Coupled-cluster theory for medium-mass nuclei

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and

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Overview

1. Coupled-cluster theory (nuclear physics peculiarities)

2. Three-nucleon forces
   [Hagen, TP, Dean, Hjorth-Jensen, arxiv:0806.3478]

3. Medium-mass nuclei from “bare” chiral interactions

4. Weakly bound and unstable nuclei – ab initio calculation of life times
   [Hagen, Dean, Hjorth-Jensen, TP, Schwenk, Phys. Rev. C 76, 044305 (2007);
   Dean, Hagen, Hjorth-Jensen, TP, Schwenk, arXiv:0709:0449]

5. Benchmark calculations
   [Hagen, Dean, Hjorth-Jensen, TP, Schwenk, Phys. Rev. C 76, 044305 (2007);
   Dean, Hagen, Hjorth-Jensen, TP, Schwenk, arXiv:0709:0449]
Ab-initio methods in nuclear structure

Green's function
Monte Carlo
Full CI

Coupled-cluster theory
Nuclear shell model

1. Traditional shell model:
   • Quantum well + strong spin-orbit force
   • “Freeze” core nucleons and work with valence nucleons

2. “Ab-initio” methods:
   • Provides basis for wave-function based methods

3. Harmonic oscillator basis allows to keep all symmetries within CI
   • Parameters: oscillator frequency, number of major oscillator shells
   • All nucleons active

4. Gamow shell model:
   • Finite well
   • Basis of bound, resonant, and scattering states
Peculiarities of coupled-cluster theory for nuclei

Interaction: One of the main questions

1. A few high-precision potentials available
2. Renormalization scale / scale of external probe provides families of interactions
3. Model-space dependencies must be examined

Hamiltonian:

1. Nucleons are fundamental degrees of freedom (orbital, spin, and isospin label single-particle states)
2. Hamiltonian is scalar under rotation
   - Cluster excitation operator is scalar, too
   - Number of j-shells $\sim A^{2/3}$ for nucleus with mass numbers $A$ (only $1/2^6$ in quantum chemistry)

\[
\hat{T} = \sum_{j_a,j_i} t^{j_a}_{j_i} \left( \hat{a}^{\dagger}_{j_a} \times \hat{a}_{j_i} \right)^{(0)} \\
+ \sum_{j_a,j_b,j_i,j_J} \sum_{J} t^{j_a,j_b}_{j_i,j_J} (J) \left( \left( \hat{a}^{\dagger}_{j_a} \times \hat{a}^{\dagger}_{j_b} \right)^{(J)} \times \left( \hat{a}_{j_j} \times \hat{a}_{j_i} \right)^{(J)} \right)^{(0)}
\]
Effective field theory: chiral potential at order $N^3$LO

Feynman diagrams

<table>
<thead>
<tr>
<th>$Q^0$</th>
<th>$Q^2$</th>
<th>$Q^3$</th>
<th>$Q^4$</th>
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<tr>
<td>LO</td>
<td>NLO</td>
<td>NNLO</td>
<td>N$^3$LO</td>
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</tbody>
</table>

$\chi^2$/datum = 1

Phase shifts reproduced to

- $^1S_0$
- $^3P_0$
- $^1P_1$
- $^3P_1$
- $^3S_1$
- $^3D_1$

About 20+ parameters


Three-nucleon forces: Why?

- Nucleons are not point particles (i.e. not elementary).
- We neglected some internal degrees of freedom (e.g. $\Delta$-resonance, “polarization effects”, …), and unconstrained high-momentum modes.

**Example from celestial mechanics:**
Earth-Moon system: point masses and modified two-body interaction

**Other tidal effects cannot be included in the two-body interaction!** Three-body force unavoidable for point masses.

Renormalization group transformation: Removal of “stiff” degrees of freedom at expense of additional forces.
A theorem for three-body Hamiltonians
Polyzou and Glöckle, Few Body Systems 9, 97 (1990)

Different two-body Hamiltonians can be made to fit two-body and three-body data by including a 3NF into one of the Hamiltonians.

**Theorem.** Let

\[ H_{ij} = H_i + H_j + V_{ij} \quad \text{and} \quad \bar{H}_{ij} = H_i + H_j + \bar{V}_{ij} \quad (1.1) \]

be two-body Hamiltonians with the same binding energies and scattering matrices for each pair of particles \( i \) and \( j \). Assume that the two-body Hamiltonians are asymptotically complete and that the unitary transformations relating these two-body Hamiltonians, which necessarily exist, have bounded Cayley transforms. Then there exists a three-body interaction, \( W \), such that the two three-body Hamiltonians

\[ H = H_1 + H_2 + H_3 + V_{12} + V_{23} + V_{31} \quad (1.2) \]

and

\[ \bar{H} = H_1 + H_2 + H_3 + \bar{V}_{12} + \bar{V}_{23} + \bar{V}_{31} \quad (1.3) \]

have the same binding energies and scattering matrix.

**Corollary.** Under the assumptions of the theorem, if \( V_{(123)} \) is a three-body interaction then there exists another three-body interaction \( \bar{V}_{(123)} \) such that

\[ H = H_1 + H_2 + H_3 + V_{12} + V_{23} + V_{31} + V_{(123)} \]

and

\[ \bar{H} = H_1 + H_2 + H_3 + \bar{V}_{12} + \bar{V}_{23} + \bar{V}_{31} + \bar{V}_{(123)} \]

have the same binding energies and scattering matrix.

**Implications:**

1. There are no experiments measuring only three-body binding energies and phase shifts that can determine if there are no three-body forces in a three-body system. The question makes no sense. The correct statement is that there may be some systems for which it is possible to find a representation in which three-body forces are not needed.
2. Different off-shell extensions of two-body forces can be equivalently realized as three-body interactions.
3. Three-body forces cannot be determined in a manner that is independent of the two-body interaction.
Low momentum potential $V_{\text{low-k}}$

\[ \frac{d}{d\Lambda} V_{\text{low-k}}(k', k) = \frac{2}{\pi} \frac{V_{\text{low-k}}(k', \Lambda) T(\Lambda, k; \Lambda^2)}{1 - (k/\Lambda)^2} \]

Different high-precision potentials

Universal low-momentum potential

Properties of $V_{\text{low-k}}$:
- No hard core
- Nonlocal
- Hartree-Fock already yields bound nuclei.

Interaction: $V_{\text{low}-k}$ from Av18 + chiral 3NF

As cutoff $\Lambda$ is varied, motion along Tjon line.

Addition of $\Lambda$-dependent three-nucleon force yields agreement with experiment.

Three-nucleon force perturbative at cutoff $\Lambda=1.9$ fm$^{-1}$ for these nuclei.

Q: Why only CCSD and not CCSDT?

A1: Expect that CCSD approximation is valid for three-nucleon force: density-dependent 2-body terms dominant

A2: CCSD with 3NF has effort $\sim v^4 o^4$ while CCSDT with 3NF $\sim v^6 o^3$

$$E = \text{Diagram 1} + \text{Diagram 2} + \text{Diagram 3} + \text{Diagram 4} + \text{Diagram 5} + \text{Diagram 6} + \text{Diagram 7} + \text{Diagram 8} + \text{Diagram 9} + \text{Diagram 10} + \text{Diagram 11} + \text{Diagram 12} + \text{Diagram 13} + \text{Diagram 14} + \text{Diagram 15}$$

Energy and 1p-1h equation as examples.
Factorization of diagrams very useful!
1p-1h: 15 diagrams
2p-2h: 51 diagrams
Correction to 1p-1h equation:

\[
0 = \frac{1}{4} \sum_{cdli} \langle kia|cede \rangle t_{kl}^d + \sum_{ce} I(6b)_{ce} t_{ki}^e + \sum_{elm} I(7)_{elm} t_{km}^e + \frac{1}{2} \sum_{ke} I(8c)_{ke} t_{ke}^e + \sum_{cm} I(9)_{cm} t_{cm}^e + \sum_{o} I(10ac)_{o} t_{io}^e - \sum_{m} I(11)_{i} t_{im}^e.
\]

Factorized diagrams:

Intermediates:

\[
I(5)_{ce}^{km} = \frac{1}{4} \sum_{dl} \langle klm|cede \rangle t_{li}^d,
\]

\[
I(6b)_{ce}^{ka} = \frac{1}{2} \sum_{dl} \langle kla|cede \rangle t_{li}^d,
\]

\[
I(7b)_{ce}^{km} = \frac{1}{2} \sum_{dl} \langle klm|cede \rangle t_{li}^d,
\]

\[
I(7)_{ce}^{km} = \frac{1}{4} \sum_{lde} \langle klm|cede \rangle t_{ie}^{de} + I(7b)_{ce}^{km} + 2 \sum_{o} I(5)_{ce}^{km} t_{oi}^e,
\]

\[
I(8c)_{ci}^{ka} = \sum_{dl} \langle kla|cede \rangle t_{li}^d,
\]

\[
I(9)_{c}^{k} = \frac{1}{4} \sum_{delm} \langle klm|cede \rangle t_{im}^{de} + 2 \sum_{cm} I(5)_{ce}^{km} t_{im}^e,
\]

\[
I(10ac)_{o}^{a} = \frac{1}{4} \sum_{skdl} \langle kla|cede \rangle t_{ki}^{ad} + \sum_{kc} I(6b)_{ce}^{ka} t_{ck}^e,
\]

\[
I(11)_{i}^{m} = \frac{1}{4} \sum_{skdl} \langle klm|cede \rangle t_{ki}^{md} + 2 \sum_{kc} I(5)_{ce}^{km} t_{ki}^e + \sum_{kc} I(7b)_{ce}^{km} t_{ki}^e + \sum_{o} I(9)_{ce}^{m} t_{oi}^e.
\]
Additional diagrams for 2p-2h cluster amplitude

<table>
<thead>
<tr>
<th>Diagram No.</th>
<th>Diagram Description</th>
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<td>21</td>
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Diagram 13:

Diagram 14:

Diagram 15:

Diagram 16:

Diagram 17:

Diagram 18:

Diagram 19:

Diagram 20:

Diagram 21:

Diagram 22:

Diagram 23:

Diagram 24:

Diagram 25:

Diagram 26:

Diagram 27:

Diagram 28:

Diagram 29:

Diagram 30:

Diagram 31:

Diagram 32:

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Diagram 102:

Diagram 103:

Diagram 104:

Diagram 105:

Diagram 106:

Diagram 107:

Diagram 108:

Diagram 109:

Diagram 110:

Diagram 111:

Diagram 112:

Diagram 113:

Diagram 114:

Diagram 115:

Diagram 116:

Diagram 117:

Diagram 118:

Diagram 119:

Diagram 120:
Coupled-cluster theory with three-nucleon forces for $^4$He

Two-body force: $V_{\text{low-k}}$ with $\Lambda=1.9$ fm$^{-1}$ from Argonne V18

Three-body force: Chiral EFT at order $N^2$LO (isospin $1/2$ only)
Important (technical) detail: normal-ordered Hamiltonian

The Hamiltonian is normal-ordered w.r.t. the vacuum state $|\Phi>$. 

\[
\hat{H} = \sum_{pq} \varepsilon_{pq} \hat{a}_p^\dagger \hat{a}_q + \frac{1}{4} \sum_{pqrs} \langle pr||sr\rangle \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_r \hat{a}_s
\]

\[
= \sum_i \varepsilon_{ii} + \frac{1}{2} \sum_{ij} \langle ij||ij\rangle
\]

\[
+ \sum_{ij} \left( \varepsilon_{pq} + \sum_i \langle pi||qi\rangle \right) \{ \hat{a}_p^\dagger \hat{a}_q \} + \frac{1}{4} \sum_{pqrs} \langle pq||sr\rangle \{ \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_r \hat{a}_s \}
\]

Similarly, the Hamiltonian of the 3NF becomes

\[
\hat{H}_3 = \frac{1}{6} \sum_{ijk} \langle ijk||ijk\rangle + \frac{1}{2} \sum_{ijpq} \langle ijp||ijq\rangle \{ \hat{a}_p^\dagger \hat{a}_q \} 
\]

\[
+ \frac{1}{4} \sum_{ipqrs} \langle ipq||irs\rangle \{ \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_r \hat{a}_s \} + \hat{h}_3
\]

\[
\hat{h}_3 \equiv \frac{1}{36} \sum_{pqrst} \langle pqr||stuv\rangle \{ \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_r^\dagger \hat{a}_u \hat{a}_t \hat{a}_s \}
\]

Note:
1. The form of the Hamiltonian is different for each nucleus under consideration.
3. "Density-dependend" terms are coherent sums over two- and three-body matrix elements.
Contributions to the binding energy of $^4$He

Main results:

- Residual 3NF can be neglected.
- Enormous reduction of computational effort
- “Two-body machinery” can be applied

Residual 3NF can be neglected!

\[ \hat{H}_3 = \frac{1}{6} \sum_{ijk} \langle ijk | ijk \rangle + \frac{1}{2} \sum_{ijpq} \langle ijpq | ij_3 \rangle \{ a_p^+ a_q^+ a_3 \} \]
\[ + \frac{1}{4} \sum_{ipqrs} \langle ipqrs | irs \rangle \{ a_p^+ a_q^+ a_s a_r \} + \hat{h}_3. \]

**FIG. 7:** (Color online) Relative contributions $|\Delta E/E|$ to the binding energy of $^4$He at the CCSD level. The different points denote the contributions from (1) low-momentum NN interactions, (2) the vacuum expectation value of the 3NF, (3) the normal-ordered one-body Hamiltonian due to the 3NF, (4) the normal-ordered two-body Hamiltonian due to the 3NF, and (5) the residual 3NFs. The dotted line estimates the corrections due to omitted three-particle–three-hole clusters.

Hagen, TP, Dean, Schwenk, Nogga, Wloch, Piecuch, PRC 76, 034302 (2007)
Déjà vu …


From the abstract:
“For nuclei two body forces as usual do not yield results in agreement with experiments. The introduction of exchange currents into the elastic electron form factor and three body forces greatly improves the situation.”


From the conclusion:
“…utilize the interesting feature that the three-body effective interaction appears to act primarily as a density-dependent two-body interaction.”

Form factor for $^{16}$O within CC: AV18 + UIX


Monopole shifts from 3NF as density-dependent NN force (Shown below: Spectrum in $^{22}$Na).

A. Zuker, PRL90, 42502 (2003).
Improved CCSD(T) results for $^4$He: perturbative 3p-3h clusters

FIG. 8: (Color online) CCSD(T) results for the binding energy of $^4$He as a function of the oscillator spacing and for model spaces consisting of $N = 3$ to $N = 6$ oscillator shells. The contributions from 3NFs are limited to the density-dependent zero-, one-, and two-body terms and exclude its residual three-body terms.

FIG. 9: (Color online) Data points: CCSD(T) results (taken at the $\hbar \omega$ minima) for the binding energy of $^4$He with 3NFs as a function of the number of oscillator shells. Dashed lines: Exponential fit to the data and asymptote of the fit. Full line: Exact result.

Center-of-mass expectation: 20 keV
Spherical (j-coupled) coupled-cluster approach

Spherical-symmetric implementation of coupled-cluster theory

1. Possible for nuclei with closed sub-shell (or cs +/- 1)
2. Relatively simple since similarity-transformed Hamiltonian is two-body (CCSD) or three-body (CCSDT) at most
3. Enormous computational reduction: $o^2u^4 \rightarrow (o^2u^4)^{2/3}$ (naïve estimate)
   - CCSD for $^{40}$Ca on a laptop (now)
   - CCSDT for $^{48}$Ca nuclei via super computers (future)
   - CCSD for $^{100}$Sn and $^{132}$Sn for “bare” chiral interaction via super computers

Avoid 9-j symbols in sums!
Keep interaction and $T_2$ amplitudes in pp and ph schemes!

in particle-particle coupled scheme

in particle-hole coupled scheme
Preliminary results $^{40}$Ca and $^{56}$Ni in j-coupled scheme

Vlowk at cutoff 1.9fm$^{-1}$ from Argonne v18

Similarity RG from $N^3$LO evolved to 2.5fm$^{-1}$
Medium-mass nuclei from chiral nucleon-nucleon forces with coupled-cluster method

Hagen, TP, Dean, Hjorth-Jensen, arXiv:0806.3478
CCSD results for $^{48}\text{Ca}$ from N$^3$LO interaction (NN only)

Densities and radii exhibit stronger model-space dependence than energies

Hagen, TP, Dean, Hjorth-Jensen, arXiv:0806.3478
Summary: CCSD results with chiral N$^3$LO (NN only)

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<tr>
<th>Nucleus</th>
<th>$E/A$</th>
<th>$V/A$</th>
<th>$\Delta E/A$</th>
<th>$R$</th>
<th>$R_{exp}$</th>
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<tr>
<td>$^4$He</td>
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<td>-22.75</td>
<td>1.08</td>
<td>1.86</td>
<td>1.64</td>
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<td>$^{16}$O</td>
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<td>$^{40}$Ca</td>
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<td>0.84</td>
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<td>$^{48}$Ca</td>
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<td>$^{48}$Ni</td>
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<td>1.21</td>
<td>3.50</td>
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Main results

1. Well converged results with respect to size of model space (< 1% change in binding energy when going from 14 to 15 oscillator shells.
2. Three-nucleon force and triples corrections expected to yield ~1MeV additional binding
3. Mirror nuclei $^{48}$Ca and exotic $^{48}$Ni differ by 1.38 MeV / A → close to mass-table predictions
4. Radii and densities exhibit stronger model-space dependence than energies
Weakly Bound nuclei away from the valley of beta-stability

~ 300 stable nuclei
N/Z~1 for light nuclei
N/Z~1.5 for $^{208}$Pb

~4000-6000 unstable nuclei
decay by $\alpha$, $\beta$, 1p, 2p, 1n, cluster emission, fission...
Helium isotopes: weakly bound and unbound quantum systems

Aim: Ab-initio description of weakly bound systems and computation of life times of particle-unstable $^5,^7\text{He}$.

Basis set: Single-particle basis of bound, resonance and scattering states: Gamow shell model $\rightarrow$ complex symmetric Hamiltonian

Two new aspects:
1. Particle-unstable nuclei $\checkmark$
2. Open-shell nuclei (✓)

Comparison with exact diagonalization

<table>
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<tr>
<th>Method</th>
<th>$^3\text{He}$</th>
<th>$^4\text{He}$</th>
<th>$^5\text{He}$</th>
<th>$^6\text{He}$</th>
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<td>CCSD (OSC)</td>
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<td>CCSD (RHF)</td>
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<td>CCSD (SC-RHF)</td>
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<tr>
<td>Exact</td>
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<td>-22.1</td>
<td>-22.7</td>
</tr>
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</table>

All fine, except $^6\text{He}$ (large T corrections); $\langle J^2 \rangle = 0.6$
CCSDT yields $\langle J^2 \rangle = 0.04$

Coupled-cluster theory for weakly bound nuclei: He-isotopes

<table>
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<tr>
<th>lj</th>
<th>$^3$He</th>
<th>$^4$He</th>
<th>$^5$He</th>
<th>$^6$He</th>
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<th>$^9$He</th>
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<td>-29.27</td>
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TABLE II: CCSD calculation of the $^3$-10He ground states with the low-momentum N3LO nucleon-nucleon interaction for increasing number partial waves. The energies $\tilde{E}$ are given in MeV for both real and imaginary parts. Experimental data are from Ref. [32]. Our calculated width of $^{10}$He is $\approx 0.002$MeV.

Interaction: $V_{\text{low-}}$ with $\Lambda$=1.9 fm$^{-1}$ from chiral N3LO potential (no three-body forces)

Main result: Converged ab-initio calculation of decay widths for unbound nuclei!
He isotopes


😊 Staggering of isotopic chain qualitatively reproduced

😊 Life times within factor 2 of data (except $^6\text{He}$)

😊 $^6\text{He}$ (open shell / three-nucleon force)
Summary and outlook

Weakly bound and unbound nuclei:
- Description of weakly bound He isotopes with Gamow states (NN only)
- Qualitative reproduction of staggering
- Semi-quantitative values for life times
- Outlook: Include 3NFs, employ spherical scheme, dripline of oxygen isotopes

3NFs:
- Developed CCSD for 3NF.
- Found that 0-, 1-, and 2-body parts of 3NF are dominant (in $^4$He).
- Residual 3-body part of 3NF can be neglected.
- Outlook: employ density-dependent contributions in medium-mass nuclei

J-coupled code:
- CCSD results for $^{40,48}$Ca, $^{48}$Ni for “softened” and “bare” interactions
- Triples corrections in progress
- Outlook: Ni, Sn, Pb isotopes, interface with DFT within UNEDF
- Outlook: Particle attached/remove, Fock space CCSD, $\rightarrow$ effective interactions