Coupled-Cluster theory for Nuclei

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1. Status and goals in microscopic nuclear structure approaches
2. Coupled Cluster approach to nuclear structure
3. Coupled-Cluster in J-coupled scheme
   - CCSD results with “bare” chiral interactions applied to $^{16}\text{O}$, $^{40}\text{Ca}$, $^{48}\text{Ca}$ and $^{48}\text{Ni}$
4. Coupled Cluster for open quantum systems
   - CCSD calculation of Helium chain
   - Charge radii and densities in $^{4}\text{He}$ and $^{8}\text{He}$
5. Conclusion and Perspectives
Ab-initio approaches to light and medium mass nuclei
1. Coupled Cluster Theory is **fully microscopic**.
2. Coupled Cluster is **size extensive**. No unlinked diagrams enters, and error scales linearly with number of particles.
3. Low computational cost (CCSD scales as $n_o^2 n_u^4$).
4. Capable of systematic improvements.
5. Amenable to parallel computing.
Exponential Ansatz for $\Psi$

$$|\Psi\rangle = e^{\hat{T}}|\Phi_0\rangle, \quad \hat{T} = \hat{T}_1 + \hat{T}_2 + \ldots + \hat{T}_A$$

$$\hat{T}_1 = \sum_{i,a} t_i^a \hat{a}_a ^\dagger \hat{a}_i, \quad \hat{T}_2 = \frac{1}{2} \sum_{i<j,a<b} t_{ij}^{ab} \hat{a}_a ^\dagger \hat{a}_b ^\dagger \hat{a}_j \hat{a}_i.$$ 

Coupled Cluster Equations

$$\Delta E = \langle \Phi_0 | (H_N \exp(T))_C | \Phi_0 \rangle$$

$$0 = \langle \Phi_p | (H_N \exp(T))_C | \Phi_0 \rangle$$

$$\tilde{H} = (H_N \exp(T))_C$$

Iterative CCSDT-n approximations to full CCSDT

$$\text{CCSDT} - 1 \quad 0 = \langle \Phi_{ijk}^{abc} | (F_N T_3 + H_N T_2)_C | \Phi_0 \rangle$$

$$\text{CCSDT} - 2 \quad 0 = \langle \Phi_{ijk}^{abc} | (F_N T_3 + H_N T_2 + H_N T_2^2/2)_C | \Phi_0 \rangle$$

$$\text{CCSDT} - 3 \quad 0 = \langle \Phi_{ijk}^{abc} | (F_N T_3 + H_N \exp(T_1 + T_2))_C | \Phi_0 \rangle$$

$$\text{CCSDT} \quad 0 = \langle \Phi_{ijk}^{abc} | (H_N \exp(T_1 + T_2 + T_3))_C | \Phi_0 \rangle$$
Motivation
Coupled-Cluster approach to nuclear structure
Spherical CCSD
Open quantum systems
Conclusion and Perspectives

Coupled Cluster in pictures

\[ |\Psi\rangle = e^{T(A)} \Phi \], \quad T^{(A)} = \sum_{k=1}^{m_A} T_k \]

\[ T_1 = \sum_{i \atop a} t^a_i |\Phi_{a i}\rangle, \quad T_2 = \sum_{i \atop a > b} t^{a b}_{i j} |\Phi_{a b i j}\rangle, \quad T_3 = \sum_{i \atop a > b > c} t^{a b c}_{i j k} |\Phi_{a b c i j k}\rangle \]
Spherical Coupled-Cluster Approach

- In a J-coupled scheme the cluster operator is a scalar under rotation, and depends only on reduced amplitudes. Thus,

\[ \hat{T}_1 = \sum_{j_i, j_a} t_{j_i}^{j_a} (a_{j_a}^\dagger \times \tilde{a}_{j_i})^{(0)}, \]

\[ \hat{T}_2 = \sum_{j_i, j_j, j_a, j_b, J} t_{j_i, j_j}^{j_a, j_b} (J) (a_{j_a}^\dagger \times a_{j_b}^\dagger)^{(J)} \cdot (\tilde{a}_{j_j} \times \tilde{a}_{j_i})^{(J)}. \]

- \( j_i \) and \( j_a \) denote the spin of the occupied and unoccupied subshells.

- A naive estimate shows that a model space of \( n_o + n_u \) single-particle states consists of \( (n_o + n_u)^{2/3} \) \( j \)-shells. Computational effort approximately reduced by a power \( 2/3 \) within the spherical scheme compared to the \( m \)-scheme.
Spherical Coupled-Cluster Approach

Speedup of J-coupled CCSD code for $^{40}\text{Ca}$ as compared to m-scheme CCSD code.

![Graph showing speedup of J-coupled CCSD code for $^{40}\text{Ca}$ as compared to m-scheme CCSD code.](image)
We have derived and implemented CCSD in a J-coupled scheme.

- Computational cost drastically reduced, from $n_o^2 n_u^4$ to $n_o^{4/3} n_u^{8/3}$.
- Large overbinding due to omitted three-body forces.

CCSD results for $^{40}$Ca and $^{56}$Ni using $V_{\text{low}-k}$.
CCSD results for $^{40}$Ca and $^{56}$Ni using V-SRG

Converged results for $^{40}$Ca and $^{56}$Ni, using N$^3$LO evolved down to $\lambda = 2.5\text{fm}^{-1}$ from similarity renormalization group theory. Large overbinding due to omitted three- and many-body forces.

![Graphs showing CCSD results for $^{40}$Ca and $^{56}$Ni](image)
$^{16}\text{O}$, $^{40}\text{Ca}$, $^{48}\text{Ca}$ and $^{48}\text{Ni}$ with "bare" chiral interactions

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Spherical CCSD

$^{16}$O, $^{40}$Ca, $^{48}$Ca and $^{48}$Ni ground state densities
Charge and matter radii / Summary of results

- Charge radii for various nuclei using the chiral N$^3$LO nucleon-nucleon potential.
- $\sim 1\text{MeV}/\text{A}$ missing for all nuclei: Size Extensivity!

<table>
<thead>
<tr>
<th>Nucleus</th>
<th>$E/A$</th>
<th>$V/A$</th>
<th>$Q$</th>
<th>$\Delta E/A$</th>
<th>$&lt;r^2&gt;_{ch}^{1/2}$</th>
<th>$&lt;r^2&gt;_{ch}^{1/2}$ (Exp)</th>
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</thead>
<tbody>
<tr>
<td>$^4\text{He}$</td>
<td>-5.99</td>
<td>-22.75</td>
<td>0.90</td>
<td>1.08</td>
<td></td>
<td>1.673(1)</td>
</tr>
<tr>
<td>$^{16}\text{O}$</td>
<td>-6.72</td>
<td>-30.69</td>
<td>1.08</td>
<td>1.25</td>
<td>2.72(5)</td>
<td>2.737(8)</td>
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<tr>
<td>$^{40}\text{Ca}$</td>
<td>-7.72</td>
<td>-36.40</td>
<td>1.18</td>
<td>0.84</td>
<td>3.25(9)</td>
<td>3.4764</td>
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<tr>
<td>$^{48}\text{Ca}$</td>
<td>-7.40</td>
<td>-37.97</td>
<td>1.21</td>
<td>1.27</td>
<td>3.24(9)</td>
<td>3.4738</td>
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<tr>
<td>$^{48}\text{Ni}$</td>
<td>-6.02</td>
<td>-36.04</td>
<td>1.20</td>
<td>1.21</td>
<td>3.52(15)</td>
<td>?</td>
</tr>
</tbody>
</table>
Ab-initio approach weakly bound and unbound nuclear states
Open Quantum systems

- \(S_n = 0\)
- Correlation dominated
- Closed QS
- Ground States
- r-process
- \(Z = \text{const}\)

Neutron number
Coupled Cluster for open quantum systems

Open Quantum System. Coupling with continuum taken into account.

Closed Quantum System. No coupling with external continuum.
Complex energies requires a generalized completeness relation

\[ |\Psi(r, t)|^2 = |\Phi(r)|^2 \exp\left(-\frac{\Gamma}{\hbar}t\right), \quad E = E_r - i\Gamma/2. \]

\[ 1 = \sum_{n=b,d} |\psi(l(k_n))\langle \tilde{\psi}_l(k_n) | + \int_{L^+} dk' k'^2 |\psi(l(k))\langle \tilde{\psi}_l(k)|. \]
How well does SR-CC describe open-shell nuclei?

Various Coupled Cluster approaches to the $^3-^6$He ground states. *Single reference Coupled-Cluster methods works!*

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<th>$\langle J^2 \rangle$, $^6$He</th>
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<td>-22.85</td>
<td>0.29</td>
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<td>CCSDT-2</td>
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<td>-22.78</td>
<td>0.25</td>
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<td>0.26</td>
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<td>CCSDT</td>
<td>-6.45</td>
<td>-26.28</td>
<td>-22.01</td>
<td>-22.52</td>
<td>0.04</td>
</tr>
<tr>
<td>FCI</td>
<td>-6.45</td>
<td>-26.3</td>
<td>-22.1</td>
<td>-22.7</td>
<td>0.00</td>
</tr>
</tbody>
</table>
CCSD results for Helium chain using $V_{\text{low}-k}$

- $V_{\text{low}-k}$ from N3LO with $\Lambda = 1.9\text{fm}^{-1}$.

- First *ab-initio* calculation of decay widths!
- CCM unique method for dripline nuclei.
- $\sim 1000$ active orbitals
- Underbinding hints at missing 3NF
**4He and 8He density distributions with V-srg**

- Single-particle density in 4He and 8He.
- Gamow-Hartree-Fock basis has correct asymptotics.
- N^3LO evolved down to \( \lambda = 2.0\text{fm}^{-1} \) from similarity renormalization group theory.

![Graphs showing density distributions](image-url)
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Partial wave decomposition of $^8$He density

- $N^3$LO evolved down to $\lambda = 2.0\text{fm}^{-1}$ from similarity renormalization group theory.
- Neutron skin in $^8$He is mainly built from $s$— and $p$—partial waves. Protons are mainly occupying $s$— partial waves.

![Graphs showing density distribution for neutrons and protons in $^8$He.](image)

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Coupled-Cluster theory for Nuclei
Matter and charge radii of $^8$He using V-srg

- $\Lambda$ dependence on $^8$He charge and matter radii indicates missing 3NF.
- Hamiltonians with two-body renormalized interactions (SRG/low-k) underestimates matter and charge radii.
Conclusion

- Coupled Cluster meets few-body benchmark calculations.
- J-coupled CCSD code has been derived and implemented.  
  Coupled cluster approach to medium mass and driplines with bare interactions!
- Derived and implemented Equation of Motion CCM; calculation of density distributions and radii.
- CCM has been successfully applied to the description of weakly bound and unbound helium isotopes.
- We have a tool to attack the structure and properties of dripline and medium mass nuclei!
Future perspectives

- Location of dripline in the Oxygen chain?
- Revisit Helium chain with 3NF. Spin-orbit splitting in He7 and He9.
- Matter and charge radii of $^{11}$Li.
- Excited states and matter densities for dripline nuclei.
- Coupled Cluster approach to nuclear matter.
- Construction of effective interaction for shell-model calculations.
- Coupled-Cluster approach to nuclear reactions; CC-LIT and construction of optical potentials from folding procedures.
- We are developing a J-coupled CCSDT code.
- Ab-initio description of $^{56}$Ni, $^{100}$Sn and $^{208}$Pb within reach!
In Shell Model approach a linear excitation operator is used instead of an exponential. $\Psi = (1 + B_1 + B_2 + \ldots)\Phi_0$

- Any particle-hole truncation introduces unlinked diagrams, and it is therefore not size extensive.
- Dimension increases dramatically with number of active particles.

**Comparison of CC with CI at given excitation level.**

**Nuclear Example (Kowalski et al PRL 2004).**
Relationship between shell model and CC amplitudes

\[ B_1 = T_1 \]
\[ B_2 = T_2 + \frac{1}{2} T_1^2 \]
\[ B_3 = T_3 + T_2 T_1 + \frac{1}{6} T_1^3 \]
\[ B_4 = T_4 + T_3 T_1 + \frac{1}{2} T_2^2 + \frac{1}{2} T_2 T_1^2 + \frac{1}{24} T_1^4 \]

Connected quadruples
Disconnected quadruples

CCSD
CCSDT
Disconnected diagrams in truncated shell model/CI models (CISD, CISDT,...) leads to wrong scaling of energy with increasing number of particles.
Coupled Cluster meets benchmarks of $^3$H and $^4$He!

CCSD(T) and Faddeev (-Yakubovsky) results for $^3$H and $^4$He using $V_{\text{low}-k}$ from AV18 with $\Lambda = 1.9\text{fm}^{-1}$. **CCSD(T) are within the errors (50 keV) of the Faddeev results!** (G. Hagen et al., Phys. Rev. C 76, 044305 (2007))
16O and 40Ca CCSD(T) ground state energies

\[
\begin{array}{c|c|c|c}
 & ^4\text{He} & ^{16}\text{O} & ^{40}\text{Ca} \\
\hline
E_0 & -11.815 & -60.204 & -347.474 \\
\Delta E_{\text{CCSD}} & -17.107 & -82.576 & -143.736 \\
\Delta E_{\text{CCSD(T)}} & -0.253 & -5.450 & -11.699 \\
E_{\text{CCSD(T)}} & -29.175 & -148.232 & -502.908 \\
\text{exact (FY)} & -29.19(5) & & \\
\end{array}
\]

40Ca converged within 1% !

Roth and Navratil PRL 99, 092501 (2007) \(E_{\text{CISDT}} = -462.7\text{MeV}\). Our comment: arXiv:0709.0449
Different contributions to $E_{CCSD}$ from 3NF in $^4$He

Three-body Hamiltonian in normal ordered form:
(G. Hagen et al., PRC (76) 034302 (2007))

\[
\hat{H}_3 = \frac{1}{6} \sum_{ijk} \langle ijk|ijk \rangle + \frac{1}{2} \sum_{ijpq} \langle ijp|ijq \rangle \{\hat{a}_p^{\dagger} \hat{a}_q\} + \frac{1}{4} \sum_{ipqrs} \langle ipq|irs \rangle \{\hat{a}_p^{\dagger} \hat{a}_q^{\dagger} \hat{a}_s \hat{a}_r\} + \hat{h}_3,
\]

Really good news!

- The “density dependent” terms of 3NF are dominant!
- $\epsilon$ from residual 3NF costs $1 - \epsilon$ of work!
- “2-body” machinery can be used.
- Residual 3NF can be neglected!
Convergence of $^4$He and $^8$He ground state energies with increasing number of partial waves in the basis.
Matter and charge radii of $^4$He using V-srg

- $\Lambda$ dependence on $^4$He charge and matter radii indicates missing 3NF.
- Hamiltonians with two-body renormalized interactions (SRG/low-k) underestimates matter and charge radii.
\( \hbar \omega \) dependence on \(^4\text{He}\) and \(^8\text{He}\) charge and matter radii.
Coupled Cluster Theory

Exponential Ansatz for $\Psi$

$$|\Psi\rangle = e^{\hat{T}}|\Phi_0\rangle, \quad \hat{T} = \hat{T}_1 + \hat{T}_2 + \ldots + \hat{T}_A$$

$$\hat{T}_1 = \sum_{i,a} t_i^a \hat{a}_a^\dagger \hat{a}_i, \quad \hat{T}_2 = \frac{1}{2} \sum_{i<j,a<b} t_{ij}^{ab} \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i.$$ 

Coupled Cluster Equations

$$\Delta E = \langle \Phi_0 | (H_N \exp(T))_C | \Phi_0 \rangle$$

$$0 = \langle \Phi_p | (H_N \exp(T))_C | \Phi_0 \rangle$$

$$\tilde{H} = (H_N \exp(T))_C$$

Iterative CCSDT-n approximations to full CCSDT

CCSDT − 1 0  =  \langle \Phi_{ijk}^{abc} | (F_N T_3 + H_N T_2)_C | \Phi_0 \rangle

CCSDT − 2 0  =  \langle \Phi_{ijk}^{abc} | \left( F_N T_3 + H_N T_2 + H_N T_2^2/2 \right)_C | \Phi_0 \rangle

CCSDT − 3 0  =  \langle \Phi_{ijk}^{abc} | (F_N T_3 + H_N \exp(T_1 + T_2))_C | \Phi_0 \rangle

CCSDT 0  =  \langle \Phi_{ijk}^{abc} | (H_N \exp(T_1 + T_2 + T_3))_C | \Phi_0 \rangle
Tripples correction to $^{16}$O and $^{40}$Ca binding energies

<table>
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$^{40}$Ca converged within 1% !

We have derived and implemented Coupled Cluster equations for three-body Hamiltonians.

Probe cutoff dependence of $V_{\text{low-k}}$ with three nucleon force in light and medium heavy nuclei.

Does 3NF provide the necessary repulsion/attraction needed to approach experimental mass values?

“Coupled-cluster theory for three-body Hamiltonians” G. Hagen et al., PRC (76) 034302 (2007).
3NF contribution to the $\hat{T}_1$ cluster equation

Energy and 1p-1h equation as examples.
Factorization of diagrams very useful!
1p-1h: 15 diagrams
2p-2h: 51 diagrams
3NF from Chiral perturbation theory

Feynman diagrams


Phase shifts reproduced to $\chi^2$/datum=1
About 24+ parameters

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Coupled Cluster Results for $^4$He with 3NF

- $V_{\text{low}_k}$ from AV18 with $\Lambda = 1.9 \text{fm}^{-1}$.
- 3NF brings in repulsion as expected!
- CCSD and CCSD(T) with 3NF meets Faddeev-Yakubovsky benchmark!
  $E_{\text{CCSD(T)}} \approx -28.24 \text{ MeV}$. F-Y $E = -28.20(5)\text{MeV}$.

![Graph showing CCSD and CCSD(T) results for different $N$ values.](image-url)
Different contributions to $E_{CCSD}$ from 3NF in $^4$He

Three-body Hamiltonian in normal ordered form:

$$\hat{H}_3 = \frac{1}{6} \sum_{ijk} \langle ijk || ijk \rangle + \frac{1}{2} \sum_{ijpq} \langle ijp || ijq \rangle \{\hat{a}_p^\dagger \hat{a}_q\} + \frac{1}{4} \sum_{ipqrs} \langle ipq || irs \rangle \{\hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_s \hat{a}_r\} + \hat{h}_3,$$

Really good news!

- The “density dependent” terms of 3NF are dominant!
- $\epsilon$ from residual 3NF costs $1 - \epsilon$ of work!
- “2-body” machinery can be used.
- Residual three-nucleon force can be neglected!
CCM vs. exact calculations for open-shell nuclei.

Various Coupled Cluster approaches to the $^3-^6$He ground states. Single reference Coupled-Cluster methods works!

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Convergence of CCSD results

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Coupled-Cluster theory for Nuclei
Convergence of CCSD energy with $2n + l \leq 10$ truncation.

- $^5$He ground state energy starting with oscillator bases given for different $\hbar \omega$ values.
- Weak $\hbar \omega$ dependence, Results are well converged. $\Delta \text{Re}[E] \sim 0.1\text{MeV}$, $\Delta \text{Im}[E] \sim 0.01\text{MeV}$
CCSD convergence of $^5$He ground state energy for the $s - d$ space (300 orbitals) using $n = 20$ discretization points for $L^+$. The calculation were performed using two very different $L^+$ contours.

- $L^+_{RT}$: $\text{Re}[E] = -23.5468$ MeV
- $L^+_{Triangle}$: $\text{Re}[E] = -23.5581$ MeV

$\Delta \text{Re}[E] = 0.0113$ MeV

- $L^+_{RT}$: $\text{Im}[E] = -0.2134$ MeV
- $L^+_{Triangle}$: $\text{Im}[E] = -0.2158$ MeV

$\Delta \text{Im}[E] = 0.0025$ MeV
Coupled Cluster Results for Helium isotopes with TNF

CC results with $V_{\text{low}-k}$ from N3LO NN-interaction. Rather limited model-space $N = 3$. Only contact term at NN2LO is retained in the three nucleon force. TNF fitted to reproduce binding energy of $^4\text{He}$.