FYS4480, NOV 24, 2022

FCI :

$$|\Psi_0\rangle = \sum_{i=0}^{\infty} C_{i0} |\Phi_i\rangle$$

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

op-ok : $|\Phi_0\rangle$

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

1p1h : $|\Phi_i^a\rangle = a_a^\dagger a_i |\Phi_c\rangle$

$$= a_a^\dagger a_i |c\rangle$$

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

$$\langle \Psi_0 | \Phi_c\rangle = C_0 = \underline{1}$$

$$|\Psi_0\rangle = |\Phi_0\rangle + \sum_{ai}^{1p1h} a_a^\dagger a_i^\dagger |\Phi_c\rangle \times C_i^a$$

$$+ \sum_{\substack{ab \\ ij}}^{2p2h} a_a^\dagger a_b^\dagger a_j a_i |\Phi_0\rangle \times C_{ij}^{ab}$$

$$+ \ldots \sum_{\substack{ab\ldots \\ ij\ldots}}^{npnh}$$

with two-body interaction only

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

$$= E - \left(W_0 + \frac{1}{2}\sum_{ij} \langle ij|v|ij\rangle_{AS}\right)$$

$$= \sum_{ai} C_i^a \langle i|f|a\rangle$$

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

Hamiltonian matrix

$$\begin{array}{c|cccccccc}
 & 0p0h & 1p1h & 2p2h & 3p3h & \ldots & & & npnh \\
\hline
0p0h & \times & \times & \times & 0 & 0 & - & - & 0 \\
1p1h & \times & \times & \times & \times & 0 & - & - & 0 \\
2p2h & \times & \times & \times & \times & \times & 0 & - & 0 \\
3p3h & 0 & \times & \times & \times & \times & \times & 0 & 0 \\
\vdots & \vdots & 0 & \times & \times & \vdots & & & \\
\vdots & \vdots & \vdots & 0 & \times & \vdots & & 0 & \\
\vdots & \vdots & \vdots & \vdots & 0 & & & & \\
npnh & 0 & 0 & 0 & \vdots & & & &
\end{array}$$

HF

Can be seen as a unitary transformation where we zero out the Block

$\langle 0p0h | H | 1p1h \rangle \Rightarrow$

$$C_i^a = 0$$

$$
\begin{array}{c|c}
 & \begin{array}{cccccc} 0p0h & 1p1h & 2p2h & - & - & - \end{array} \\
\begin{array}{c} 0p0h \\ 1p1h \\ 2p2h \\ \vdots \\ \vdots \\ \vdots \\ \vdots \end{array} &
\begin{bmatrix}
\tilde{x} & 0 & \tilde{x} & 0 & \cdots & 0 \\
0 & \tilde{x} & \tilde{x} & \tilde{x} & & \vdots \\
\tilde{x} & \tilde{x} & \tilde{x} & & & \vdots \\
0 & \tilde{x} & \tilde{x} & & & \vdots \\
\vdots & 0 & \tilde{x} & & & \vdots \\
\vdots & \vdots & 0 & & & \vdots \\
0 & \vdots & \vdots & & & 0
\end{bmatrix}
\end{array}
$$

$$|c'\rangle = \exp(\hat{T}_1)|c\rangle$$

(Thouless' theorem)

$$\hat{T}_1 = \left(\sum c_i^a a_a^\dagger a_i \right)$$

MBPT

$$\Delta E_{MBPT} = E - W_0$$

$$= \sum_{i=1}^{\infty} \Delta E^{(i)}$$

$$\Delta E^{(1)} = \frac{1}{2} \sum_{ij} \langle ij | v | ij \rangle_{AS}$$

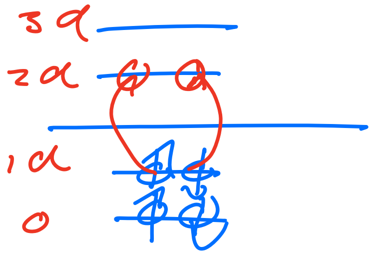
$$\Delta E^{(2)}(\text{HF-basis}) =$$

$$\frac{1}{4} \sum_{\substack{ab \\ ij}} \frac{\langle ij | v | ab \rangle \langle ab | v | ij \rangle}{\varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_b}$$

Midterm 2:

$$\langle ij | v | ab \rangle = -g$$

$$\Delta E^{(2)} = \frac{1}{4} g^2 \sum_{\substack{ab \\ ij}} \frac{1}{\varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_b}$$



$|\Phi_0\rangle$

$$C_{ij}^{ab}(2) \simeq \frac{1}{4} \frac{\langle ab | v | ij \rangle_{AS}}{\varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_b}$$

$$\hat{T}_1 = \sum_{ai} t_i^a a_a^\dagger a_i \qquad 1p1h$$

$$\hat{T}_2 = \frac{1}{4} \sum_{\substack{ab\\ij}} t_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i \qquad 2p2h$$

$$\vdots$$

$$\hat{T}_n = \frac{1}{(n!)^2} \sum_{\substack{abcd\ldots\\ ijkl\ldots}} t_{ijkl\ldots}^{abcd\ldots} a_a^\dagger a_b^\dagger \ldots a_j a_i \ldots$$

npnh

Exponential ansatz

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

$$\hat{T} = \hat{T}_1 + \hat{T}_2 + \hat{T}_3 + \ldots \hat{T}_n$$

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

FCI: $\hat{C} = \sum c_i^a a_a^\dagger a_i$

$$+ \sum c_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i + \ldots$$

npnh

Classical truncation:

Singles and doubles

$\hat{T} \simeq \hat{T}_1 + \hat{T}_2$

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

Need to solve:

(i) $\Delta E = E - E_0^{Ref} =$

$$\sum_{ai} t_i^a \langle i|f|a\rangle + \sum_{\substack{ab\\ij}} t_{ij}^{ab} \langle ij|ab\rangle_{AS}$$

(ii) $\langle 1p1h|\bar{H}|0p0h\rangle =$

$\langle 1p1h|\bar{H}|\Phi_0\rangle = 0$ gives t_i^a

(iii) $\langle 2p2h|\bar{H}|\Phi_0\rangle = 0$ gives t_{ij}^{ab}

$A x = \lambda x$

$$SS^T = S^TS = \mathbb{1}$$

$$SAS^T = D = \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_d \end{bmatrix}$$

$$A \in \mathbb{R}^{d \times d}$$

$$SAx = \lambda Sx$$

$$\underbrace{SAS^T}_{D}\underbrace{Sx}_{y} = \lambda \underbrace{Sx}_{y}$$

$$D \cdot y = \lambda y$$

$$S_m S_{m-1} \dots S_1 A S_1^T \dots S_m^T = D$$

$$v = S_m S_{m-1} \dots S_1 x$$

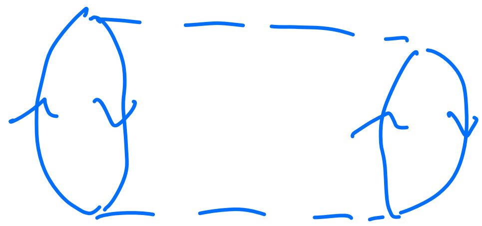
$$A = \begin{bmatrix} x & x & x \\ x & x & x \\ x & x & x \end{bmatrix}$$

$$S_1 \begin{bmatrix} x & x & x \\ x & x & x \\ x & x & x \end{bmatrix} S_1^T = \begin{bmatrix} \tilde{x} & \tilde{x} & 0 \\ \tilde{x} & \tilde{x} & \tilde{x} \\ 0 & \tilde{x} & \tilde{x} \end{bmatrix}$$

$$\begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix}\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}\begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}$$

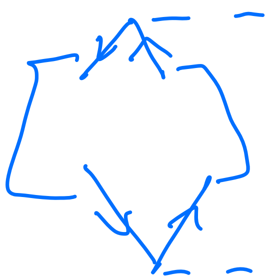
$$= \begin{bmatrix} b_{11} & 0 \\ 0 & b_{22} \end{bmatrix} = \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix}$$

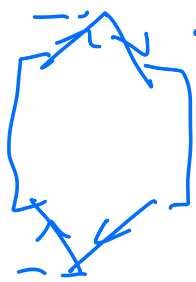
MBPT



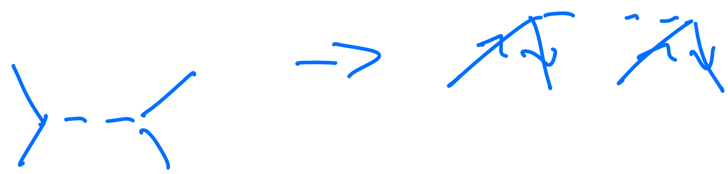
$$t_{ij}^{ab}$$

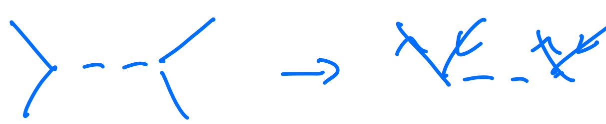
$$= \frac{1}{4} \sum_{\substack{ab \\ ij}} \frac{\langle ij|v|ab\rangle \langle ab|v|ij\rangle}{\varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_b}$$

 ~ -2 2p2h

 $+2$ 2p2h

$\langle \Phi_c |$



 2p2h

$| \Phi_c \rangle$

$$\frac{1}{4}\sum_{\substack{ab\\ij}} \langle ij|v|ab\rangle\, t_{ij}^{ab}$$

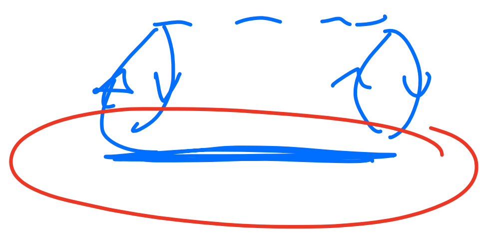
$$\frac{\langle ab|v|ij\rangle}{\varepsilon_i+\varepsilon_j-\varepsilon_a-\varepsilon_b}$$

$$\underline{\hat{t}_{ij}^{ab}\,|\Phi_0\rangle}$$

wave operator

$\approx$ $\hat{T}_2$ repr

MBPT(2)



MBPT(3)