FYS4480/9480, Lecture October 25, 2024

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Reminder from our FCI discussions.

$$|\Psi_0\rangle = \sum_i C_i |\Phi_i\rangle$$

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

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

$$= |\Phi_0\rangle + \sum_{ai} C_i^a |\Phi_i^a\rangle +$$

$$\sum_{\substack{ab\\ij}} c_{ij}^{ab} |\Phi_{ij}^{ab}\rangle + \ldots \; O(N \phi N H)$$

$$|\Phi_i^a\rangle = a_a^\dagger a_i |\Phi_0\rangle \quad 1p1h$$

$$|\Phi_{ij}^{ab}\rangle = a_a^\dagger a_b^\dagger a_j a_i |\Phi_0\rangle \; 2p2h$$

$$\langle \Phi_0 | H | \Psi_0\rangle =$$

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

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

$$E_0 - \underbrace{\langle \Phi_0 | H | \Phi_0 \rangle}_{E_0^{Ref}} = \underbrace{\Delta E}_{\text{correlation energy}}$$

$$= \sum_{ai} c_i^a \underbrace{\langle a | f | i \rangle}_{\left(\langle a | h_0 | i \rangle + \sum_{j \leq F} \langle aj | v | ij \rangle_{AS} \right)}$$

$$c_i^a = \frac{\langle i | f | a \rangle}{\varepsilon_i - \varepsilon_a}$$

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

$$c_{ij}^{ab} = \frac{\langle ij | v | ab \rangle_{AS}}{\varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_b}$$

PT to 2nd order

Simple problem

$$H_0 = \sum_p \varepsilon_p a_p^+ a_p$$

$$H_1 = g \sum_{pq} a_p^+ a_q$$

$$\langle p | H_0 | q \rangle = \delta_{pq} \varepsilon_p$$

Two states $\varepsilon_1 < \varepsilon_2$

$p = 1$ Model space $p = 2$

$$\hat{P} = |1\rangle\langle 1| \qquad \hat{Q} = |2\rangle\langle 2|$$

$$\mathbb{1} = \sum_{i=1}^{2} |i\rangle\langle i|$$

$$|\Phi_0\rangle = a_1^\dagger |0\rangle$$

$$|\Phi_1\rangle = a_2^\dagger |0\rangle$$

$$\langle p | H_1 | q \rangle \rightarrow$$

$$\langle \Phi_0 | H_1 | \Phi_0 \rangle$$

$$\langle \Phi_0 | H_1 | \Phi_1 \rangle$$

$$\langle \Phi_1 | H_1 | \Phi_1 \rangle$$

$$\langle \Phi_0 | H_0 | \Phi_0 \rangle = \langle 0 | \overbrace{a_1 \sum_p \varepsilon_p a_p^\dagger}^{\delta_{p1}} \overbrace{a_p a_1^\dagger}^{\delta_{p1}} |0\rangle$$

$= \quad \varepsilon_1$

$$\langle \Phi_0 | H_1 | \Phi_1 \rangle =$$

$$\langle 0 | a_1 \, g \sum_{pq} a_p^\dagger a_q \, a_2^\dagger | 0 \rangle = g$$

$$\langle \Phi_0 | H_1 | \Phi_0 \rangle =$$

$$\langle 0 | a_1 \, g \sum_{pq} a_p^\dagger a_q \, a_1^\dagger | 0 \rangle$$

$$= g$$

$$\langle \Phi_1 | H_1 | \Phi_1 \rangle = g \qquad \Rightarrow$$

$$\begin{bmatrix} \varepsilon_1 + g & g \\ g & \varepsilon_2 + g \end{bmatrix} = \hat{H}$$

eigenvalue

$$\det(\hat{H} - \lambda) = 0$$

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

$$= \frac{\varepsilon_1 + \varepsilon_2}{2} + g \pm \sqrt{\frac{(\varepsilon_1+\varepsilon_2)^2}{4} + g^2}$$

$$\Rightarrow \frac{\varepsilon_1 + \varepsilon_2}{2}\left[1 + \frac{2g}{\varepsilon_1+\varepsilon_2} - \sqrt{1 + \left(\frac{2g}{\varepsilon_1+\varepsilon_2}\right)^2}\,\right]$$

$$x = \left(\frac{2g}{\varepsilon_1 + \varepsilon_2}\right)^2$$

$$\sqrt{1+x} = 1 + \frac{x}{2} - \frac{x^2}{8} + \frac{x^3}{16} + \cdots$$

$$= 1 + 2\frac{g^2}{(\varepsilon_1+\varepsilon_2)^2} - 2\frac{g^4}{(\varepsilon_1+\varepsilon_2)^4} + \cdots$$

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

1st-order

2nd-order

Fourth-order

Rayleigh-schrödinger theory

Many-body PT (MBPT)

$$|\Psi_0\rangle = |\Phi_0\rangle + \sum_{m=1}^{D} a_m |\Phi_m\rangle$$

$$H_0 |\Phi_0\rangle = \varepsilon_0 |\Phi_0\rangle$$

$$H |\Psi_0\rangle = E_0 |\Psi_0\rangle$$

$$H_0 |\Phi_0\rangle = \varepsilon_0 |\Phi_0\rangle$$

$$H = H_0 + \underline{H_1}$$

$$\langle \Phi_0 | \Psi_0 \rangle = \underline{1}$$

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

$$\langle \Psi_0 | H_0 | \Phi_0 \rangle = \varepsilon_0$$

$$\langle \Phi_0 | H_0 | \Psi_0 \rangle^* = \varepsilon_0 \underbrace{\langle \Phi_0 | \Psi_0 \rangle^*}_{=1}$$

$$\langle \Phi_0 | H_0 | \Psi_0 \rangle = \varepsilon_0 \langle \Phi_0 | \Psi_0 \rangle$$

$$\langle \Phi_0 | H | \Psi_0 \rangle - \langle \Phi_0 | H_0 | \Psi_0 \rangle =$$

$$(E_0 - \varepsilon_0) \langle \Phi_0 | \Psi_0 \rangle$$

$$= \langle \Phi_0 | H_1 | \Psi_0 \rangle$$

$$E_0 - \varepsilon_0 = \frac{\langle \Phi_0 | H_1 | \Psi_0 \rangle}{\langle \Phi_0 | \Psi_0 \rangle}$$

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

$$\Delta E_0 = E_0 - \varepsilon_0 = \langle \Phi_0 | H_1 | \Psi_0 \rangle$$

$$\hat{P} | \Psi_0 \rangle = | \Phi_0 \rangle \qquad \hat{P} = | \Phi_0 \rangle \langle \Phi_0 |$$

$$\hat{G} = \underbrace{\sum_{m=1}^{D} | \Phi_m \rangle \langle \Phi_m |}_{\text{excluded space}} \qquad \hat{P}^2 = P$$

model space

$$[\hat{P}, \hat{Q}] = 0 \qquad \hat{P}^2 = \hat{P}$$

$$\hat{Q}^2 = \hat{Q}$$

$$\hat{P} + \hat{Q} = \mathbb{1}$$

$$|\Psi_0\rangle = (\hat{P} + \hat{Q})|\Psi_0\rangle =$$

$$|\Phi_0\rangle + Q|\Psi_0\rangle$$

$$(H_0 + H_1)|\Psi_0\rangle = E_0|\Psi_0\rangle$$

$$(\omega - H_0)|\Psi_0\rangle = (\omega - E_0 + H_1)|\Psi_0\rangle$$

$$(\omega - \hat{H}_0)^{-1} = \frac{1}{\omega - \hat{H}_0}$$

$$\hat{Q}\,|\Psi_i\rangle = \frac{1}{\omega - \hat{H}_0}(\omega - E_0 + \hat{H}_1)|\Psi_i\rangle$$

$$\hat{Q}\hat{H}_0 - \hat{H}_0\hat{Q} = [H_0, \hat{Q}] \qquad H_0|\Phi_i\rangle$$

$$= 0 \qquad\qquad = E_i|\Phi_i\rangle$$

$$[\hat{P}, \hat{H}_0] = 0$$

$$\hat{Q}\frac{1}{\omega - \hat{H}_0} = \hat{Q}\frac{1}{\omega - H_0}\hat{Q}$$

$$= \frac{\hat{Q}}{\omega - H_0}$$

$$|\Psi_0\rangle = |\Phi_0\rangle + \frac{\hat{G}}{\omega - \hat{H}_0}(\omega - E_0 + \hat{H}_1)|\Psi_0\rangle$$

$$|\Psi_0\rangle = \sum_{n=0}^{\infty} \left\{ \frac{\hat{G}}{\omega - \hat{H}_0}(\omega - E_0 + H_1) \right\}^n |\Phi_0\rangle$$

$$\langle \Phi_0 | H_1 | \Psi_0 \rangle = \Delta E_0 =$$

$$\sum_{n=0}^{\infty} \langle \Phi_0 | H_1 \left\{ \frac{\hat{G}}{\omega - \hat{H}_0} (\omega - E_0 + \hat{H}_1) \right\}^n$$

$$\times |\Phi_0\rangle$$