Role of the continuum in Coupled-Cluster theory

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Weakly-Bound Systems in Atomic and Nuclear Physics
INT, March 10, 2010
1. The driplines - the limit of nuclear existence

2. Coupled Cluster approach to nuclear structure
   - Single-Reference Coupled-Cluster theory
   - Coupled-Cluster approach to open quantum systems and Helium isotopes

3. Equation-of-Motion Coupled-Cluster approach to open-shell nuclei
   - Equation-of-Motion Coupled-Cluster theory
   - Microscopic description of resonances and halo states in $^{17}$F and $^{17}$O
   - Low-lying states in $^{17}$O and the Center of Mass
   - Shell evolution in the oxygen and fluorine isotopes

4. Conclusion and Perspectives
Peculiarities at the nuclear driplines

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

~ 4000-6000 unstable nuclei
decay by $\alpha$, $\beta$, 1p, 2p, 1n, cluster emission, fission...
Peculiarities at the nuclear driplines

- Motivation
- Ab-initio Coupled-Cluster approach
- Open-shell nuclei and CCM
- Conclusion and Perspectives

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Coupled-Cluster approach to nuclear structure
“If you want more accuracy, you have to use more theory (more orders)”

Effective Lagrangian $\rightarrow$ obeys QCD symmetries (spin, isospin, chiral symmetry breaking)

Lagrangian $\rightarrow$ infinite sum of Feynman diagrams.

Expand in $O(Q/\Lambda_{QCD})$

Weinberg, Ordonez, Ray, van Kolck

NN amplitude uniquely determined by two classes of contributions: contact terms and pion exchange diagrams.

24 parameters (rather than 40 from meson theory) to describe 2400 data points with
Low-momentum nucleon-nucleon interaction: $V_{\text{low}-k}$

A-body nuclear Hamiltonian

$$H^A = T - T_{CM} + V_2(\Lambda) + V_3(\Lambda) + \cdots V_A(\Lambda) \approx T - T_{CM} + V_2(\Lambda) + V_3(\Lambda)$$

**Single-Reference Coupled Cluster Theory**

### Exponential Ansatz for $\Psi$

\[
|\psi\rangle = e^{\hat{T}}|\Phi_0\rangle, \quad \hat{T} = \hat{T}_1 + \hat{T}_2 + \ldots + \hat{T}_A
\]

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

### Coupled Cluster Equations

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

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

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

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.
Coupled Cluster in pictures

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

\[ T_1 = \sum_{i,a} t_i^a |\Phi^a_i\rangle, \quad T_2 = \sum_{i,j,a>b} t_{ij}^{ab} |\Phi^{ab}_{ij}\rangle, \quad T_3 = \sum_{i,j,k,a>b>c} t_{ijk}^{abc} |\Phi^{abc}_{ijk}\rangle \]
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.

<table>
<thead>
<tr>
<th>Method</th>
<th>$^3$He</th>
<th>$^4$He</th>
<th>$^5$He</th>
<th>$^6$He</th>
<th>$\langle J^2 \rangle$, $^6$He</th>
</tr>
</thead>
<tbody>
<tr>
<td>CCSD</td>
<td>-6.21</td>
<td>-26.19</td>
<td>-21.53</td>
<td>-20.96</td>
<td>0.61</td>
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<tr>
<td>CCSD(T)</td>
<td>-6.40</td>
<td>-26.27</td>
<td>-21.88</td>
<td>-22.60</td>
<td>0.65</td>
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<tr>
<td>CCSDT-1</td>
<td>-6.41</td>
<td>-28.27</td>
<td>-21.89</td>
<td>-22.85</td>
<td>0.29</td>
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<tr>
<td>CCSDT-2</td>
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<td>-22.78</td>
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</tr>
<tr>
<td>CCSDT-3</td>
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<td>-26.27</td>
<td>-21.92</td>
<td>-22.90</td>
<td>0.26</td>
</tr>
<tr>
<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>
Coupled-cluster approach to open quantum systems

- SR Coupled-Cluster theory
- Coupled-Cluster theory for open quantum systems

Coupled-cluster approach to nuclear structure

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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 of a whole isotopic chain.
- CCM unique method for dripline nuclei.
- $\sim 1000$ active orbitals
- Underbinding hints at missing 3NF
Helium isotopes with $V_{\text{low}-k}$


<table>
<thead>
<tr>
<th>$\Lambda$ [fm$^{-1}$]</th>
<th>$E_0(^4\text{He})$</th>
<th>$E_0^\infty(^6\text{He})$ [for $K_{\text{max}} = 14$]</th>
<th>$E_0(^8\text{He})$ $\Lambda$-CCSD(T) [CCSD]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.8</td>
<td>$-29.30(2)$</td>
<td>$-30.28(3)$ $[-30.13]$</td>
<td>$-31.21$ $[-30.33]$</td>
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<tr>
<td>2.0</td>
<td>$-28.65(2)$</td>
<td>$-29.35(13)$ $[-29.13]$</td>
<td>$-29.84$ $[-28.72]$</td>
</tr>
<tr>
<td>2.4</td>
<td>$-27.40(2)$</td>
<td>$-27.62(19)$ $[-26.91]$</td>
<td>$-27.54$ $[-25.88]$</td>
</tr>
</tbody>
</table>
Single-particle density in $^4$He and $^8$He.

Gamow-Hartree-Fock basis has correct asymptotics.

$N^3$LO evolved down to $\lambda = 2.0\text{fm}^{-1}$ from similarity renormalization group theory.

\begin{itemize}
  \item Full density
  \item Proton density
  \item Neutron density
\end{itemize}
Most nuclei are open-shell. How to access these nuclei with coupled-cluster method?
Single-reference or Multi-reference Coupled-Cluster theory?

**Single-Reference CC**
- Single-Reference Coupled-Cluster (SR CC) theory can in principle be applied to open-shell nuclei.
- SR CC cannot define a unique reference function.
- SR CC breaks rotational invariance for truly open shell systems like $^6\text{He}$.
- SR CC requires uncoupled basis (m-scheme), must use soft interactions due to explosion of basis states.

**Equation-of-Motion (Multi-Reference) CC:**
- Equation-of-Motion provides us with a consistent approach to open-shell nuclei.
- Equation-of-Motion can be implemented in a spherical scheme, can apply basis sets large enough to accommodate "bare" interactions.
Equation-of-Motion CC for open-shell nuclei

Equation-of-Motion Coupled-Cluster theory

The idea of Equation-of-Motion Coupled-Cluster theory is to calculate ground- and excited states of system $B$ by acting with a excitation operator $\Omega_k$ on the ground state of system $A$

$$|\psi_k^B\rangle = \Omega_k |\psi_0^A\rangle, \quad |\psi^A\rangle = \exp(T) |\phi_0^A\rangle$$

Define the non-particle conserving excitation operators $\Omega_k = R_k^{(A\pm1)}$

$$R_k^{(A+1)} = r^a a_a^\dagger + \frac{1}{2} r_{ij}^{ab} a_a^\dagger a_b^\dagger a_j + \ldots,$$

$$R_k^{(A-1)} = r_i a_i + \frac{1}{2} r_{ij}^{ba} a_b^\dagger a_i a_j + \ldots,$$

Particle-Attached/Removed EOM-CC equations

$$\left[ H, R_k^{(A\pm1)} \right] |\phi_0\rangle = \left( HR_k^{(A\pm1)} \right)_C |\phi_0\rangle = \omega_k R_k^{(A\pm1)} |\phi_0\rangle.$$
Low-lying single-particle states in $^{17}$F using a Gamow-Hartree-Fock basis (GHF) and a Oscillator-Hartree-Fock (OHF) basis.

Very weak dependence on the oscillator frequency $\hbar \omega$ for calculations done in a GHF basis.

Significant effect of continuum coupling on the $1/2^+$ and $3/2^+$ states in $^{17}$F.
Cutoff dependence on the low-lying states in $^{17}$F.

- Spin-orbit splitting increases between the $d_{5/2}$-$d_{3/2}$ orbitals with decreasing cutoff $\lambda$.
- $s_{1/2}$ state show very weak dependence on the cutoff.
- The $1/2^+$ state is a *halo* state which extends far beyond the range of the interaction. Renormalizing the interaction by integrating out high momentum modes does not alter the long range physics.
Low-lying states in $^{17}$F and $^{17}$O using a Gamow-Hartree-Fock basis and a Oscillator-Hartree-Fock basis.
Summary of results for $^{17}\text{O}$ and $^{17}\text{F}$

- Our calculations for the $1/2^+$ states in $^{17}\text{F}$ and $^{17}\text{O}$ agree remarkably well with experiment.
- Spin-orbit splitting between $d_{5/2}-d_{3/2}$ orbitals too compressed without three-nucleon forces.
- Our calculations of the widths of the $3/2^+$ resonant states compare reasonably well with experiment.

<table>
<thead>
<tr>
<th></th>
<th>$^{17}\text{O}$</th>
<th></th>
<th>$^{17}\text{F}$</th>
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</thead>
<tbody>
<tr>
<td></td>
<td>$(1/2)^+_1$</td>
<td>$(5/2)^+_1$</td>
<td>$E_{\text{s.o.}}$</td>
</tr>
<tr>
<td>OHF</td>
<td>-1.888</td>
<td>-2.955</td>
<td>4.891</td>
</tr>
<tr>
<td>GHF</td>
<td>-2.811</td>
<td>-3.226</td>
<td>4.286</td>
</tr>
<tr>
<td>Exp.</td>
<td>-3.272</td>
<td>-4.143</td>
<td>5.084</td>
</tr>
</tbody>
</table>

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<tr>
<th></th>
<th>$^{17}\text{O}$ $(3/2)^+_1$</th>
<th></th>
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</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Re[$E_{\text{sp}}$]</td>
<td>$\Gamma$</td>
<td>Re[$E_{\text{sp}}$]</td>
</tr>
<tr>
<td>PA-EOMCCSD</td>
<td>1.059</td>
<td>0.014</td>
<td>3.859</td>
</tr>
<tr>
<td>Experiment</td>
<td>0.942</td>
<td>0.096</td>
<td>4.399</td>
</tr>
</tbody>
</table>
Low-lying states in $^{17}$O with $V_{srg}$ (2.8/fm) and the center of mass

- Low-lying $1/2^+$, $3/2^+$ and $5/2^+$ states in $^{17}$O calculated using PA-EOM-CCSD in 13 major oscillator shells.

- The expectation value of $H_{cm}(\omega) = T_{cm} + \frac{1}{2} m A \omega^2 R_{cm}^2 - \frac{3}{2} \hbar \omega$ measures to what degree the CoM is a Gaussian with oscillator frequency $\omega$. 

![Graph showing low-lying states in $^{17}$O and $^{17}$F with $V_{srg}$ (2.8/fm) and the center of mass.](image-url)
Motivation
Ab-initio Coupled-Cluster approach
Open-shell nuclei and CCM
Conclusion and Perspectives

PA-EOMCC
Low-lying states in $^{17}$F and $^{17}$O
PA-EOM and Center of Mass
Shell-evolution in oxygen and fluor

Coupled-Cluster wave function factorizes: $\psi_{int}\psi_{cm}$

- Assumption: CoM wave function is always a gaussian (approximately).
- Take expectation value of the generalized CoM Hamiltonian $H_{cm}(\tilde{\omega}) = T_{cm} + \frac{1}{2} mA\tilde{\omega}^2 R_{cm}^2 - \frac{3}{2} \hbar\tilde{\omega}$.
- CC wave function factorizes and the CoM wave function is a Gaussian with almost constant width $\hbar\tilde{\omega} \sim 16\,\text{MeV}$ for all different $\hbar\omega$ values of the basis.
Shell evolution towards the drip line

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Coupled-Cluster approach to nuclear structure

25O neutron separation energy: -820 keV
the width was measured to be 90(30) keV
giving a lifetime of $t \sim 7 \times 10^{-21}$ sec

C. Hoffman PRL 100 (2008) 152502

FIG. 4 (color online). The experimental [25,26] (data points) and theoretical [13–15] (lines) one- and two-neutron separation energies for the $N = 15$–18 oxygen isotopes. The experimental error is shown if it is larger than the symbol size.
Low lying states in oxygen and fluorine isotopes calculated using PA/PR-EOMCCSD with “bare” chiral interactions.

Model space consists of 15 major harmonic oscillator shells with fixed oscillator frequency $\hbar \omega = 32\text{MeV}$.

$^{25}\text{O}$ is stable with respect to neutron emission. Interesting inversion of ground state in $^{25}\text{F}$.

What is the role of continuum and three-body forces?
Cutoff dependence in $^{24}\text{O}$ and $^{25}\text{F}$

- Variation of the cutoff as a tool to probe the effects of missing many-body forces.
- No unique cutoff that will reproduce data in $^{24}\text{O}$ and $^{25}\text{F}$ simultaneously.
- Three-nucleon forces are needed. Continuum coupling might bring additional binding in the low-lying states in $^{25}\text{F}$. 
Cutoff dependence in $^{25}\text{O}$

- Cutoff dependence on the $3/2^+$ state in $^{25}\text{O}$.
- Calculations done in 15 major oscillator shells with fixed oscillator frequency $\hbar \omega = 32\text{MeV}$.
- There are no two-body forces within the family of phase-equivalent low-momentum interactions derived from N$^3$LO that will make $^{25}\text{O}$ unstable.
- Three-nucleon forces are needed to match theory with experiment in $^{25}\text{O}$!
Conclusion

- Coupled-Cluster theory has been successfully applied to weakly bound and unbound helium isotopes.
- Derived and implemented Equation of Motion CCM; calculation of open-shell systems, excited states, density distributions and radii.
- PA-EOM Coupled-cluster method has been successfully applied to the description of weakly bound and unbound states in $^{17}\text{O}$ and $^{17}\text{F}$.
- Coupling to the continuum plays a significant role on states close to the particle emission threshold.
- PR/PA-EOM Coupled-Cluster theory allows for *ab initio* calculations of single-particle states and the study of shell-evolution in neutron rich nuclei.
- Provide realistic single-particle energies for shell-model calculations with a core.
Future perspectives

- 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.
- Ab-initio description of $^{56}$Ni, $^{100}$Sn and $^{208}$Pb within reach.
Coupled Cluster for open quantum systems

Open Quantum System.
Coupling with continuum taken into account.

Closed Quantum System.
No coupling with external continuum.
Berggren Single-particle basis

Complex energies requires a generalized completeness relation

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

$$1 = \sum_{n=b,d} |\psi_l(k_n)\rangle\langle \tilde{\psi}_l(k_n)| + \int_{L^+} dk \, k^2 |\psi_l(k)\rangle\langle \tilde{\psi}_l(k)|.$$
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.
Matter and charge radii of $^8\text{He}$ using V-srg

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

\[ R_{\text{rms}} \text{ [fm]} \]

\begin{align*}
\text{for } l_{\text{max}} = 1.375, 1.4, 1.425, 1.45 \text{ and } \Lambda = 1.43, 1.435, 1.44, 1.445, 1.45, 1.455, 1.46
\end{align*}
\( \hbar \omega \) dependence on \(^4\text{He}\) and \(^8\text{He}\) charge and matter radii.
Shell model calculations of oxygen isotopes using two-body effective interactions and second order perturbation theory.

Calculations starting from a $^{16}\text{O}$ core gives $^{25}\text{O}$ bound.

Starting from a $^{22}\text{O}$ core gives $^{25}\text{O}$ unbound in both HO and Gamow basis.

Inclusion of many-body effects crucial, continuum plays a role in the description of excited states.

**Motivation**

Ab-initio Coupled-Cluster approach
Open-shell nuclei and CCM

**Conclusion and Perspectives**

$^4-^8\text{He}$ with smooth $v$-lowk

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**Figure**: Graphs showing the energy $E_0$ as a function of $K_{\text{max}}$ for $^4\text{He}$, $^6\text{He}$, and $^8\text{He}$, with different values of $\Lambda$. The graphs are compared with experimental data.

<table>
<thead>
<tr>
<th>$\Lambda$ [fm$^{-1}$]</th>
<th>$E_0(^4\text{He})$</th>
<th>$E_0^\infty(^6\text{He})$</th>
<th>$E_0(K_{\text{max}} = 14)$</th>
<th>$E_0(^8\text{He})$</th>
<th>$A$-CCSD(T)</th>
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Convergence of CCSD results
Convergence of CCSD energy with $2n + I \leq 10$ truncation.

- $^5$He ground state energy starting with oscillator bases given for different $\hbar \omega$ values.
- Weak $\hbar \omega$ dependence, Results are well converged.
  \[ \Delta \text{Re}[E] \sim 0.1\text{MeV}, \Delta \text{Im}[E] \sim 0.01\text{MeV} \]
Convergence of CCSD energy.

CCSD convergence of $^5$He ground state energy for the $s - d$ space (300 orbitals) using $n = 20$ discretization points for $L^+$. The calculation where performed using two very different $L^+$ contours.

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

$\Delta \text{Im}[E] = 0.0025 \text{MeV}$