) = \langle \Psi_0 | H | \Psi_0 \rangle - E_0 \langle \Psi_0 | \Psi_0 \rangle$$

$$= \sum_{PH} \sum_{P'H'} (C_H^P)^* C_{H'}^{P'} \langle \Phi_H^P | H | \Phi_{H'}^{P'} \rangle$$

$$- \sum_{PH} \sum_{P'H'} (C_H^P)^* C_{H'}^{P'} E_0 \langle \Phi_H^P | \Phi_{H'}^{P'} \rangle$$

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

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

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

$$= 0$$

$$\sum_{P'H'} \rightarrow \sum_j$$

$$\langle \Phi_H^P | \Phi_{H'}^{P'} \rangle = \langle \Phi_i | \Phi_j \rangle$$

$$= S_{ij} \ (\delta_{ij})$$

$$\langle \Phi_H^P | H | \Phi_{H'}^{P'} \rangle = H_{ij}$$

$C_H^{p} = C_i'$ $\quad C_H^{p'} = C_j'$

we can rewrite the previous eq. 95

$$\sum_j C_j' (H_{ij} - E_0 S_{ij}) = 0$$

Solution if $\det(H - E_0 S) = 0$

we will have $S_{ij} = \delta_{ij}$

$$\boxed{\sum_j C_j H_{ij} = E_0 C_i'}$$

FCI eq 5

$$\Rightarrow \quad HC = \lambda C$$

$$
\begin{array}{c|cccccc}
 & |\Phi_0\rangle & |\Phi_i^a\rangle & |\Phi_{ij}^{ab}\rangle & \cdots & NPNH \\
 & 0p0h & 1p1h & 2p2h & & \\
\hline
\langle\Phi_0| & \times & \times & \times & 0 & \cdots \\
\langle\Phi_i^a| & \times & \times & \times & 0 & \cdots\ 0 \\
\langle\Phi_{ij}^{ab}| & \times & \times & & \vdots & \\
\vdots & 0 & \times & & \vdots & \\
\vdots & \vdots & 0 & & \vdots & \\
NPNH & 0 & \vdots & & &
\end{array}
\quad
\begin{bmatrix} c_0 \\ c_i^a \\ c_{ij}^{ab} \\ \vdots \\ c_{NH}^{NP} \end{bmatrix}
$$

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

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

$$+ \sum_{\substack{ab \\ ij}} c_{ij}^{ab} |\Phi_{ij}^{ab}\rangle + \ldots \text{NPNH} \Big\}$$

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

$$+ \sum_{ai} \langle \Phi_0 | H | \Phi_i^a \rangle c_i^a = 0$$

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