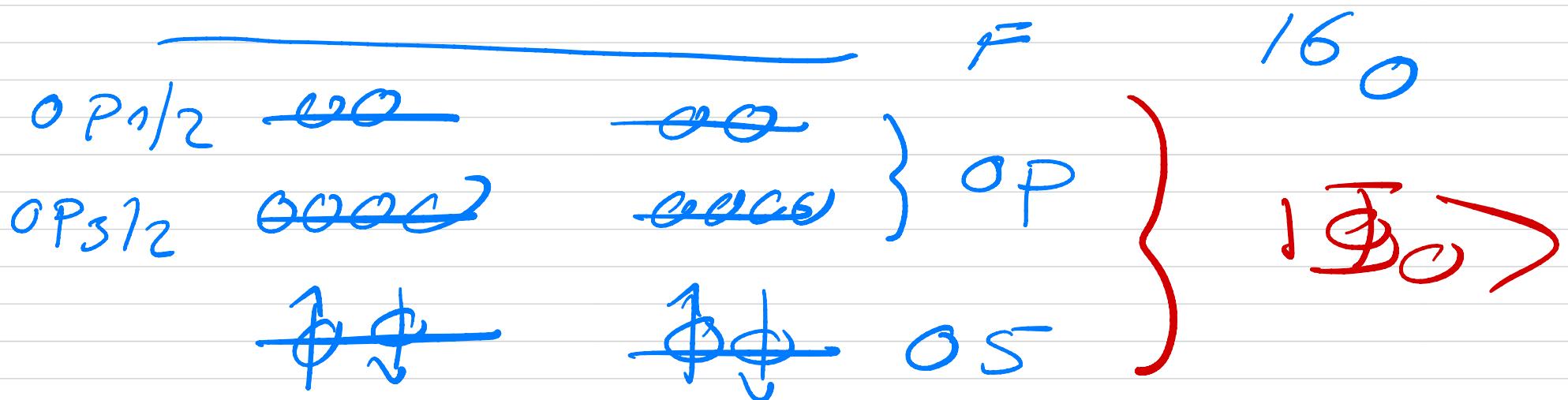


FYS4480/9480
lecture, November
21, 2024

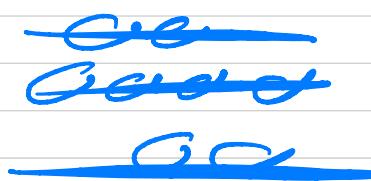
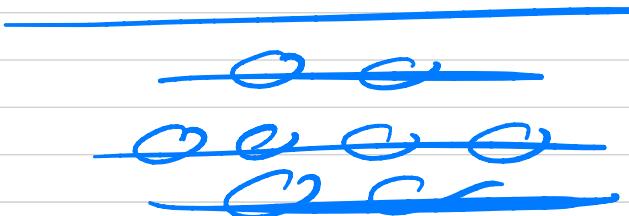
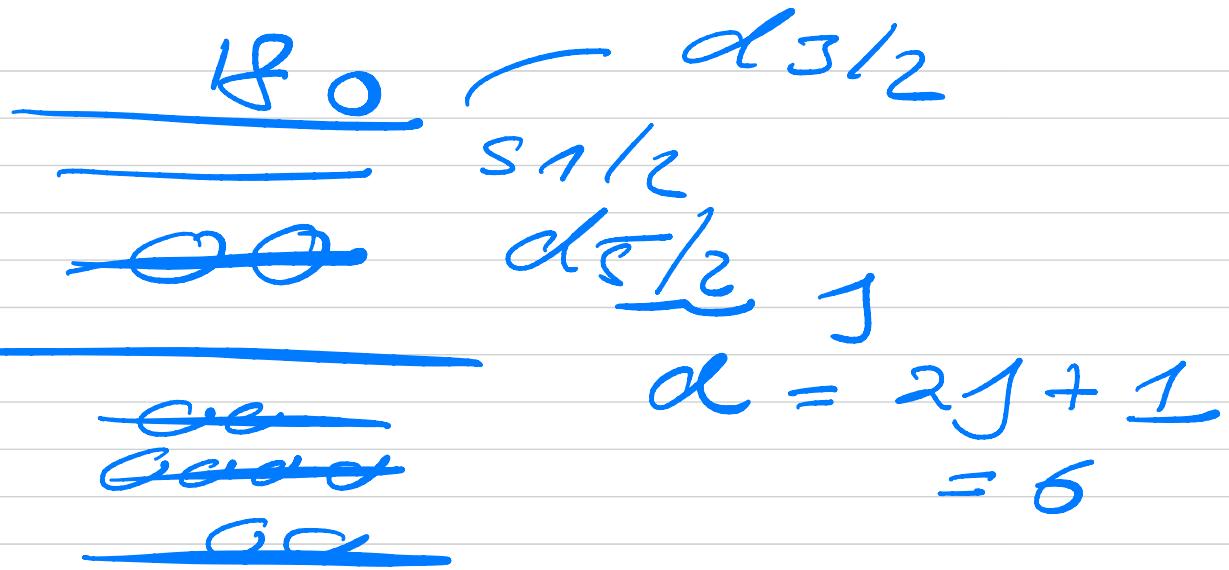
FYS 4480/9480, NOV 21



moons

neutrinos

$$M_S = 0 = \sum_{SP} m_{SP} + \sum_{SA} m_{SA}$$



protons

neutrons

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

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FC i Reminder, step 1

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

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

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

$$H = H_0 + H_1$$

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

$$\sum_{i=1}^n \varepsilon_i \cdot a_i^\dagger a_i$$

$$g \sum_{ij} a_i^\dagger a_j$$

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

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

$$\bar{E}_1 = \frac{1}{2}(\varepsilon_1 + \varepsilon_2 - \sqrt{(\varepsilon_1 - \varepsilon_2)^2 + 4g^2})$$

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

intermediate normalized states

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

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

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

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

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

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

$$g + \varepsilon_{1/2} \Delta E/g = \bar{E}_1 \Delta E/g \Rightarrow$$

$$\frac{g^2}{\bar{E}_1 - \varepsilon_1} = \bar{E}_1 - \varepsilon_2 \Rightarrow$$

$$g^2 = (\bar{E}_1 - \varepsilon_2)(\bar{E}_1 - \varepsilon_1)$$

$$\det \begin{bmatrix} \varepsilon_1 - \bar{E}_1 & g \\ s & \varepsilon_2 - \bar{E}_1 \end{bmatrix} = 0$$

Taylor-expand \bar{E}_1

$$\tilde{\varepsilon}_1 = \varepsilon_1 - \frac{g^2}{\varepsilon_2 - \varepsilon_1} + \frac{g^4}{(\varepsilon_2 - \varepsilon_1)^3} - \dots$$

at second order

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

$$w_1 \approx N \left[\frac{1}{\frac{g}{\varepsilon_1 - \varepsilon_2}} \right] \Rightarrow$$

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

$$w_1^T w_1 = \frac{(1 + \beta)^2}{1 + \beta^2} = 1$$

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

(FCI)

$$(1 + \hat{c})|\Psi_0\rangle = \sum_{PH} C_H^P |\Psi_H^P\rangle$$

$$= (|0\rangle + \underbrace{\sum_{ai} c_i^a |\Psi_i^a\rangle}_{q_a + q_i} + |0\rangle)$$

$$\sum_{ab} \sum_{ij} c_{ij}^{ab} |\Psi_{ij}^{ab}\rangle + \dots NPNH$$

$$\langle \underline{\Phi}_0 | H | \Psi_0 \rangle = E_0 \underbrace{\langle \underline{\Phi}_0 | \Psi_0 \rangle}_{=1}$$

$$\langle \underline{\Phi}_0 | H | \underline{\Phi}_0 \rangle +$$

$$\sum_{ai} c_i^a \langle \underline{\Phi}_0 | H | \underline{\Phi}_i^a \rangle +$$

$$\sum_{\substack{ab \\ ij}} c_{ij}^{ab} \langle \underline{\Phi}_0 | H | \underline{\Phi}_{ij}^{ab} \rangle$$

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

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

$$\Delta E = E_0 - \bar{E}_0^{\text{Ref}} =$$

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

$$\left\langle \sum_n c_n^a | H | \psi_0 \right\rangle = 0$$

$$c_i^a = 0 = c_{ijk}^{abc} = c_{ijke}^{abcd} \dots$$

$$c_{N+}^{NP} = 0$$

$$\left\langle \sum_{ij} c_{ij}^{ab} | H | \psi_0 \right\rangle = \left\langle \sum_{ij} c_{ij}^{ab} | H | \psi_0 \right\rangle +$$

$$+ \sum_{\substack{cd \\ ke}} C_{ke}^{ca} \langle \hat{\Phi}_{ij}^{ab} | H | \hat{\Phi}_{ke}^{cd} \rangle$$

$$= \bar{E}_0 C_{ij}^{ab}$$

\Rightarrow

$$\langle ab/v/v_j \rangle + \sum_{\substack{cd \\ ke}} C_{ke}^{cd} \langle \hat{\Phi}_{ij}^{ab} |$$

$$(E_0^{\text{ref}} + \hat{F}_N + \hat{V}_N) | \hat{\Phi}_{ke}^{ca} \rangle$$

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

$$\langle ab|v|ij\rangle + \sum_{\substack{ca \\ ke}} C_{ke}^{ca} \langle \Phi_{ij}^{ab} | F_N | v_N |$$

$$x | \Phi_{ke}^{cd} \rangle$$

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

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

$$\langle \Phi_0 | a_i^+ q_j^+ a_k q_a \sum_{pq} \langle p | g | q \rangle a_p^+ q_q$$

$$x a_c^+ q_d^+ a_e q_k | \Phi_0 \rangle$$

$$\langle p | f | q \rangle = \langle p | h_0 | q \rangle + \sum_j \underbrace{\langle p j | h_0 | q j \rangle}_{\mathcal{H}^{HF}}$$

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

only h_0

$$\varepsilon_p (a_i^+ a_i^- a_b a_a a_p^+ a_p^- a_c^+ a_c^- a_e a_k)$$

δ_{ap} δ_{pc} ε_a
 δ_{ec} ε_e

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

$$\langle ab|v|i\rangle + (\epsilon_a + \epsilon_b - \epsilon_j - \epsilon_i) C_{ij}^{ab}$$

$$+ \sum_{cd} C_{ke}^{cd} \langle \hat{\psi}_i^a | u^{HF} + v_N | \hat{\psi}_{ke}^{cq} \rangle$$

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

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

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

$$c_{ij}^{ab}(\omega) = \frac{\langle ab|v|ij\rangle}{\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b}$$

(wave operator to first order
in RSPT)

$$\Delta E(\omega) = \sum_{\substack{ab \\ ij}} c_{ij}^{ab}(\omega) \langle ab|v|ij\rangle$$

$$\langle \hat{\epsilon}_{ij}^{ab} | H - E_0 | \psi_0 \rangle = 0$$

$$\langle \hat{\epsilon}_{ij}^{ab} | H | \psi_0 \rangle = E_0 c_{ij}^{ab}$$

	opoh	1p1h	2p2L	3p5L	-	NpNL
opoh	$\langle \Phi_0 H \Phi_0 \rangle$	$\langle \Phi_0 H \Phi_n^a \rangle$	$\langle \Phi_0 H \Phi_{ij}^{ab} \rangle$			
1p1h	$\langle \Phi_n^a H \Phi_0 \rangle$			X	X	X C.
2p2L		$\langle \Phi_{ij}^{ab} H \Phi_0 \rangle$	X		—	—
3p5L			\approx_0			
/						
)						
)						
NpNL						

when we diagonalize

$$|N_0\rangle = u|\Phi_0\rangle$$

$$u^+ u = uu^+ = \underline{1}$$

$$|\Phi_0\rangle =$$

$$u^+ |N_0\rangle$$

$$u^+ H |N_0\rangle = u^+ E_0 |N_0\rangle$$

$$\overset{\uparrow}{uu^+} = \underline{1}$$

$$\underline{u^+ H u} |\Phi_0\rangle = E_0 |\Phi_0\rangle$$

D

in F_C

$$\hat{w} = (1 + \hat{c}) | \Phi_0 \rangle$$

in MBPT (2s)

$$\hat{c} |\Phi_0 \rangle = \sum_{k=1}^{\infty} \left[\underbrace{(R + H_1)^k}_{\uparrow} | \Phi_0 \rangle \right]_L$$

$$\sum_{M>1} \frac{|\phi_M\rangle \langle \phi_M|}{E_0 - E_M}$$

wave operator to 1st order

$$\frac{\sum_{a,i} \langle \psi_a^a | \hat{E}_i^a \rangle \langle \hat{E}_i^a | H_1 | \psi_0 \rangle}{\epsilon_i - \epsilon_a}$$
$$+ \frac{\sum_{a,b,i,j} \langle \psi_{ij}^{ab} | \hat{E}_{ij}^{ab} \rangle \langle \hat{E}_{ij}^{ab} | H_1 | \psi_0 \rangle}{\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b}$$

$$\sum_i t_i^a \langle a_a^+ q_i | \hat{E}_0 \rangle$$

$$t_i^a = \frac{\langle \hat{E}_i^a | H_1 | \psi_0 \rangle}{\epsilon_i - \epsilon_a}$$

1p1h excitations

$$\sum_{ai} t_a^a a_a^+ q_i | \Phi_0 \rangle / \sum_{ai} C_a^a q_a^+ q_i | \Phi_0 \rangle$$

Thouless theorem

$$| \Phi_0' \rangle = \exp \left\{ \sum_{ai} c_i^a a_a^+ q_i \right\} | \Phi_0 \rangle$$

$$| \Psi_0 \rangle = \exp(\bar{\tau}_1) | \Phi_0 \rangle$$

$$= (1 + \bar{\tau}_1 + \frac{1}{2!} \bar{\tau}_1^2 + \frac{1}{3!} \bar{\tau}_1^3 + \dots) | \Phi_0 \rangle$$

$$|\Psi_C\rangle = e^{\frac{T_1}{k}} |\Phi_C\rangle$$

$$\boxed{\overline{T}_1 = \sum_{a_i} t_i^a a_i a_i^\dagger}$$

1PI h excitation (singular)

General $\overline{T} = \overline{T}_1 + \overline{T}_2 + \overline{T}_3 + \dots + \overline{T}_{NPNT}$

$$|\Psi_0\rangle = e^{\frac{\overline{T}}{k}} |\Phi_0\rangle = e^{\overline{T}_1 + \overline{T}_2 + \dots + \overline{T}_{NPNT}} \times |\Phi_0\rangle$$

exponential ansatz

$$\begin{aligned}
 |\psi_0\rangle &= (1 + \bar{\tau}_1 + \bar{\tau}_2 + \bar{\tau}_3 + \dots \\
 &\quad + \frac{1}{2} \bar{\tau}_1^2 + \bar{\tau}_1 \bar{\tau}_2 + \frac{1}{2} \bar{\tau}_2^2 \\
 &\quad + \frac{1}{3!} \bar{\tau}_1^3 + \frac{1}{2} \frac{\bar{\tau}_1^2}{\bar{\tau}_2} + \frac{1}{2} \frac{\bar{\tau}_1}{\bar{\tau}_2} + \\
 &\quad \frac{1}{3!} \frac{\bar{\tau}_1^3}{\bar{\tau}_2} + \dots \\
 &\quad \dots) |E_0\rangle
 \end{aligned}$$

$$[\bar{\tau}_1, \bar{\tau}_2] = 0$$

approximations

(i) $T = \bar{T}_1$ singlet (CCS)

(ii) $T = \bar{T}_2$ doublet (CCD)

(iii) $T = \bar{T}_1 + \bar{T}_2$ singlet
+ doublet (CCSD)

(IV) $T = \bar{T}_1 + \bar{T}_2 + \bar{T}_3$
(singlet + doublet
+ triplet)
CCSDT