Coupled-cluster computations of neutron-rich nuclei

Gaute Hagen
Oak Ridge National Laboratory

ECT*, Trento, April 10th, 2017
Collaborators

@ ORNL / UTK: G. R. Jansen, T. Morris, T. Papenbrock, M. Schuster, Z. H. Sun

@ MSU: W. Nazarewicz, F. Nunes, J. Rotureau

@ Chalmers: B. Carlsson, A. Ekström, C. Forssén

@ Hebrew U: N. Barnea, D. Gazit

@ MSU/ U Oslo: M. Hjorth-Jensen

@ Trento: G. Orlandini

@ TRIUMF: S. Bacca, J. Holt, M. Miorelli, P. Navratil, S. R. Stroberg

@ TU Darmstadt: C. Drischler, C. Stumpf, K. Hebeler, R. Roth, A. Schwenk, J. Simonis

@ LLNL: K. Wendt

@ U. Manchester: R. F. Garcia-Ruiz
Outline

- Inclusive electron scattering and Coulomb sum rule
- The neutron skin and dipole polarizability of $^{48}$Ca and $^{68}$Ni
- Structure of $^{78}$Ni and $^{100}$Sn
- Optical potentials from coupled-cluster theory
Trend in realistic ab-initio calculations

**Explosion of many-body methods** (Coupled clusters, Green’s function Monte Carlo, In-Medium SRG, Lattice EFT, MCSM, No-Core Shell Model, Self-Consistent Green’s Function, UMOA, ...)

**Application of ideas from EFT and renormalization group** ($V_{\text{low-}k}$, Similarity Renormalization Group, ...)

![Graph showing trend in realistic ab-initio calculations](image)

- Realistic: BEs within 5% and starts from NN + 3NFs
Reach of ab-initio computations of nuclei

Computational capabilities (for some observables) exceed accuracy of available interactions

Nuclei for which ab-initio computations have been attempted

H. Hergert et al, Physics Reports 621, 165-222 (2016)
**Coupled-cluster method (CCSD approximation)**

**Ansatz:**

\[
|\Psi\rangle = e^T|\Phi\rangle \\
T = T_1 + T_2 + \ldots \\
T_1 = \sum_{ia} t_i^a a^\dagger_a a_i \\
T_2 = \sum_{ijab} t_{ij}^{ab} a^\dagger_a a^\dagger_b a_j a_i
\]

- Scales gently (polynomial) with increasing problem size \( o^2u^4 \).
- Truncation is the only approximation.
- Size extensive (error scales with \( A \))
- Most efficient for closed (sub-)shell nuclei

**Correlations are exponentiated** 1p-1h and 2p-2h excitations. Part of np-nh excitations included!

**Coupled cluster equations**

\[
E = \langle \Phi | \overline{H} | \Phi \rangle \\
0 = \langle \Phi_i^a | \overline{H} | \Phi \rangle \\
0 = \langle \Phi_{ij}^{ab} | \overline{H} | \Phi \rangle 
\]

\[
\overline{H} \equiv e^{-T}He^T = (He^T)_c = \left(H + HT_1 + HT_2 + \frac{1}{2}HT_1^2 + \ldots\right)_c
\]

Alternative view: CCSD generates similarity transformed Hamiltonian with no 1p-1h and no 2p-2h excitations.
Coupled-cluster method

- CCSD captures most of the 3p3h and 4p4h excitations (scales as $n_o^2n_u^4$)
- In order to describe $\alpha$-cluster states, need to include full quadruples (CCSDTQ) (scales $n_o^4n_u^6$)

Correlations are *exponentiated* 1p-1h and 2p-2h excitations. Part of np-nh excitations included!
Success: BEs of oxygen chain

- Calculations based on chiral NN and 3NF
- Agreement between different methods

Challenge: Collectivity and transition strengths

- $^{14}$C computed in FCI and CC with psd effective interaction
- As effective charge is varied from 0 to 1 CCSD fails
- Need excitations beyond 4p4h to describe $B(E2)$ even if 2+ energy is reproduced
**Accurate nuclear binding energies and radii from a chiral interaction**

**Solution:** Simultaneous optimization of NN and 3NFs. Include charge radii and binding energies of $^3$H, $^3,^4$He, $^{14}$C, $^{16}$O in the optimization ($\text{NNLO}_{\text{sat}}$).


**Not new:** GFMC with AV18 and Illinois-7 are fit to 23 levels in nuclei with $A < 10$. 
Accurate BEs from light → heavy → infinite matter from a chiral interaction

1.8/2.0 (EM) from K. Hebeler et al PRC (2011)
The other chiral NN + 3NFs are from Binder et al, PLB (2014)

- Accurate binding energies up to mass 100 from a chiral NN + 3NF
- Fit to nucleon-nucleon scattering and BEs and radii of A=3,4 nuclei
- Reproduces saturation point in nuclear matter within uncertainties
- Deficiencies: Radii are less accurate
Inclusive electron scattering and the Coulomb sum rule

The CSR is the total integrated strength of inelastic longitudinal response function

\[ \text{CSR}(q) = \int d\omega \frac{R_L^{\text{in}}(\omega, q)}{G_p^2(Q^2)} \]

\[ R_L^{\text{in}}(\omega, q) = \sum_f |\langle f | \rho(q) | 0 \rangle|^2 \delta(\omega - E_f + E_0) \]

Here \( \rho(q) \) is the nuclear charge operator
Final state different from g.s. since we want the inelastic response

We approached the problem as we do for the calculation of the total strength of the dipole response function in PRL 111, 122502 (2013).
Inclusive electron scattering and the Coulomb sum rule

$$CSR(q) = Z + \langle 0 | \sum_{i \neq j} e^{i \mathbf{q} \cdot (\mathbf{r}_i - \mathbf{r}_j)} | 0 \rangle - |F(q)|^2 Z^2$$

Benchmark with “exact” Hyperspherical Harmonics for $^4\text{He}$

Very nice agreement!
Comparison to data in $^4$He and $^{16}$O

- Good agreement in $^4$He
- CSR for $^{16}$O based on NNLO$_{sat}$ and N3LO(EM)
- Comparison to data in $^{12}$C and to Mihaila and Heisenberg (PRL 2000)
Comparison to data in $^{40}$Ca with NNLO$_{\text{sat}}$

- Excellent agreement with elastic charge form factor up to momentum transfers of ~500MeV/c
- Very little data for the CSR
- To exhaust the sum rule need to integrate longitudinal response over large energy range
Comparison to data in $^{48}$Ca

Data from Ingo Sick
Neutron radius and skin of $^{48}$Ca

- Neutron skin significantly smaller than in DFT
- Neutron skin almost independent of the employed Hamiltonian
- Our predictions for $^{48}$Ca are consistent with existing data


Uncertainty estimates from family of chiral interactions: K. Hebeler et al PRC (2011)

DFT: SkM*, SkP, Sly4, SV-min, UNEDF0, and UNEDF1

Dispersive Optical Model

- $\bar{p}$ atoms - Trzcinski
- $\pi$ - Friedman
- $\pi$ - Gibbs & Dedonder
- $\alpha$-scattering - Gils
- Theory - Hagen
Weak charge form-factor of $^{48}\text{Ca}$

\textbf{Ab-initio predictions:}

$0.195 \lesssim F_W(q_c) \lesssim 0.222$, $3.59 \lesssim R_W \lesssim 3.71$ fm, $0.12 \lesssim R_{\text{skin}} \lesssim 0.15$ fm

\textbf{DFT predictions:}

SV-min: $F_W(q_C) = 0.1986$, $R_{\text{skin}} = 0.1830$ fm

FSUBJ: $F_W(q_C) = 0.205$, $R_{\text{skin}} = 0.1925$ fm

Can we reliably extract the neutron skin from a single measurement?
Weak skin of $^{48}\text{Ca}$ at $q_c = 0.778\text{fm}^{-1}$
**Dipole response from coupled-cluster**

S. Bacca, N. Barnea, G. Hagen, M. Miorelli, G. Orlandini, T. Papenbrock, PRC 90, 064610 (2014)

![Graph showing dipole response](image)

- **Lorentz Integral transform from coupled-cluster benchmarked with “exact” hyper-spherical harmonics for $^4$He**

![Graph showing dipole response](image)

- **CCSD agrees within 1% of Hyper-spherical harmonics**

$$\alpha_D = 2\alpha \int_{\omega_{th}}^{\infty} d\omega \frac{S(\omega)}{\omega}$$

Dipole polarizability of $^{48}\text{Ca}$

- DFT results are consistent and within band of ab-initio results
- Data has been analyzed by Osaka-Darmstadt collaboration
- Ab-initio prediction overlaps with experimental uncertainty

\begin{align*}
\alpha_D \text{ (fm}^3\text{)} &\approx 2.0 \\
R_p \text{ (fm)} &\approx 3.4
\end{align*}

\textit{Ab-initio} prediction from correlation with $R_p$:
\[2.19 \leq \alpha_D \leq 2.60 \text{ fm}^3\]


J. Birkhan \textit{et al} (submitted).
Neutron skin/dipole polarizability of $^{68}\text{Ni}$

- Charge radii have been measured by the the COLLAPS collaboration at ISOLDE, CERN
- Neutron skin larger than RPA results

Measuremet of dipole strength in $^{68}\text{Ni}$:
D. Rossi et al, PRL 111 242503 (2013)


<table>
<thead>
<tr>
<th>Nucleus</th>
<th>$\Delta r_{np}$ (a)</th>
<th>$\Delta r_{np}$ (b)</th>
<th>$\Delta r_{np}$ (c)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{68}\text{Ni}$</td>
<td>0.15–0.19</td>
<td>0.18 ± 0.01</td>
<td>0.16 ± 0.04</td>
</tr>
<tr>
<td>$^{120}\text{Sn}$</td>
<td>0.12–0.16</td>
<td>0.14 ± 0.02</td>
<td>0.12 ± 0.04</td>
</tr>
<tr>
<td>$^{208}\text{Pb}$</td>
<td>0.13–0.19</td>
<td>0.16 ± 0.02</td>
<td>0.16 ± 0.03</td>
</tr>
</tbody>
</table>

![Graph showing dipole polarizability and charge radii](image-url)
A high $2^+$ energy in $^{78}$Ni indicates that this nucleus is doubly magic

A measurement of this state has been made at RIBF, RIKEN
R. Taniuchi et al., in preparation

Consistent with recent shell-model studies
F. Nowacki et al., PRL 117, 272501 (2016)

- From an observed correlation we predict the $2^+$ excited state in $^{78}$Ni using the experimental data for the $2^+$ state in $^{48}$Ca
- Similar correlations have been observed in other nuclei, e.g. Tjon line in light nuclei

G. Hagen, G. R. Jansen, and T. Papenbrock
Excited states in $^{78}\text{Ni}$ and its neighbors

- $4^+/2^+ = 1.2$ consistent with $^{78}\text{Ni}$ being a doubly magic
- Continuum impacts level ordering in $^{79}\text{Ni}$
- Dripline is beyond $^{80}\text{Ni}$

F. Nowacki et al., PRL 117, 272501 (2016)

N=50 isotones
\( {^{100}}\text{Sn} \) – a nucleus of superlatives

- Heaviest self-conjugate doubly magic nucleus
- Largest known strength in allowed nuclear \( \beta \)-decay
- In the closest proximity to the proton dripline
- At the endpoint of the rapid proton capture process (Sn-Sb-Te cycle)
- Unresolved controversy regarding s.p. structure of \( {^{101}}\text{Sn} \)

Sewernyiak et al PRL (2007) predicted a 5/2+ ground-state as presumably in \( {^{103}}\text{Sn} \)


Darby et al, PRL (2010)
Structure of the lightest tin isotopes

- High $2^+$ energy in $^{100}$Sn
- Predict $7/2^+$ ground-state in $^{101}$Sn
- Experimental splitting between $7/2^+$ and $5/2^+$ reproduced
- Ground-state spins of $^{101-121}$Sn will be measured at CERN (CRIS collaboration)
Structure of the lightest tin isotopes
Optical potentials from coupled-cluster theory


\[
G^{CC}(\alpha, \beta, E) \equiv \\
\langle \Phi_{0,L} | \overline{a_\alpha} \frac{1}{E - (\overline{H} - E^A_{gs}) + i\eta} \overline{a_\beta} | \Phi_0 \rangle \\
+ \langle \Phi_{0,L} | \overline{a_\beta} \frac{1}{E - (E^A_{gs} - \overline{H}) - i\eta} \overline{a_\alpha} | \Phi_0 \rangle 
\]

Coupled-cluster Green’s function:

Solve for A±1 systems with PA/PR-EOMCCSD truncated at 2p1h and 1p2h

\[
\begin{align*}
\left[ E - (\overline{H} - E^A_{gs}) \right] | \Psi^{A+1}_{R,\beta}(E) \rangle &= \overline{a_\beta} | \Phi_{0,R} \rangle \\
\left[ E - (E^A_{gs} - \overline{H}) \right] | \Psi^{A-1}_{R,\alpha}(E) \rangle &= \overline{a_\alpha} | \Phi_{0,R} \rangle 
\end{align*}
\]

The coupled-cluster Green’s function can then be written:

\[
G(\alpha, \beta, E) = \langle \phi_{0,L} | \overline{a_\alpha} | \Psi^{A+1}_{R,\beta}(E) \rangle + \langle \phi_{0,L} | \overline{a_\beta} | \Psi^{A-1}_{R,\alpha}(E) \rangle 
\]

Optical potentials from coupled-cluster theory

Using a Berggren basis allows stable results for $\eta \to 0$

$$\sum_i |u_i\rangle \langle \tilde{u}_i| + \int_{L^+} dk |u(k)\rangle \langle u(\tilde{k})| = \hat{1}$$

See also Hagen 04, Kruppa 07, Carbonell 2014, Papadimitriou 2015 for few-body applications

Inverting the Dyson equation we obtain the self-energy:

$$\Sigma^*(E) = [G^{(0)}(E)]^{-1} - G^{-1}(E)$$

Scattering phase shifts are obtained by the solving the equation:

$$-\frac{\hbar^2}{2\mu} \nabla^2 \xi(r) + \int dr' \Sigma'(r, r', E^+) \xi(r') = E^+ \xi(r)$$

Imaginary part of the neutron s-wave Green’s function
Neutron elastic scattering on $^{16}\text{O}$ with $\text{NNLO}_\text{opt}$


Consistent results between computed phase shifts and resonances computed directly in the Berggren basis via PA-EOMCCSD

<table>
<thead>
<tr>
<th>$N_{\text{max}}$</th>
<th>$E(5/2^+)$</th>
<th>$E(1/2^+)$</th>
<th>$E(3/2^+)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>-4.35</td>
<td>-2.62</td>
<td>2.68-i0.32</td>
</tr>
<tr>
<td>10</td>
<td>-4.49</td>
<td>-2.73</td>
<td>2.24-i0.25</td>
</tr>
<tr>
<td>12</td>
<td>-4.56</td>
<td>-2.76</td>
<td>2.34-i0.21</td>
</tr>
<tr>
<td>14</td>
<td>-4.57</td>
<td>-2.80</td>
<td>2.26-i0.12</td>
</tr>
</tbody>
</table>
Neutron elastic scattering on $^{40}$Ca

- Diffraction minima in good agreement with data
- Cross section overestimated due to lack of absorption (e.g. $0^+$ state in $^{40}$Ca too high)
- Using a Berggren basis allows for stable results as $\epsilon \rightarrow 0$. 
Summary

- Promising results for electron scattering and Coulomb sum rule
- Predictions of dipole polarizability of $^{48}\text{Ca}$ and $^{68}\text{Ni}$ are consistent with data
- $^{78}\text{Ni}$ and $^{100}\text{Sn}$ are predicted to be doubly magic
- Optical potentials from coupled-cluster theory – promising first results for $^{40}\text{Ca}+n$ with $\text{NNLO}_{\text{sat}}$