Open-shell nuclei from coupled-cluster theory

Gustav R. Jansen$^{1,2}$

gustav.jansen@utk.edu

$^1$University of Tennessee, Knoxville

$^2$Oak Ridge National Laboratory

April 09. 2013
Collaborators and acknowledgements

- Andreas Ekström (UiO, MSU)
- Christian Forrsen (Chalmers)
- Gaute Hagen (ORNL)
- Morten Hjorth-Jensen (UiO, MSU)
- Gustav R. Jansen (UTK, ORNL)
- Ruprecht Machleidt (UI)
- Hai Ah Nam (ORNL)
- Witold Nazarewicz (UTK, ORNL)
- Thomas Papenbrock (UTK, ORNL)
Outline

- Coupled cluster theory.
- Two-particles attached EOMCC.
- Shell evolution in oxygen isotopes.
- $^{26}$F with 2PA-EOMCC.
- Shell evolution in calcium isotopes.
- NNLO (POUNDerS)
The nuclear manybody problem

Need to solve the Schrödinger equation

\[ \hat{H} |\psi\rangle = \left( \hat{T} + \hat{V}_1 + \hat{V}_2 + \hat{V}_3 \ldots \right) |\psi\rangle = E |\psi\rangle \]

Two ingredients

1. The nuclear interaction.
2. A method to solve the many body problem.
Chiral effective field theory

<table>
<thead>
<tr>
<th>LO $(Q/\Lambda_{\chi})^0$</th>
<th>2N Force</th>
<th>3N Force</th>
<th>4N Force</th>
</tr>
</thead>
</table>
|                         | ![Diagram](image)
|                         | ![Diagram](image)
|                         | ![Diagram](image)
|                         | ![Diagram](image)

- Direct link to QCD.
- Perturbative expansion in momentum.
- Chiral symmetry is spontaneously and explicitly broken.
- The hierarchy of nuclear forces unfolds automatically.
The wavefunction is expanded in Slater determinants

\[ |\psi\rangle = \sum_{i}^{D} c_i |\Phi_i\rangle. \]

The number of possible Slater determinants is \( \binom{n}{A} \), where \( n \) is the number of single particle states and \( A \) is the number of nucleons.
Curse of dimensionality

![Graph showing the curse of dimensionality](image-url)
Coupled-cluster summary

Reduction of the number of degrees of freedom

\[ \hat{T} = \hat{T}_1 + \hat{T}_2 + \ldots + \hat{T}_A \]

\[ = \sum_{ia} t_i^a \left\{ a_a^\dagger a_i \right\} + \sum_{ijab} t_{ij}^{ab} \left\{ a_a^\dagger a_b^\dagger a_j a_i \right\} + \ldots + \]

\[ + \sum_{i_1,\ldots,i_A, a_1,\ldots,a_A} t_{i_1,\ldots,i_A}^{a_1,\ldots,a_A} a_a^\dagger a_{a_1} \ldots a_a^\dagger a_{a_A} a_{i_A} \ldots a_{i_1} \]
Coupled-cluster summary

Exponential ansatz

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

Include terms like

\[ e^{\hat{T}} \leftarrow \frac{1}{6} \hat{T}_1^3 + \frac{1}{2} \hat{T}_1 \hat{T}_2 + \frac{1}{A!} \hat{T}_A \]
### Coupled-cluster summary

Similarity transformed Hamiltonian

\[ \bar{H} = e^{-\hat{T}} \hat{H}_N e^{\hat{T}} \]

\[
\begin{pmatrix}
\langle \Phi_0 | \bar{H} | \Phi_0 \rangle & \cdots & \langle \Phi_0 | \bar{H} | \Phi_{a_1, \ldots, a_A} \rangle \\
\langle \Phi_a | \bar{H} | \Phi_0 \rangle & \cdots & \langle \Phi_a | \bar{H} | \Phi_{a_1, \ldots, a_A} \rangle \\
\langle \Phi_{ij} | \bar{H} | \Phi_0 \rangle & \cdots & \langle \Phi_{ij} | \bar{H} | \Phi_{a_1, \ldots, a_A} \rangle \\
\langle \Phi_{ijk} | \bar{H} | \Phi_0 \rangle & \cdots & \langle \Phi_{ijk} | \bar{H} | \Phi_{a_1, \ldots, a_A} \rangle \\
\vdots & \ddots & \vdots \\
\langle \Phi_{i_1, \ldots, i_A} | \bar{H} | \Phi_0 \rangle & \cdots & \langle \Phi_{i_1, \ldots, i_A} | \bar{H} | \Phi_{i_1, \ldots, i_A} \rangle \\
\end{pmatrix}
\]
Coupled-cluster summary
Similarity transformed Hamiltonian

CCS

\[
\begin{pmatrix}
E_{\text{CCS}} & \cdots & \langle \Phi_0 | \bar{H} | \Phi_{a_1, \ldots, a_A} \rangle \\
0 & \cdots & \langle \Phi_i | \bar{H} | \Phi_{a_1, \ldots, a_A} \rangle \\
\langle \Phi_{ij}^{ab} | \bar{H} | \Phi_0 \rangle & \cdots & \langle \Phi_{ij}^{ab} | \bar{H} | \Phi_{a_1, \ldots, a_A} \rangle \\
\langle \Phi_{ijk}^{abc} | \bar{H} | \Phi_0 \rangle & \cdots & \langle \Phi_{ijk}^{abc} | \bar{H} | \Phi_{a_1, \ldots, a_A} \rangle \\
\vdots & \ddots & \vdots \\
\langle \Phi_{i_1, \ldots, i_A}^{a_1, \ldots, a_A} | \bar{H} | \Phi_0 \rangle & \cdots & \langle \Phi_{i_1, \ldots, i_A}^{a_1, \ldots, a_A} | \bar{H} | \Phi_{a_1, \ldots, a_A} \rangle 
\end{pmatrix}
\]
Coupled-cluster summary
Similarity transformed Hamiltonian

CCSD

\[
\begin{pmatrix}
E_{\text{CCSD}} & \ldots & \langle \Phi_0 | \bar{H} | \Phi^{a_1,\ldots,a_A}_{i_1,\ldots,i_A} \rangle \\
0 & \ldots & \langle \Phi^a_i | \bar{H} | \Phi^{a_1,\ldots,a_A}_{i_1,\ldots,i_A} \rangle \\
0 & \ldots & \langle \Phi^{ab}_{ij} | \bar{H} | \Phi^{a_1,\ldots,a_A}_{i_1,\ldots,i_A} \rangle \\
\langle \Phi^{abc}_{ijk} | \bar{H} | \Phi_0 \rangle & \ldots & \langle \Phi^{abc}_{ijk} | \bar{H} | \Phi^{a_1,\ldots,a_A}_{i_1,\ldots,i_A} \rangle \\
\vdots & \ddots & \vdots \\
\langle \Phi^{a_1,\ldots,a_A}_{i_1,\ldots,i_A} | \bar{H} | \Phi_0 \rangle & \ldots & \langle \Phi^{a_1,\ldots,a_A}_{i_1,\ldots,i_A} | \bar{H} | \Phi^{a_1,\ldots,a_A}_{i_1,\ldots,i_A} \rangle
\end{pmatrix}
\]
Coupled-cluster summary
Similarity transformed Hamiltonian

\[ E_{\text{CCSDT}} \begin{pmatrix} \langle \Phi_0 \vert \bar{H} \vert \Phi_{a_1, \ldots, a_A} \rangle \\ \langle \Phi_{i_1, \ldots, i_A} \vert \bar{H} \vert \Phi_{a_1, \ldots, a_A} \rangle \\ \langle \Phi_{i_1, \ldots, i_A} \vert \bar{H} \vert \Phi_{a_1, \ldots, a_A} \rangle \\ \vdots \\ \langle \Phi_{i_1, \ldots, i_A} \vert \bar{H} \vert \Phi_{a_1, \ldots, a_A} \rangle \end{pmatrix} \]
Coupled-cluster summary

Similarity transformed Hamiltonian

FCI

\[
\begin{pmatrix}
E & \ldots & \langle \Phi_0 | \bar{H} | \Phi_{a_1, \ldots, a_A} \rangle \\
0 & \ldots & \langle \Phi_{a_i} | \bar{H} | \Phi_{a_1, \ldots, a_A} \rangle \\
0 & \ldots & \langle \Phi_{a_{ij}} | \bar{H} | \Phi_{a_1, \ldots, a_A} \rangle \\
0 & \ldots & \langle \Phi_{a_{ijk}} | \bar{H} | \Phi_{a_1, \ldots, a_A} \rangle \\
\vdots & \ddots & \vdots \\
0 & \ldots & \langle \Phi_{a_1, \ldots, a_A} | \bar{H} | \Phi_{a_1, \ldots, a_A} \rangle
\end{pmatrix}
\]
Excited states using EOM-CC

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

$\left( \bar{H}\hat{R} \right)_c = \omega \hat{R}$

Properties of $\bar{H}$.

- 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 $\left( \bar{H}\hat{R} \right)_c$ is key.
Two particles attached (2PA-EOM-CCSD)

Why?

- Access to additional isotopes.
- Possibility of effective interactions for shell model.
Two particles attached (2PA-EOM-CCSD)

Eigenvalue problem

\[
\left( \bar{H}\hat{R} \right)_c = \omega \hat{R}
\]

2PA-EOM-CCSD(2p0h)

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

2PA-EOM-CCSD(3p1h)

\[
\hat{R} = \hat{R}_2 + \hat{R}_3 = \frac{1}{2} \sum_{a,b} r^{ab} a_a \dagger a_b \dagger + \frac{1}{6} \sum_{a,b,c,i} r^{abc}_i a_a \dagger a_b \dagger a_c \dagger a_i
\]
**Testcase - \(^6\)He**

GRJ, M. Hjorth-Jensen, G. Hagen, and T. Papenbrock,

<table>
<thead>
<tr>
<th>Method</th>
<th>(0^+_1)</th>
<th>(2^+_1)</th>
<th>(0^+ \langle J \rangle)</th>
<th>(2^+_1 \langle J \rangle)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CCSD</td>
<td>(-22.732)</td>
<td>(-20.905)</td>
<td>0.78</td>
<td>2</td>
</tr>
<tr>
<td>CCSDT-1</td>
<td>(-24.617)</td>
<td>(-21.586)</td>
<td>0.25</td>
<td>2</td>
</tr>
<tr>
<td>CCSDT</td>
<td>(-24.530)</td>
<td>(-21.786)</td>
<td>0.01</td>
<td>2</td>
</tr>
<tr>
<td>2PA-EOM-CCSD(2(p)-0(h))</td>
<td>(-21.185)</td>
<td>(-18.996)</td>
<td>0</td>
<td>2</td>
</tr>
<tr>
<td>2PA-EOM-CCSD(3(p)-1(h))</td>
<td>(-24.543)</td>
<td>(-21.634)</td>
<td>0</td>
<td>2</td>
</tr>
<tr>
<td>FCI</td>
<td>(-24.853)</td>
<td>(-21.994)</td>
<td>0</td>
<td>2</td>
</tr>
</tbody>
</table>

**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.
Convergence

$^6\text{Li} (1^+)$

$^6\text{Li} (3^+)$

$^{18}\text{O} (0^+)$

$^{18}\text{O} (3^+)$
4p-2h states in $^{18}\text{O}$

Density dependent chiral threebody force

Our strategy: $C_D$ is given by fit to triton half-life, we fix $C_E$ and $k_F$ from fit to binding energy in selected medium mass nuclei:

Schematic three-nucleon forces

Integrating over the third leg in infinite nuclear matter and derive density dependent corrections to the nucleon-nucleon interaction.

K. Hebeler and A. Schwenk (2010)
Oxygen isotopes from chiral interaction

- Inclusion of effective 3NF places dripline at $^{25}$O.
- Overall the odd-even staggering in the neutron rich oxygen is well reproduced.
- We find $^{26}$O to unbound with respect to $^{24}$O by $\sim$100keV, agreement with E. Lunderberg et al., Phys. Rev. Lett. 108 (2012) 142503.
- We find $^{28}$O to be unbound with a resonance width of $\sim$2MeV.

Chiral three-nucleon force at order N2LO. $k_f=1.05$fm$^{-1}$, $C_D = 0.2$, $C_E = 0.71$ ($k_f$ and $c_E$ fitted to the binding energy of $^{16}$O and $^{22}$O).

Oxygen isotopes from chiral interaction

The effects of three-nucleon forces decompress the spectra and brings it in good agreement with experiment.

We find several states (4+,3+,2+) near the observed peak at ~7.5MeV in $^{24}$O

Matter and charge radii for $^{21-24}$O
Computed from intrinsic densities and Compared to experiment.

Excited states in $^{24}$O computed with EOM-CCSD and compared to experiment

<table>
<thead>
<tr>
<th>$J^\pi$</th>
<th>2$^+$</th>
<th>1$^+$</th>
<th>4$^+$</th>
<th>3$^+$</th>
<th>2$^+$/2</th>
<th>1$^+$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_{CC}$</td>
<td>4.56</td>
<td>5.2</td>
<td>6.2</td>
<td>6.9</td>
<td>7.0</td>
<td>8.4</td>
</tr>
<tr>
<td>$E_{Exp}$</td>
<td>4.7(1)</td>
<td>5.33(10)</td>
<td>0.03</td>
<td>0.04</td>
<td>0.005</td>
<td>0.01</td>
</tr>
<tr>
<td>$\Gamma_{CC}$</td>
<td>0.05$^{+0.21}_{-0.05}$</td>
<td>0.03$^{+0.12}_{-0.03}$</td>
<td>0.005</td>
<td>0.01</td>
<td>0.04</td>
<td>0.56</td>
</tr>
<tr>
<td>$\Gamma_{Exp}$</td>
<td>0.05$^{+0.21}_{-0.05}$</td>
<td>0.03$^{+0.12}_{-0.03}$</td>
<td>0.005</td>
<td>0.01</td>
<td>0.04</td>
<td>0.56</td>
</tr>
</tbody>
</table>
Threebody forces in $^{26}$F


Technical details

- Chiral interaction at N$^3$LO.
- Identical threebody force as established in the oxygen chain.
- 17 major harmonic oscillator shells with a Gamow-Hartree-Fock basis for $\nu s_{1/2}$ and $\nu d_{3/2}$.
- CCSD with triples corrections (A-CCSD(T)) for $^{24}$O, with 2PA-EOMCC.
- $^{26}$F$_{\text{free}} = B(^{25}$O) + $B(^{25}$F) − $B(^{24}$O)

Threebody forces are crucial for correct levels spacing.
Evolution of single particle energies

Technical details

- Relativistic mean-field including continuum effects.

Main features

- Bunching of single-particle energies outside the $pf$-shell.
- No shell-gap in $^{60}\text{Ca}$ - $^{70}\text{Ca}$.
- Large deformations and no shell-closure.
- Continuum effects responsible for bound $^{60}\text{Ca}$ - $^{72}\text{Ca}$. 

![Graph of single particle energies](image)
Main features

- Shell-model calculation in the $pf$-shell including $0g_{9/2}$ and $2d_{5/2}$ for neutrons.
- Inversion of the $0g_{9/2}$ and the $2d_{5/2}$ single particle states in $^{60}$Ca.
- Bunching of levels including the $0f_{5/2}$ state indicates no shell-closure.
Binding energies in calcium isotopes

G. Hagen, M. Hjorth-Jensen, GRJ, R. Machleidt, and T. Papenbrock
PRL109 032502 (2012)

Technical details

- Chiral interaction at $N^3$LO.
- Density dependent three body force with $k_F = 0.95\text{fm}^{-1}$, $c_D = -0.2$ and $c_E = 0.735$. $N_{\text{max}} = 18$ and $\hbar \omega = 26 \text{MeV}$.
- Mass of $^{51}\text{Ca}$ and $^{52}\text{Ca}$ from A. T. Gallant et al., PRL 109, 032506 (2012)

Main features

- Total binding energies agree well with experimental masses.
- $^{60}\text{Ca}$ is not magic.
- Three nucleon force is repulsive.
Shell evolution in neutron rich calcium isotopes.

Details


- $J^\pi = 2^+$ systematics in even calcium isotopes.

Main features

- Threebody forces needed to make $^{48}$Ca magic.
- Different models have $^{54}$Ca magic, semi magic and not magic at all.
$J^\pi = 2^+$ systematics in even calcium isotopes
G. Hagen, M. Hjorth-Jensen, GRJ, R. Machleidt, and T. Papenbrock,
PRL109 032502 (2012)

Technical details
- Chiral interaction at N$^3$LO.
- Density dependent three body force with $k_F = 0.95\text{fm}^{-1}$, $c_D = -0.2$ and $c_E = 0.735$. $N_{\text{max}} = 18$ and $\hbar\omega = 26\text{ MeV}$.

Main features
- Good agreement between theory and experiment.
- Shell closure in $^{48}$Ca.
- Sub-shell closure in $^{52}$Ca.
- Predict weak sub-shell closure in $^{54}$Ca.
Spectra in calcium isotopes
G. Hagen, M. Hjorth-Jensen, GRJ, R. Machleidt, and T. Papanbrook
PRL109 032502 (2012)

Technical details
- Chiral interaction at $N^3$LO.
- Density dependent three body force with $k_F = 0.95 \text{fm}^{-1}$, $c_D = -0.2$ and $c_E = 0.735$. $N_{\text{max}} = 18$ and $\hbar \omega = 26 \text{ MeV}$.
- Continuum included for selected weakly bound and resonant states.

Main features
- Inversion of $g_9/2$ and $d_5/2$.
- $1/2^+$ groundstate in $^{61}\text{Ca}$.
- Continuum effects are crucial.
NNLO (POUNDerS)

- Want to derive consistent forces.
- All contributions at a given order are evaluated.
- Currently NNLO.
- Apply numerical optimization algorithms to find the optimal parameters.
Triton binding energy
$^4$He binding energy
Oxygen isotopes with NNLO (POUNDerS)

Oxygen spectra with NNLO (POUNDerS)
$J^\pi = 2^+$ systematics with NNLO (POUNDerS)

$J^\pi = 2^+$ systematics with NNLO (POUNDerS)

Calcium isotopes with NNLO (POUNDerS)
Calcium isotopes with NNLO (POUNDerS)
Calcium isotopes with NNLO (POUNDerS)
Calcium isotopes with NNLO (POUNDerS)

Questions?

Gustav R. Jansen
gustav.jansen@utk.edu

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).

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.