Coupled-Cluster for open-shell nuclei

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Overview of close-shell coupled-cluster(by T.P)

- Starting from a Hamiltonian normal ordered to a reference state(new definition of vacuum)

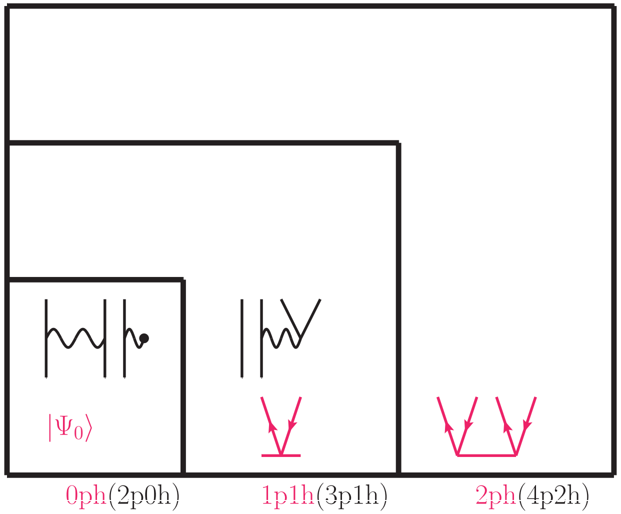
$$\mathcal{H} = H - E_{\text{ref}} = \sum_{pq} f_{pq}\{p^\dagger q\} + \frac{1}{4}\sum_{pqrs} V_{pqrs}\{p^\dagger q^\dagger sr\}.$$

- Coupled-cluster(CC) is similarity transformation(result in a non-Hermitian Hamiltonian)

$$\begin{aligned}\overline{\mathcal{H}} &\equiv \exp(-T)\mathcal{H}\exp(T) \\ &= (\mathcal{H}\exp(T))_C \\ &= \Delta E + \sum_{pq} \overline{\mathcal{H}}_{pq}\{p^\dagger q\} + \sum_{pqrs} \overline{\mathcal{H}}_{pqrs}\{p^\dagger q^\dagger sr\} \\ &\quad + \sum_{pqrstu} \overline{\mathcal{H}}_{pqrstu}\{p^\dagger q^\dagger r^\dagger uts\} + \cdots .\end{aligned}$$

$$\langle \Psi_i | \mathcal{H} | \Psi_j \rangle \neq \langle \Psi_j | \mathcal{H} | \Psi_i \rangle$$

- One-body , two-body , etc. excitations decoupled from the system. Ground state and any excited states are not linked after the transformation by definition of CC.



$$\Psi = \Phi_{\mathrm{SCF}} + \sum_{i,a} C_i^a \Phi_i^a + \sum_{i<j,\, a<b} C_{ij}^{ab} \Phi_{ij}^{ab} + \cdots \qquad \text{(up to } N \text{ excitations)},$$

$$\hat{C}_4 = \hat{T}_4 + \tfrac{1}{2}\hat{T}_2{}^2 + \tfrac{1}{4!}\hat{T}_1{}^4 + \hat{T}_1\hat{T}_3 + \tfrac{1}{2}\hat{T}_1{}^2\hat{T}_2\,.$$

- CC is extensive(FCI, CC, MBPT, etc.)

  computational less expensive compared with CI

Approximation of CC

Truncation of high-rank ops.

$$\overline{\mathcal{H}} \equiv \exp(-T)\mathcal{H}\exp(T)$$
$$= (\mathcal{H}\exp(T))_C$$
$$= \Delta E + \sum_{pq} \overline{\mathcal{H}}_{pq}\{p^\dagger q\} + \sum_{pqrs} \overline{\mathcal{H}}_{pqrs}\{p^\dagger q^\dagger sr\}$$
$$+ \sum_{pqrstu} \overline{\mathcal{H}}_{pqrstu}\{p^\dagger q^\dagger r^\dagger uts\} + \cdots .$$

$$\hat{T} = \sum_{m=1}^{N} \hat{T}_m .$$

$$\hat{T}_m = \frac{1}{(m!)^2} \sum_{\substack{i_1 i_2 \ldots i_m \\ a_1 a_2 \ldots a_m}} \langle a_1 a_2 \cdots a_m | \hat{t}_m | i_1 i_2 \cdots i_m \rangle_{\mathrm{A}} \{\hat{a}_1^\dagger \hat{a}_2^\dagger \cdots \hat{a}_m^\dagger \hat{i}_m \cdots \hat{i}_2 \hat{i}_1\}$$
$$= \frac{1}{(m!)^2} \sum_{\substack{i_1 i_2 \ldots i_m \\ a_1 a_2 \ldots a_m}} t_{i_1 i_2 \ldots i_m}^{a_1 a_2 \ldots a_m} \{\hat{a}_1^\dagger \hat{i}_1 \hat{a}_2^\dagger \hat{i}_2 \cdots \hat{a}_m^\dagger i_m \cdots\}, \qquad (9.82)$$

$T = T_1$ HF

$T = T_1 + T2$ CCSD

$T = T1 + T2 + T3$ CCSDT

Ground state decoupling, Coupled-cluster effective Hamiltonian

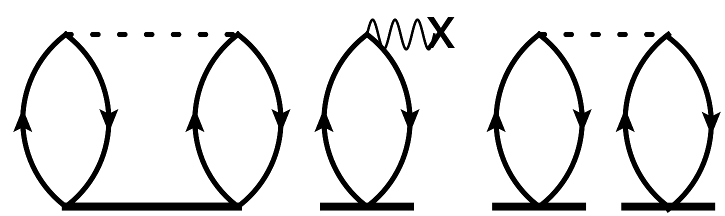
$$|\Psi_0\rangle = e^{\hat{T}}|\Phi_0\rangle \qquad \hat{T} = \sum_i T_i$$

$$\hat{T}_1 = \sum_{ia} t_i \alpha_a^\dagger \alpha_i, \quad \hat{T}_2 = \frac{1}{2}\sum_{i<j,a<b} t_{ij}^{ab} \alpha_a^\dagger \alpha_b^\dagger \alpha_i \alpha_j$$

$$\bar{H} = e^{-T} H e^{T} = H + [H,T] + \frac{1}{2!}[[H,T],T] + ... = (He^T)_C$$

$$\langle \Psi_0 | e^{-T} H e^{T} | \Psi_0 \rangle = E$$

$$\langle \Psi_{ij\ldots}^{ab\ldots} | e^{-T} H e^{T} | \Psi_0 \rangle = 0$$



CCSD

Expectation of observables

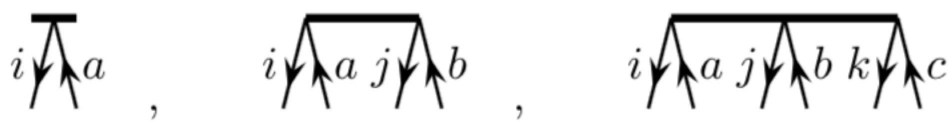
The expectation value in quantum mechanics

$$\bar{O} = \frac{\langle \Psi | O | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

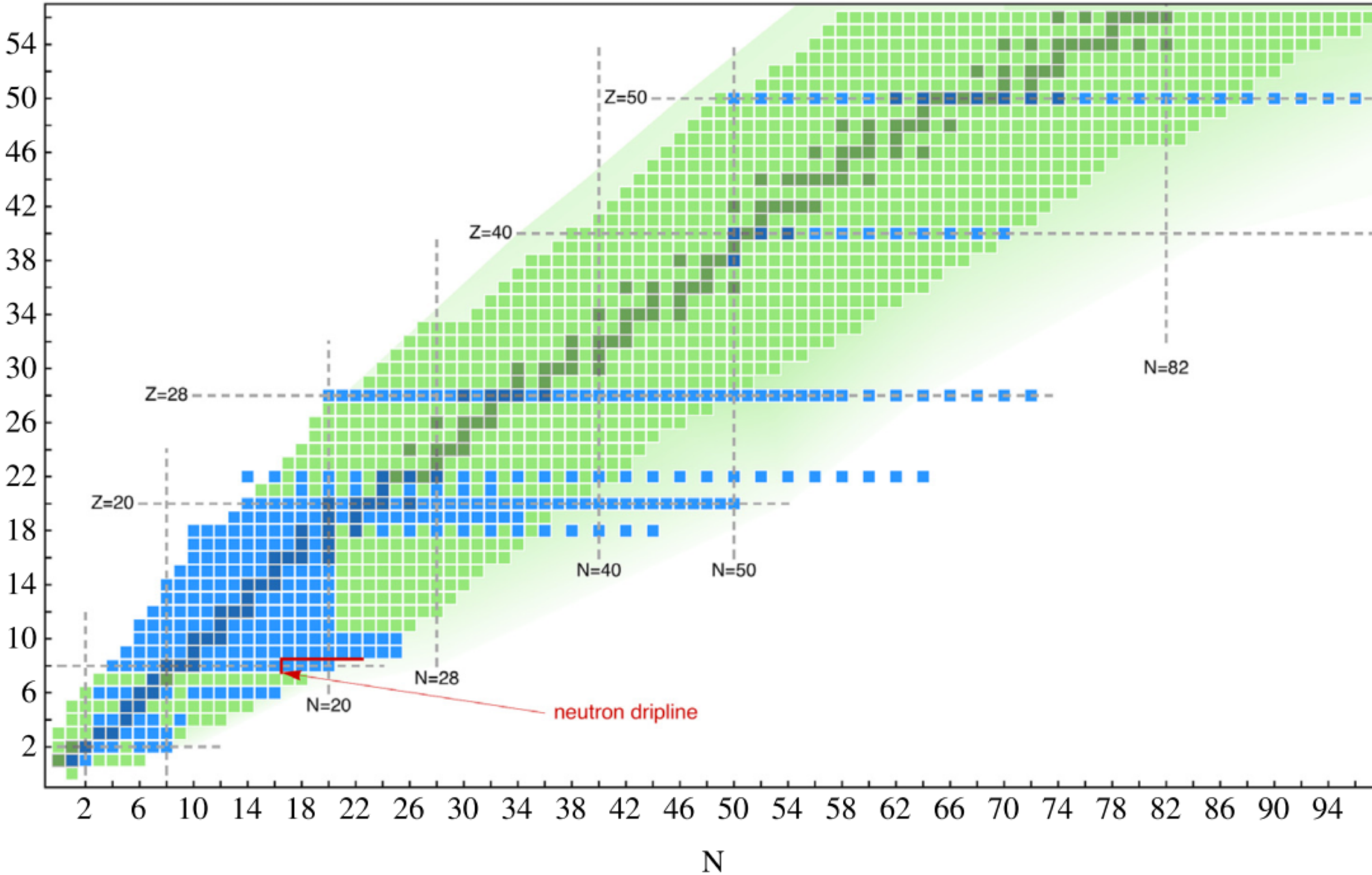
$$\bar{O} = \frac{\langle 0 | e^{T^\dagger} O e^{T} | 0 \rangle}{\langle 0 | e^{T^\dagger} e^{T} | 0 \rangle} = \frac{\langle 0 | e^{T^\dagger} e^{T} e^{-T} O e^{T} | 0 \rangle}{\langle 0 | e^{T^\dagger} e^{T} | 0 \rangle} = \frac{\langle 0 | e^{T^\dagger} e^{T}}{\langle 0 | e^{T^\dagger} e^{T} | 0 \rangle} \bar{O} | 0 \rangle$$

For CC:

$$\langle O \rangle = P(1+\Lambda)\bar{O}P \qquad\qquad P(1+\Lambda Q)(\bar{H} - \delta E)Q = 0$$



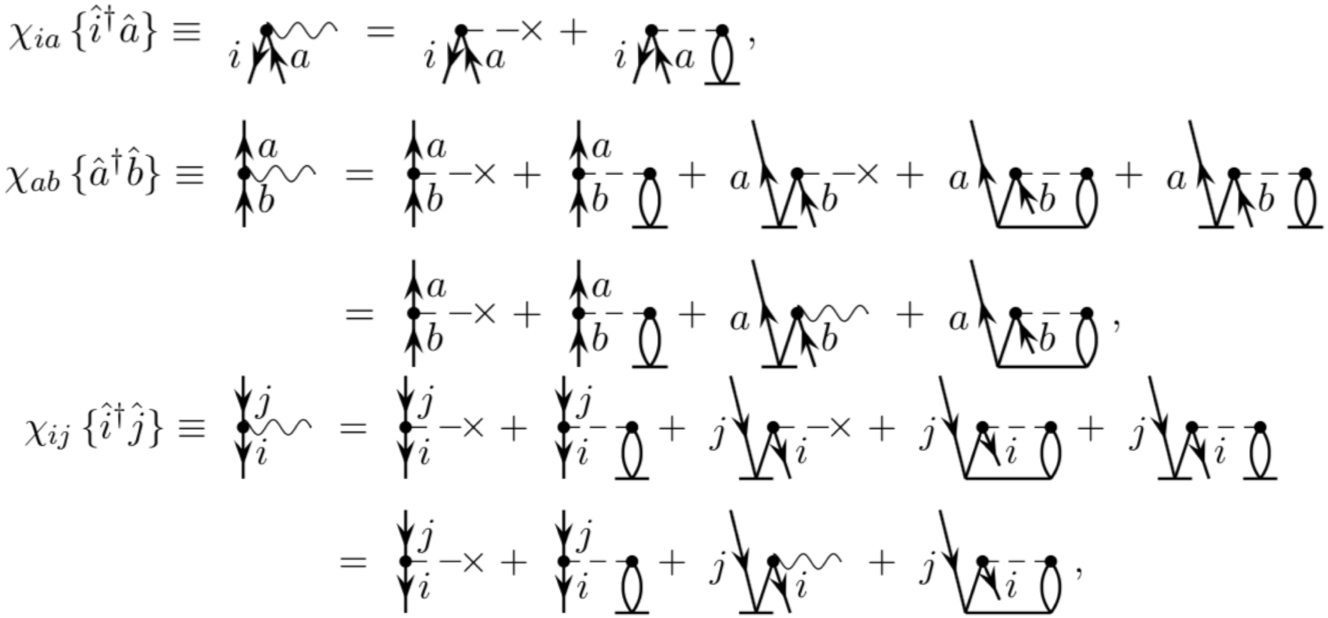
$$\lambda_a^i \{\hat{i}^\dagger \hat{a}\}, \qquad \lambda_{ab}^{ij} \{\hat{i}^\dagger \hat{a} \hat{j}^\dagger \hat{b}\}, \qquad \lambda_{abc}^{ijk} \{\hat{i}^\dagger \hat{a} \hat{j}^\dagger \hat{b} \hat{k}^\dagger \hat{c}\}$$



Z=50
Z=40
Z=28
Z=20
N=20
N=28
N=40
N=50
N=82
neutron dripline
N

Equation of motion CC

- Coupled-cluster effective Hamiltonian



$$
\begin{aligned}
\overline{\mathcal{H}} &\equiv \exp(-T)\mathcal{H}\exp(T) \\
&= (\mathcal{H}\exp(T))_C \\
&= \Delta E + \sum_{pq} \overline{\mathcal{H}}_{pq}\{p^\dagger q\} + \sum_{pqrs} \overline{\mathcal{H}}_{pqrs}\{p^\dagger q^\dagger s r\} \\
&\quad + \sum_{pqrstu} \overline{\mathcal{H}}_{pqrstu}\{p^\dagger q^\dagger r^\dagger u t s\} + \cdots .
\end{aligned}
$$

Configuration interaction with CC Hamiltonian

- The coupled cluster transformation is a similarity transformation even if the T operator is truncated.
- The CC Hamiltonian is fully renormalized. Truncations in CI is a good approximation

reference state: $\hat{H}\Psi_0 = E_0\Psi_0$

excited state: $\hat{H}\Psi_k = E_k\Psi_k$

$$|\Psi_k\rangle = Q_k|\Psi_0\rangle$$

EOM

$$\begin{aligned} H|\Psi_k\rangle &= HQ_k|\Psi_0\rangle = E_kQ_k|\Psi_0\rangle \\ &= [H, Q_k]|\Psi_0\rangle + Q_kH|\Psi_0\rangle \\ &= [H, Q_k]|\Psi_0\rangle + E_0Q_k|\Psi_0\rangle \end{aligned}$$

$$\begin{aligned} [H, Q_k]|\Psi_0\rangle &= (E_k - E_0)Q_k|\Psi_0\rangle \\ &= \omega_k Q_k|\Psi_0\rangle \end{aligned}$$

EOM-CC

Ground state:

$$|\Psi_0\rangle = e^T|HF\rangle$$

k-th excited state:

$$|\Psi_k\rangle = \hat{R}_k|\Psi_0\rangle$$

Close shell nuclei

$$\hat{R}_k = r_0 + \sum_{i,a} r_i^a\{\hat{a}^\dagger\hat{i}\} + \sum_{i<j,\ a<b} r_{ij}^{ab}\{\hat{a}^\dagger\hat{i}\hat{b}^\dagger\hat{j}\} + \cdots .$$

One particle attached(core + 1 system)

$$\hat{R} = \sum_a r^a\hat{a}^\dagger + \sum_{a>b,\ j} r_j^{ba}\hat{b}^\dagger\hat{j}\hat{a}^\dagger + \cdots$$

$$[T_k, R_k] = 0$$

One particle removed(core -1 system)

$$\hat{R} = \sum_i r_i\hat{i} + \sum_{b,\ j>i} r_{ji}^b\hat{b}^\dagger\hat{j}\hat{i} + \sum_{b>c,\ j>k>i} r_{jki}^{bc}\hat{b}^\dagger\hat{j}\hat{c}^\dagger\hat{k}\hat{i} + \cdots .$$

Two particle attached/removed(core +2/-2 system)

EOM-CC

$$H_N R_k e^T|HF\rangle = \Delta E_k R_k e^T|HF\rangle$$

R_k Commutes with T_k

$$\mathcal{H}R_k|HF\rangle = \Delta E_k R_k|HF\rangle$$

$$[\mathcal{H}, R_k]|HF\rangle = (\Delta E_k - \Delta E_0)R_k|HF\rangle$$

H can only contract with. R_k from right side(same as T_k) as it contains only particle Or hole generation operator.

$$(\mathcal{H}R_k)_C|HF\rangle = \omega_k R_k|HF\rangle$$

Good Eigenvalue problem

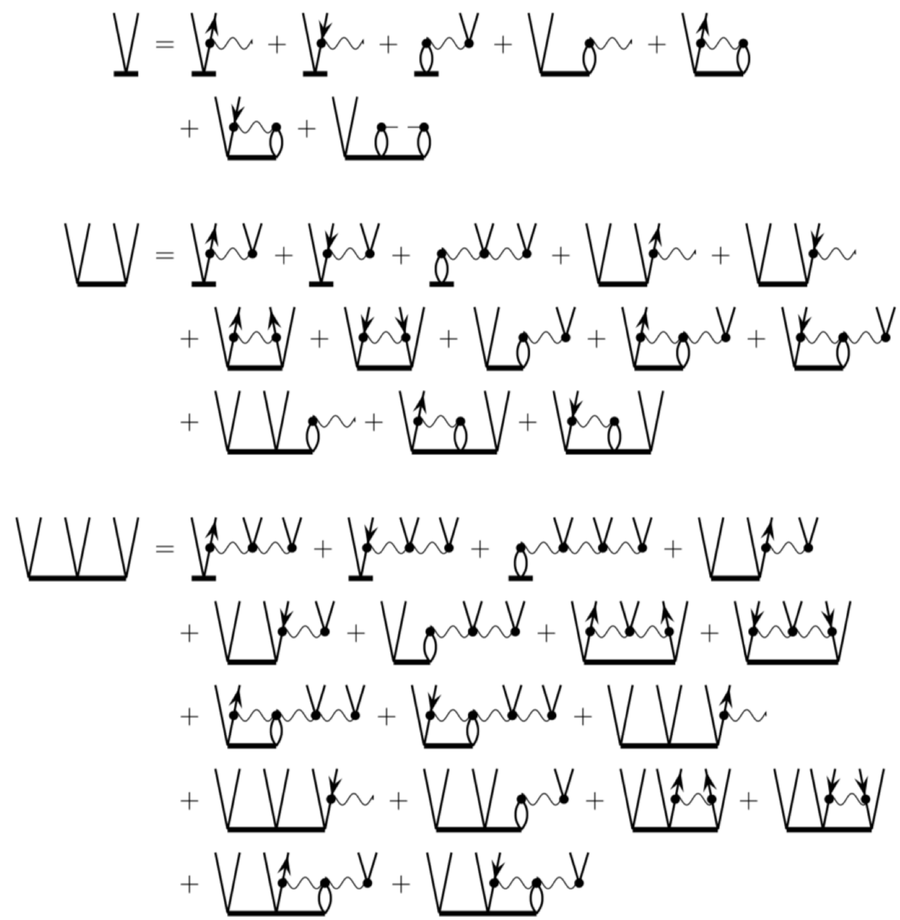
$$(\mathcal{H}R_k)_C|HF\rangle = \omega_k R_k|HF\rangle$$

$$\left(\hat{P}\mathcal{H}\hat{Q}\hat{R}_k\hat{P}\right)_{\mathrm{C}} = \omega_k r_0 \hat{P}\,,$$

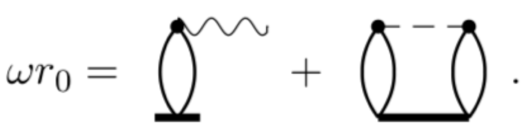
$$\left(\hat{Q}\mathcal{H}\hat{Q}\hat{R}_k\hat{P}\right)_{\mathrm{C}} = \omega_k \hat{Q}\hat{R}_k\hat{P}\,.$$

$$\sum_d \chi_{ad} r_i^d - \sum_l \chi_{li} r_l^a + \sum_{dl} \chi_{ladi} r_l^d + \sum_{dl} \chi_{ld} r_{il}^{ad} + \tfrac{1}{2}\sum_{del} \chi_{alde} r_{il}^{de}$$
$$- \tfrac{1}{2}\sum_{dlm} \chi_{lmid} r_{lm}^{ad} + \tfrac{1}{4}\sum_{delm} \langle lm\|de\rangle r_{ilm}^{ade} = \omega r_i^a \qquad \text{(for all } i, a\text{)},$$

$$\hat{P}(ij)\sum_d \chi_{abej} r_i^d - \hat{P}(ab)\sum_l \chi_{lbij} r_l^a + \sum_{dl} \chi_{labdij} r_l^d + \hat{P}(ab)\sum_d \chi_{bd} r_{ij}^{ad}$$
$$- \hat{P}(ij)\sum_l \chi_{lj} r_{il}^{ab} + \tfrac{1}{2}\sum_{de} \chi_{abde} r_{ij}^{de} + \tfrac{1}{2}\sum_{lm} \chi_{lmij} r_{lm}^{ab}$$
$$+ \hat{P}(ab|ij)\sum_{dl} \chi_{lbdj} r_{il}^{ad} + \tfrac{1}{2}\hat{P}(ij)\sum_{del} \chi_{albdej} r_{il}^{de} - \tfrac{1}{2}\hat{P}(ab)\sum_{dlm} \chi_{lmbidj} r_{lm}^{ae}$$
$$+ \sum_{dl} \chi_{ld} r_{ijl}^{abd} + \tfrac{1}{2}\hat{P}(ab)\sum_{del} \chi_{alde} r_{ilj}^{deb} - \tfrac{1}{2}\hat{P}(ij)\sum_{dlm} \chi_{lmid} r_{lmj}^{adb}$$
$$= \omega r_{ij}^{ab} \qquad \text{(for all } i > j,\ a > b\text{)},$$



$$\omega r_0 = \sum_{dl} \chi_{ld} r_l^d + \tfrac{1}{4}\sum_{delm} \langle lm\|de\rangle r_{lm}^{de}\,.$$



Operator expectation of EOM-CC

Left wavefunction:

$$\langle 0|\hat{L}_k\mathcal{H} = \langle 0|\hat{L}_k\Delta E_k\,.$$

$$\hat{L}_k = l_0 + \sum_{i,a} l_a^i\{\hat{i}^\dagger\hat{a}\} + \sum_{i<j,\ a<b} l_{ab}^{ij}\{\hat{i}^\dagger\hat{a}\hat{j}^\dagger\hat{b}\} + \cdots$$

Nether left wf or right wf are normalized to one:

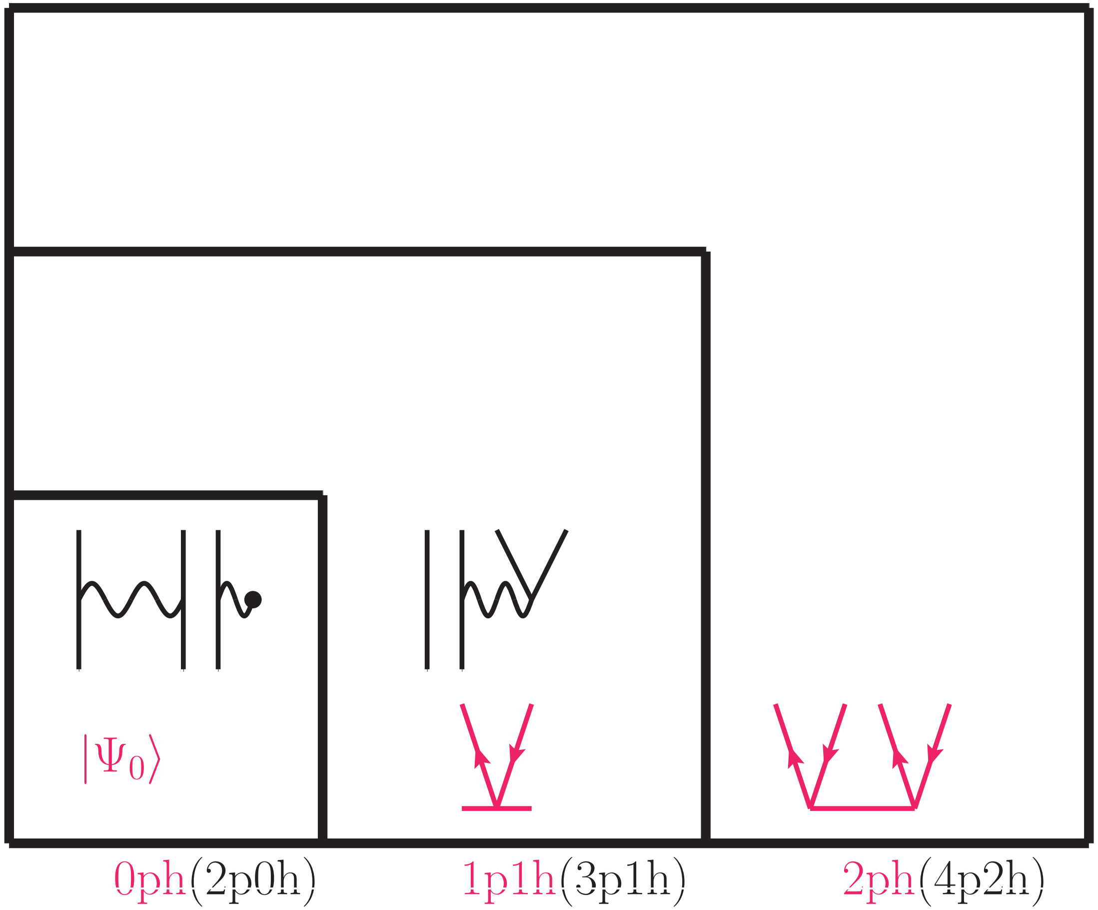
$$\langle 0|\hat{L}_k\hat{R}_l|0\rangle = \delta_{kl}\,.$$

$$\overline{O} = \frac{\langle\Psi|\hat{O}|\Psi\rangle}{\langle\Psi|\Psi\rangle}\,.$$

For energy: $$\langle 0|\hat{L}_k\mathcal{H}\hat{R}_l|0\rangle = E_l\delta_{lk}$$

For other observables: $$\langle 0|\hat{L}_k\mathcal{O}\hat{R}_l|0\rangle = \langle\mathcal{O}\rangle$$

Other method: SMCC



Thanks

Non-Hermitian Hamiltonian

- Expectation value of coupled cluster

$$\overline{O} = \frac{\langle\Psi|\hat{O}|\Psi\rangle}{\langle\Psi|\Psi\rangle}\,.$$

$$\begin{aligned}\overline{O} &= \frac{\langle 0|e^{\hat{T}^\dagger}\hat{O}e^{\hat{T}}|0\rangle}{\langle 0|e^{\hat{T}^\dagger}e^{\hat{T}}|0\rangle} \\ &= \frac{\langle 0|\left[1+T^\dagger+\frac{1}{2!}(T^\dagger)^2+\frac{1}{3!}(T^\dagger)^3+\cdots\right]\hat{O}\left[1+T+\frac{1}{2!}T^2+\frac{1}{3!}T^3+\cdots\right]|0\rangle}{\langle 0|\left[1+\hat{T}^\dagger+\frac{1}{2!}(\hat{T}^\dagger)^2+\frac{1}{3!}(\hat{T}^\dagger)^3+\cdots\right]\left[1+\hat{T}+\frac{1}{2!}\hat{T}^2+\frac{1}{3!}\hat{T}^3+\cdots\right]|0\rangle}\,.\end{aligned}$$

$$\begin{aligned}\Delta E &= \frac{\langle 0|e^{\hat{T}^\dagger}\hat{H}_{\mathrm{N}}e^{\hat{T}}|0\rangle}{\langle 0|e^{\hat{T}^\dagger}e^{\hat{T}}|0\rangle} = \frac{\langle 0|e^{\hat{T}^\dagger}e^{\hat{T}}(\hat{P}+\hat{Q})e^{-\hat{T}}\hat{H}_{\mathrm{N}}e^{\hat{T}}|0\rangle}{\langle 0|e^{\hat{T}^\dagger}e^{\hat{T}}|0\rangle} \\ &= \frac{\langle 0|e^{\hat{T}^\dagger}e^{\hat{T}}|0\rangle\langle 0|e^{-\hat{T}}\hat{H}_{\mathrm{N}}e^{\hat{T}}|0\rangle}{\langle 0|e^{\hat{T}^\dagger}e^{\hat{T}}|0\rangle} = \langle 0|e^{-\hat{T}}\hat{H}_{\mathrm{N}}e^{\hat{T}}|0\rangle = \langle 0|\mathcal{H}|0\rangle\,.\end{aligned}$$

- CC decoupled the Hamiltonian only for energy

Failure of Feynman-Hellman

Solution to Left wave function of CC

$$\hat{P}(1+\Lambda\hat{Q})(\mathcal{H}-\Delta E)=0$$

$$\Lambda = \Lambda_1 + \Lambda_2 + \Lambda_3 + \cdots ,$$

where

$$\Lambda_1 = \sum_{ia} \lambda_a^i \{i^\dagger a\} ,$$

$$\Lambda_2 = \tfrac{1}{4} \sum_{ijab} \lambda_{ab}^{ij} \{i^\dagger a j^\dagger b\} ,$$

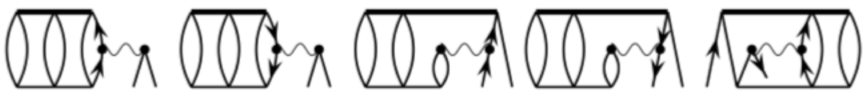
$$\Lambda_n = \frac{1}{(n!)^2} \sum_{\substack{ij\dots \\ ab\dots}} \lambda_{ab\dots}^{ij\dots} \{i^\dagger a j^\dagger b \cdots\} ,$$

$$\hat{P}\mathcal{H}\hat{Q} + \hat{P}(\Lambda\mathcal{H})_{\mathrm{C}}\hat{Q} + \hat{P}\mathcal{H}\hat{Q}\Lambda\hat{Q} = 0$$

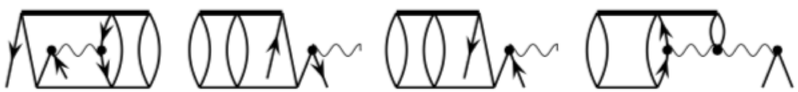
$$\begin{aligned}
&\langle 0|\hat{H}_{\mathrm{N}} e^{\hat{T}}|\Phi_{ij\dots}^{ab\dots}\rangle_{\mathrm{C}} + \langle 0|\Lambda\big(\hat{H}_{\mathrm{N}} e^{\hat{T}}\big)_{\mathrm{C}}|\Phi_{ij\dots}^{ab\dots}\rangle_{\mathrm{C}} \\
&+ \sum_{\substack{k<l<\cdots \\ c<d<\cdots}} \langle 0|\hat{H}_{\mathrm{N}} e^{\hat{T}}|\Phi_{kl\dots}^{cd\dots}\rangle_{\mathrm{C}} \langle \Phi_{kl\dots}^{cd\dots}|\Lambda|\Phi_{ij\dots}^{ab\dots}\rangle = 0 .
\end{aligned}$$

1 3 4 5 18 19 26 27

48 49 50 51 52



53 54 55 56 57



58 59 60 75

1 2 4 5 8 9 10

11 12 23 24 33 34

45 46 47 48 55

56 57 58 59