FYS4480 OCT 27, 2022

Thouless' theorem

$$|\Phi_0\rangle = \prod_{i=1}^{n} a_i^{\dagger}|0\rangle = |c\rangle$$

$$|c'\rangle = \exp\left\{\sum_{ai} c_{ai}\, a_a^{\dagger} a_i\right\}|c\rangle$$

assumption $\langle c'|c\rangle \neq 0$

$$\exp(ny) = \exp\left(\sum_{k=1}^{n} y\right)$$

$$= \prod_{k=1}^{n} \exp(y)$$

$$|c'\rangle = \prod_{i\leq F}\Big[1 + \sum_{a>F} c_{ai}\, a_a^{\dagger} a_i + \frac{1}{2!}\Big(\sum_{a>F} c_{ai}\, a_a^{\dagger} a_i\Big)^2 + \cdots\Big]|c\rangle$$

$$[a_a^{\dagger} a_i, a_b^{\dagger} a_j] = 0$$

$$e^A e^B = e^{A+B} \text{ if } [A,B]=0$$

$$\sum_{a>F} c_{ai}\, a_a^{\dagger} a_i \sum_{b>F} c_{bi}\, a_b^{\dagger} a_i\, |c\rangle$$

$$\propto (a_i)^2 |c\rangle = 0$$

$$(a_i)^n |c\rangle = 0$$

when $n > 1$

$$|c'\rangle = \prod_i \left(1 + \sum_a c_{ai}\, a_a^\dagger a_i\right)|c\rangle$$

$$= \prod_i \left(1 + \sum_a c_{ai}\, a_a^\dagger a_i\right) a_{i_1}^\dagger a_{i_2}^\dagger \cdots a_{i_n}^\dagger |0\rangle$$

$$= \left[\left(1 + \sum_a c_{ai_1}\, a_a^\dagger a_{i_1}\right) a_{i_1}^\dagger\right]$$

$$\times \left[\left(1 + \sum_a c_{ai_2}\, a_a^\dagger a_{i_2}\right) a_{i_2}^\dagger\right]$$

$$\vdots$$

$$\left[\left(1 + \sum_a c_{ai_n}\, a_a^\dagger a_{i_n}\right) a_{i_n}^\dagger\right]$$

$$\times |0\rangle$$

$$= \prod_i \left(\underbrace{a_i^\dagger + \sum_a c_{ai}\, a_a^\dagger}_{b_i^\dagger}\right)|0\rangle$$

$$= \prod_i b_i^{+} |0\rangle$$

1p1h

$$|\Psi_0\rangle = c_0 |\Phi_0\rangle + \sum_{ai} c_i^a |\Phi_i^a\rangle$$

$$+ \sum_{\substack{ab \\ ij}} c_{ij}^{ab} |\Phi_{ij}^{ab}\rangle + \cdots$$

2p2h

$$|c'\rangle = \exp\left\{ \sum_{ai} c_{ai}\, a_a^{+} a_i \right\} |c\rangle$$

$$\langle c' | c \rangle$$

$$\hat{T}_1 = \sum_{ai} c_{ai}\, a_a^{+} a_i = \sum_{ai} t_i^a a_a^{+} a_i$$

$$|c'\rangle = e^{\hat{T}_1} |c\rangle$$

$$\hat{T} = \underset{\text{1p1h}}{\hat{T}_1} + \underset{\text{2p2h}}{\hat{T}_2} + \underset{\text{3p3h}}{\hat{T}_3} + \cdots + \underset{\text{NpNh}}{\hat{T}_N}$$

$$|\Psi_0\rangle = e^{\hat{T}} |\Phi_0\rangle$$

$$|\Psi_0\rangle \simeq |c'\rangle = e^{\hat{T}_1} |\Phi_0\rangle$$

$$|\Psi_0\rangle \simeq e^{\hat{T}_1+\hat{T}_2}|\Phi_0\rangle$$

1p1h = single
2p2h = double

MBPT

Many-body perturbation theory.

$$|\Psi_0\rangle = C_0|\Phi_0\rangle + \sum_m C_{0m}|\Phi_m\rangle$$

correlation energy

FCI

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

$$\hat{H}|\Psi_0\rangle = E|\Psi_0\rangle$$

$$E_0^{Ref} = \sum_i \langle i|\hat{h}_0|i\rangle + \frac{1}{2}\sum_{ij}\langle ij|\hat{v}|ij\rangle_{AS}$$

$$\Delta E = \sum_{ai} C_i^a \langle\Phi_0|\hat{H}|\Phi_i^a\rangle + \sum_{\substack{ab\\ ij}} C_{ij}^{ab}\langle\Phi_0|\hat{H}|\Phi_{ij}^{ab}\rangle$$

$$= \sum_{ai} c_i^a \underbrace{\langle i|\hat{f}|a\rangle}_{\text{with HF } = 0}$$

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

Define ;

$$\hat{H}_0 |\Phi_0\rangle = W_0 |\Phi_0\rangle$$

intermediate normalization

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

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

$$H|\Psi_0\rangle = E|\Psi_0\rangle$$

multiply from the left with $\langle \Phi_0 \rangle$

$$\langle \Phi_0 | \hat{H} | \Psi_0 \rangle = E \qquad \hat{H} = \hat{H}_0 + \hat{H}_I$$

$$\langle \Psi_0 | \hat{H}_0 | \Phi_0 \rangle = W_0 = \sum_i \varepsilon_i$$

$$\Delta E(\text{MBPT}) = E - W_0$$

$$= \langle \Phi_0 | \hat{H}_I | \Psi_0 \rangle$$

$$\hat{P} = |\Phi_0\rangle\langle\Phi_0| \qquad \hat{P}^2 = \hat{P}$$

$$\hat{Q} = \sum_{m=1}^{\infty} |\Phi_m\rangle\langle\Phi_m|$$

$$\hat{Q}^2 = \hat{Q} \qquad \hat{P} + \hat{Q} = \mathbb{1}$$

$$\hat{P}\hat{Q} = \hat{Q}\hat{P} = 0$$

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

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

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

introduce a constant ω add and subtract

$$\omega|\Psi_0\rangle$$

$$(\omega - \hat{H}_0)|\Psi_0\rangle = (\omega - E + H_I)|\Psi_0\rangle$$

assume that

$$\frac{1}{\omega - \hat{H}_0} \quad \text{exists (Resolvent)}$$

$$\left(\frac{1}{E - \hat{H}}\right)$$

$(\omega - H_0)^{-1}$ exists

$$|\Psi_0\rangle = \frac{1}{\omega - \hat{H}_0}\left(\omega - E + \hat{H}_1\right)|\Psi_0\rangle$$

$$Q|\Psi_0\rangle = \hat{Q}\frac{1}{\omega - \hat{H}_0}(\hat{P} + \hat{Q})(\omega - E + \hat{H}_1)$$

$$\times |\Psi_0\rangle$$

$$Q\frac{1}{\omega - \hat{H}_0}(\hat{P} + \hat{Q}) = \hat{Q}\frac{1}{\omega - \hat{H}_0}\hat{Q}$$

$$Q\hat{H}_0 P = \underbrace{\hat{Q}\hat{P}}_{=0}\hat{H}_0 \quad = \hat{Q}^2\frac{1}{\omega - \hat{H}_0}$$

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

$$= \sum_{m=1}^{\infty} \frac{|\Phi_m\rangle\langle\Phi_m|}{\omega - \hat{H}_0}$$

$$Q|\Psi_0\rangle = \frac{Q}{\omega - \hat{H}_0}(\omega - E + \hat{H}_1)|\Psi_0\rangle$$

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

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

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

$$|\Psi_0^{(0)}\rangle = |\Phi_0\rangle$$

$$|\Psi_0^{(1)}\rangle = |\Phi_0\rangle + \frac{Q}{\omega - \hat{H}_0}(\omega - E + H_1)|\Phi_0\rangle$$

$$|\Psi_0^{(2)}\rangle = |\Phi_0\rangle + \frac{\hat{Q}}{\omega - \hat{H}_0}(\omega - E + H_I) \times |\Phi_0\rangle$$

$$+ \left(\frac{\hat{Q}}{\omega - \hat{H}_0}(\omega - E + \hat{H}_I)\right)^2 |\Phi_0\rangle$$

$$\vdots$$

$$|\Psi_0\rangle = \sum_{i=1}^{\infty} \left\{\frac{\hat{Q}}{\omega - \hat{H}_0}(\omega - E + \hat{H}_I)\right\}^i |\Phi_0\rangle$$

$$\Delta E = \sum_{n=1}^{\infty} \langle \Phi_0 | \hat{H}_1 \left\{ \frac{\hat{Q}}{\omega - \hat{H}_0} (\omega - E + \hat{H}_I) \right\}^{n} \times | \Phi_0 \rangle$$

(i) $\omega = E$ Brillouin–Wigner

$$\Delta E = \langle \Phi_0 | \left\{ H_I + H_I \hat{Q} \frac{1}{E - \hat{H}_0} \hat{Q} H_I + \hat{H}_1 \hat{Q} \frac{1}{E - \hat{H}_0} \hat{Q} \hat{H}_1 \hat{Q} \frac{1}{E - \hat{H}_0} \hat{Q} H_I + \ldots \right\} | \Phi_0 \rangle$$

(ii) $\omega = W_0$ Rayleigh–Schrödinger MBPT