Coupled cluster theory for open shell nuclei

Two particles attached to a closed-shell reference

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Outline

- Coupled-cluster theory.
- Two particles attached EOM.
- Preliminary results for $A = 18$ nuclei.
- Outlook

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Coupled Cluster summary

Wavefunction:

$$|\Psi\rangle \approx |\Psi_{CC}\rangle = e^{\hat{\mathrm{T}}}|\Phi_0\rangle \qquad \hat{\mathrm{T}} = \hat{\mathrm{T}}_1 + \hat{\mathrm{T}}_2 + \ldots + \hat{\mathrm{T}}_A$$

$$\hat{\mathrm{T}}_n = \left(\frac{1}{n!}\right)^2 \sum_{\substack{i_1,i_2,\ldots i_n \\ a_1,a_2,\ldots a_n}} t_{i_1 i_2 \ldots i_n}^{a_1 a_2 \ldots a_n} a_{a_1}^\dagger a_{a_2}^\dagger \ldots a_{a_n}^\dagger a_{i_n} \ldots a_{i_2} a_{i_1}.$$

Energy equation:

$$E_{\mathrm{CC}} = \langle \Phi_0 | \bar{\mathrm{H}} | \Phi_0 \rangle, \qquad \bar{\mathrm{H}} = e^{-\hat{\mathrm{T}}} \hat{\mathrm{H}} e^{\hat{\mathrm{T}}} - \langle \Phi_0 | \hat{\mathrm{H}} | \Phi_0 \rangle$$

Amplitude equations:

$$0 = \langle \Phi_{i_1 \ldots i_n}^{a_1 \ldots a_n} | \bar{\mathrm{H}} | \Phi_0 \rangle$$

Coupled cluster wavefunction

Manybody basis - All possible Slater determinants that can be constructed out of a given set of single particle wavefunctions.

$$|\Psi\rangle = \hat{\mathrm{C}}|\Phi_0\rangle \qquad \hat{\mathrm{C}} = \hat{1} + \hat{\mathrm{C}}_1 + \hat{\mathrm{C}}_2 + \ldots + \hat{\mathrm{C}}_A$$

$$\hat{\mathrm{C}}_n = \left(\frac{1}{n!}\right)^2 \sum_{\substack{i_1, i_2, \ldots i_n \\ a_1, a_2, \ldots a_n}} c_{i_1 i_2 \ldots i_n}^{a_1 a_2 \ldots a_n} a_{a_1}^\dagger a_{a_2}^\dagger \ldots a_{a_n}^\dagger a_{i_n} \ldots a_{i_2} a_{i_1} .$$

Reparametrization of $\hat{\mathrm{C}}_n$, not a change of basis.

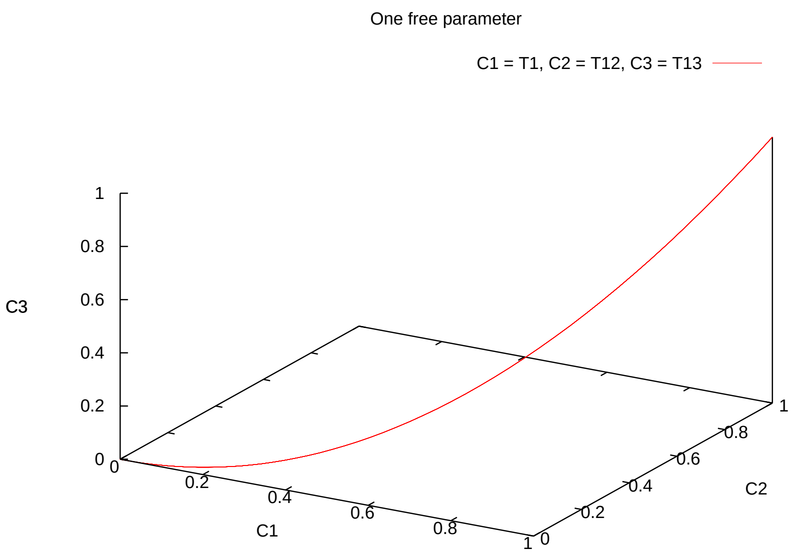
$$\hat{\mathrm{C}}_1 = \hat{\mathrm{T}}_1 \qquad \hat{\mathrm{C}}_2 = \frac{1}{2}\hat{\mathrm{T}}_1^2 + \hat{\mathrm{T}}_2$$

$$\hat{\mathrm{C}}_3 = \frac{1}{6}\hat{\mathrm{T}}^3 + \hat{\mathrm{T}}_1\hat{\mathrm{T}}_2 + \hat{\mathrm{T}}_3 \qquad \hat{\mathrm{C}}_4 = \frac{1}{24}\hat{\mathrm{T}}_1^4 + \frac{1}{2}\hat{\mathrm{T}}_1^2\hat{\mathrm{T}}_2 + \frac{1}{2}\hat{\mathrm{T}}_2^2 + \hat{\mathrm{T}}_1\hat{\mathrm{T}}_3 + \hat{\mathrm{T}}_4$$

$$\vdots \qquad\qquad \vdots$$

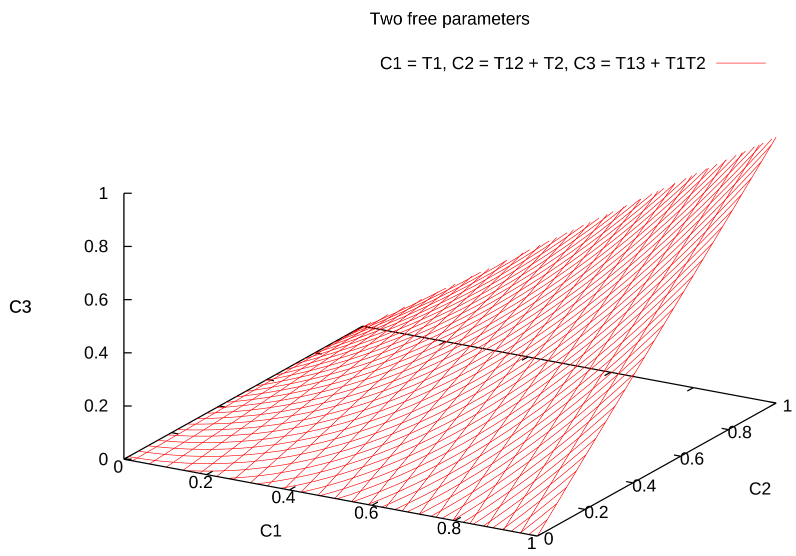
A simple picture

A line in $\mathbb{R}^3$



$$\hat{C}_1 = \hat{T}_1$$
$$\hat{C}_2 = \hat{T}_1^2$$
$$\hat{C}_3 = \hat{T}_1^3$$

A surface in $\mathbb{R}^3$



$$\hat{C}_1 = \hat{T}_1$$
$$\hat{C}_2 = \hat{T}_1^2 + \hat{T}_2$$
$$\hat{C}_3 = \hat{T}_1^3 + \hat{T}_1\hat{T}_2$$

Theory - 1

Suppose $|\Psi_0\rangle$ is the coupled-cluster wavefunction, so that

$$|\Psi_0\rangle = e^{\hat{\mathrm{T}}}|\Phi_0\rangle, \qquad \hat{\mathrm{T}} = \hat{\mathrm{T}}_1 + \hat{\mathrm{T}}_2 + \cdots + \hat{\mathrm{T}}_N,$$

where N is the number of particles in the system, $\hat{\mathrm{T}}_n$ is a n-particle, n-hole excitation operator and $|\Phi_0\rangle$ is the reference determinant in your chosen basis.

Theory - 2

Any other $N \pm k$-particle state $|\Psi_\mu^{N\pm k}\rangle$, can be reached by applying the proper excitation operator - $\hat{\mathrm{R}}_\mu^{N\pm k}$ - to this reference state

$$|\Psi_\mu^{N\pm k}\rangle = \hat{\mathrm{R}}_\mu^{N\pm k}|\Psi_0\rangle = \hat{\mathrm{R}}_\mu^{N\pm k} e^{\hat{\mathrm{T}}}|\Phi_0\rangle.$$

Theory - 3

We write a separate Schrødinger equation for these two states

$$\hat{\mathrm{H}}|\Psi_0\rangle = E_0|\Psi_0\rangle$$
$$\hat{\mathrm{H}}|\Psi_\mu^{N\pm k}\rangle = E_\mu^{N\pm k}|\Psi_\mu^{N\pm k}\rangle$$

and take the difference where the top Schrødinger equation has been left-multiplied with $\hat{\mathrm{R}}_\mu^{N\pm k}$

$$\hat{\mathrm{H}}|\Psi_\mu^{N\pm k}\rangle - \hat{\mathrm{R}}_\mu^{N\pm k}\hat{\mathrm{H}}|\Psi_0\rangle = E_\mu^{N\pm k}|\Psi_\mu^{N\pm k}\rangle - \hat{\mathrm{R}}_\mu^{N\pm k}E_0|\Psi_0\rangle$$

Theory - 4

The EOM-CC equations are derived by a short calculation

$$
\begin{aligned}
\hat{\mathrm{H}}|\Psi_\mu^{N\pm k}\rangle - \hat{\mathrm{R}}_\mu^{N\pm k}\hat{\mathrm{H}}|\Psi_0\rangle &= E_\mu^{N\pm k}|\Psi_\mu^{N\pm k}\rangle - \hat{\mathrm{R}}_\mu^{N\pm k}E_0|\Psi_0\rangle \\
\hat{\mathrm{H}}\hat{\mathrm{R}}_\mu^{N\pm k}e^{\hat{\mathrm{T}}}|\Phi_0\rangle - \hat{\mathrm{R}}_\mu^{N\pm k}\hat{\mathrm{H}}e^{\hat{\mathrm{T}}}|\Phi_0\rangle &= E_\mu^{N\pm k}\hat{\mathrm{R}}_\mu^{N\pm k}e^{\hat{\mathrm{T}}}|\Phi_0\rangle - \hat{\mathrm{R}}_\mu^{N\pm k}E_0 e^{\hat{\mathrm{T}}}|\Phi_0\rangle \\
\left(e^{-\hat{\mathrm{T}}}\hat{\mathrm{H}}e^{\hat{\mathrm{T}}}\hat{\mathrm{R}}_\mu^{N\pm k} - \hat{\mathrm{R}}_\mu^{N\pm k}e^{-\hat{\mathrm{T}}}\hat{\mathrm{H}}e^{\hat{\mathrm{T}}}\right)|\Phi_0\rangle &= \omega_\mu^{N\pm k}\hat{\mathrm{R}}_\mu^{N\pm k}e^{-\hat{\mathrm{T}}}e^{\hat{\mathrm{T}}}|\Phi_0\rangle
\end{aligned}
$$

$$
\left[\bar{\mathrm{H}}, \hat{\mathrm{R}}\right]|\Phi_0\rangle = \omega\hat{\mathrm{R}}|\Phi_0\rangle \tag{1}
$$

where $\omega_\mu^{N\pm k} = E_\mu^{N\pm k} - E_0$ and $\bar{\mathrm{H}} = e^{-\hat{\mathrm{T}}}\hat{\mathrm{H}}e^{\hat{\mathrm{T}}}$. The cumbersome sub- and superscripts has been suppressed in the last equation.

Theory - 5

The commutator form allows us to use the connected cluster theorem and ensures only contributions from terms where $\bar{\mathrm{H}}$ and $\hat{\mathrm{R}}$ are connected. The EOM-CC equations can now be written

$$\left(\bar{\mathrm{H}}\hat{\mathrm{R}}\right)_c |\Phi_0\rangle = \omega\hat{\mathrm{R}}|\Phi_0\rangle$$

By rewriting $\hat{\mathrm{R}}$ as a vector **R** the EOM-CC equations (1)now become an eigenvalue problem

$$(\bar{\mathrm{H}}\mathbf{R})_c = \omega\mathbf{R} \tag{2}$$

The form of $\hat{\mathrm{R}}$ determines what target system we are looking at and also the specific form of the matrix to diagonalize. We solve the eigenvalue problem using the Implicitly Restarted Arnoldi Method (IRAM), where only the matrix-vector product is used to solve for the eigenpairs.

Two particles attached (2PA-EOM-CCSD)

The reference wavefunction is calculated using $\hat{\mathrm{T}} = \hat{\mathrm{T}}_1 + \hat{\mathrm{T}}_2$ and $\hat{\mathrm{R}}$ is parametrized

$$\hat{\mathrm{R}} = \hat{\mathrm{R}}_2 + \ldots \hat{\mathrm{R}}_{N+2},$$

where N is the number of particles in the reference wavefunction and

$$\hat{\mathrm{R}}_n = \frac{1}{n!(n-2)!} \sum_{\substack{a_1,\ldots a_n \\ i_1,\ldots i_{n-2}}} r_{i_1\ldots i_{n-2}}^{a_1\ldots a_n} a_{a_1}^\dagger \ldots a_{a_n}^\dagger a_{i_{n-2}} \ldots a_{i_1},$$

We want to solve for the $n_p^n n_h^{n-2}$ unknowns $r_{i_1\ldots i_{n-2}}^{a_1\ldots a_n}$.

Two particles attached (2PA-EOM-CCSD)

Introduce approximations by a truncation in $\hat{\mathrm{R}}$.

2PA-EOM-CCSD(2p0h)

$$\hat{\mathrm{R}} = \hat{\mathrm{R}}_2 = \frac{1}{2}\sum_{a,b} r^{ab} a_a^\dagger a_b^\dagger$$

2PA-EOM-CCSD(3p1h)

$$\hat{\mathrm{R}} = \hat{\mathrm{R}}_2 + \hat{\mathrm{R}}_3 = \frac{1}{2}\sum_{a,b} r^{ab} a_a^\dagger a_b^\dagger + \frac{1}{6}\sum_{a,b,c,i} r_i^{abc} a_a^\dagger a_b^\dagger a_c^\dagger a_i$$

Two particles attached (2PA-EOM-CCSD)

The n'th element of the matrix-vector product in (2) is defined

2PA-EOM-CCSD(2p0h) - $N = n_p^2$

$$R_n = \langle \Phi^{ab} | \left(\bar{\mathrm{H}} \hat{\mathrm{R}}_1 \right)_c | \Phi_0 \rangle, \quad n = (a-1) * n_p + b$$

2PA-EOM-CCSD(3p1h) - $N = n_p^2 + n_p^3 n_h$

$$R_n = \langle \Phi^{ab} | \left(\bar{\mathrm{H}} \hat{\mathrm{R}}_1 \right)_c | \Phi_0 \rangle + \langle \Phi^{ab} | \left(\bar{\mathrm{H}} \hat{\mathrm{R}}_2 \right)_c | \Phi_0 \rangle$$

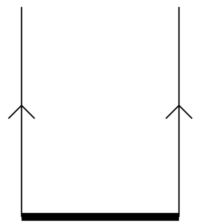
$$n = (a-1) * n_p + b$$

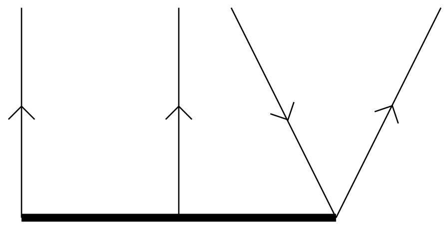
$$R_n = \langle \Phi_i^{abc} | \left(\bar{\mathrm{H}} \hat{\mathrm{R}}_1 \right)_c | \Phi_0 \rangle + \langle \Phi_i^{abc} | \left(\bar{\mathrm{H}} \hat{\mathrm{R}}_2 \right)_c | \Phi_0 \rangle$$

$$n = n_p^2 + (i-1) * n_p^3 + (c-1) * n_p^2 + (b-1) * n_p + c$$

Two particles attached (2PA-EOM-CCSD)

Diagram forms of $\hat{\mathrm{R}}$.

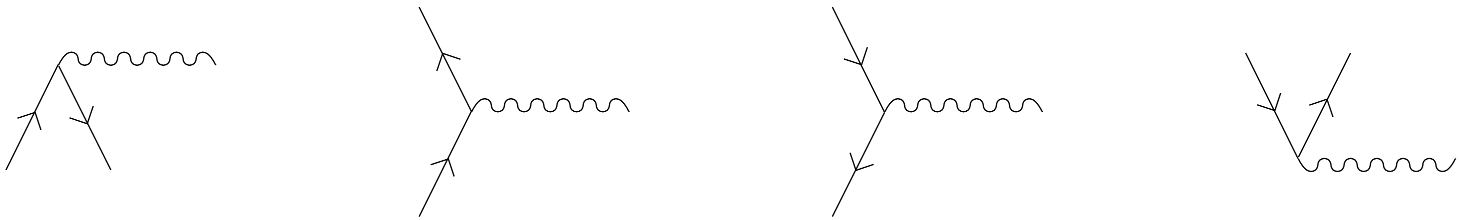
$\hat{\mathrm{R}}_1 =$ 

$\hat{\mathrm{R}}_2 =$ 

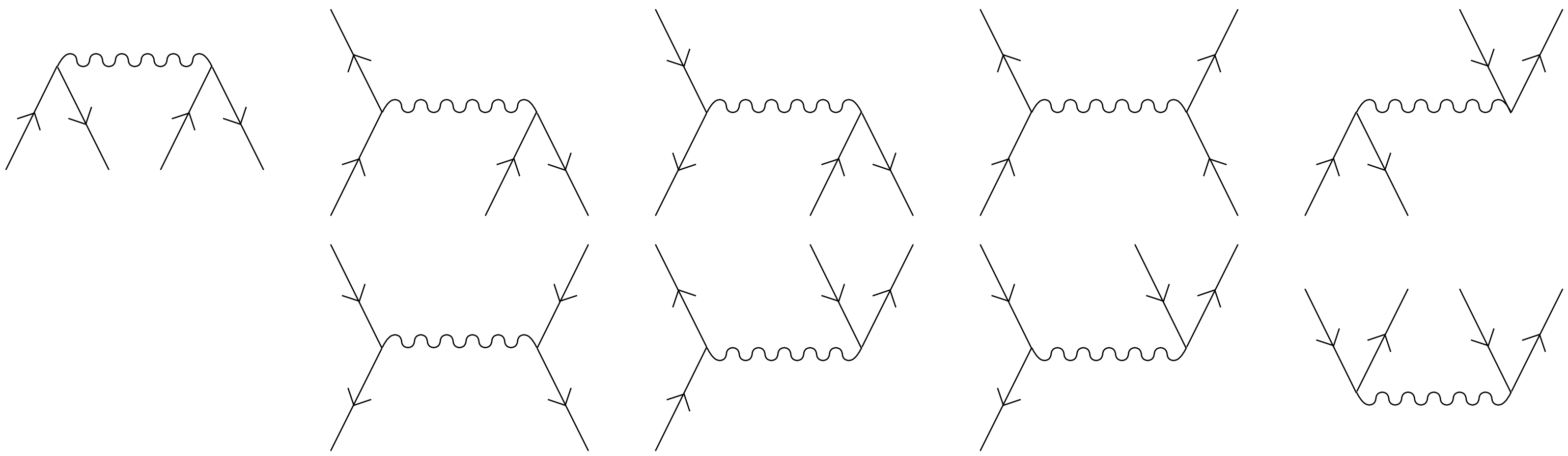
Two particles attached (2PA-EOM-CCSD)

Diagram forms of $\bar{\mathrm{H}}$.

One-body part



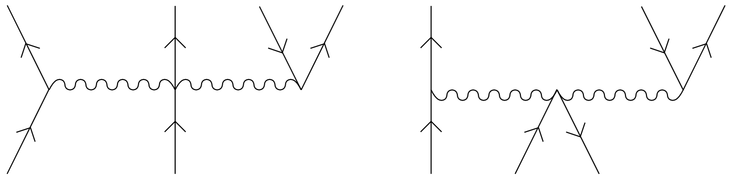
Two-body part



Two particles attached (2PA-EOM-CCSD)

Diagram forms of $\bar{\mathrm{H}}$.

Three-body part

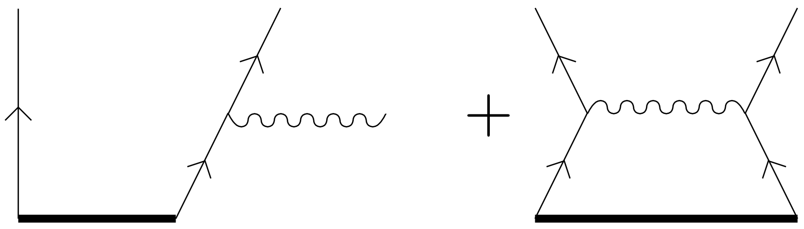


Two particles attached (2PA-EOM-CCSD)

Working equations for 2PA-EOM-CCSD(2p0h)

Diagram equations

$$\langle \Phi^{ab} | \left(\bar{\mathrm{H}} \hat{\mathrm{R}}_1 \right)_c | \Phi_0 \rangle =$$



Algebraic equations

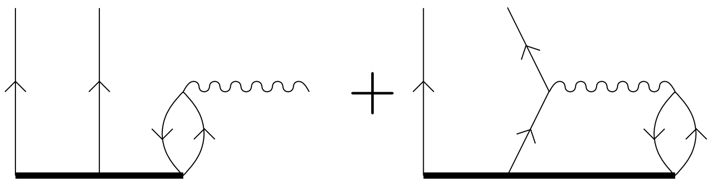
$$\langle \Phi^{ab} | \left(\bar{\mathrm{H}} \hat{\mathrm{R}} \right)_c | \Phi_0 \rangle = P(ab) \bar{\mathrm{H}}_e^b r^{ae} + \frac{1}{2} \bar{\mathrm{H}}_{ef}^{ab} r^{ef}$$

Two particles attached (2PA-EOM-CCSD)

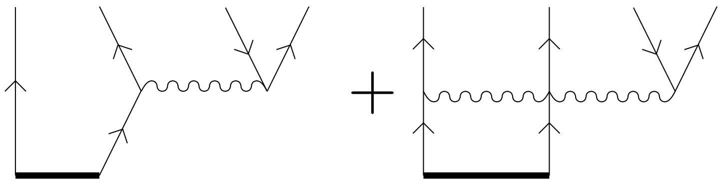
Working equations for 2PA-EOM-CCSD(3p1h)

Diagram equations

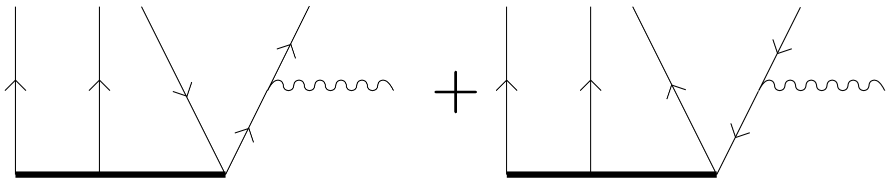
$$\langle \Phi^{ab} | \left(\bar{\mathrm{H}} \hat{\mathrm{R}}_2 \right)_c | \Phi_0 \rangle =$$

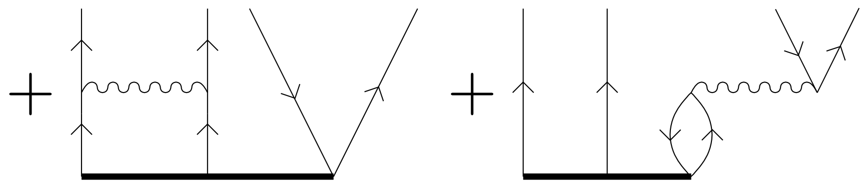


$$\langle \Phi_i^{abc} | \left(\bar{\mathrm{H}} \hat{\mathrm{R}}_1 \right)_c | \Phi_0 \rangle =$$



$$\langle \Phi_i^{abc} | \left(\bar{\mathrm{H}} \hat{\mathrm{R}}_2 \right)_c | \Phi_0 \rangle =$$





Two particles attached (2PA-EOM-CCSD)

Working equations for 2PA-EOM-CCSD(3p1h)

Algebraic equations

$$
\begin{aligned}
\langle \Phi^{ab} | \left(\bar{\mathrm{H}} \hat{\mathrm{R}} \right)_c | \Phi_0 \rangle &= P(ab) \bar{\mathrm{H}}_e^b r^{ae} + \frac{1}{2} \bar{\mathrm{H}}_{ef}^{ab} r^{ef} + \bar{\mathrm{H}}_e^m r_m^{abe} \\
&+ \frac{1}{2} P(ab) \bar{\mathrm{H}}_{ef}^{bm} r_m^{aef} \\
\langle \Phi_i^{abc} | \left(\bar{\mathrm{H}} \hat{\mathrm{R}} \right)_c | \Phi_0 \rangle &= P(a,bc) \bar{\mathrm{H}}_{ei}^{bc} r^{ae} + P(ab,c) \bar{\mathrm{H}}_e^c r_i^{abe} - \bar{\mathrm{H}}_i^m r_m^{abc} \\
&+ \frac{1}{2} P(ab,c) \bar{\mathrm{H}}_{ef}^{ab} r_i^{efc} + P(ab,c) \bar{\mathrm{H}}_{ei}^{mc} r_m^{abe} \\
&+ \frac{1}{2} \bar{\mathrm{H}}_{efi}^{abc} r^{ef}
\end{aligned}
$$

Testcase - ^{6}He

The Hamiltonian and the modelspace

- Intrinsic Hamiltonian

$$\begin{aligned}\hat{\mathrm{H}} &= \hat{\mathrm{T}} - \hat{\mathrm{T}}_{cm} + \hat{\mathrm{V}} \\ &= \left(1 - \frac{1}{A'}\right)\sum_{i=1}^{A}\frac{p_i^2}{2m} + \sum_{i<j=1}^{A}\hat{\mathrm{V}}_{ij} - \frac{\hat{\mathrm{p}}_i \cdot \hat{\mathrm{p}}_j}{mA'},\end{aligned} \tag{3}$$

- Interaction renormalized with SRG (PRC75,061001) using a cutoff of 1.9fm^{-1} and $\hbar\omega = 24$ MeV.
- Four major harmonic oscillator shells, with some modifications.
  - $0s_{1/2}$, $0p_{3/2}$, $0p_{1/2}$, $0d_{5/2}$, $0d_{3/2}$, $1s_{1/2}$ - s, p and sd shell
  - $1p_{3/2}$, $1p_{1/2}$ - pf shell, No $0f_{7/2}$ or $0f_{5/2}$
  - $1d_{5/2}$, $1d_{3/2}$, $2s_{1/2}$
  - Total of 76 basis states, 4 hole states and 72 particle states using approx 500Mb of memory.
  - Resulting in a matrix rank of 5184 and $1.5 \cdot 10^6$ for 2p0h and 3p1h respectivly.

Testcase - ^{6}He

Results

	0_1^+	2_1^+	0^+ $\langle J \rangle$	2_1^+ $\langle J \rangle$
CCSD	-22.732	-20.905	0.78	2
CCSDT-1	-24.617	-21.586	0.25	2
CCSDT	-24.530	-21.786	0.01	2
2PA-EOM-CCSD(2p-0h)	-21.185	-18.996	0	2
2PA-EOM-CCSD(3p-1h)	-24.543	-21.634	0	2
FCI	-24.853	-21.994	0	2

Table: Energies (in MeV) for the ground state and first excited state of ^{6}He and the expectation value of the total angular momentum, calculated with coupled-cluster methods truncated at the 2-particle-2-hole (CCSD) level, 3-particle-3-hole (CCSDT) and a hybrid (CCSDT-1) where the 3-particle-3-hole amplitudes are treated perturbatively.

Preliminary results - $A = 18$ nuclei.

The Hamiltonian and the modelspace

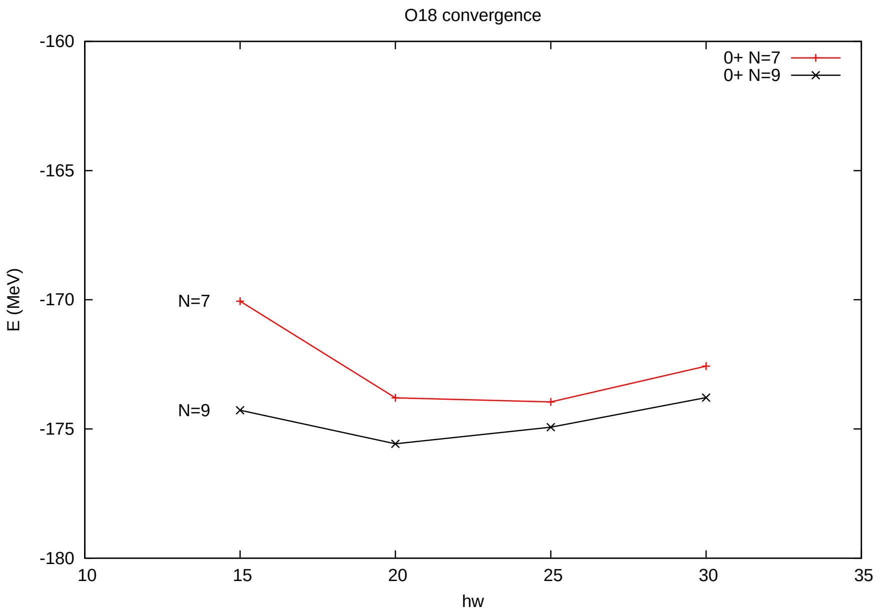
- Intrinsic Hamiltonian

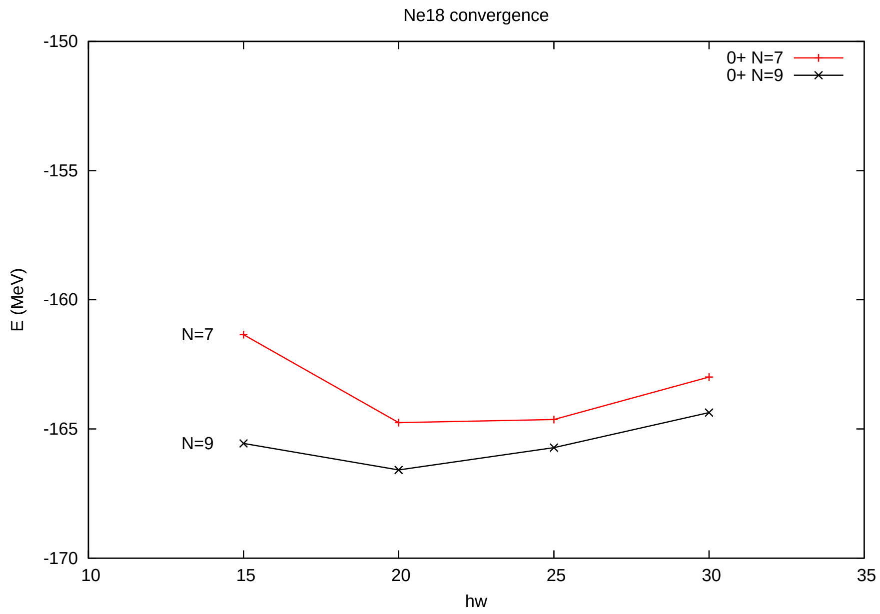
$$\hat{\mathrm{H}} = \hat{\mathrm{T}} - \hat{\mathrm{T}}_{cm} + \hat{\mathrm{V}}$$
$$= \left(1 - \frac{1}{A'}\right) \sum_{i=1}^{A} \frac{p_i^2}{2m} + \sum_{i<j=1}^{A} \hat{\mathrm{V}}_{ij} - \frac{\hat{\mathrm{p}}_i \cdot \hat{\mathrm{p}}_j}{mA'}, \qquad (4)$$

- Chiral interaction (Machleidt, Entem), renormalized using SRG (PRC75,061001) using a cutoff of 1.9fm^{-1} - 2.1fm^{-1} and $\hbar\omega = 15, 20, 25, 30$ MeV.
- Spherical basis
- 8 major oscillator shells for 6 lowest eigenvalues.
- 10 major oscillator shells for 0+ eigenvalues of ^{18}O and ^{18}Ne.
- Matrix rank of $0.5 \cdot 10^6$-$3.5 \cdot 10^6$.

Total energies as a function of $\hbar\omega$

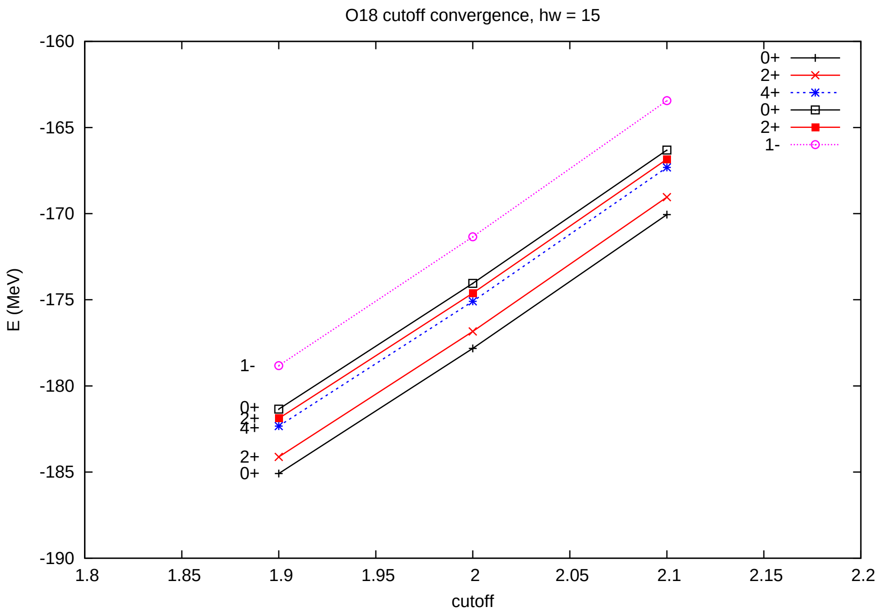
^{18}O ^{18}Ne



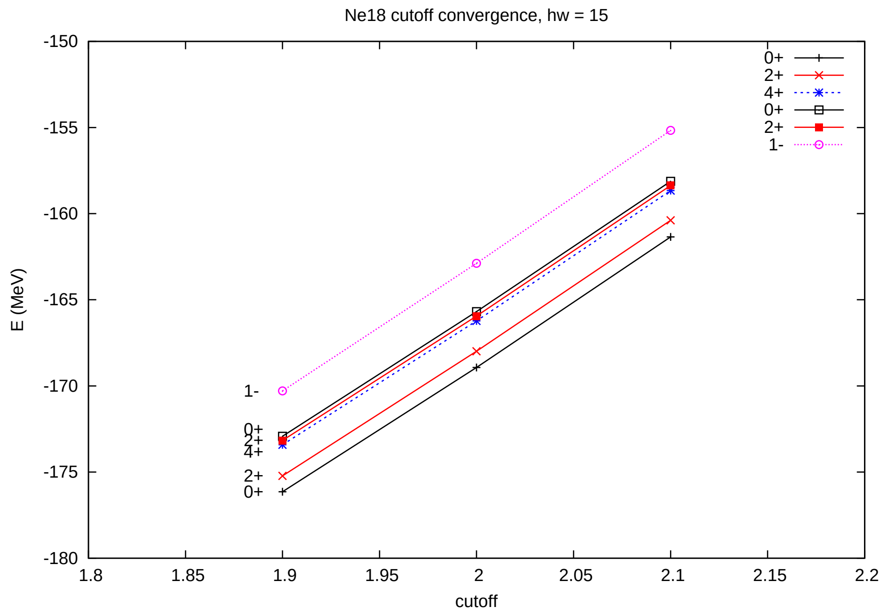


Total energies as a function of cutoff

^{18}O

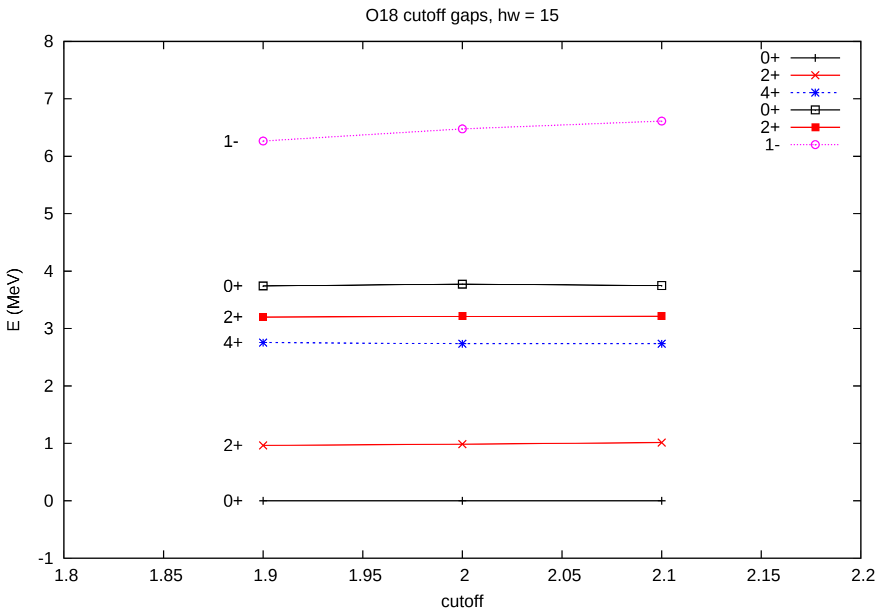


^{18}Ne

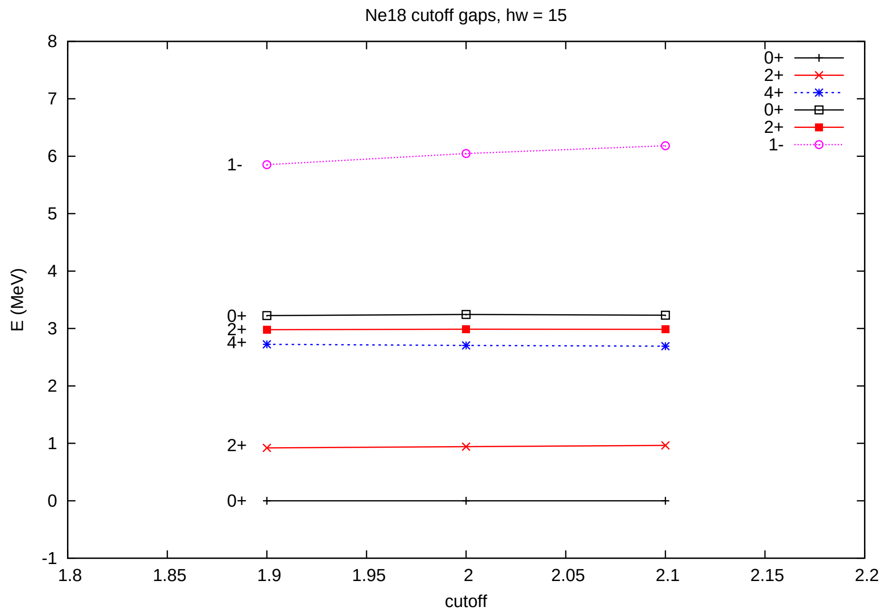


Level spacing as a function of cutoff.

^{18}O

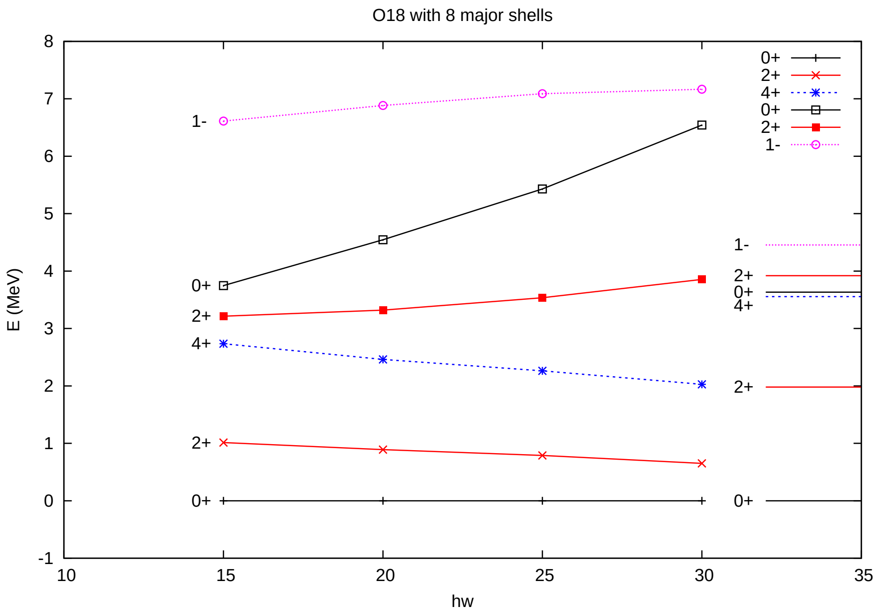


^{18}Ne

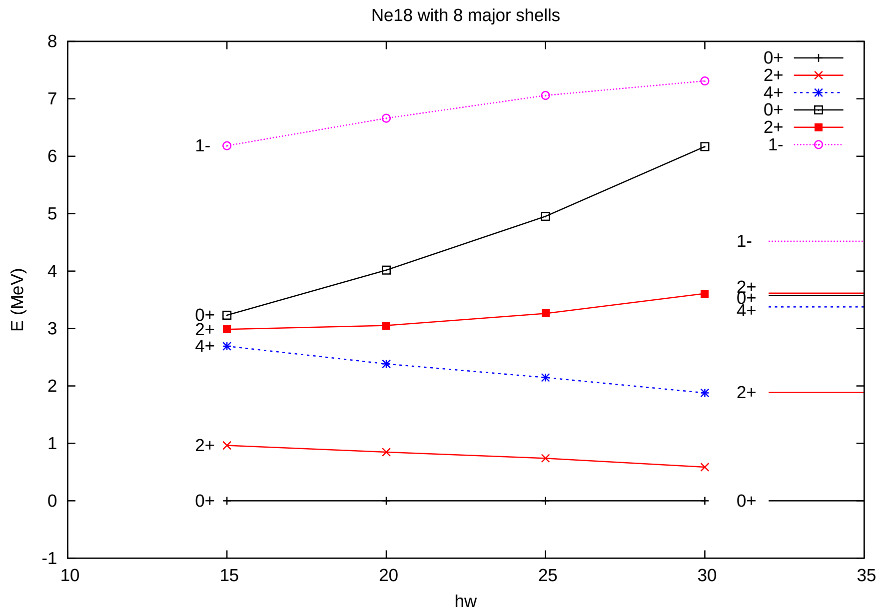


Level spacing as a function of $\hbar\omega$

^{18}O

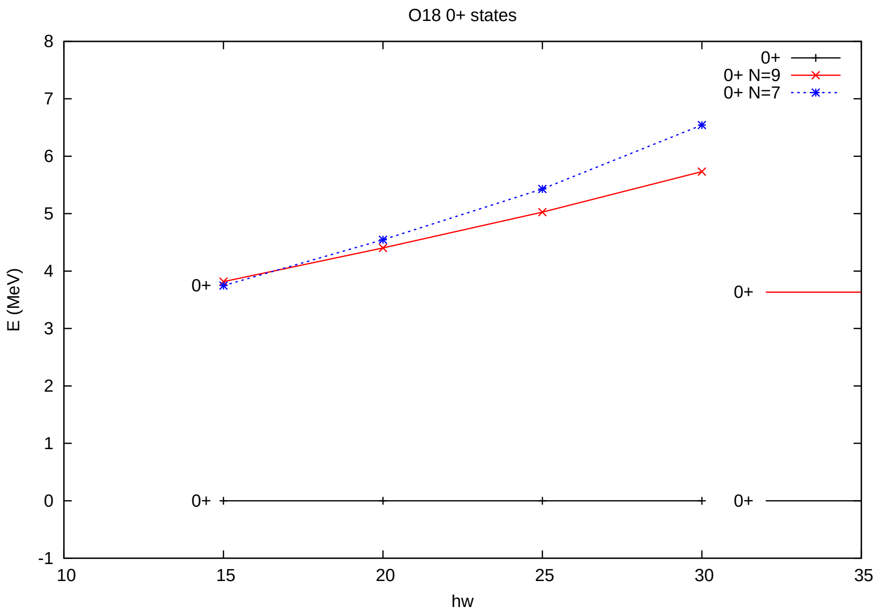


^{18}Ne

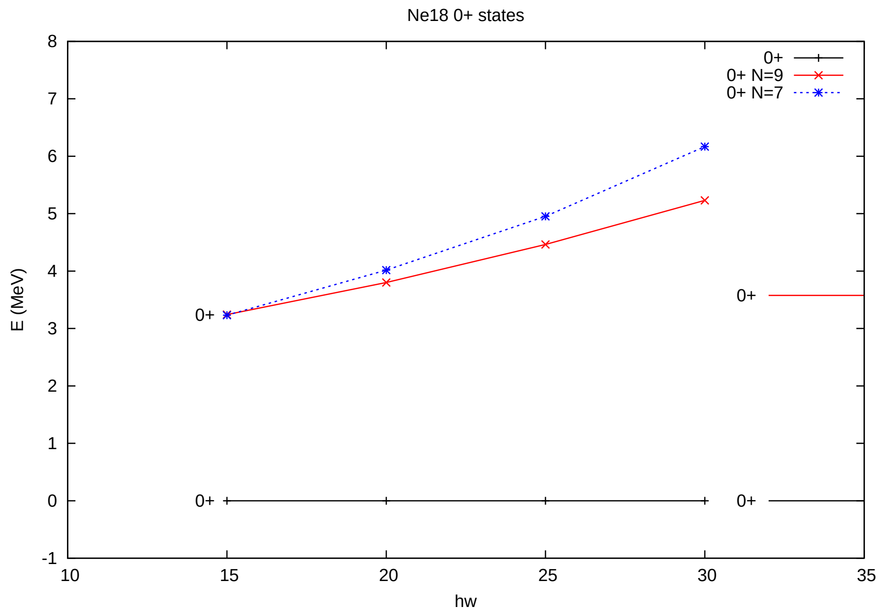


Convergence properties of the second 0+ state

^{18}O



^{18}Ne

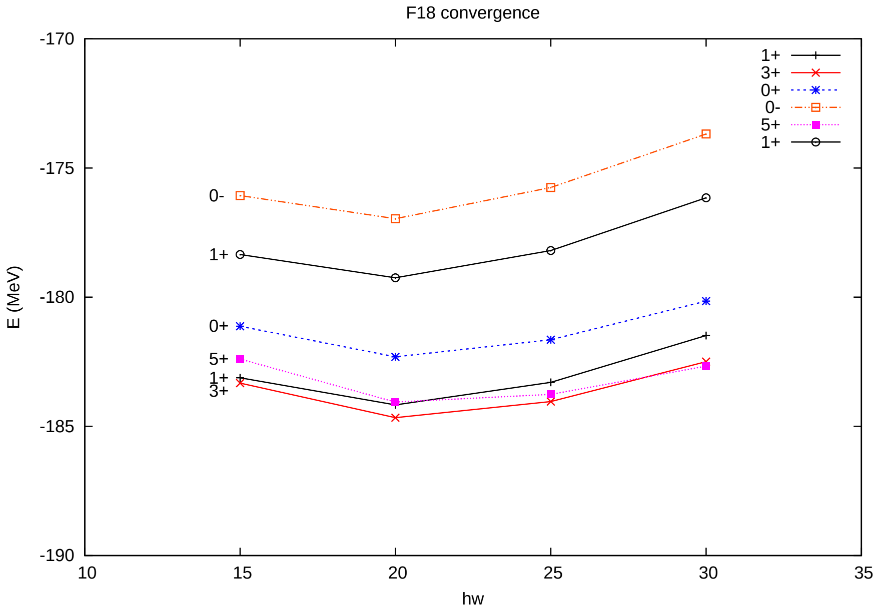


Outlook

- Spherical basis up to 14-15 major oscillator shells (shared memory)
- Shell model effective interaction
- Parallellized for distributed memory
- Include 4p-2h configurations
- Three-body Hamiltonian (without residual)
- CCSDT for the reference wavefunction
- Include hyperon degrees of freedom

JIT calculation ^{18}F

Total energies



Level spacing