$$H = \sum_{pq} h_{pq} c_p^\dagger c_q + \frac{1}{2} \sum_{pqrs} V_{pqrs} \, c_p^\dagger c_q^\dagger c_s c_r$$

spin orbitals $\{ \phi_1(\vec{x}), \cdots, \phi_d(\vec{x}) \}$.

$$h_{pq} = \int d\vec{x} \; \phi_p^*(\vec{x}) \left(-\frac{1}{2} \Delta_r + V_{ext}(\vec{r}) \right) \phi_q(\vec{x})$$

$$V_{pqrs} \equiv \langle pq | rs \rangle = \int d\vec{x} \, d\vec{x}' \; \frac{\phi_p^*(\vec{x}) \phi_q^*(\vec{x}') \phi_r(\vec{x}) \phi_s(\vec{x}')}{|\vec{r} - \vec{r}'|}$$

Simplified model.

Hubbard $\quad H = \sum_{\sigma} \sum_{\langle pq \rangle} h_{pq} \, c_{p\sigma}^\dagger c_{q\sigma} + \sum_p U_p \, n_{p\uparrow} n_{p\downarrow}$

$$n_{p\sigma} = c_{p\sigma}^\dagger c_{p\sigma}$$

Hartree-Fock theory.

$$\underbrace{\phi_1, \cdots, \phi_N}_{\text{occupied}}, \underbrace{\phi_{N+1}, \cdots, \phi_d}_{\text{unoccupied.}} : \text{already HF orbitals.}$$

i, j, k, l $\qquad$ a, b, c, d

$$|\Psi_0\rangle = c_1^\dagger \cdots c_N^\dagger |0\rangle$$

$$\mathcal{E}_{HF} = \langle \Psi_0 | H | \Psi_0 \rangle \Rightarrow \text{compute.}$$

① $\langle \Psi_0 | c_p^\dagger c_q | \Psi_0 \rangle$

$$= \langle 0 | c_N \cdots c_1 \, c_p^\dagger c_q \, c_1^\dagger \cdots c_N^\dagger | 0 \rangle$$

to be non zero, $1 \le p, q \le N$.

$$\theta_p = \begin{cases} 1, & 1 \le p \le N \\ 0, & p > N \end{cases}$$

$$[c_p^\dagger c_q, c_i^\dagger] = c_p^\dagger \delta_{qi}$$

$$\Rightarrow c_p^\dagger c_q c_1^\dagger \cdots c_N^\dagger |0\rangle = \sum_{i=1}^{N} c_1^\dagger \cdots \underset{\overset{\uparrow}{i}}{c_p^\dagger} \cdots c_N^\dagger |0\rangle \delta_{qi}$$

$p = i$ to be non zero.

$$\langle \Psi_0 | c_p^\dagger c_q | \Psi_0 \rangle = \theta_p \theta_q \delta_{pq} \langle \Psi_0 | c_p^\dagger c_q | \Psi_0 \rangle$$

$$\langle \Psi_0 | \sum_{pq} h_{pq} c_p^\dagger c_q | \Psi_0 \rangle = \sum_{i=1}^{N} h_{ii}$$

② $\frac{1}{2}\sum_{pqrs} \langle \Psi_0 | c_p^\dagger c_q^\dagger c_s c_r | \Psi_0 \rangle V_{pqrs}$

$= \frac{1}{2}\sum_{pqrs} \langle 0 | c_N \cdots c_1 \; c_p^\dagger c_q^\dagger c_s c_r \; c_1^\dagger \cdots c_N^\dagger | 0 \rangle V_{pqrs}$

$\{p, q\} = \{r, s\} \subset \{1, \cdots, N\}, \quad p \neq q, \quad s \neq r.$

① $p = r, \; q = s$ ② $p = s, \; q = r.$

recall

$\frac{1}{2}\sum_{pqrs} V_{pqrs} \; c_p^\dagger c_q^\dagger c_s c_r \; c_1^\dagger \cdots c_N^\dagger | 0 \rangle$

$= \sum_{pq} \sum_{1 \le i < j \le N} V_{pqij} \; c_1^\dagger \cdots \underset{\substack{\uparrow \\ i}}{c_p^\dagger} \cdots \underset{\substack{\uparrow \\ j}}{c_q^\dagger} \cdots c_N^\dagger | 0 \rangle$

2-particle energy

$$= \sum_{i<j} \left(V_{ijij} - V_{ijji} \right)$$

$$= \frac{1}{2} \sum_{i,j} \left(\langle ij|ij\rangle - \langle ij|ji\rangle \right)$$

$$:= \frac{1}{2} \sum_{i,j} \langle ij||ij\rangle$$

$$\mathcal{E}_{HF} = \sum_i h_{ii} + \frac{1}{2} \sum_{ij} \langle ij||ij\rangle .$$

interpret back to integrals.

$$E_{HF} = \sum_{i=1}^{N} \int \phi_i(\vec{x}) \left(-\frac{1}{2}\Delta_{\vec{r}} + V_{ext}(\vec{r})\right) \phi_i(\vec{x})$$

$$+ \frac{1}{2} \sum_{i,j} \int \frac{\phi_i^*(\vec{x})\, \phi_j^*(\vec{x}')\, \phi_i(\vec{x})\, \phi_j(\vec{x}')}{|\vec{r}-\vec{r}'|} d\vec{r}\, d\vec{r}'$$

$$- \frac{1}{2} \sum_{i,j} \int \frac{\phi_i^*(\vec{x})\, \phi_j^*(\vec{x}')\, \phi_j(\vec{x})\, \phi_i(\vec{x}')}{|\vec{r}-\vec{r}'|} d\vec{r}\, d\vec{r}'$$

$$= \sum_{i=1}^{N} \frac{1}{2} \int |\nabla_{\vec{r}} \phi_i(\vec{x})|^2 d\vec{r} + \int V_{ext}(\vec{r})\, \rho(\vec{r})\, d\vec{r}$$

$$+ \frac{1}{2} \int \frac{\rho(\vec{r})\, \rho(\vec{r}')}{|\vec{r}-\vec{r}'|} d\vec{r}\, d\vec{r}' - \frac{1}{2} \int \frac{|P(\vec{x},\vec{x}')|^2}{|\vec{r}-\vec{r}'|} d\vec{r}\, d\vec{r}'$$

E-L to optimize orbital. $\Rightarrow$ H-F eq.

$$\left(-\frac{1}{2}\Delta + V_{ext}(\vec{r}) + \int \frac{\rho(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|}\right)\varphi_i(\vec{x})$$

$$-\int \frac{P(\vec{x},\vec{x}\,')}{|\vec{r}-\vec{r}\,'|}\varphi_i(\vec{x}\,')\,d\vec{x}\,' = \varepsilon_i\,\varphi_i(\vec{r})$$

Fock matrix. op. in the HF basis.

Galerkin projection.

$$F = \sum_{pq} f_{pq}\, c_p^\dagger c_q$$

$$
\begin{aligned}
f_{pq} &= \int \phi_p^* \left(-\frac{1}{2}\Delta + V_{ext} \right) \phi_q \, d\vec{x} \\
&\quad + \sum_{j=1}^{N} \int \frac{\phi_p^*(\vec{x})\, \phi_j(\vec{x}')\, \phi_j^*(\vec{x}')\, \phi_q(\vec{x})}{|\vec{r}-\vec{r}'|} \, d\vec{x}\, d\vec{x}' \\
&\quad - \sum_{j=1}^{N} \int \frac{\phi_p^*(\vec{x})\, \phi_j(\vec{x})\, \phi_j^*(\vec{x}')\, \phi_q(\vec{x}')}{|\vec{r}-\vec{r}'|} \, d\vec{x}\, d\vec{x}' \\
&= h_{pq} + \sum_{j=1}^{N} V_{pjqj} - V_{pjjq} \\
&\equiv h_{pq} + \sum_{j=1}^{N} \langle pj || qj \rangle
\end{aligned}
$$

self-consistency: $f_{pq} = \epsilon_p \delta_{pq}$

$\downarrow$

diagonal matrix.

In the HF basis

Fock op. $F = \sum_p \epsilon_p c_p^\dagger c_p$

chemical potential. $\mu \hat{N} = \mu \sum_p c_p^\dagger c_p$

Fact 1. $F - \mu N = \sum_p (\epsilon_p - \mu) c_p^\dagger c_p$.

μ controls the # el. of the ground state.

w.l.o.g. assume $\mu = 0$.

$$\epsilon_1 \le \cdots \le \epsilon_N < 0 < \epsilon_{N+1} \le \cdots \le \epsilon_d.$$

Fact 2. Any quadratic Hamiltonian is easy.

$$H = \sum_{pq} h_{pq} c_p^\dagger c_q$$

$\downarrow$ diagonalize $d \times d$ matrix h

rotate. redefine $a_p^\dagger$, a_q

$$H = \sum_p \epsilon_p a_p^\dagger a_p$$

Møller - Plesset perturbation theory.

Same perturbation of eigenvalues applied to this setting.

Recall

$$H = H_0 + \lambda H_1$$

$$(H_0 + \lambda H_1)(\psi_0 + \lambda \psi_1 + \lambda^2 \psi_2 + \cdots)$$

$$= (E_0 + \lambda E_1 + \lambda^2 E_2 + \cdots)(\psi_0 + \lambda \psi_1 + \cdots)$$

$$E_1 = \langle \psi_0 | H_1 | \psi_0 \rangle \qquad Q = I - |\psi_0\rangle\langle\psi_0|$$

$$|\psi_1\rangle = Q\,(E_0 - H_0)^{-1} Q\, H_1 |\psi_0\rangle\,, \qquad \langle \psi_0 | \psi_1 \rangle = 0$$

$$E_2 = \langle \psi_0 | H_1 | \psi_1 \rangle$$

$$= \langle \psi_0 | H_1\, Q\,(E_0 - H_0)^{-1} Q\, H_1 | \psi_0 \rangle$$

$$H_0 |\varphi_j\rangle = \varepsilon_j |\varphi_j\rangle\,, \qquad |\varphi_0\rangle = |\psi_0\rangle$$

$$\Rightarrow \quad E_2 = \sum_{j \neq 0} \frac{|\langle \varphi_0 | H_1 | \varphi_j \rangle|^2}{\varepsilon_0 - \varepsilon_j}$$

Perturbation $\quad H_0 = F + \langle \Psi_0 | H - F | \Psi_0 \rangle$

$$\langle \Psi_0 | H_0 | \Psi_0 \rangle = \langle \Psi_0 | H | \Psi_0 \rangle = \text{HF energy.}$$

$$W = H - H_0 = H - F - \langle \Psi_0 | H - F | \Psi_0 \rangle$$

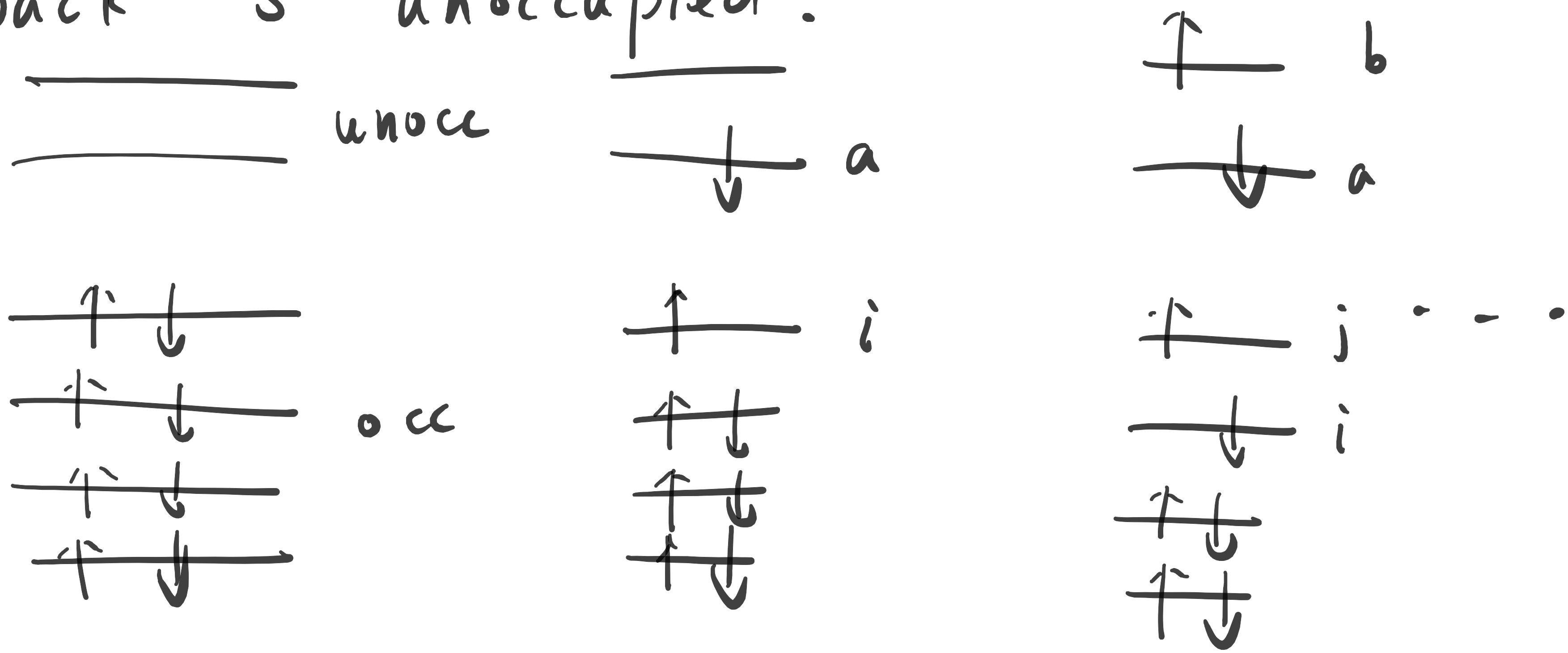
$$E_1 = \langle \Psi_0 | W | \Psi_0 \rangle = 0.$$

what are φ_j's.

Fact 1: Only neutral excitation matter

(W preserves # els).

Fact 2: all neutral excited states can be created by removing s occupied, and put back s unoccupied.



$|\Phi_0\rangle$

$|\Phi_i^a\rangle = c_a^\dagger c_i |\Phi_0\rangle$

$|\Phi_{ij}^{ab}\rangle = c_a^\dagger c_b^\dagger c_j c_i |\Phi_0\rangle$

(exer) $\langle \Psi_i^a | H_0 | \Psi_i^a \rangle = E_{HF} + \epsilon_a - \epsilon_i$

$$\langle \Psi_{ij}^{ab} | H_0 | \Psi_{ij}^{ab} \rangle = E_{HF} + \epsilon_a + \epsilon_b - \epsilon_i - \epsilon_j$$

$$\cdots$$

$$E_{MP2} = \sum_{ia} \frac{|\langle \Psi_0 | W | \Psi_i^a \rangle|^2}{\epsilon_i - \epsilon_a} + \sum_{\substack{i<j \\ a<b}} \frac{|\langle \Psi_0 | W | \Psi_{ij}^{ab} \rangle|^2}{\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b}$$

$+ \cdots$

$\downarrow$

high order vanish

$\nearrow$

not double counting excited states

① $\langle \Psi_0 | W | \Psi_i^a \rangle$

$= \langle \Psi_0 | H - F | \Psi_i^a \rangle$

1) $h_{pq} \; c_p^\dagger c_q$

2) $V_{pqrs} \; c_p^\dagger c_q^\dagger c_s c_r$

3) $-\epsilon_p \; c_p^\dagger c_p$

1) $\langle \Psi_0 | c_p^\dagger c_q | \Psi_i^a \rangle$

$= \langle 0 | c_N \cdots c_1 \underbrace{c_p^\dagger c_q \; c_a^\dagger c_i} \; c_1^\dagger \cdots c_N^\dagger | 0 \rangle$

$= \delta_{pi} \, \delta_{qa}$

$$\langle \Phi_0 | \sum_{pq} h_{pq} \, c_p^\dagger c_q | \Phi_i^a \rangle = h_{ia}$$

$$\langle \Phi_0 | \sum_{p} \epsilon_p \, c_p^\dagger c_p | \Phi_i^a \rangle = 0 \quad \longrightarrow)))$$

2) $$\langle \Phi_0 | c_p^\dagger c_q^\dagger c_s c_r | \Phi_i^a \rangle$$

$$= \langle 0 | c_N \cdots c_1 \, c_p^\dagger c_q^\dagger c_s c_r \underbrace{c_a^\dagger c_i} c_1^\dagger \cdots c_N^\dagger | 0 \rangle$$

commute to the right

$$= \delta_{pi} \delta_{ra} \delta_{qs} \theta_q - \delta_{qi} \delta_{ra} \delta_{ps} \theta_p$$

$$+ \delta_{qi} \delta_{sa} \delta_{pr} \theta_p - \delta_{pi} \delta_{sa} \delta_{qr} \theta_q$$

$$\langle \Psi_0 | H - F | \Psi_i^a \rangle$$

$$= h_{ia} + \frac{1}{2} \sum_{pqrs} V_{pqrs} \left(\delta_{pi} \delta_{ra} \delta_{qs} \theta_q - \cdots \right)$$

$$= h_{ia} + \frac{1}{2} \sum_j \left(V_{ijaj} - V_{jiaj} + V_{jija} - V_{ijja} \right)$$

$$= h_{ia} + \sum_j \left(V_{ijaj} - V_{ijja} \right)$$

$$= h_{ia} + \sum_j \langle ij || aj \rangle = F_{ia} = 0$$

off-diagonal.

Fock operator

Only remaining term.

$$\langle \Psi_0 | H - F | \Psi_{ij}^{ab} \rangle$$

$$\langle \Psi_0 | c_p^\dagger c_q | \Psi_{ij}^{ab} \rangle = 0.$$

$$\langle \Psi_0 | c_p^\dagger c_q^\dagger c_s c_r | \Psi_{ij}^{ab} \rangle$$

$$= \langle 0 | c_N \cdots c_1 \underbrace{c_p^\dagger c_q^\dagger c_s c_r \, c_a^\dagger c_b^\dagger c_j c_i} c_i^\dagger \cdots c_N^\dagger | 0 \rangle$$

$$= \delta_{pi} \delta_{qj} \delta_{ra} \delta_{sb} - \delta_{qi} \delta_{pj} \delta_{ra} \delta_{sb}$$

$$- \delta_{pi} \delta_{qj} \delta_{sa} \delta_{rb} + \delta_{qi} \delta_{pj} \delta_{sa} \delta_{rb}$$

$$\langle \Phi_0 | H - F | \Phi_{ij}^{ab} \rangle = V_{ijab} - V_{ijba} \equiv \langle ij || ab \rangle$$

$$E_{MP2} = \sum_{\substack{i<j \\ a<b}} \frac{|\langle ij || ab \rangle|^2}{\varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_b} < 0$$

$$E_{MP2} = \sum_{\substack{i<j \\ a<b}} \frac{V_{ijab}^2 + V_{ijba}^2 - 2 V_{ijab} V_{ijba}}{\varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_b}$$

$$= \frac{1}{4} \sum_{\substack{ij \\ ab}} \frac{V_{ijab}^2 + V_{ijba}^2 - 2 V_{ijab} V_{ijba}}{\varepsilon_i + \varepsilon_j - \varepsilon_a - \epsilon_b}$$

$$= \frac{1}{2} \sum_{ijab} \frac{V_{ijab}^2 - V_{ijab} V_{ijba}}{\varepsilon_i + \varepsilon_j - \varepsilon_b - \varepsilon_a}.$$

direct mp2   exchange mp2.

exer: RHF. spatial orbitals.

$$E_{MP2} = \sum_{ijab} \frac{2 V_{ijab}^2 - V_{ijab} V_{ijba}}{\varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_b}.$$

Configuration interaction.

Use HF orbitals as well as HF ground / excited states.

CIS

$$|\Psi\rangle = c_0 |\Psi_0\rangle + \sum_{ia} c_i^a |\Psi_i^a\rangle$$

$$+ \frac{1}{(2!)^2} \sum_{ijab} c_{ij}^{ab} |\Psi_{ij}^{ab}\rangle + \cdots$$

CISD

Compute matrix elements

$$\langle \Psi^{a'b'c'\cdots}_{i'j'k'\cdots} | H | \Psi^{abc\cdots}_{ijk\cdots} \rangle$$

Sparse matrix. Ψ, Ψ' cannot differ by >2 pairs of indices

- exp. scaling (FCI)
- size extensivity (truncated CI)

Coupled cluster. (CC).

ansatz

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

amplitudes

$$T = \sum_{ia} t_i^a \, c_a^\dagger c_i + \frac{1}{4} \sum_{\substack{ij\\ab}} t_{ij}^{ab} \, c_a^\dagger c_b^\dagger c_j c_i + \cdots$$

CCS　　　　CCSD

"Golden standard"　　CCSD(T) ← perturbatively

Apply variational principle

$$\inf_{\hat{T}} \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} = \frac{\langle \Psi_0 | e^{\hat{T}^\dagger} H e^{\hat{T}} | \Psi_0 \rangle}{\langle \Psi_0 | e^{\hat{T}^\dagger} e^{\hat{T}} | \Psi_0 \rangle}$$

exp. scaling even for truncated CC.

Projected CC

$$H e^{\hat{T}} | \Psi_0 \rangle = E_{cc} e^{\hat{T}} | \Psi_0 \rangle$$

$$e^{-\hat{T}} H e^{\hat{T}} | \Psi_0 \rangle = E_{cc} | \Psi_0 \rangle$$

$$\langle \Phi_0 | e^{-\hat{T}} H e^{\hat{T}} | \Phi_0 \rangle = E_{cc}$$

But how to find $\hat{T}$?

$$\begin{cases} \langle \Phi_i^a | e^{-\hat{T}} H e^{\hat{T}} | \Phi_0 \rangle = 0 \\ \langle \Phi_{ij}^{ab} | e^{-\hat{T}} H e^{\hat{T}} | \Phi_0 \rangle = 0 \\ \cdots \end{cases}$$

← not variational.

Baker-Campbell-Hausdorff (BCH) expansion.

$$e^{A} B e^{-A} = B + [A,B] + \frac{1}{2!}[A,[A,B]] + \cdots$$

$$= \sum_{n=0}^{\infty} \frac{1}{n!} [A,[A,\cdots[A,B]]] := [A,B]_n$$

pf: $f(\lambda) = e^{\lambda A} B e^{-\lambda A}$

$$f(1) = \sum_{n=0}^{\infty} \frac{1}{n!} f^{(n)}(0) \qquad \square$$

Use BCH

$$e^{-\hat{T}} H e^{\hat{T}} = H - [T, H] + \frac{1}{2!}[T, [T, H]] + \cdots$$

Fact: ① $\hat{T}$ only contains excitation operators.

$c_a^+ c_i$, $c_a^+ c_b^+ c_j c_i$

② H only contains up to 2 body interaction. at most 4 general indices.

$[T, H]$. at most 3 general indices.

$[T, H]_2$ " " 2 " "

$\vdots$

$[T, H]_4$ " " 0 " " → all excitation operators.

$[T, H]_n \equiv 0$, $n \geq 5$ (excitation ops commute)

CC eq.

$$\left(H - [T, H] + \frac{1}{2!}[T, H]_2 - \frac{1}{3!}[T, H]_3 + \frac{1}{4!}[T, H]_4\right)|\Phi_0\rangle$$

$$= E_{cc}|\Phi_0\rangle$$

CCD. $\hat{T} = \frac{1}{4} \sum_{\substack{ij \\ ab}} t_{ij}^{ab} c_a^{+} c_b^{+} c_j c_i$

Only project to $\langle \Psi_{ij}^{ab} |$

(exer). $[T, H]_n$ contribution is 0

$n \geq 3$.

Assume $\hat{T}$ is obtained.

$$E_{CCD} = \langle \Psi_0 | e^{-\hat{T}} H e^{\hat{T}} | \Psi_0 \rangle$$

$$= E_{HF} - \langle \Psi_0 | \hat{T} \cancel{H} | \Psi_0 \rangle + \underbrace{\langle \Psi_0 | H \hat{T} | \Psi_0 \rangle}$$

$$+\frac{1}{2}\langle\Psi_0|\cancel{\hat{T}^2 H}-\cancel{\hat{T}H\hat{T}}+\cancel{H\hat{T}^2}|\Psi_0\rangle$$

$$=E_{HF}+\frac{1}{4}\sum_{\substack{ij\\ab}}\langle ij||ab\rangle t_{ij}^{ab}$$

$$t_{ij}^{ab}\hat{\approx}\frac{\langle ij||ab\rangle}{\varepsilon_i+\varepsilon_j-\varepsilon_a-\varepsilon_b} \Rightarrow \text{MP2 energy.}$$

$$t_{ij}^{ab}=-t_{ji}^{ab}=-t_{ij}^{ba}=t_{ji}^{ba}$$

CCD: Algebraic Expressions

CC energy:

$$\Delta E = \frac{1}{4} \sum_{ij} \sum_{ab} \langle ij||ab \rangle \, t_{ij}^{ab}$$

CC equations:

$$0 = \langle ab||ij \rangle + P_-(ab) \sum_{e} f_{ae} \, t_{ij}^{eb} - P_-(ij) \sum_{m} f_{mi} \, t_{mj}^{ab}$$

MP2.

$$+ \frac{1}{2} \sum_{mn} \langle mn||ij \rangle \, t_{mn}^{ab} + \frac{1}{2} \sum_{ef} \langle ab||ef \rangle \, t_{ij}^{ef}$$

$$+ P_-(ij) P_-(ab) \sum_{m} \sum_{e} \langle mb||ej \rangle \, t_{im}^{ae}$$

$$- \frac{1}{2} P_-(ab) \sum_{mn} \sum_{ef} \langle mn||ef \rangle \, t_{mn}^{af} \, t_{ij}^{eb} - \frac{1}{2} P_-(ij) \sum_{mn} \sum_{ef} \langle mn||ef \rangle \, t_{in}^{ef} \, t_{mj}^{ab}$$

$$+ \frac{1}{4} \sum_{mn} \sum_{ef} \langle mn||ef \rangle \, t_{mn}^{ab} \, t_{ij}^{ef} + \frac{1}{2} P_-(ij) P_-(ab) \sum_{mn} \sum_{ef} \langle mn||ef \rangle \, t_{im}^{ae} \, t_{jn}^{bf}$$

The CCSD Amplitude Equations

$$
\begin{aligned}
0 \quad = \quad & \langle ab||ij\rangle + \sum_c \left(f_{bc}t_{ij}^{ac} - f_{ac}t_{ij}^{bc}\right) - \sum_k \left(f_{kj}t_{ik}^{ab} - f_{ki}t_{jk}^{ab}\right) + \frac{1}{2}\sum_{kl}\langle kl||ij\rangle t_{kl}^{ab} \\
& + \frac{1}{2}\sum_{cd}\langle ab||cd\rangle t_{ij}^{cd} + P(ij)P(ab)\sum_{kc}\langle kb||cj\rangle t_{ik}^{ac} + P(ij)\sum_c\langle ab||cj\rangle t_i^c - P(ab)\sum_k\langle kb||ij\rangle t_k^a \\
& + \frac{1}{2}P(ij)P(ab)\sum_{klcd}\langle kl||cd\rangle t_{ik}^{ac}t_{lj}^{db} + \frac{1}{4}\sum_{klcd}\langle kl||cd\rangle t_{ij}^{cd}t_{kl}^{ab} - P(ab)\frac{1}{2}\sum_{klcd}\langle kl||cd\rangle t_{ij}^{ac}t_{kl}^{bd} \\
& - P(ij)\frac{1}{2}\sum_{klcd}\langle kl||cd\rangle t_{ik}^{ab}t_{jl}^{cd} + P(ab)\frac{1}{2}\sum_{kl}\langle kl||ij\rangle t_k^a t_l^b + P(ij)\frac{1}{2}\sum_{cd}\langle ab||cd\rangle t_i^c t_j^d \\
& P(ab)\sum_{kc} f_{kc}t_k^a t_{ij}^{bc} + P(ij)\sum_{kc} f_{kc}t_i^c t_{jk}^{ab} P(ij)\sum_{klc}\langle kl||ci\rangle t_k^c t_{lj}^{ab} + P(ab)\sum_{kcd}\langle ka||cd\rangle t_k^c t_{ij}^{db} + \\
& P(ij)P(ab)\sum_{kcd}\langle ak||dc\rangle t_i^d t_{jk}^{bc} + P(ij)P(ab)\sum_{klc}\langle kl||ic\rangle t_l^a t_{jk}^{bc} - P(ij)P(ab)\sum_{kc}\langle kb||ic\rangle t_k^a t_j^c + \\
& P(ij)\frac{1}{2}\sum_{klc}\langle kl||cj\rangle t_i^c t_{kl}^{ab} - P(ab)\frac{1}{2}\sum_{kcd}\langle kb||cd\rangle t_k^a t_{ij}^{cd} - \\
& P(ij)P(ab)\frac{1}{2}\sum_{kcd}\langle kb||cd\rangle t_i^c t_k^a t_j^d + P(ij)P(ab)\frac{1}{2}\sum_{klc}\langle kl||cj\rangle t_i^c t_k^a t_l^b - \\
& P(ij)\sum_{klcd}\langle kl||cd\rangle t_k^c t_i^d t_{lj}^{ab} - P(ab)\sum_{klcd}\langle kl||cd\rangle t_k^c t_l^a t_{ij}^{db} + \\
& P(ij)\frac{1}{4}\sum_{klcd}\langle kl||cd\rangle t_i^c t_j^d t_{kl}^{ab} + P(ab)\frac{1}{4}\sum_{klcd}\langle kl||cd\rangle t_k^a t_l^b t_{ij}^{cd} + \\
& P(ij)P(ab)\sum_{klcd}\langle kl||cd\rangle t_i^c t_l^b t_{kj}^{ad} + P(ij)P(ab)\frac{1}{4}\sum_{klcd}\langle kl||cd\rangle t_i^c t_k^a t_j^d t_l^b .
\end{aligned} \qquad (123)
$$