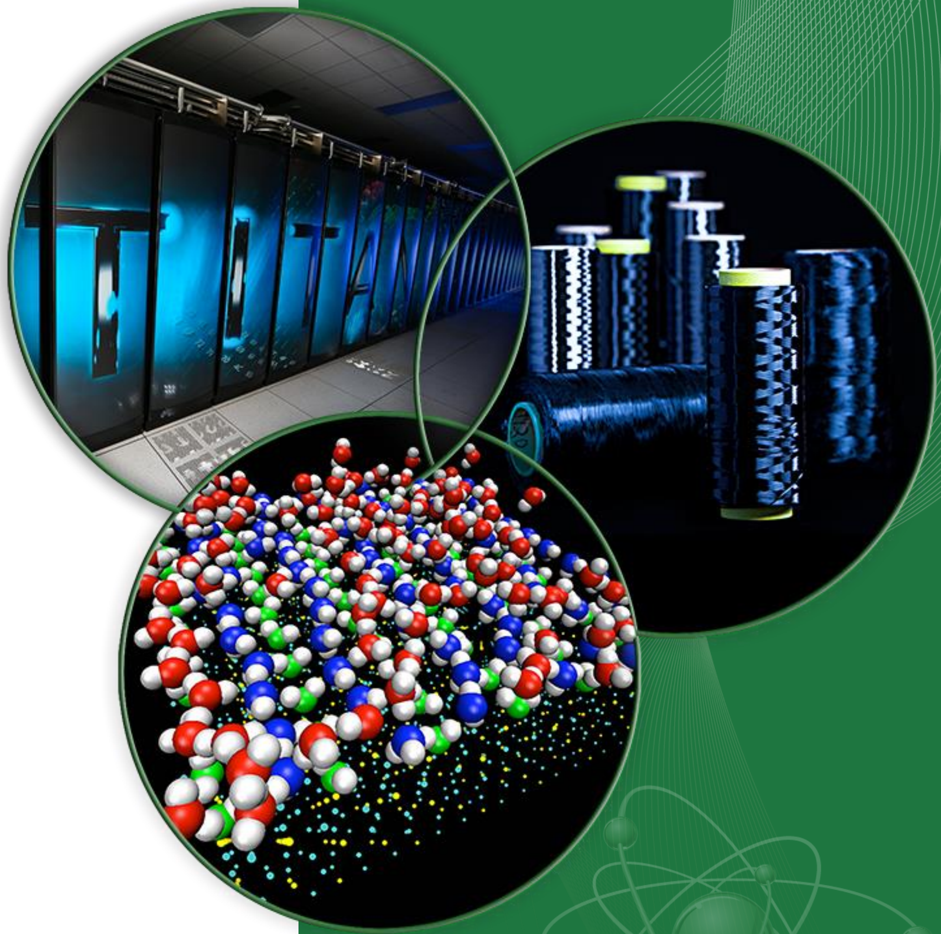
Near closed-shell nuclei from equation-of-motion coupled-cluster theory



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Outline

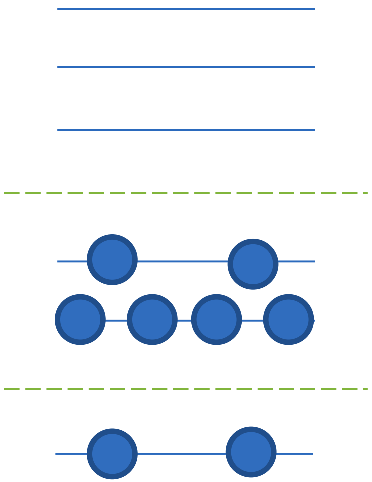
- Hamiltonian
- Three-nucleon forces
- Coupled-cluster summary
- Examples from spherically coupled EOM-CCSD

The nuclear Schrödinger equation

$$H\Psi = E\Psi$$

The basis

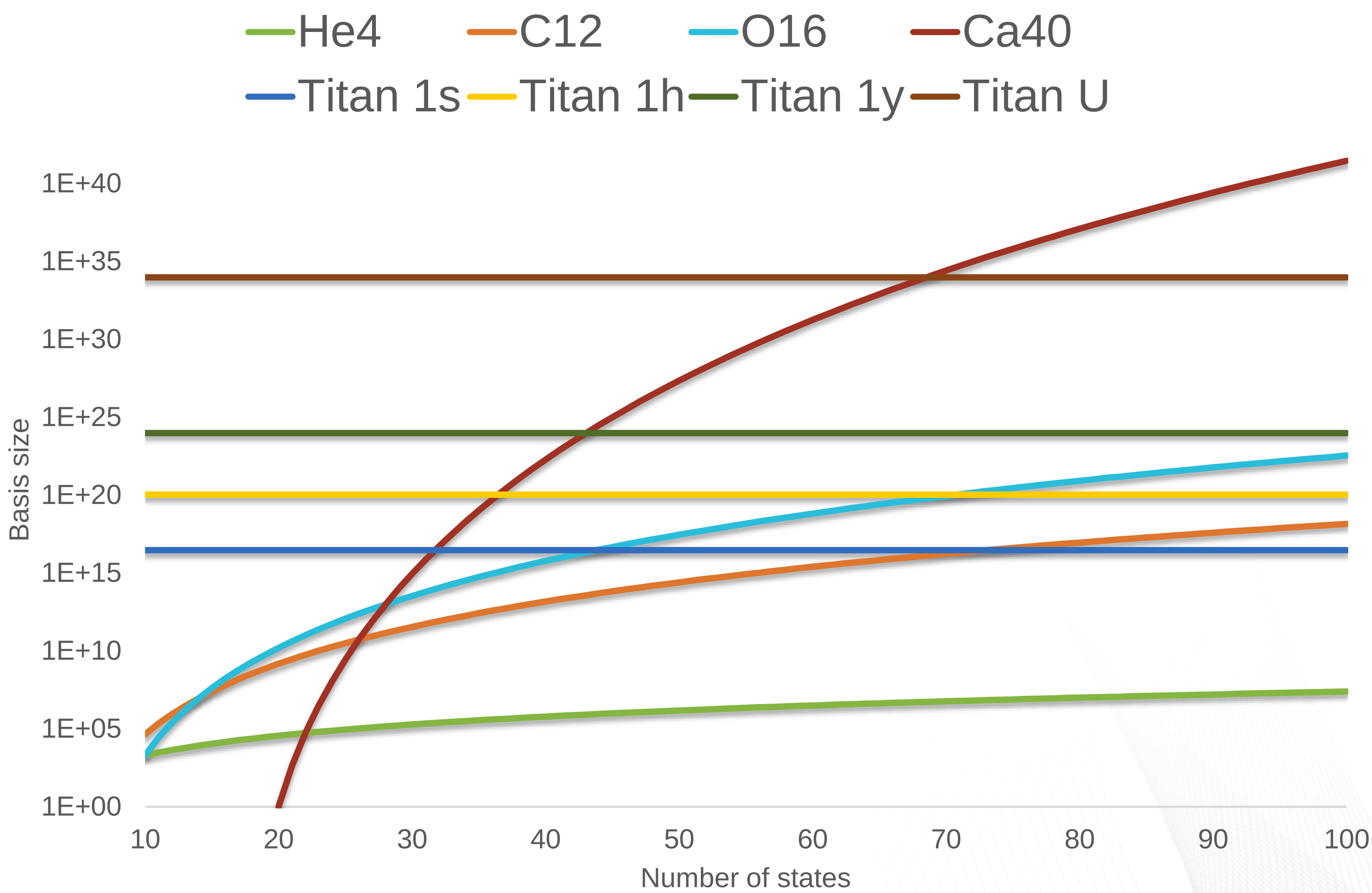
Single particle picture



Fermions

$$\binom{N}{A}$$

Basis size



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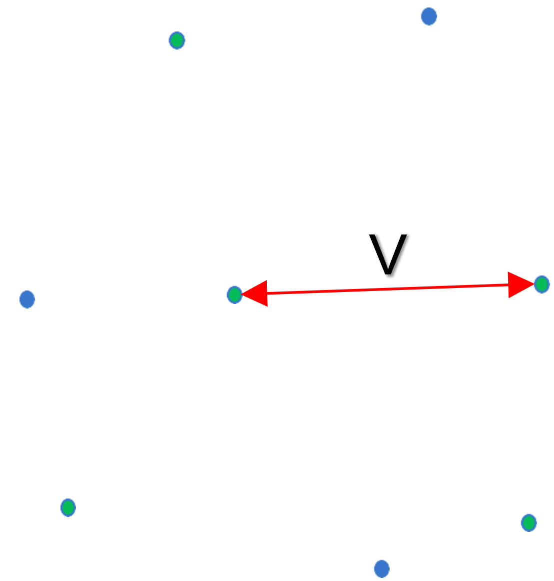
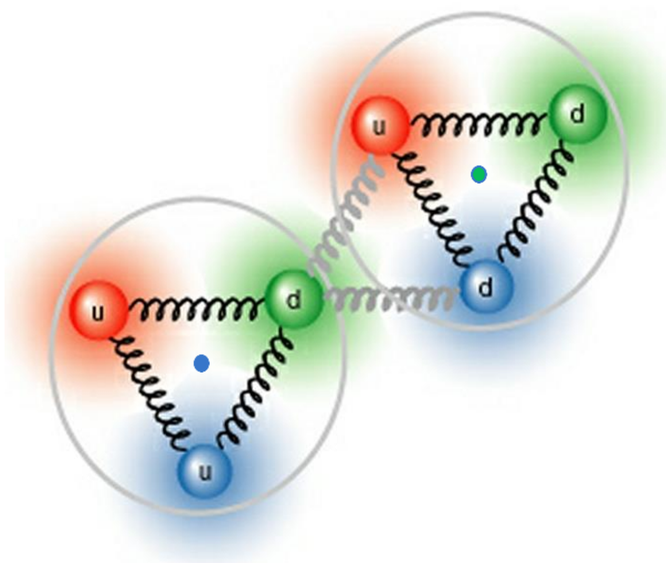
Hamiltonian

The interaction

Interactions between point particles

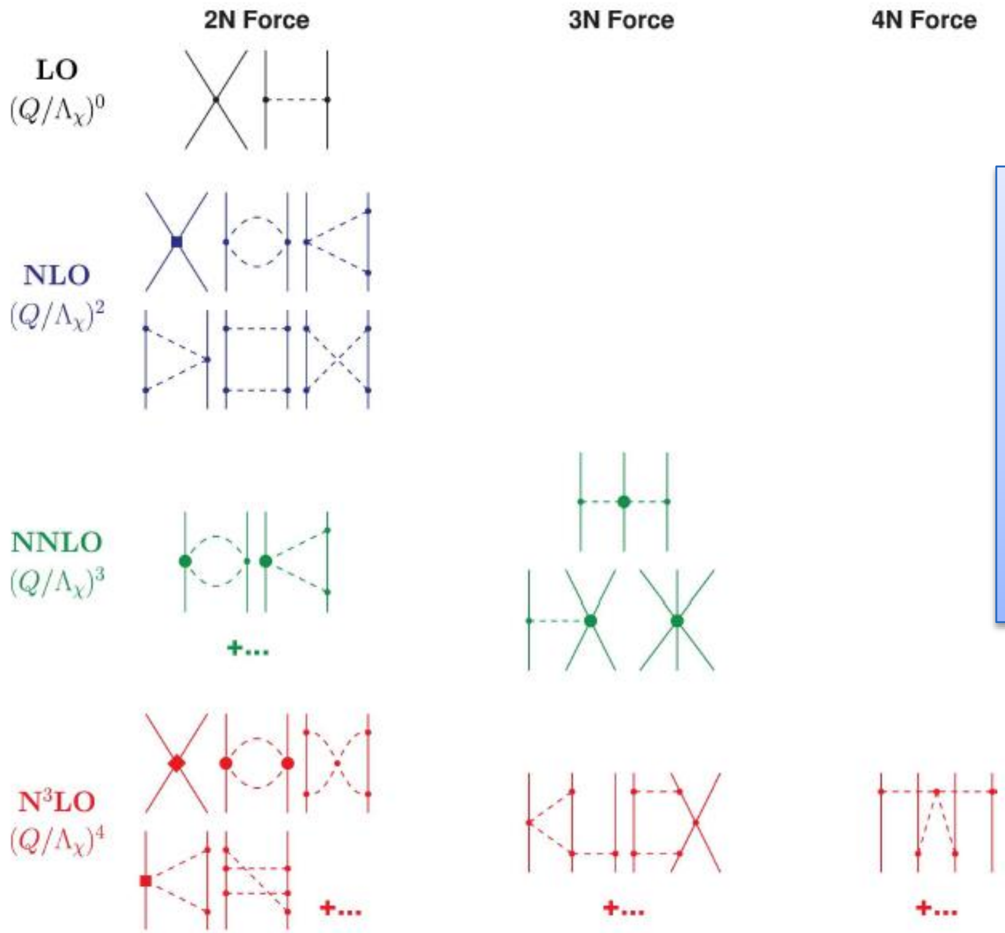




Complicated many-body forces

Three-nucleon forces are crucial!

Chiral effective field theory



- Direct link to QCD
- Perturbative expansion in momentum
- Hierarchy of nuclear forces

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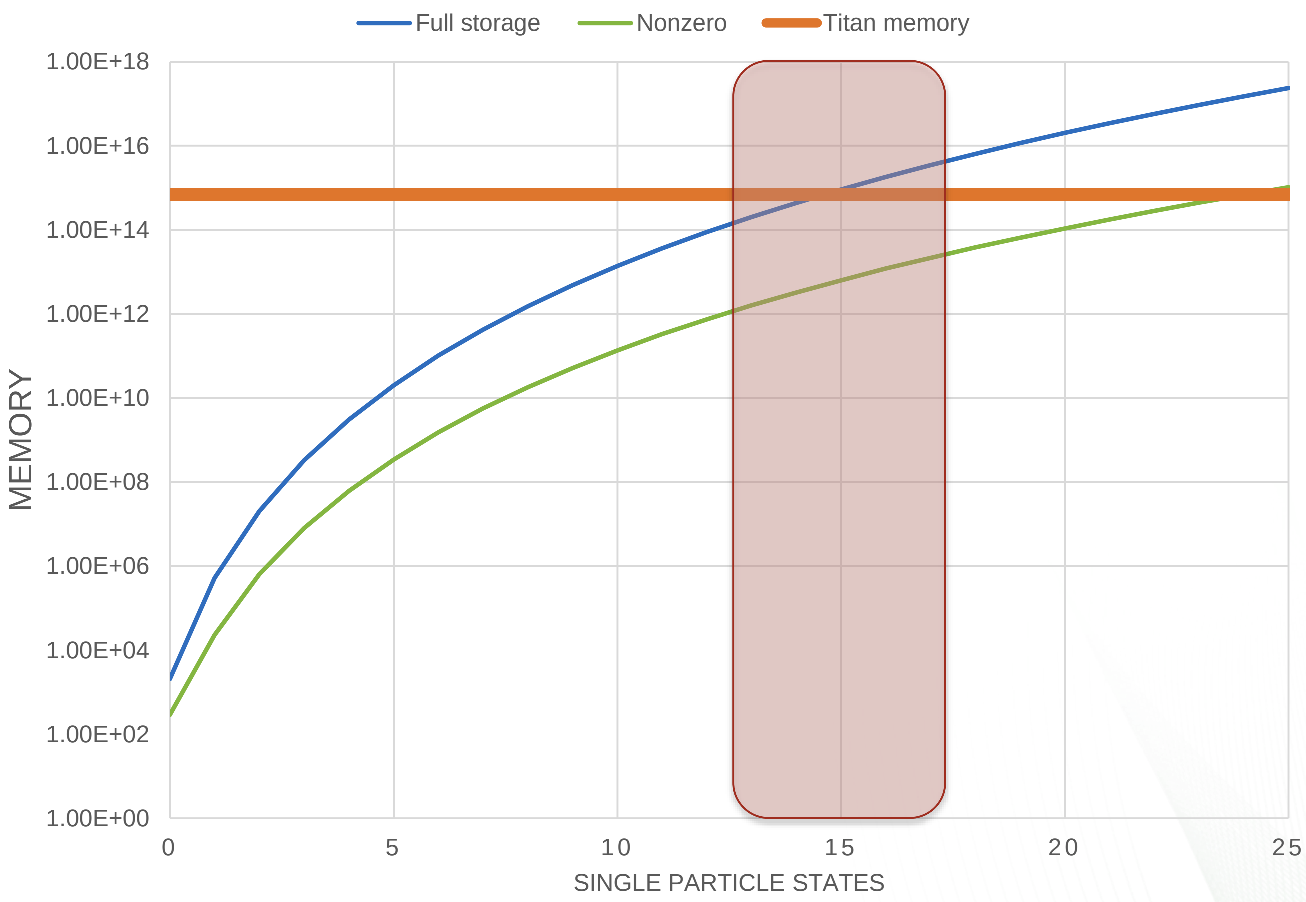
Computing the interaction

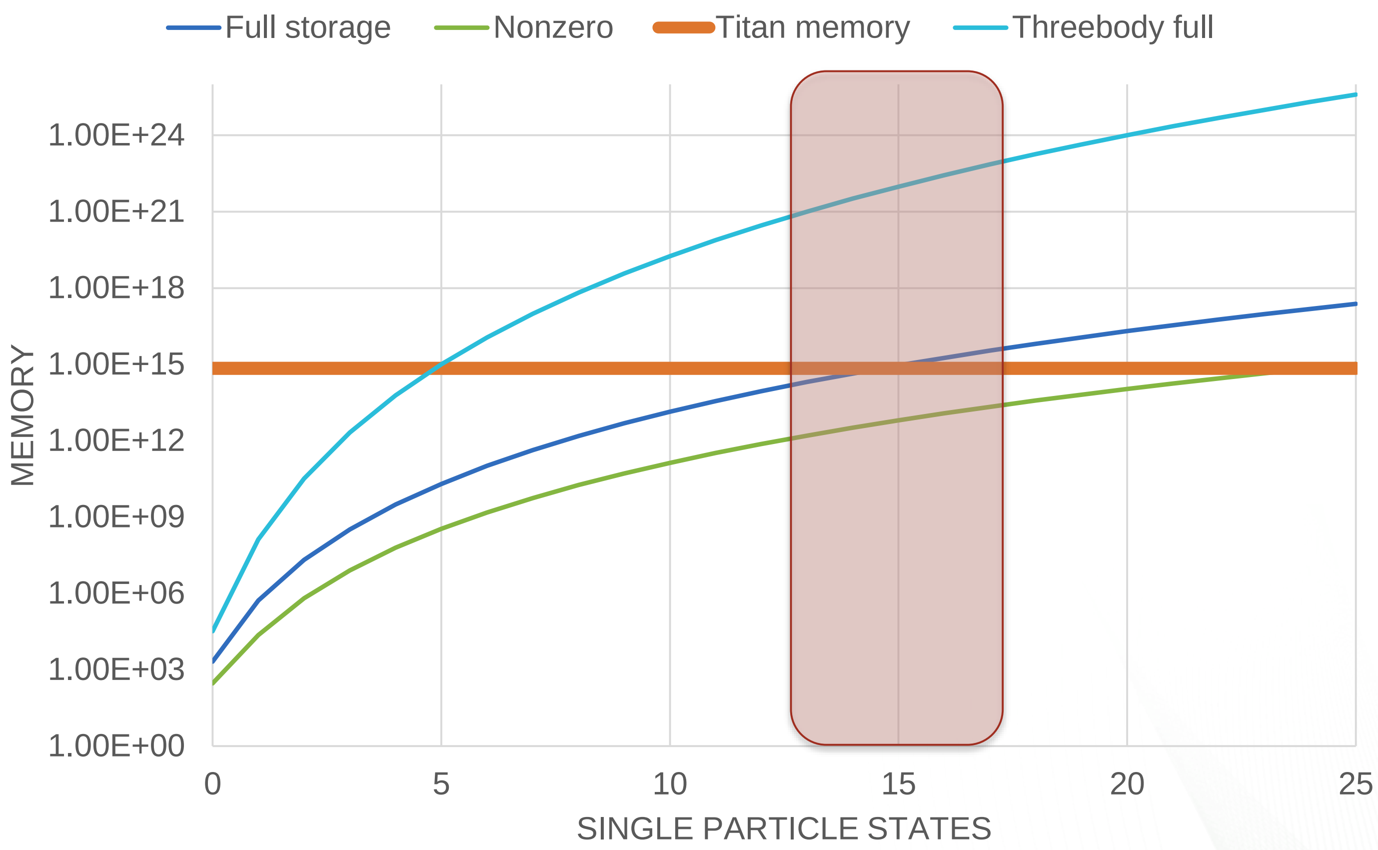
- Not possible to do “on the fly”.
- Three-nucleon forces takes weeks to transform to single particle coordinates.

The interaction elements have to be stored in memory!

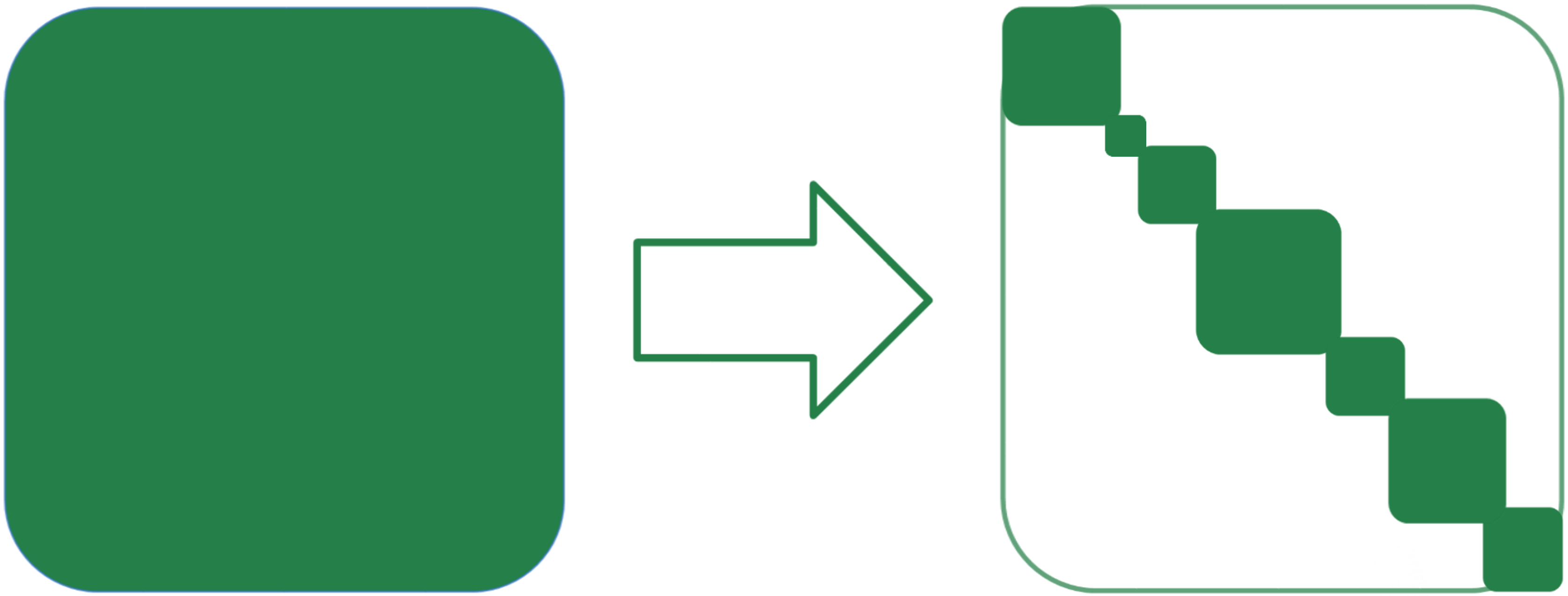
Memory usage



Memory usage



Spherically coupled scheme



Expose invariant subspaces labelled by the total angular momentum

Transformation of a twobody scalar operator

$$\langle ab; j_a m_a j_b m_b | X | cd; j_c m_c j_d m_d \rangle =$$

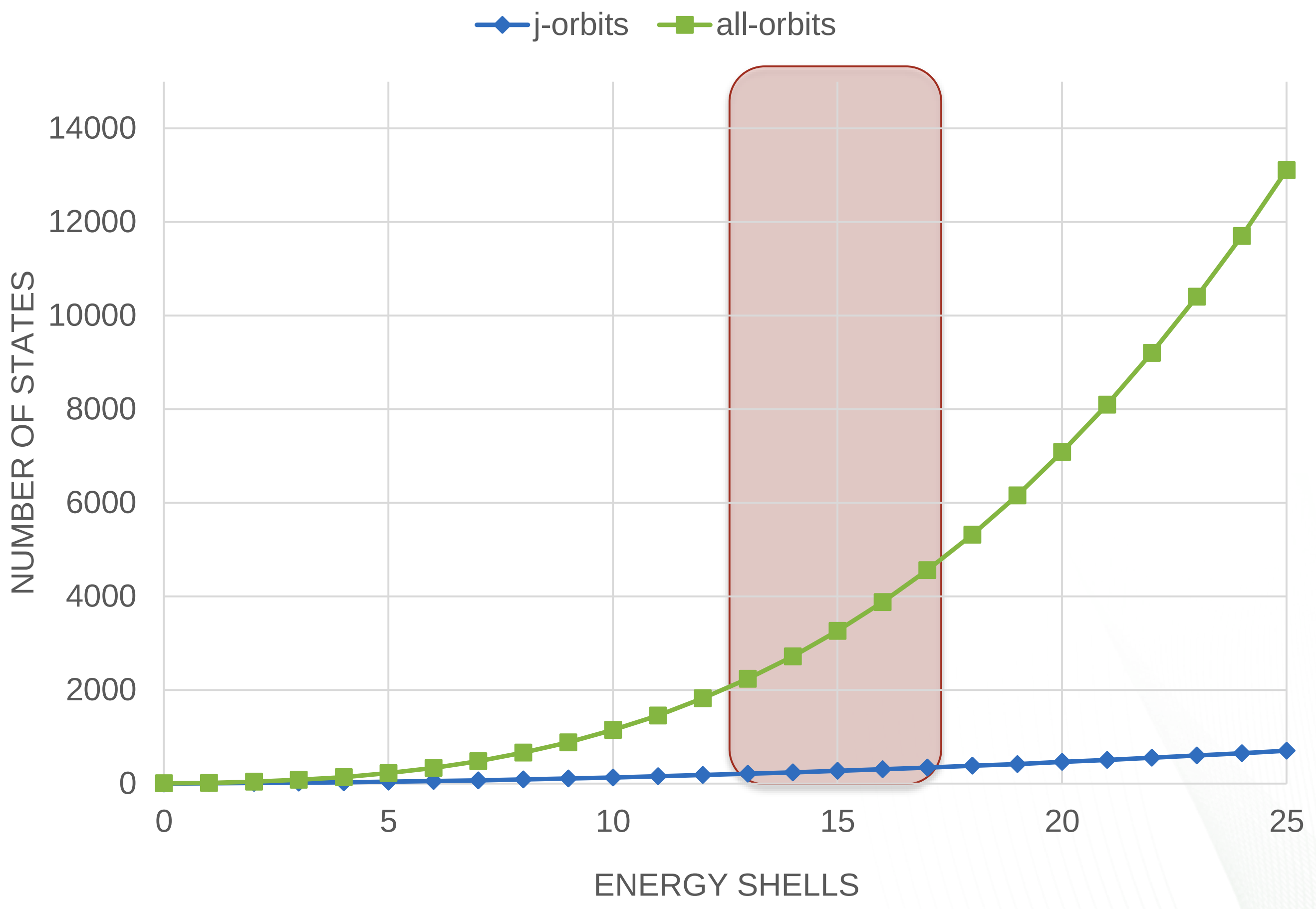
$$\sum_{JM} C^{j_a j_b J}_{m_a m_b M} C^{j_c j_d J}_{m_c m_d M} \langle ab; j_a j_b J || X || cd; j_c j_d J \rangle$$

$$\langle ab; j_a j_b J || X || cd; j_c j_d J \rangle =$$

$$\frac{1}{2J+1} \sum_{m_a m_b m_c m_d M} C^{j_a j_b J}_{m_a m_b M} C^{j_c j_d J}_{m_c m_d M} \langle ab; j_a m_a j_b m_b | X | cd; j_c m_c j_d m_d \rangle$$

1. Different single particle spaces.
2. Matrix elements are independent of projections.

Single particle states



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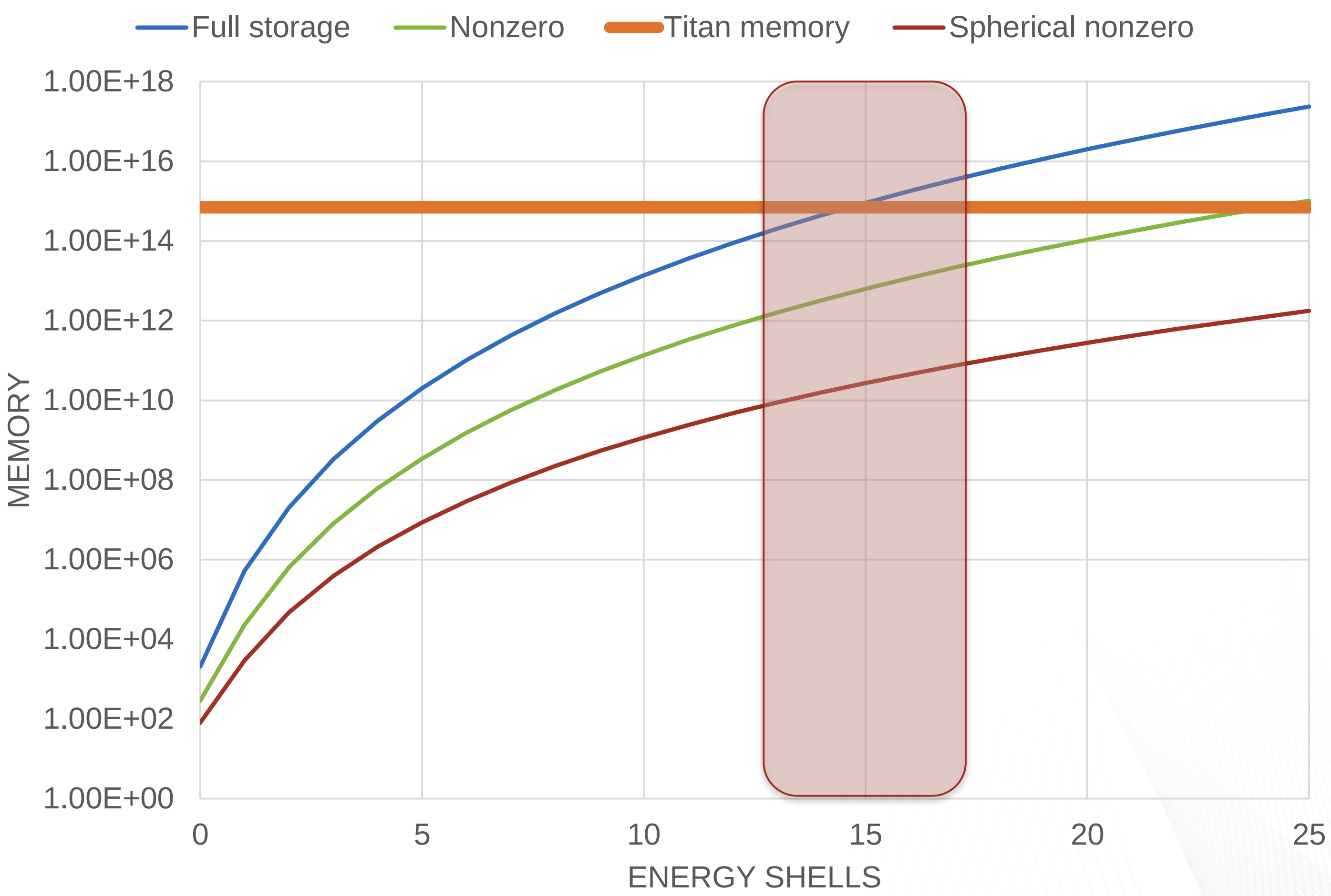
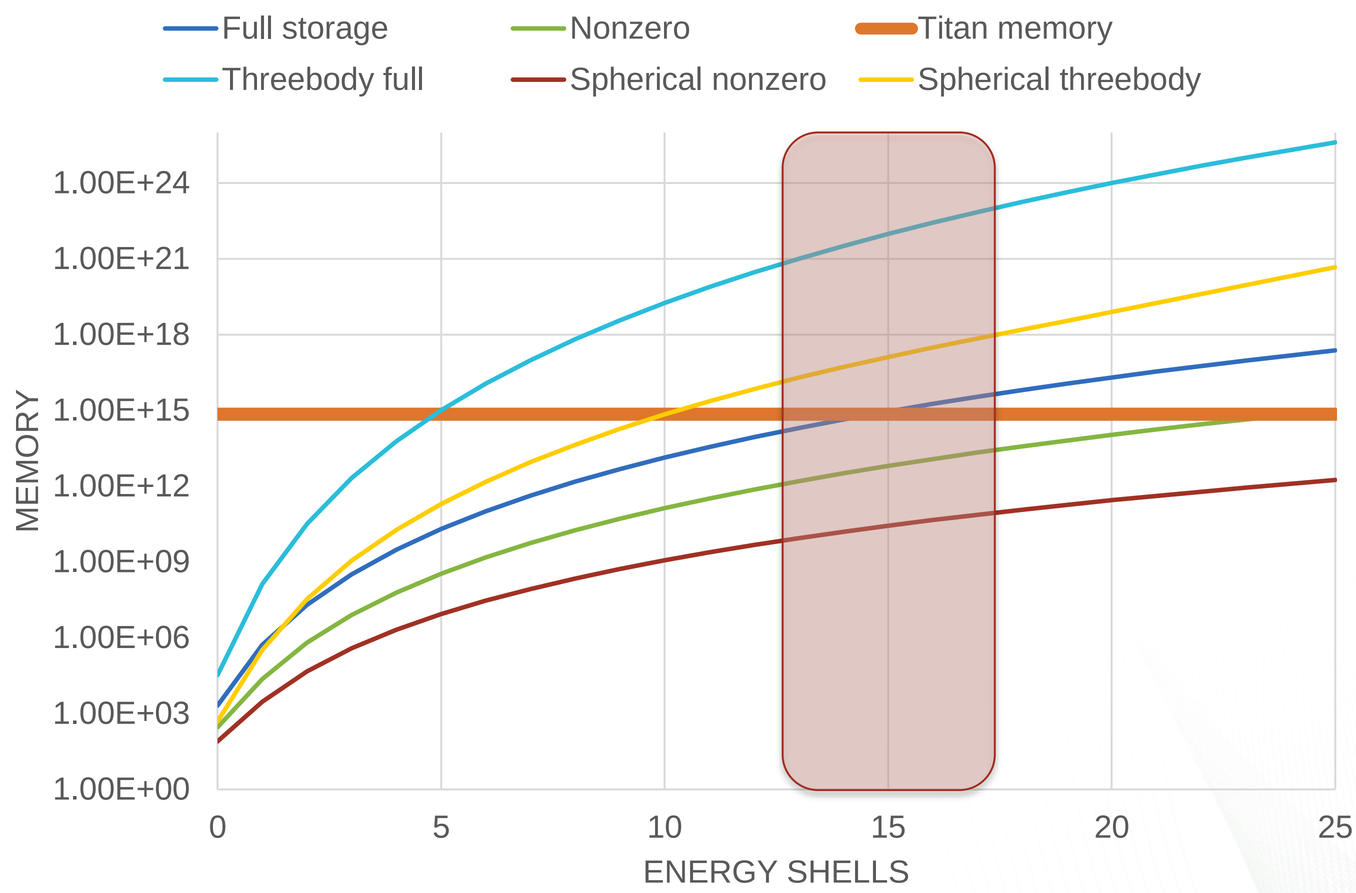
Memory usage



Memory usage



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Three nucleons forces

- Hartree-Fock with full three-nucleon force
  - Current limit: Nmax=14, E3max=18
    - ~10 TB total memory
    - Titan : 10-20% for 1 hour
    - Need larger modelspaces beyond ^{52}Ca
- Normal-ordered twobody approximation (NO2B)
  - Keep only contributions to:
    - Vacuum energy
    - Onebody operator
    - Twobody operator
- Residual three-nucleon force with $T_3^{(1)}$ (MBPT2).
  - 1 % effect (0.1 MeV per Nucleon)

Pros and cons

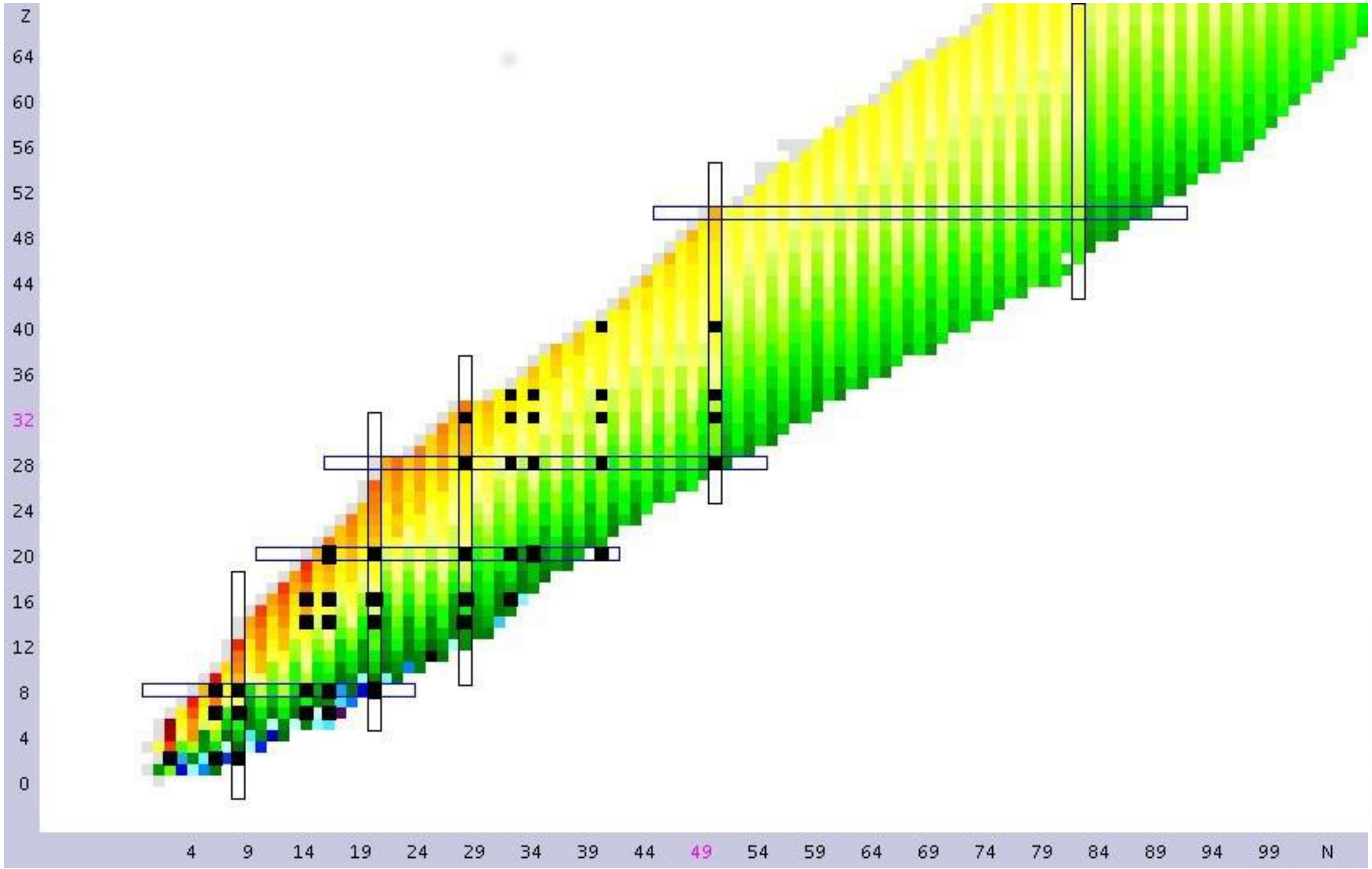
Pros

- Preserve symmetries.
- Dramatic reduction in memory usage.
- Dramatic reduction in computational cost.

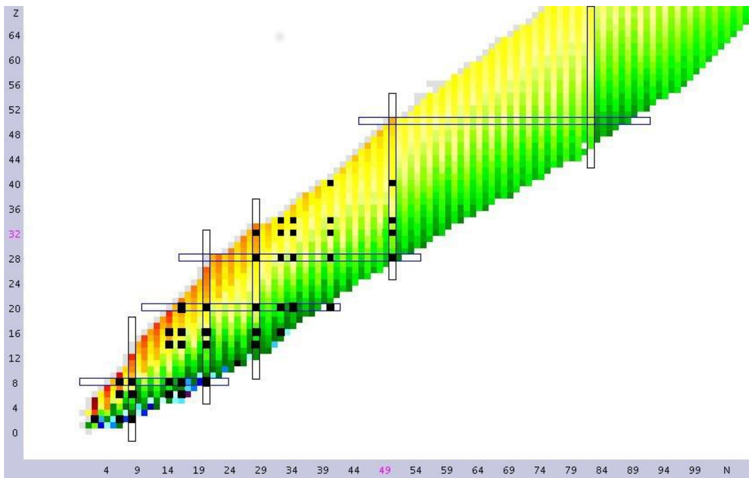
Cons

- Complicated algebra.
- Every diagram is coupled differently.
- Antisymmetry is non-trivial.
- Lots of opportunities for bugs.
- Limited set of nuclei are accessible.

NUCCOR coverage



Closed (sub-)shell nuclei

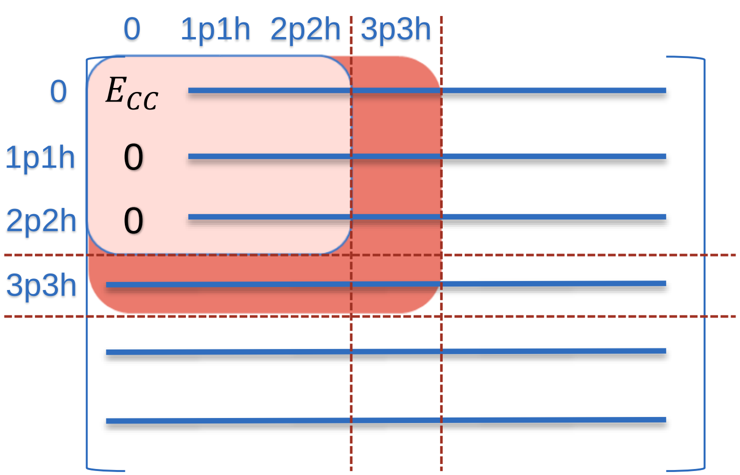


Coupled-cluster summary

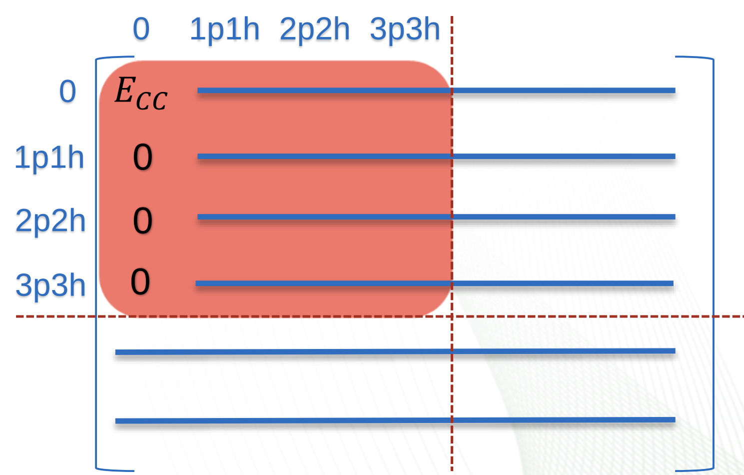
$$|\Psi\rangle = e^{T}|\Phi_0\rangle$$

$$T = 1 + T_h^p + T_{2h}^{2p} + T_{3h}^{3p} + \cdots$$

$$\overline{H} = e^{-T} H e^{T}$$

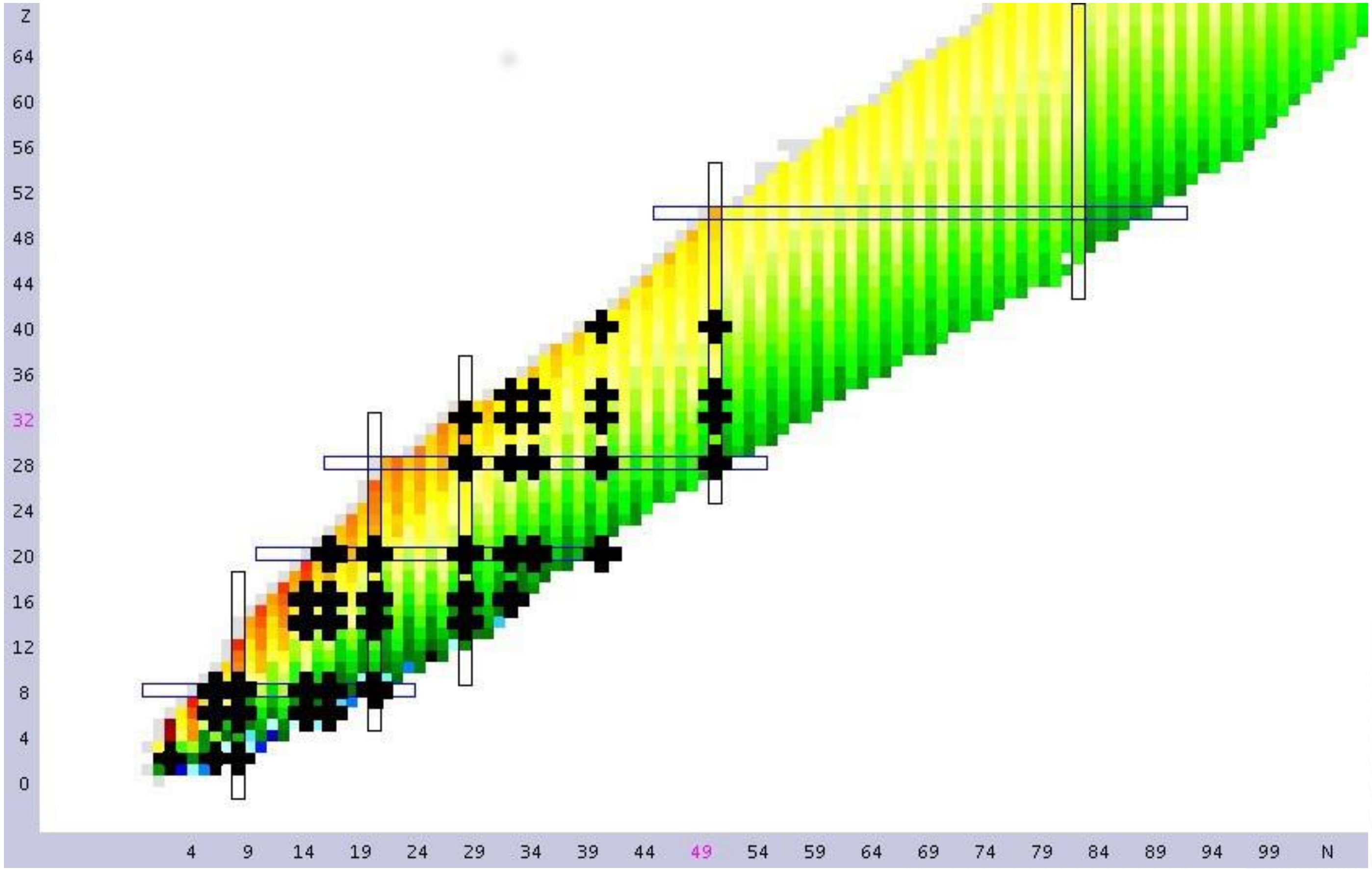


CCSD

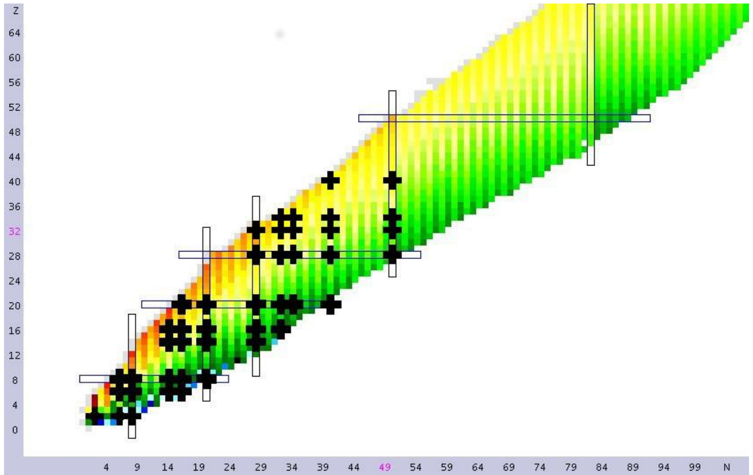


CCSDT

NUCCOR coverage (PA/PR)



One particle attached or removed

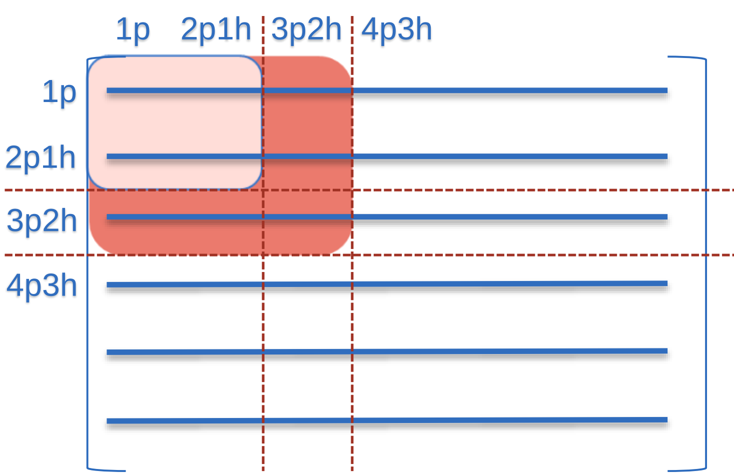


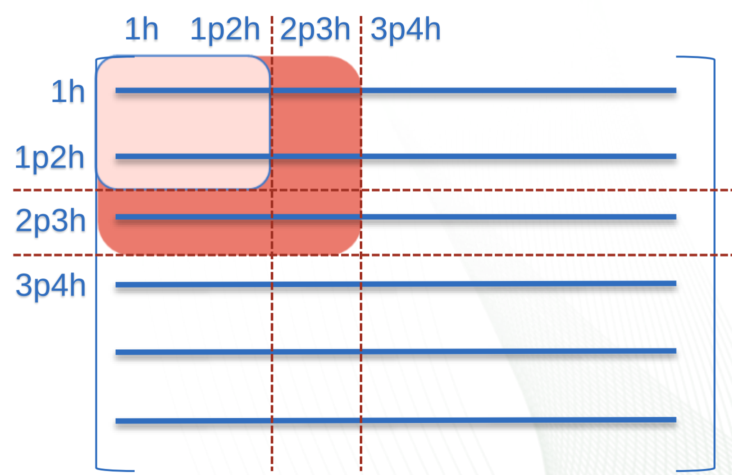
PA/PR-EOM operators

$$\overline{H} = e^{-T} H e^{T}$$

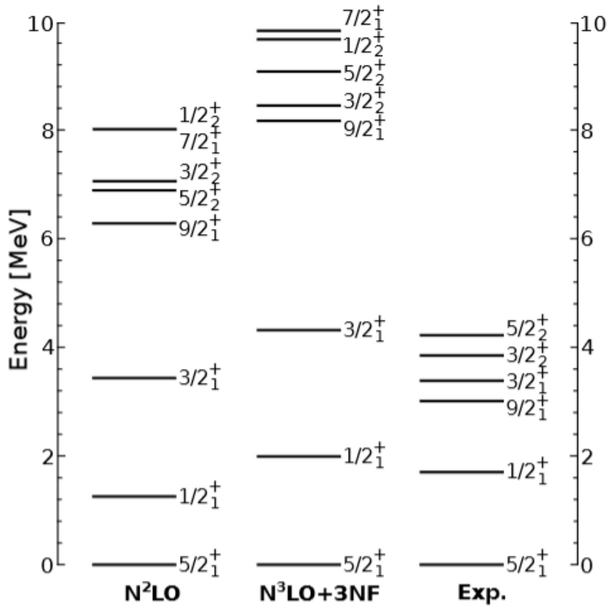
$$R^{A+1} = R^{p} + R_{h}^{2p} + R_{2h}^{3p} + R_{3h}^{4p} + \cdots$$

$$R^{A-1} = R_{h} + R_{2h}^{p} + R_{3h}^{2p} + R_{4h}^{3p} + \cdots$$





Excited states in ^{25}F



	1p	2p1h	3p2h
$5/2_1^+$	0.63	0.30	0.07
$1/2_1^+$	0.56	0.36	0.08
$9/2_1^+$	0.00	0.74	0.26
$3/2_1^+$	0.47	0.42	0.11
$3/2_2^+$	0.01	0.72	0.27
$5/2_2^+$	0.01	0.73	0.26
$1/2_2^+$	0.03	0.72	0.25
$7/2_1^+$	0.00	0.73	0.27

Zs. Vajta *et al.*
Phys. Rev. C 89, 054323 (2014)

- Assumed ^{24}O with a proton attached.
- Ground state and first excited states have significant 2p1h component.
- Collection of states with significant 3p2h components.
- 4p3h amplitudes are necessary.
- Already at computational limit with 3p2h amplitudes.

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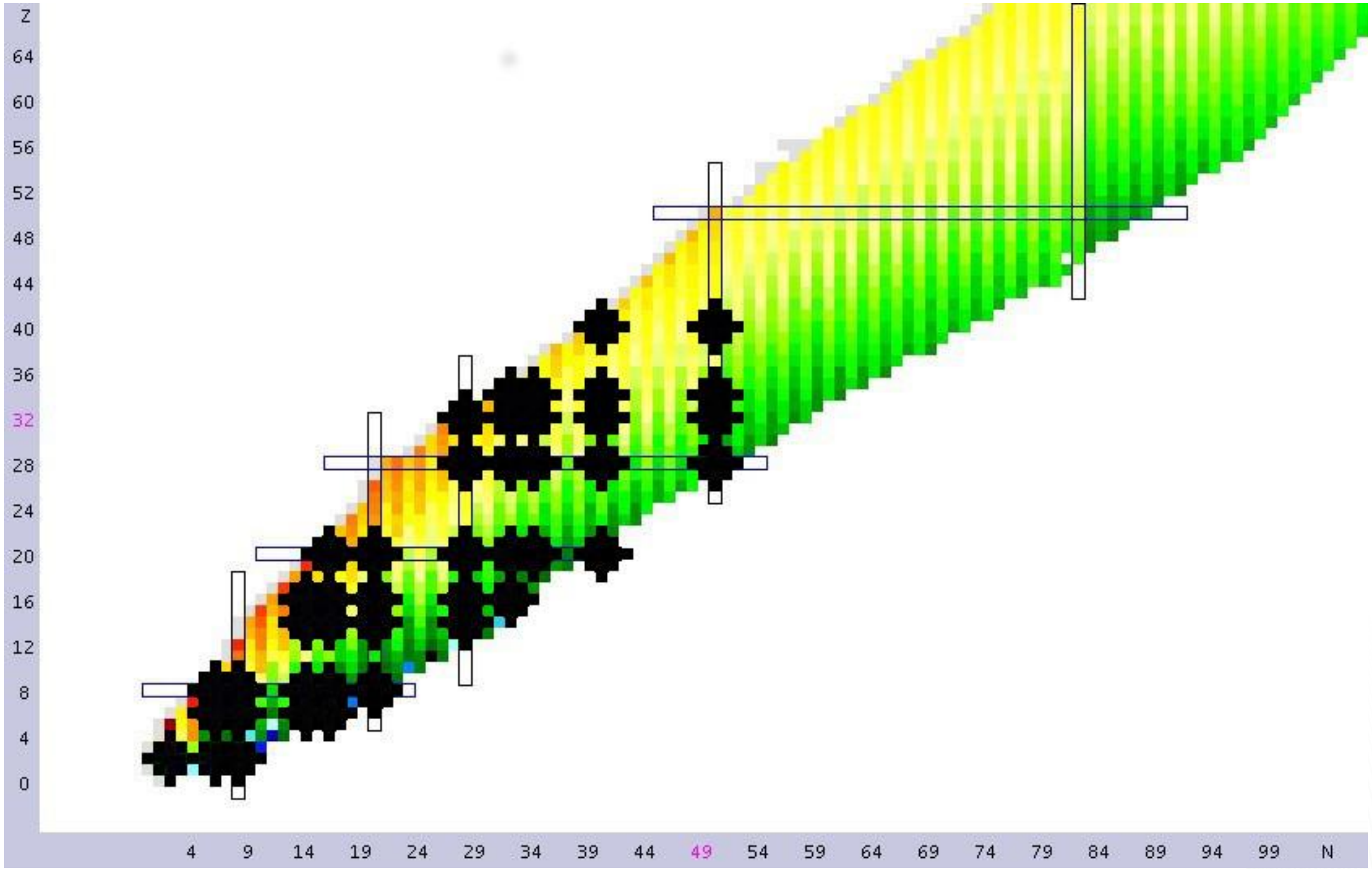
NUCCOR coverage (2PA/2PR)



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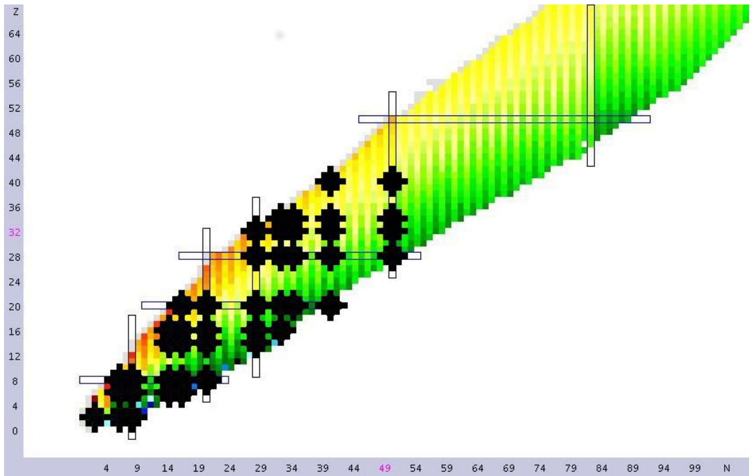
Two particles attached or removed

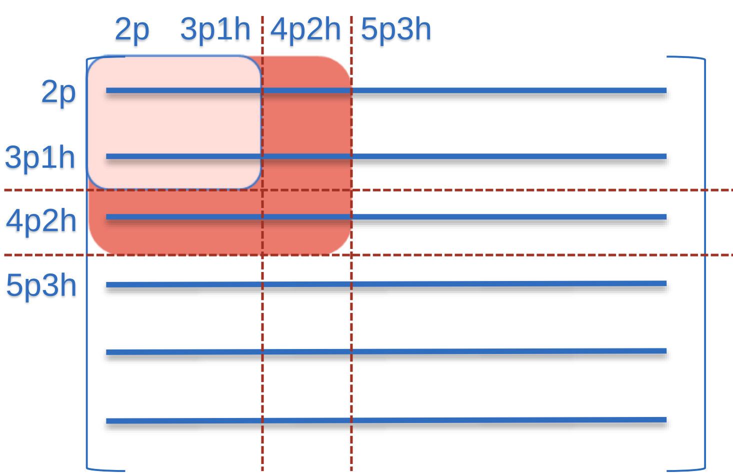


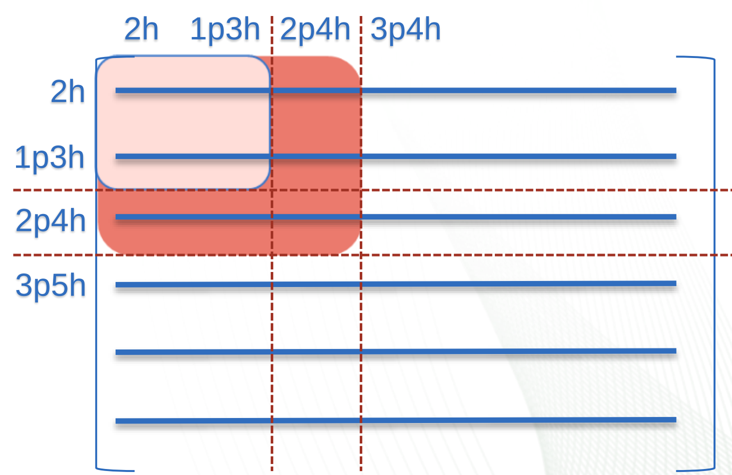
2PA/2PR-EOM operators

$$\overline{H} = e^{-T} H e^{T}$$

$$R^{A+2} = R^{2p} + R_{h}^{3p} + R_{2h}^{4p} + R_{3h}^{5p} + \cdots$$

$$R^{A-2} = R_{2h} + R_{3h}^{p} + R_{4h}^{2p} + R_{5h}^{3p} + \cdots$$

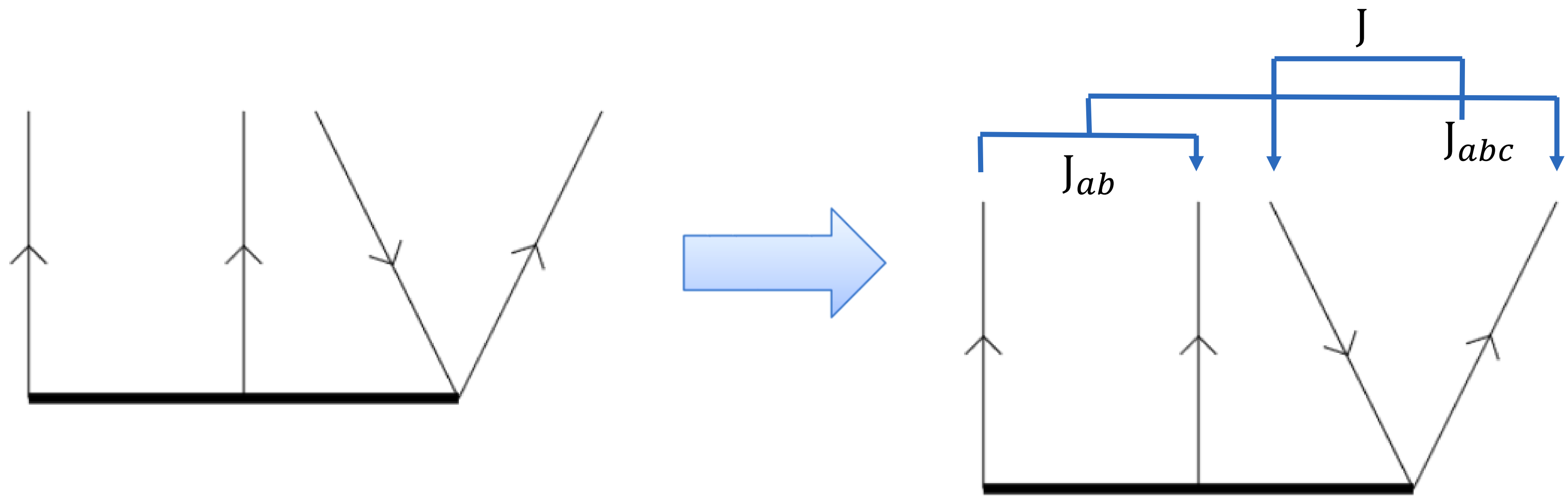




Strategy (j-scheme)

1. Define transformations between m-scheme and j-scheme elements/amplitudes.
2. Take the original equations and replace m-scheme elements/amplitudes with the transformations from 1.
3. Eliminate projections (m's) by finding the correct Wigner coefficients

3p1h (R_3) transformations

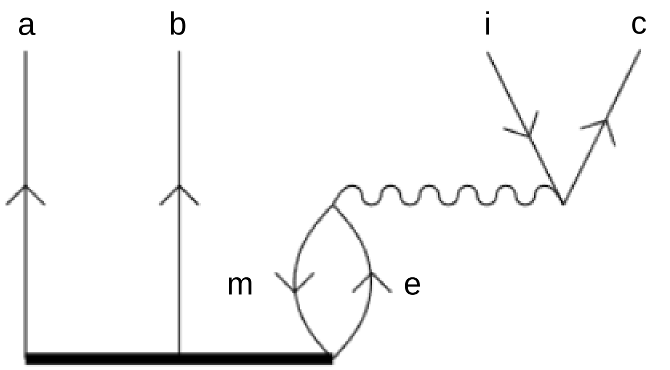


$$r_i^{abc} = \sum_{\substack{J_{abc}M_{abc}\\ J_{ab}M_{ab}}} r_i^{abc}(J, J_{abc}, J_{ab}) \times C^{j_a j_b M_{ab}}_{m_a m_b M_{ab}} C^{J_{ab} j_c J_{abc}}_{M_{ab} m_c M_{abc}} C^{J j_i J_{abc}}_{M m_i M_{abc}}.$$

$$r_i^{abc}(J, J_{abc}, J_{ab}) = \frac{1}{\hat{J}^2_{abc}} \sum_{\substack{M M_{abc} M_{ab}\\ m_a m_b m_c m_i}} r_i^{abc} C^{j_a j_b J_{ab}}_{m_a m_b M_{ab}} \times C^{J_{ab} j_c J_{abc}}_{M_{ab} m_c M_{abc}} C^{J j_i J_{abc}}_{M m_i M_{abc}}.$$

Example diagram (2PA-EOMCCSD)

GRJ Phys. Rev. C 88, 024305 (2013



$$\hat{\mathrm{P}}(ab,c)\bar{\mathrm{H}}^{mc}_{ei} r^{abe}_{m}$$

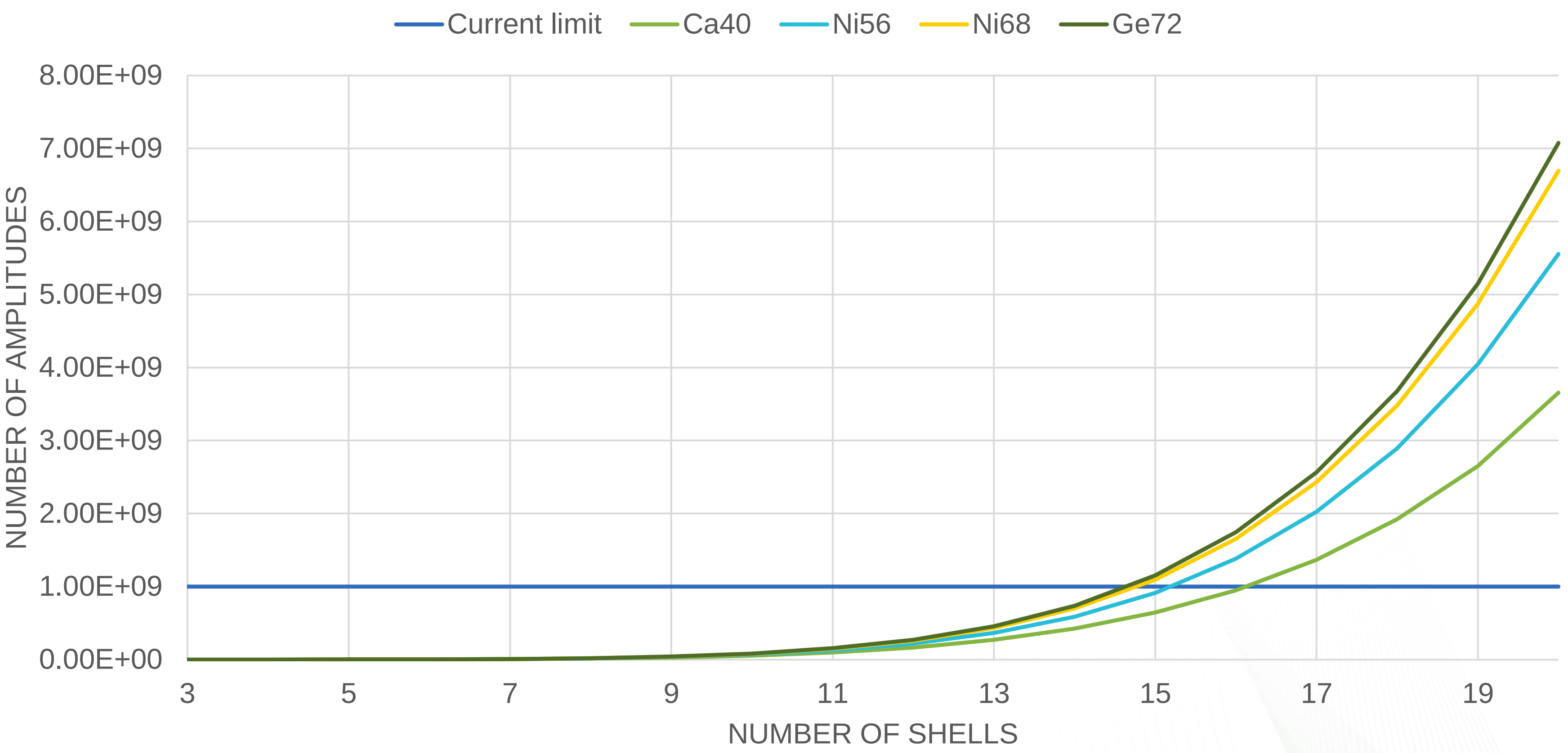
$$\hat{\mathrm{P}}(ab,c)\sum_{J_{abe},J_{mc}}(-1)^{1+j_e+j_m+J_{abe}+J_{abc}+J_{mc}}\hat{J}^2_{abe}\hat{J}^2_{mc}\begin{Bmatrix} J_{ab} & j_e & J_{abe} \\ j_c & J_{mc} & j_m \\ J_{abc} & j_i & J \end{Bmatrix}$$

$$\times\bar{\mathrm{H}}^{mc}_{ei}(J_{mc})r^{abe}_{m}(J_{ab},J_{abe},J)$$

$$\hat{\mathrm{P}}(ab,c) = \hat{1} + \sum_{J_{cb}}\hat{J}_{cb}\hat{J}_{ab}\begin{Bmatrix} j_c & j_b & J_{cb} \\ j_a & J_{abc} & J_{ab} \end{Bmatrix}\hat{\mathrm{P}}_{a,c} -$$

$$\sum_{J_{ac}}(-1)^{j_b+j_c-J_{ab}+J_{ac}}\hat{J}_{ab}\hat{J}_{ac}\times\begin{Bmatrix} j_c & j_a & J_{ac} \\ j_b & J_{abc} & J_{ab} \end{Bmatrix}\hat{\mathrm{P}}_{b,c}$$

2PA EOM-CCSD amplitudes



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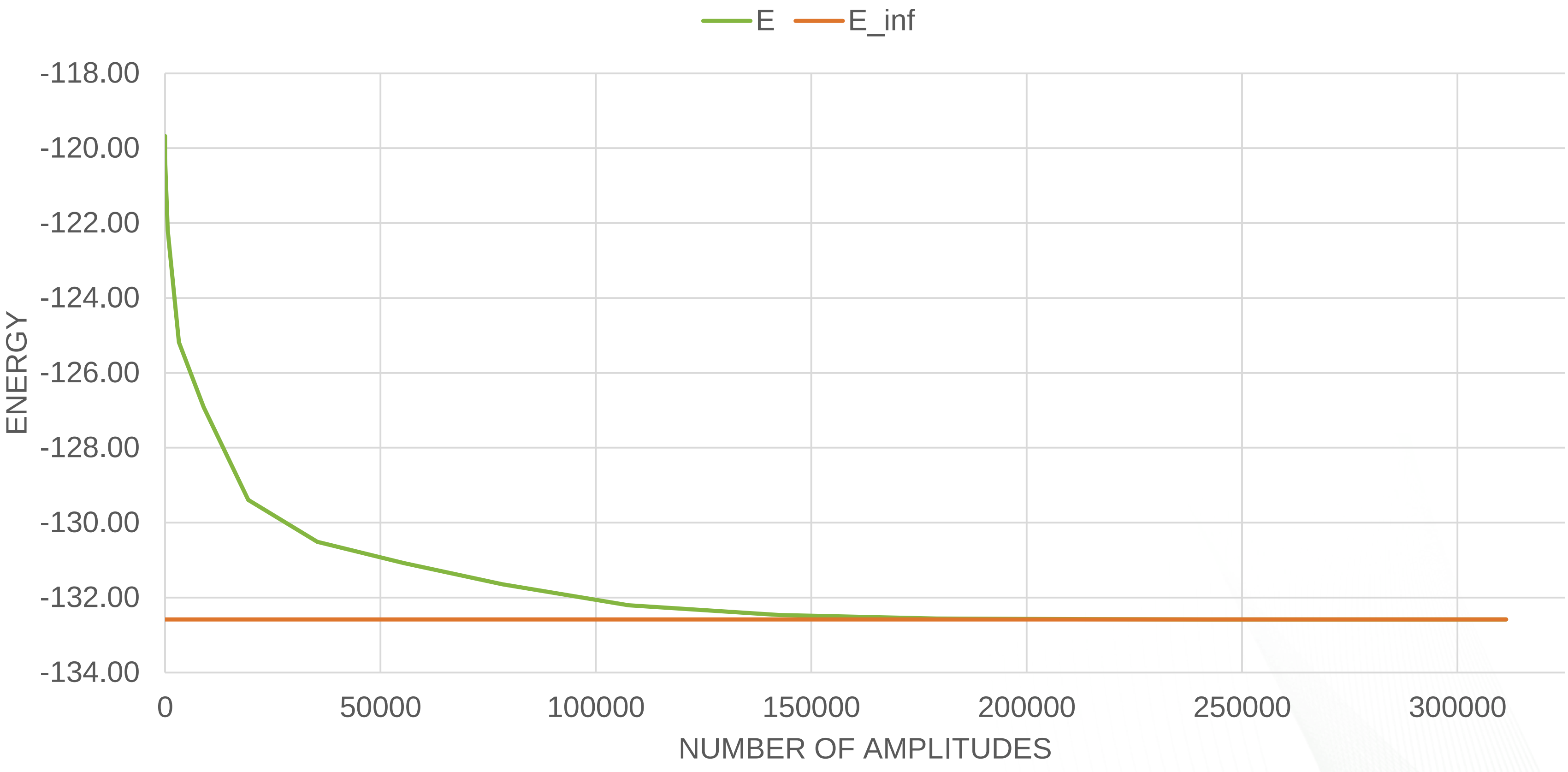
Active space (preliminary)



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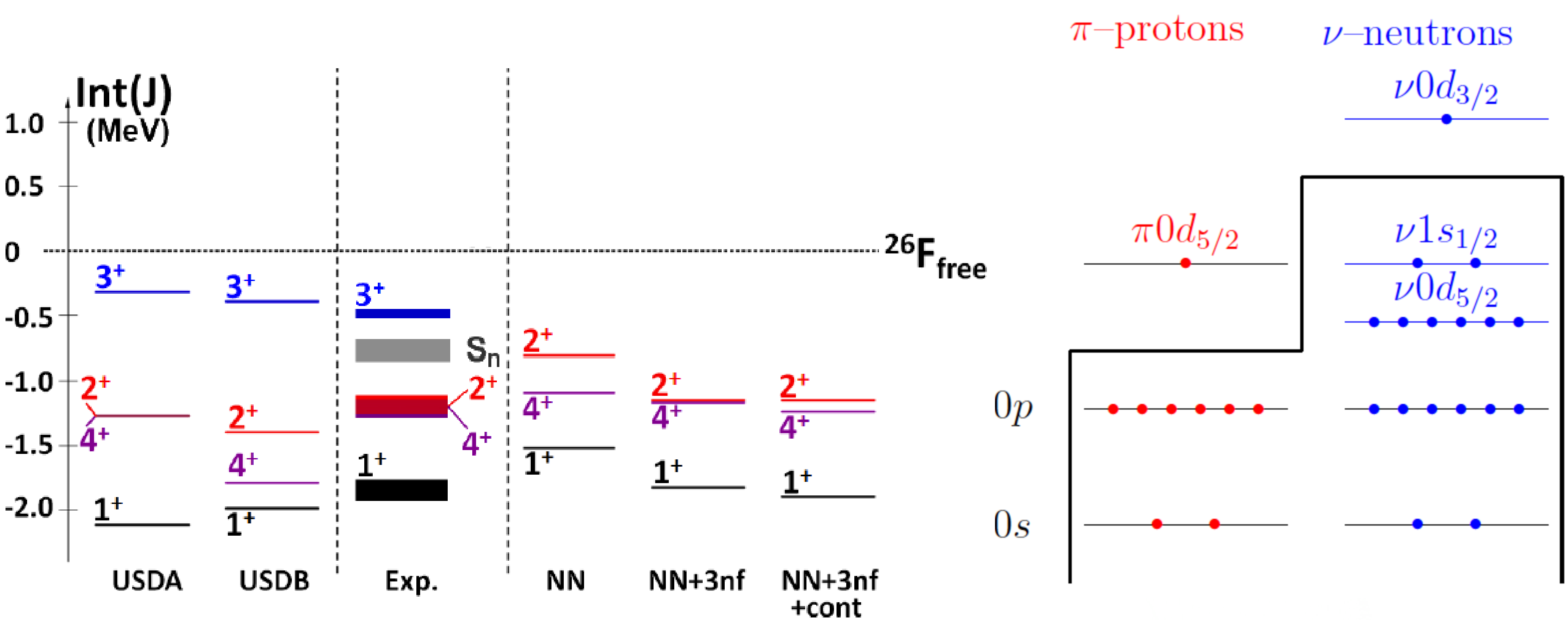
Computing nuclei with A+2: Example Fluorine-26

GRJ et al. PRC 2011, GRJ PRC 2013, J. Shen and P. Piecuch J. Chem. Phys (2013)



Experimental spectra in ^{26}F compared with phenomenological USD shell-model calculations and coupled-cluster calculations.

A. Lepailleur et al (2012)

Benchmark in ^{6}He

GRJ, M. Hjorth-Jensen, G. Hagen, T. Papenbrock Phys. Rev. C 83, 054306, 2011

	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

- Uncoupled scheme
- Tiny modelspace
- Good agreement between FCI and 2PA-EOMCCSD with 3p1h amplitudes.

Challenges

- Three-nucleon forces in HF, CC and EOM-CC.
  - Residual three-nucleon forces contribute > 1%
  - Needs to be included in CC.
- Additional correlations in EOM-CC.
  - Not possible to include the full set of amplitudes.
  - Active spaces?
- Larger modelspaces (three-nucleon force).
  - Nmax=14, E3max=18 not enough
  - Quickly saturates the available computational resources.

Questions?

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