# Effective interactions from coupled-cluster theory

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TRIUMF
February 21. 2014

# Outline

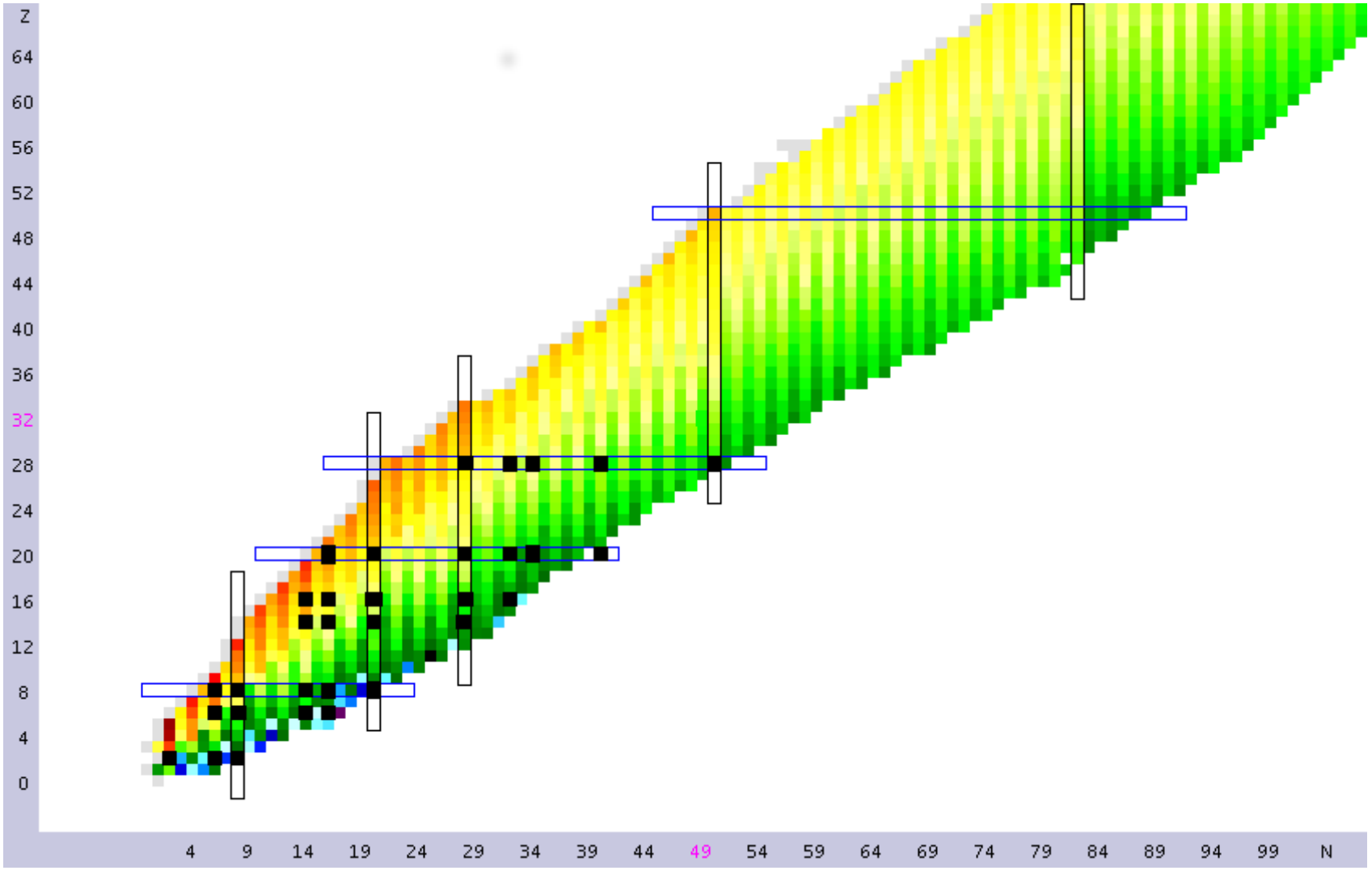
- Who - Collaborators.
- Why - Motivation.
- How - Formalism.
- What - Results.
- When - Outlook.

# Collaborators and acknowledgements

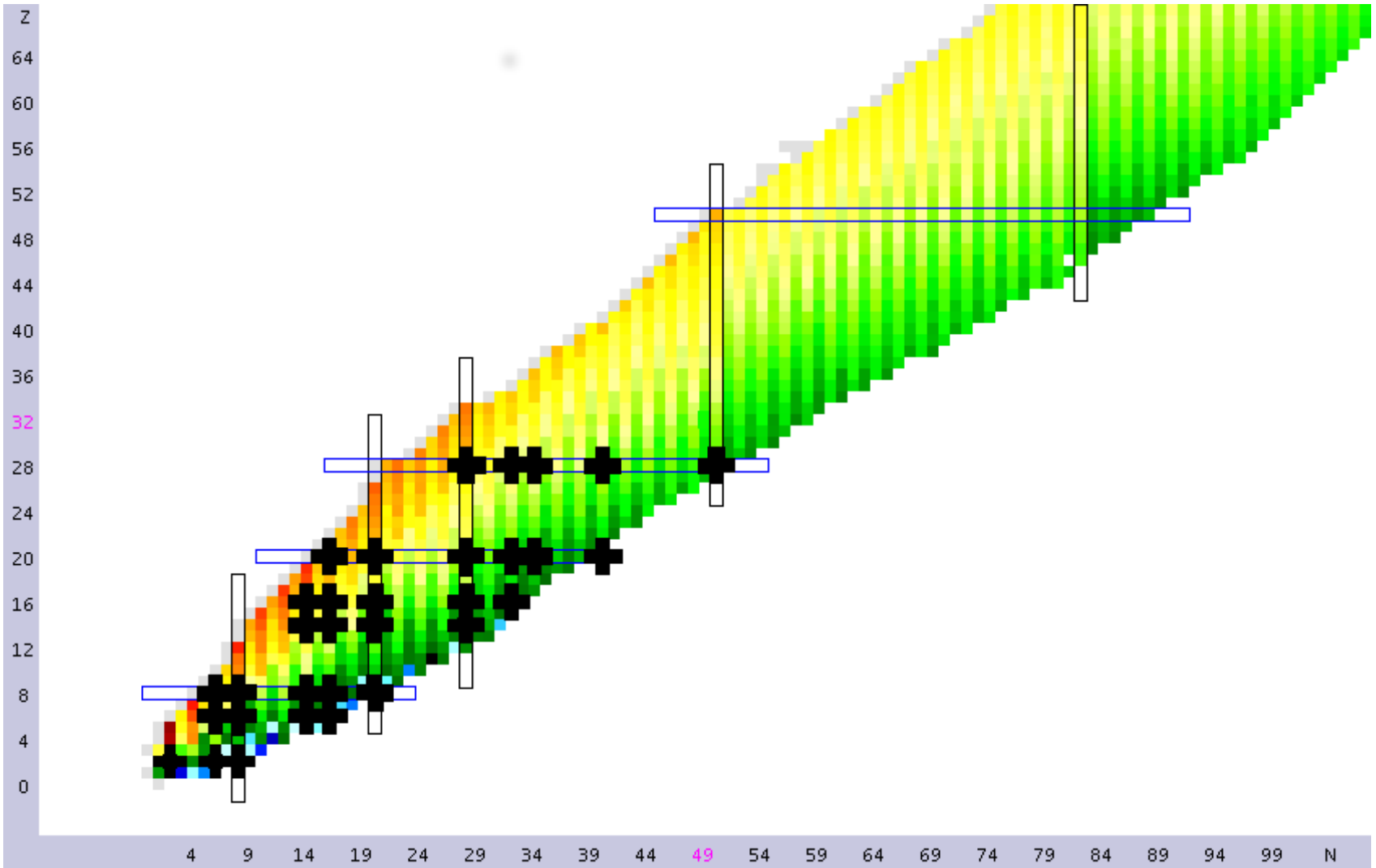
- Gaute Hagen (ORNL)
- Gustav R. Jansen (UTK, ORNL)
- Jon Engel (UNC)
- Petr Navratil (TRIUMF)
- Angelo Signoracci (UTK, ORNL)



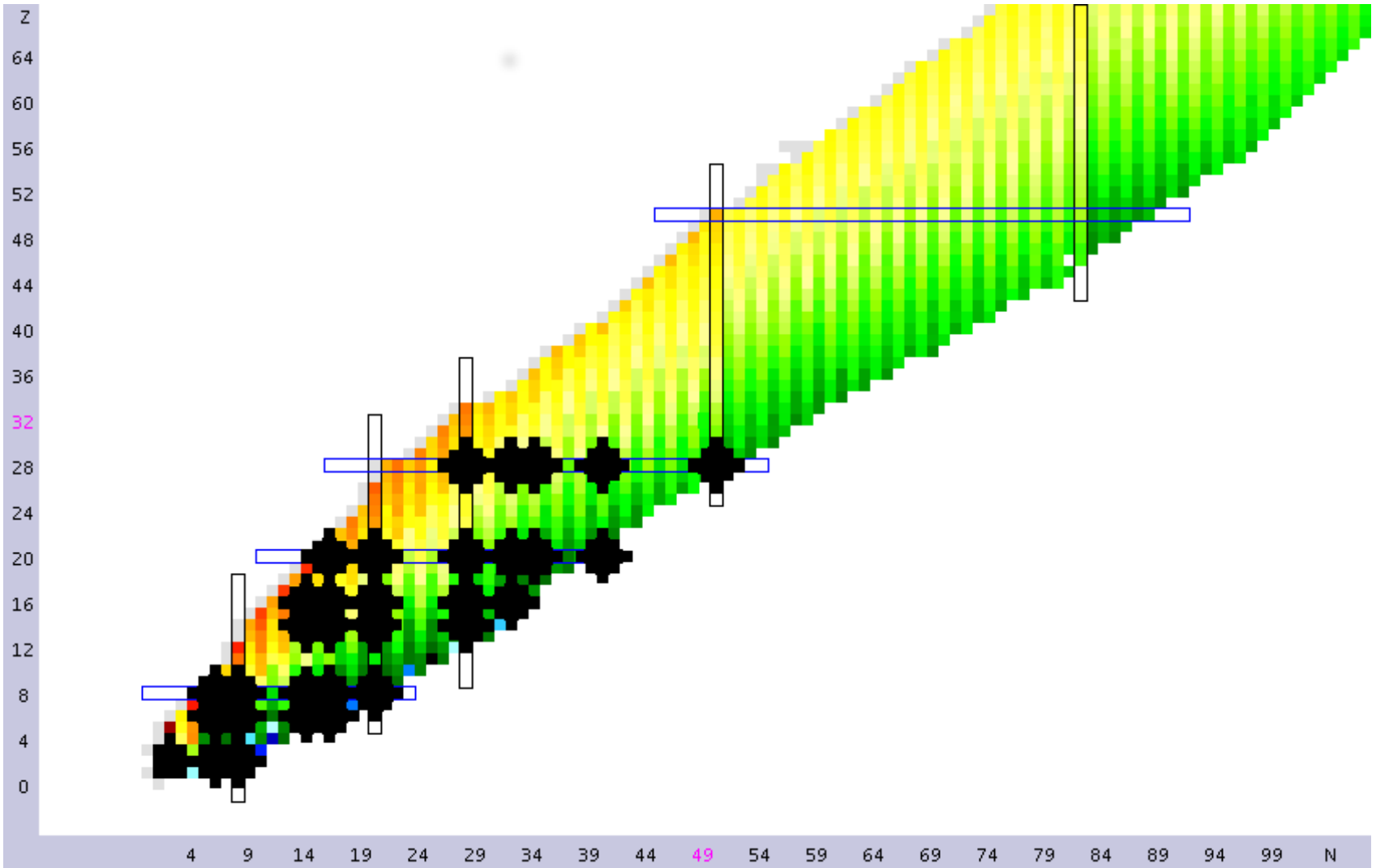
# Coupled-cluster coverage (CC)



# Coupled-cluster coverage (CC + PA/PR)



# Coupled-cluster coverage (CC + PA/PR + 2PA/2PR)

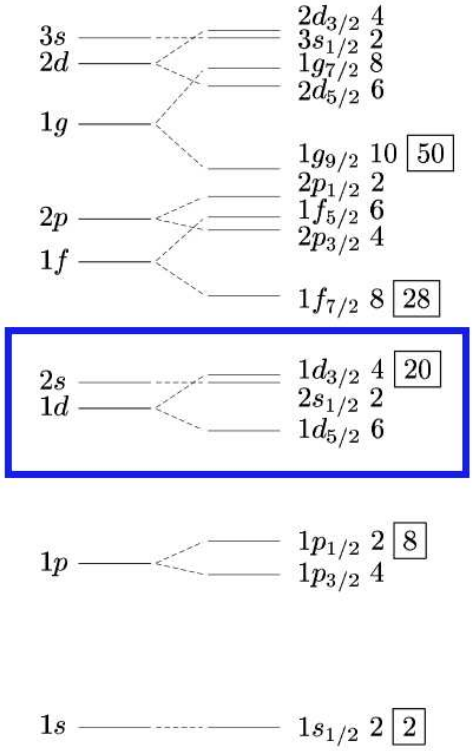


# Valence cluster expansion

A. F. Lisetskiy, B. R. Barrett, M. K. G. Kruse, P. Navratil, I. Stetcu, and J. P. Vary Phys. Rev. C 78, 044302 (2008)

$$\hat{\mathrm{H}}_{\mathrm{eff}}^{A_c}(A) = E_c(A) + H_1^{A_c}(A) + H_2^{A_c}(A) + \ldots$$

- Effective Hamiltonian operating in a very reduced modelspace where full diagonalization is possible.
- Solves the $A_c + 2$-body system exactly.
- Used for more than 2 nucleons in the valence space.



# Okubo-Lee-Suzuki transformation

- Choose the wanted eigenpairs and define

$$\langle p|\hat{\mathrm{M}}_R|k\rangle = \langle p|\Psi_k\rangle$$

and

$$\langle k|\hat{\mathrm{E}}|k\rangle$$

- The non-hermitian effective Hamiltonian is given by

$$\hat{\mathrm{H}}'_{eff} = \hat{\mathrm{M}}_R\hat{\mathrm{E}}\hat{\mathrm{M}}_R^{-1}$$

- Equivalent to

$$\hat{\mathrm{H}}'_{eff} = \hat{\mathrm{P}}\hat{\mathrm{H}}\left(\hat{\mathrm{P}}+\omega\right), \qquad \langle q|\omega|p\rangle = \sum_k \langle q|R_k\rangle \mathrm{inv}\{\langle p|R_k\rangle\}$$

- Symmetric orthogonalization procedure to get an hermitian effective interaction (I. Mayer, Int. J. Quantum Chem., 90: 63–65)

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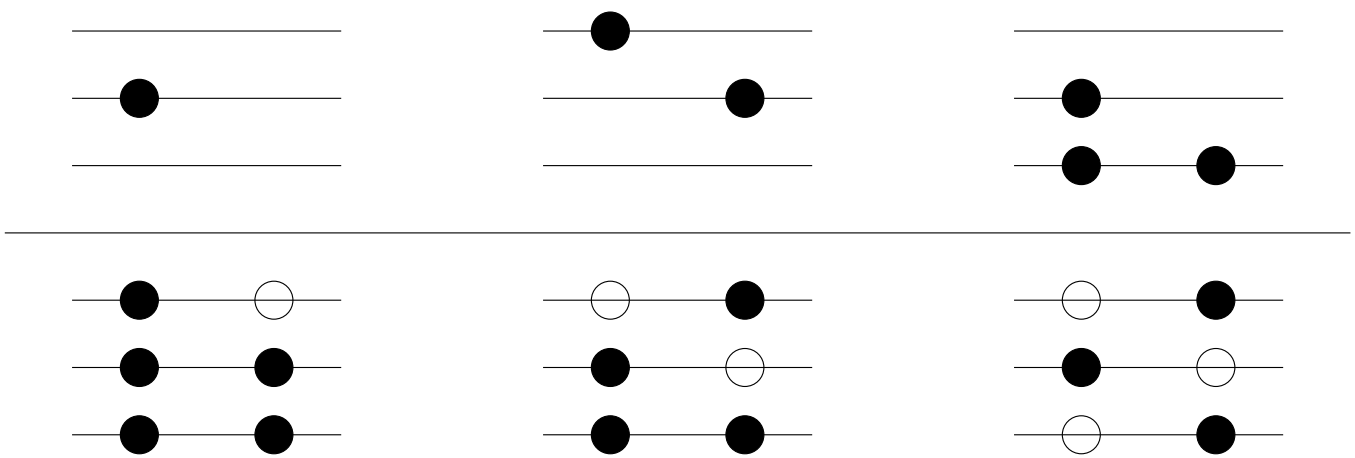
# Necessary ingredients

- Good description of the core especially the ground state energy.
- $A_c + 1$ eigenvalues for single particle energies.
- $A_c + 2$ wavefunctions and energies for constructing the effective interaction.

# Coupled-cluster summary

## The cluster operator

$$\hat{\mathrm{T}} = \hat{\mathrm{T}}_1 + \hat{\mathrm{T}}_2 + \ldots + \hat{\mathrm{T}}_A$$
$$= \sum_{ia} t_i^a \left\{ a_a^\dagger a_i \right\} + \sum_{ijab} t_{ij}^{ab} \left\{ a_a^\dagger a_b^\dagger a_j a_i \right\} + \ldots +$$
$$\sum_{\substack{i_1,\ldots i_A \\ a_1,\ldots a_A}} t_{i_1,\ldots i_A}^{a_1,\ldots a_A} a_{a_1}^\dagger \ldots a_{a_A}^\dagger a_{i_A} \ldots a_{i_1}$$



# Coupled-cluster summary

## Exponential ansatz

$$|\Psi\rangle \approx |\Psi_{CC}\rangle = e^{\hat{\mathrm{T}}}|\Phi_0\rangle = \left(\sum_{n=1}^{\infty} \frac{1}{n!}\hat{\mathrm{T}}^n\right)|\Phi_0\rangle,$$

Include terms like

$$e^{\hat{\mathrm{T}}} \leftarrow \frac{1}{6}\hat{\mathrm{T}}_1^3 + \frac{1}{2}\hat{\mathrm{T}}_1\hat{\mathrm{T}}_2 + \frac{1}{A!}\hat{\mathrm{T}}_1^A$$

# Coupled-cluster summary

## Similarity transformed Hamiltonian

$$\bar{\mathrm{H}} = e^{-\hat{\mathrm{T}}} \hat{\mathrm{H}}_N e^{\hat{\mathrm{T}}}$$

$$\begin{pmatrix}
\langle \Phi_0 | \bar{\mathrm{H}} | \Phi_0 \rangle & \dots & \langle \Phi_0 | \bar{\mathrm{H}} | \Phi_{i_1,\dots i_A}^{a_1,\dots a_A} \rangle \\
\langle \Phi_i^a | \bar{\mathrm{H}} | \Phi_0 \rangle & \dots & \langle \Phi_i^a | \bar{\mathrm{H}} | \Phi_{i_1,\dots i_A}^{a_1,\dots a_A} \rangle \\
\langle \Phi_{ij}^{ab} | \bar{\mathrm{H}} | \Phi_0 \rangle & \dots & \langle \Phi_{ij}^{ab} | \bar{\mathrm{H}} | \Phi_{i_1,\dots i_A}^{a_1,\dots a_A} \rangle \\
\langle \Phi_{ijk}^{abc} | \bar{\mathrm{H}} | \Phi_0 \rangle & \dots & \langle \Phi_{ijk}^{abc} | \bar{\mathrm{H}} | \Phi_{i_1,\dots i_A}^{a_1,\dots a_A} \rangle \\
\vdots & \ddots & \vdots \\
\langle \Phi_{i_1,\dots i_A}^{a_1,\dots a_A} | \bar{\mathrm{H}} | \Phi_0 \rangle & \dots & \langle \Phi_{i_1,\dots i_A}^{a_1,\dots a_A} | \bar{\mathrm{H}} | \Phi_{i_1,\dots i_A}^{a_1,\dots a_A} \rangle
\end{pmatrix}$$

# Coupled-cluster summary

## Similarity transformed Hamiltonian

### CCS: $\hat{\mathrm{T}} = \hat{\mathrm{T}}_1$

$$\begin{pmatrix} E_{\mathrm{CCS}} & \dots & \langle \Phi_0 | \bar{\mathrm{H}} | \Phi_{i_1,\dots i_A}^{a_1,\dots a_A} \rangle \\ 0 & \dots & \langle \Phi_i^a | \bar{\mathrm{H}} | \Phi_{i_1,\dots i_A}^{a_1,\dots a_A} \rangle \\ \langle \Phi_{ij}^{ab} | \bar{\mathrm{H}} | \Phi_0 \rangle & \dots & \langle \Phi_{ij}^{ab} | \bar{\mathrm{H}} | \Phi_{i_1,\dots i_A}^{a_1,\dots a_A} \rangle \\ \langle \Phi_{ijk}^{abc} | \bar{\mathrm{H}} | \Phi_0 \rangle & \dots & \langle \Phi_{ijk}^{abc} | \bar{\mathrm{H}} | \Phi_{i_1,\dots i_A}^{a_1,\dots a_A} \rangle \\ \vdots & \ddots & \vdots \\ \langle \Phi_{i_1,\dots i_A}^{a_1,\dots a_A} | \bar{\mathrm{H}} | \Phi_0 \rangle & \dots & \langle \Phi_{i_1,\dots i_A}^{a_1,\dots a_A} | \bar{\mathrm{H}} | \Phi_{i_1,\dots i_A}^{a_1,\dots a_A} \rangle \end{pmatrix}$$

$$\langle \Phi_i^a | \bar{\mathrm{H}} | \Phi_0 \rangle = 0$$

**Similarity transformation is exact independent of truncation.**

# Coupled-cluster summary

## Similarity transformed Hamiltonian

$$\text{CCSD: } \hat{\mathrm{T}} = \hat{\mathrm{T}}_1 + \hat{\mathrm{T}}_2$$

$$\begin{pmatrix} E_{\mathrm{CCSD}} & \dots & \langle \Phi_0 | \bar{\mathrm{H}} | \Phi_{i_1,\dots i_A}^{a_1,\dots a_A} \rangle \\ 0 & \dots & \langle \Phi_i^a | \bar{\mathrm{H}} | \Phi_{i_1,\dots i_A}^{a_1,\dots a_A} \rangle \\ 0 & \dots & \langle \Phi_{ij}^{ab} | \bar{\mathrm{H}} | \Phi_{i_1,\dots i_A}^{a_1,\dots a_A} \rangle \\ \langle \Phi_{ijk}^{abc} | \bar{\mathrm{H}} | \Phi_0 \rangle & \dots & \langle \Phi_{ijk}^{abc} | \bar{\mathrm{H}} | \Phi_{i_1,\dots i_A}^{a_1,\dots a_A} \rangle \\ \vdots & \ddots & \vdots \\ \langle \Phi_{i_1,\dots i_A}^{a_1,\dots a_A} | \bar{\mathrm{H}} | \Phi_0 \rangle & \dots & \langle \Phi_{i_1,\dots i_A}^{a_1,\dots a_A} | \bar{\mathrm{H}} | \Phi_{i_1,\dots i_A}^{a_1,\dots a_A} \rangle \end{pmatrix}$$

$$\langle \Phi_{ij}^{ab} | \bar{\mathrm{H}} | \Phi_0 \rangle = 0$$

**Similarity transformation is exact independent of truncation.**

# Coupled-cluster summary

## Similarity transformed Hamiltonian

$$\text{CCSDT: } \hat{\mathrm{T}} = \hat{\mathrm{T}}_1 + \hat{\mathrm{T}}_2 + \hat{\mathrm{T}}_3$$

$$\begin{pmatrix} E_{\mathrm{CCSDT}} & \dots & \langle \Phi_0 | \bar{\mathrm{H}} | \Phi_{i_1,\dots i_A}^{a_1,\dots a_A} \rangle \\ 0 & \dots & \langle \Phi_i^a | \bar{\mathrm{H}} | \Phi_{i_1,\dots i_A}^{a_1,\dots a_A} \rangle \\ 0 & \dots & \langle \Phi_{ij}^{ab} | \bar{\mathrm{H}} | \Phi_{i_1,\dots i_A}^{a_1,\dots a_A} \rangle \\ 0 & \dots & \langle \Phi_{ijk}^{abc} | \bar{\mathrm{H}} | \Phi_{i_1,\dots i_A}^{a_1,\dots a_A} \rangle \\ \vdots & \ddots & \vdots \\ \langle \Phi_{i_1,\dots i_A}^{a_1,\dots a_A} | \bar{\mathrm{H}} | \Phi_0 \rangle & \dots & \langle \Phi_{i_1,\dots i_A}^{a_1,\dots a_A} | \bar{\mathrm{H}} | \Phi_{i_1,\dots i_A}^{a_1,\dots a_A} \rangle \end{pmatrix}$$

$$\langle \Phi_{ijk}^{abc} | \bar{\mathrm{H}} | \Phi_0 \rangle = 0$$

**Similarity transformation is exact independent of truncation.**

# Excited states using EOM-CC

Eigenvalues of $\bar{\mathrm{H}} = e^{-\hat{\mathrm{T}}} \hat{\mathrm{H}} e^{\hat{\mathrm{T}}} - \langle \Phi_0 | \hat{\mathrm{H}} | \Phi_0 \rangle$

$$\left( \bar{\mathrm{H}} \hat{\mathrm{R}} \right)_c |\Phi_0\rangle = (E - E_c)\, \hat{\mathrm{R}} |\Phi_0\rangle$$

Properties of $\bar{\mathrm{H}}$.

- Non-symmetric (non-hermetian) operator.
- For CCSD and a twobody hamiltonian - six-body operator.
- The matrix representation is very sparse.
- Generally too large to store and diagonalize exactly.

*Efficient implementation of* $\left( \bar{\mathrm{H}} \hat{\mathrm{R}} \right)_C$ *is key.*

# Adding particles with EOM

- Diagonalize the similarity transformed hamiltonian in the appropriate space

$$\bar{\mathrm{H}}|R_k\rangle = (E_k - E_c)\,|R_k\rangle \qquad |R_k\rangle = \hat{\mathrm{R}}|\Phi_0\rangle$$
$$\langle L_k|\bar{\mathrm{H}} = \langle L_k|\,(E_k - E_c) \qquad \langle L_k| = \langle \Phi_0|\hat{\mathrm{L}}$$
$$\langle L_k|R_{k'}\rangle = \delta_{kk'}$$

## PA-EOM-CCSD ($A_c + 1$)

$$\hat{\mathrm{R}} = \sum_a r^a \left\{a_a^\dagger\right\} + \frac{1}{2}\sum_{a,b,i} r_i^{ab} \left\{a_a^\dagger a_b^\dagger a_i\right\}$$
$$\hat{\mathrm{L}} = \sum_a l_a \left\{a_a\right\} + \frac{1}{2}\sum_{a,b,i} l_{ab}^i \left\{a_i^\dagger a_b a_a\right\}$$

## 2PA-EOM-CCSD ($A_c + 2$)

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

# Toolchain

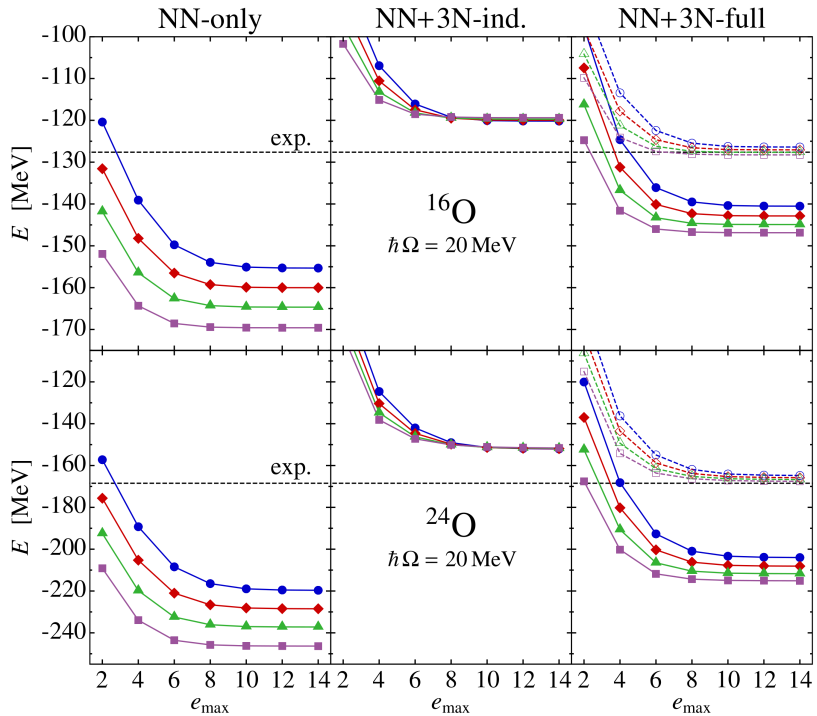
$$\hat{\mathrm{H}} = \sum_{i<j} \left( \frac{(\mathbf{p}_i - \mathbf{p}_j)^2}{2mA} + \hat{\mathrm{V}}_{NN}^{(i,j)} \right) + \sum_{i<j<k} \hat{\mathrm{V}}_{3\mathrm{N}}^{(i,j,k)}$$

1. Solve Hartree-Fock equations with full threebody interaction.
2. Discard the residual threebody elements to get a twobody Hamiltonian (NO2B).
3. CCSD to get the similarity transformed Hamiltonian.
4. Λ-CCSD(T) to get the core energy $E_c(A)$.
5. PA-EOM-CCSD to get the single particle energies.
6. 2PA-EOM-CCSD to get the $A_c + 2$-body energies and wavefunctions.
7. Okubo-Lee-Suzuki to get the non-Hermitian effective interaction.
8. Symmetric orthogonalization to get the final Hermitian effective interaction.
9. Shell-model calculation to get the energies.

# Interaction

## Benchmark interaction for the oxygen chain

- Chiral NN interaction at N$^3$LO from EM with cutoff at 500 MeV.
- Chiral 3N interaction at NNLO with $c_D = -0.2$, $c_E = 0.098$ and a cutoff at 400 MeV.
- Evolved to $\lambda = 2.0$ fm$^{-1}$ with SRG.
- $N_{max} = 12$ for NN interaction and $E3_{max} = 12, 14$ for 3N interaction.
- Fixed $\hbar\omega$ at 20 MeV.




R. Roth, S. Binder, K. Vobig, A. Calci, J. Langhammer, and P. Navratil, PRL 109 052501 (2012).

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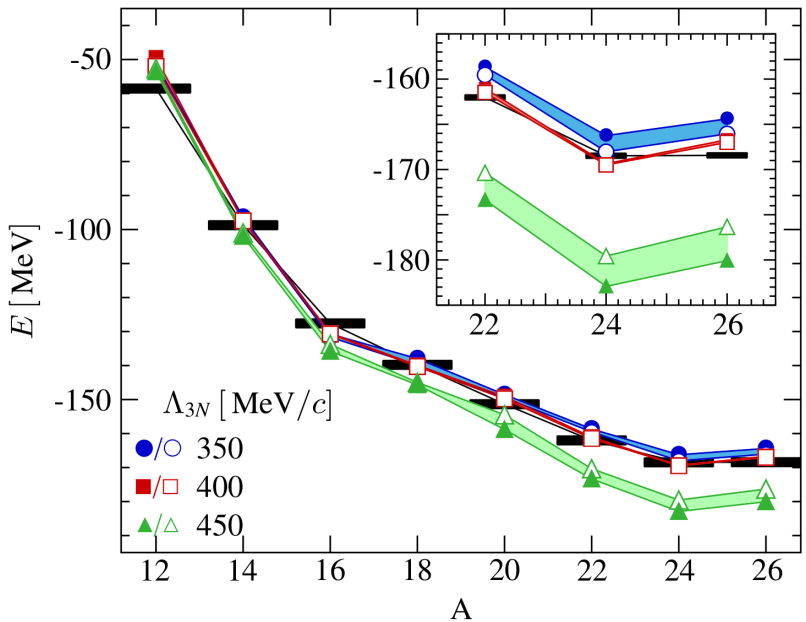


H. Hergert, S. Binder, A. Calci, J. Langhammer and R. Roth, PRL 110 242501 (2013).

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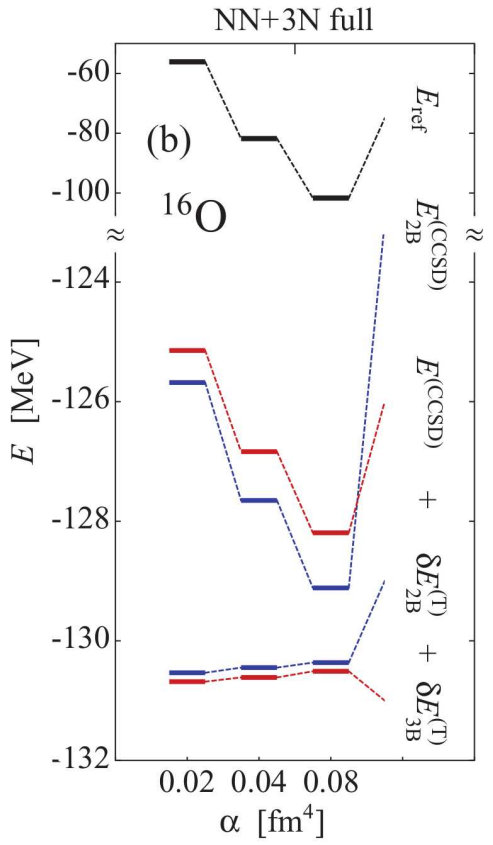


S. Binder, P. Piecuch, A. Calci, J. Langhammer, P. Navratil and R. Roth, PRC 88 054319 (2013).

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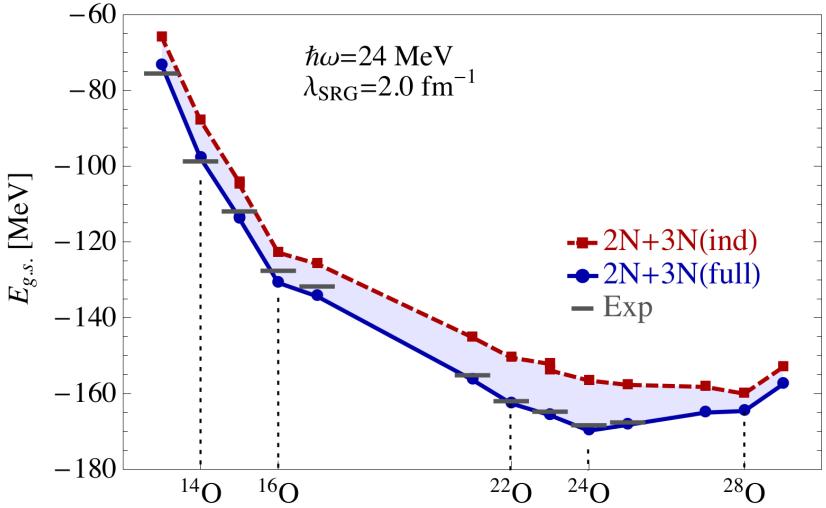
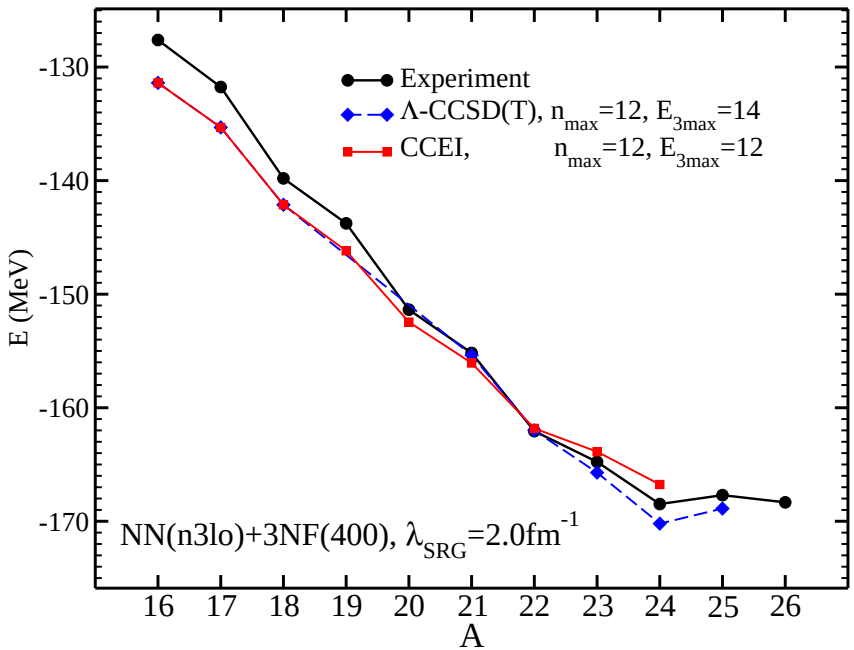



A. Cipollone, C. Barbieri and P. Navr´atil, arXiv:1303.4900v2 (2013).

# Oxygen isotopes

## Total binding energy

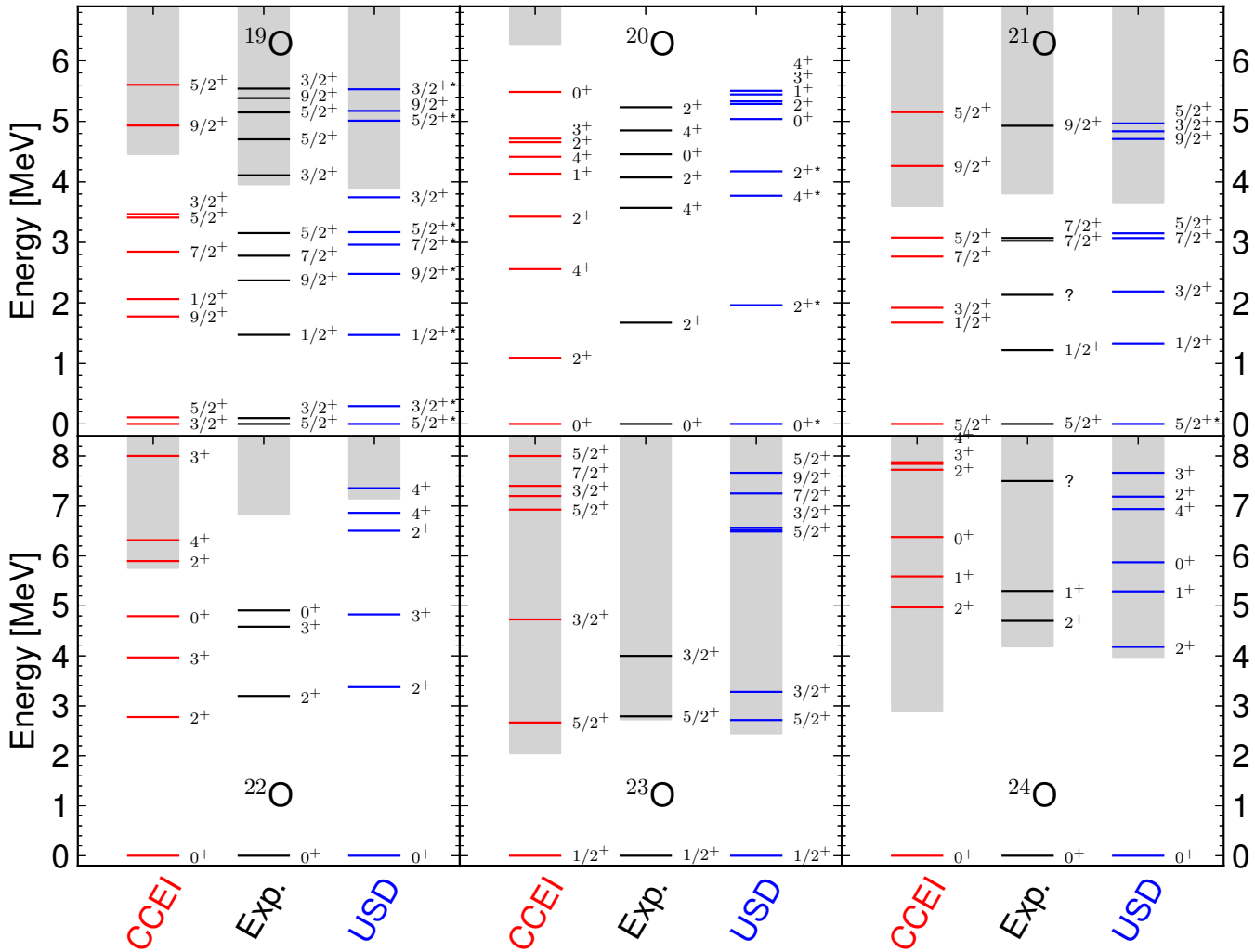
- Overall good agreement with experiment.
- CCEI and Λ-CCSD(T) agree very well.
- CCEI starts to deviate at $^{23}$O.
  - Convergence issues
  - Missing many-body forces in the valence space.
  - Additional correlations in the CCEI wavefunction than accessible with CCSD.




GRJ, J. Engel, G. Hagen, P. Navratil and A. Signoracci, arXiv:1402.2563 (2014).

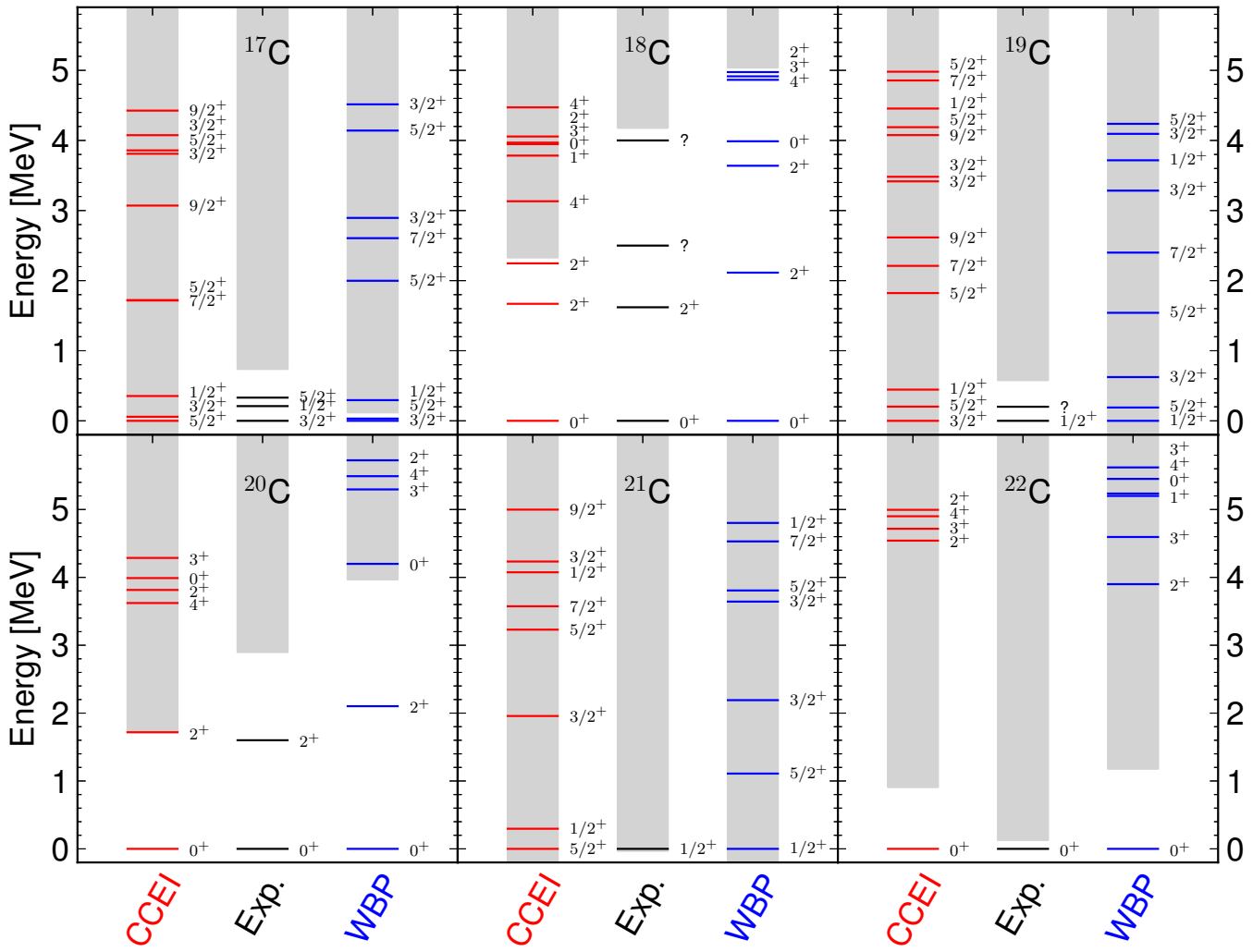
# Oxygen isotopes

## Exitation energies



# Carbon isotopes

## Exitation energies



# Outlook

- Include continuum degrees of freedom.
- Effective operators.
- Threebody interactions in the valence space.

# Questions?

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This work was partly supported by the Office of Nuclear Physics, U.S. Department of Energy (Oak Ridge National Laboratory), under Contracts No. DE-FG02-96ER40963 (University of Tennessee) and No.DE-SC0008499 (NUCLEI SciDAC-3 Collaboration), and the Field Work Proposal ERKBP57 at Oak Ridge National Laboratory.

An award of computer time was provided by the Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program. This research used resources of the Oak Ridge Leadership Computing Facility located in the Oak Ridge National Laboratory, which is supported by the Office of Science of the Department of Energy under Contract DE-AC05-00OR22725 and used computational resources of the National Center for Computational Sciences, the National Institute for Computational Sciences, and the Notur project in Norway.