FYS4480/9480 lecture, November 21, 2024

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			F	16O
$0p_{1/2}$	$\cancel{\circ\circ}$	$\cancel{\circ\circ}$	$0p$	$\|\Phi_0\rangle$
$0p_{3/2}$	$\cancel{\circ\circ\circ\circ}$	$\cancel{\circ\circ\circ\circ}$		
	$\cancel{\uparrow\downarrow}$	$\cancel{\uparrow\downarrow}$	$0s$	
	protons	neutrons		

$$M_S = 0 = \sum_{sp} m_{sp} + \sum_{sn} m_{sn}$$

^{18}O

$d_{3/2}$

$s_{1/2}$

$d_{5/2}$

j

$d = 2j + 1$
$= 6$

protons neutrons

$$\binom{6}{2} = \frac{6!}{2!\,4!} = \frac{5 \cdot 6}{2} = 15$$

FCI Reminder, step 1

$$\begin{bmatrix} \varepsilon_1 & g \\ g & \varepsilon_2 \end{bmatrix}$$

$$\langle \phi_1 | H | \phi_1 \rangle = \varepsilon_1$$

$$\langle \phi_1 | H | \phi_2 \rangle = g$$

$$\langle \phi_2 | H | \phi_2 \rangle = \varepsilon_2$$

$$H = H_0 + H_1$$

$$H_0 = \sum_{i=1}^{2} \varepsilon_i \, a_i^\dagger a_i \qquad H_1 = g \sum_{ij} a_i^\dagger a_j$$

$$H_0 | \phi_1 \rangle = \varepsilon_1 | \phi_1 \rangle$$

$$H_0 | \phi_2 \rangle = \varepsilon_2 | \phi_2 \rangle$$

$$E_1 = \frac{1}{2}\left(\varepsilon_1 + \varepsilon_2 - \sqrt{(\varepsilon_1 - \varepsilon_2)^2 + 4g^2}\right)$$

$$|\psi_1\rangle = \alpha|\phi_1\rangle + \beta|\phi_2\rangle$$

intermediate normalization

$$\langle \psi_1 | \phi_1 \rangle = 1 = \alpha$$

$$|\psi_1\rangle = (1 + \hat{C})|\phi_1\rangle$$

$$\begin{bmatrix} \varepsilon_1 & g \\ g & \varepsilon_2 \end{bmatrix} \begin{bmatrix} 1 \\ \beta \end{bmatrix} = E_1 \begin{bmatrix} 1 \\ \beta \end{bmatrix}$$

$$\varepsilon_1 + g\beta = E_1$$

$$g + \varepsilon_2 \beta = E_1 \beta$$

$$E_1 - \varepsilon_1 = \Delta E \Rightarrow \beta = \Delta E / g$$

$$g + \varepsilon_2 \Delta E / g = E_1 \Delta E / g \Rightarrow$$

$$\frac{g^2}{E_1 - \varepsilon_1} = E_1 - \varepsilon_2 \Rightarrow$$

$$g^2 = (E_1 - \varepsilon_2)(E_1 - \varepsilon_1)$$

$$\det \begin{bmatrix} \varepsilon_1 - E_1 & g \\ g & \varepsilon_2 - E_1 \end{bmatrix} = 0$$

Taylor-expand E_1

$$E_1 = \varepsilon_1 - \frac{g^2}{\varepsilon_2-\varepsilon_1} + \frac{g^4}{(\varepsilon_2-\varepsilon_1)^3} - + \dots$$

at second order

$$\beta = \frac{g}{\varepsilon_1-\varepsilon_2} \qquad \frac{g}{\varepsilon_1-\varepsilon_2} - \frac{g^3}{(\varepsilon_1-\varepsilon_2)^3}$$

$$v_1 \simeq N \begin{bmatrix} 1 \\ \frac{g}{\varepsilon_1-\varepsilon_2} \end{bmatrix} \Rightarrow$$

$$N = 1 \Big/ \sqrt{1+\beta^2}$$

$$v_1^T v_1 = \frac{1+\beta^2}{1+\beta^2} = \underline{1}$$

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

(FCI)

$$(1+\hat{C})|\Phi_0\rangle = \sum_{PH} C_H^P |\Phi_H^P\rangle$$

$$= \Big(|\Phi_0\rangle + \sum_{ai} C_i^a \underbrace{|\Phi_i^a\rangle}_{a_a^\dagger a_i|\Phi_0\rangle} + \sum_{\substack{ab\\ij}} C_{ij}^{ab} |\Phi_{ij}^{ab}\rangle + \ldots NPNH\Big)$$

$$\langle \Phi_0 | H | \Psi_0 \rangle = E_0 \underbrace{\langle \Phi_0 | \Psi_0 \rangle}_{=1}$$

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

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

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

$$= E_0^{Ref} + \sum_{ai} c_i^a \langle i | f | a \rangle$$

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

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

$$\sum_{ai} c_i^a \cancel{\langle i|f|a\rangle} + \sum_{\substack{ab\\ ij}} c_{ij}^{ab} \langle ab||ij\rangle$$

$$\langle \Phi_i^a | H | \Psi_0 \rangle = 0$$

$$c_i^a = 0 = c_{ijk}^{abc} = c_{ijkl}^{abcd} \cdots$$

$$c_{NH}^{NP} = 0$$

$$\langle \Phi_{ij}^{ab} | H | \Psi_0 \rangle = \langle \Phi_{ij}^{ab} | H | \Phi_0 \rangle$$

$$+$$

$$+ \sum_{\substack{cd \\ ke}} C_{ke}^{cd} \langle \Phi_{ij}^{ab} | H | \Phi_{ke}^{cd} \rangle$$

$$= E_0 \, C_{ij}^{ab}$$

$$\Rightarrow$$

$$\langle ab | v | ij \rangle + \sum_{\substack{cd \\ ke}} C_{ke}^{cd} \langle \Phi_{ij}^{ab} | \left(E_0^{Ref} + \hat{F}_N + \hat{V}_N \right) | \Phi_{ke}^{cd} \rangle$$

$$= E_0 \, C_{ij}^{ab}$$

$$\langle ab|v|ij\rangle + \sum_{\substack{cd\\ke}} C_{ke}^{cd} \langle \Phi_{ij}^{ab} | F_N + V_N | \times | \Phi_{ke}^{cd} \rangle = \Delta E \, C_{ij}^{ab}$$

$$\langle \Phi_{ij}^{ab} | F_N | \Phi_{ke}^{cd} \rangle =$$

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

$$\langle p|f|q\rangle = \underbrace{\langle p|h_0|q\rangle}_{h_0} + \underbrace{\sum_j \langle pj|v|qj\rangle}_{u^{HF}}$$

$$h_0|q\rangle = \varepsilon_q|q\rangle$$

only h_0

$$\varepsilon_p \left(a_j^\dagger a_i^\dagger a_b a_a a_p^\dagger a_p a_c^\dagger a_d^\dagger a_e a_k \right)$$

δ_{ap} δ_{pc} ε_a

ε_b

$$(\varepsilon_a + \varepsilon_b - \varepsilon_i - \varepsilon_j)\, C_{ij}^{ab}$$

$$\langle ab|v|ij\rangle + (\varepsilon_a+\varepsilon_b-\varepsilon_j-\varepsilon_i)\,C_{ij}^{ab}$$

$$+ \sum_{\substack{cd\\ke}} C_{ke}^{cd} \langle \Phi_{ij}^{ab} | u^{HF} + V_N | \Phi_{ke}^{cd} \rangle$$

$$= \Delta E \; C_{ij}^{ab}$$

$$\Delta E = \sum_{\substack{ab\\ij}} C_{ij}^{ab} \langle ab|v|ij\rangle$$

set of coupled non-linear eqs in C_{ij}^{ab}

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

(wave operator to first order in RSPT)

$$\Delta E(0) = \sum_{\substack{ab \\ ij}} C_{ij}^{ab}(0) \langle ab \| ij \rangle$$

$$\langle \Phi_{ij}^{ab} | H - E_0 | \Psi_0 \rangle = 0$$

$$\langle \Phi_{ij}^{ab} | H | \Psi_0 \rangle = E_0 C_{ij}^{ab}$$

$$
\begin{array}{c|cccccc}
 & 0p0h & 1p1h & 2p2h & 3p3h & \cdots & NpNh \\
\hline
0p0h & \langle \Phi_0 | H | \Phi_0 \rangle & \langle \Phi_0 | H | \Phi_i^a \rangle & \langle \Phi_0 | H | \Phi_{ij}^{ab} \rangle & & & \\
1p1h & \langle \Phi_i^a | H | \Phi_0 \rangle & \times & \times & \times & 0 - & \\
2p2h & \langle \Phi_{ij}^{ab} | H | \Phi_0 \rangle & \times & - & - & & \\
3p3h & & & & & & \\
\vdots & & & & & & \\
NpNh & & & & & &
\end{array}
$$

$\Rightarrow 0$

when we diagonalize

$$|\Psi_0\rangle = U|\Phi_0\rangle$$

$$U^\dagger U = UU^\dagger = \mathbb{1}$$

$$|\Phi_0\rangle = U^\dagger|\Psi_0\rangle$$

$$U^\dagger H|\Psi_0\rangle = U^\dagger E_0|\Psi_0\rangle$$

$$UU^\dagger = \mathbb{1}$$

$$\underbrace{U^\dagger H U}_{D}|\Phi_0\rangle = E_0|\Phi_0\rangle$$

in FCI

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

in MBPT (RS)

$$\hat{C}|\Phi_0\rangle = \sum_{k=1}^{\infty} \left[(R H_1)^k |\Phi_0\rangle \right]_L$$

$$R = \sum_{M>1} \frac{|\Phi_M\rangle\langle\Phi_M|}{E_0 - E_M}$$

wave operator to 1st-order

$$\sum_{ai} \frac{|\Phi_i^a\rangle\langle\Phi_i^a|H_1|\Phi_0\rangle}{\varepsilon_i - \varepsilon_a}$$

$$+ \sum_{\substack{ab\\ij}} \frac{|\Phi_{ij}^{ab}\rangle\langle\Phi_{ij}^{ab}|H_1|\Phi_0\rangle}{\varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_b}$$

$$\sum t_i^a \; a_a^\dagger a_i \, |\Phi_0\rangle$$

$$t_i^a = \langle\Phi_i^a|H_1|\Phi_0\rangle / \varepsilon_i - \varepsilon_a$$

1p1h excitations

$$\sum_{ai} t_i^a a_a^\dagger a_i |\Phi_0\rangle \Big/ \sum_{ai} C_i^a a_a^\dagger a_i |\Phi_0\rangle$$

FCI

Thouless theorem

$$|\Phi_0'\rangle = \exp\left\{\sum_{ai} C_i^a a_a^\dagger a_i\right\} |\Phi_0\rangle$$

$$|\Psi_0\rangle = \exp(T_1) |\Phi_0\rangle$$

$$= \left(1 + T_1 + \frac{1}{2!} T_1^2 + \frac{1}{3!} T_1^3 + \cdots\right) |\Phi_0\rangle$$

$$|\Psi_0\rangle = e^{T_1}|\Phi_0\rangle$$

$$\boxed{T_1 = \sum_{ai} t_i^a a_a^\dagger a_i}$$

1p1h excitation (singles)

General $T = T_1 + T_2 + T_3 + \cdots + T_{NPNH}$

$$|\Psi_0\rangle = e^{T}|\Phi_0\rangle = e^{T_1 + T_2 + \cdots T_{NPNH}} \times |\Phi_0\rangle$$

exponential ansatz

$$|\Psi_0\rangle = \Big(1 + T_1 + T_2 + T_3 + \cdots$$

$$+ \frac{1}{2} T_1^2 + T_1 T_2 + \frac{1}{2} T_2^2 \cdots$$

$$+ \frac{1}{3!} T_1^3 + \frac{1}{2} T_1^2 T_2 + \frac{1}{2} T_1 T_2^2 +$$

$$\frac{1}{3!} T_2^3 + \cdots$$

$$\cdots \Big) |\Phi_0\rangle$$

$$[T_i, T_j] = 0$$

approximations

(i) $T = T_1$ singles (CCS)

(ii) $T = T_2$ doubles (CCD)

(iii) $T = T_1 + T_2$ singles + doubles (CCSD)

(iv) $T = T_1 + T_2 + T_3$ (singles + doubles + triples) CCSDT