Medium-mass atomic and lattice nuclei with pionless EFT

with
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Goals

1. Study $^{16}\text{O}$ and $^{40}\text{Ca}$ nuclei with NLO pionless EFT at physical (140 MeV) and heavier (806 MeV) pion mass.

2. Formulate pionless EFT directly in harmonic oscillator (HO) basis.
   - Make potentials from pion less EFT readily available in HO basis for many-body calculations.

(LO for $4 \leq A \leq 16$ - Stetcu et al. 2007; Kirscher et al. 2015; Barnea et al. 2015; Contessi et al. 2017)
Discrete Variable Representation (DVR) in Harmonic Oscillator basis

1. Eigenstates of $p^2$ operator in finite spherical oscillator basis
   - localized at discrete momenta, zero at other discrete values -> DVR
   - facilitates computation of matrix elements

3. UV cutoff varied by changing oscillator frequency at fixed $N$.
   - [Reviews: Littlejohn et al. 2002; Light et al. 2003]
Pionless Effective field theory

[Bedaque, van Kolck, Hammer; Kaplan, Savage, Wise; Griesshammer, Kirscher; Phillips; Platter; König …]

**LO**

\[ V_{ct}^{(0)}(1S_0) = \tilde{C}_{1S_0} \]

\[ V_{ct}^{(0)}(3S_1) = \tilde{C}_{3S_1} \]

**NLO**

\[ V_{3\text{NF}} = c_E \sum_{j \neq i} \vec{\tau}_i \cdot \vec{\tau}_j. \]

\[ V_{ct}^{(2)}(3S_1) = C_{3S_1}(p^2 + p'^2) \]

\[ V_{ct}^{(2)}(1S_0) = C_{1S_0}(p^2 + p'^2) \]

LO NN: 2 LECs

LO NNN: 1 LEC

NLO NN: 2 LECs
Calibration

<table>
<thead>
<tr>
<th>Nature</th>
<th>Lattice</th>
</tr>
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<tbody>
<tr>
<td>$m_\pi$</td>
<td>806. ± 1</td>
</tr>
<tr>
<td>$m$</td>
<td>1634. ± 18</td>
</tr>
<tr>
<td>$B_{nn}$</td>
<td>15.9 ± 4</td>
</tr>
<tr>
<td>$B_d$</td>
<td>19.5 ± 5</td>
</tr>
<tr>
<td>$B_t$</td>
<td>53.9 ± 10.7</td>
</tr>
<tr>
<td>$n_p a_s^{-1}$</td>
<td>84.7 ± 18</td>
</tr>
<tr>
<td>$n_p r_s^{-1}$</td>
<td>174.6 ± 25</td>
</tr>
<tr>
<td>$a_t^{-1}$</td>
<td>108. ± 13</td>
</tr>
<tr>
<td>$r_t^{-1}$</td>
<td>217.8 ± 46</td>
</tr>
</tbody>
</table>

Input to fit LECs

[Lattice data : NPLQCD collaboration(2013)]
Results for $A \leq 4$ nuclei

Method: No-Core Shell Model in Jacobi Basis
[Reviews: Navratil et al 2009; Barrett et al 2013]

<table>
<thead>
<tr>
<th>$h\omega$</th>
<th>$\Lambda$</th>
<th>$E(^3H)$</th>
<th>$r(^3H)$</th>
<th>$E(^3He)$</th>
<th>$r(^3He)$</th>
<th>$E(^4He)$</th>
<th>$r(^4He)$</th>
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<td>8.482</td>
<td>1.59</td>
<td>7.755</td>
<td>1.75</td>
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<tr>
<td>22</td>
<td>487.38</td>
<td>8.482</td>
<td>1.63</td>
<td>7.77</td>
<td>1.83</td>
<td>29.30</td>
<td>1.44</td>
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<tr>
<td>40</td>
<td>657.19</td>
<td>8.482</td>
<td>1.64</td>
<td>7.82</td>
<td>1.80</td>
<td>27.30</td>
<td>1.57</td>
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<table>
<thead>
<tr>
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<th>$\Lambda$</th>
<th>$E(^3H)$</th>
<th>$r(^3H)$</th>
<th>$E(^3He)$</th>
<th>$r(^3He)$</th>
<th>$E(^4He)$</th>
<th>$r(^4He)$</th>
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<tr>
<td>10</td>
<td>433.48</td>
<td>53.9</td>
<td>1.14</td>
<td>52.9</td>
<td>1.16</td>
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<td>1.16</td>
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<tr>
<td>22</td>
<td>642.96</td>
<td>53.9</td>
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<td>1.13</td>
<td>89.7</td>
<td>1.34</td>
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<tr>
<td>40</td>
<td>866.97</td>
<td>53.9</td>
<td>1.17</td>
<td>53.1</td>
<td>1.29</td>
<td>109.7</td>
<td>1.33</td>
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• At NLO, $E(^4He)$ binding energy
  (i) close to experimental value for physical nuclei $E(^4He) = 28.3$ MeV.
  (ii) Within the uncertainty of LQCD calculations for lattice $^4He$, $E(^4He) = 107 \pm 34$ MeV.

[LO results consistent with Barnea et al 2015, Kirscher et al 2015, Contessi et al 2017]
Physical $^{16}$O, $^{40}$Ca nuclei

- At NLO, $^{16}$O and $^{40}$Ca bound.

- $E/A(^{16}$O) $\sim$ 9 MeV, $E/A(^{40}$Ca) $\sim$ 10 MeV

- Mild cutoff dependence.

Method: Coupled Cluster with singles and doubles (CCSD) approximation.

[Review: Hagen et al 2014]
Lattice $^{16}$O, $^{40}$Ca nuclei

All quantities are in MeV.

<table>
<thead>
<tr>
<th>$\hbar \omega$</th>
<th>$\Lambda$</th>
<th>$E(^{16}$O$)$</th>
<th>$E(^{40}$Ca$)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>433.46</td>
<td>371</td>
<td>832</td>
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<td>1187</td>
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<td>40</td>
<td>866.97</td>
<td>548</td>
<td>1252</td>
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</table>

- This work,
  $E/A(^{16}$O$) \sim 23 - 35$ MeV
  $E/A(^{40}$Ca$) \sim 21 - 36$ MeV

- $E/A(^{4}$He$) \sim 25$ MeV from LQCD / pionless EFT
- Stronger cutoff dependence.

Method: Coupled Cluster with singles and doubles (CCSD) approximation.
[Review: Hagen et al 2014]
Summary

- Build infrastructure for pionless EFT directly in harmonic oscillator basis-UV convergence by construction; facilitates many-body calculations.

- First NLO pionless EFT calculations for $^{16}$O and $^{40}$Ca nuclei.
  - At physical pion mass
    - $E/A(^{16}$O) $\sim$ 9 MeV
    - $E/A(^{40}$Ca) $\sim$ 10 MeV
    - Results comparable to NLO Chiral HO EFT calculation.
  
  - At 806 MeV pion mass
    - $E/A(^{16}$O) $\sim$ 23 - 35 MeV
    - $E/A(^{40}$Ca) $\sim$ 21 - 36 MeV

- Outlook: Higher orders in pionless EFT; apply to future (and more accurate) results from lattice QCD; explore pionless EFT in p-shell nuclei.
For more details ...
Background

• At LO it is known,
  1. Physical/Real Nuclei ($m_\pi \sim 140$ MeV)
    • $^6$Li unbound w.r.t. $^4$He [Stetcu et al. 2007]
    • $^{16}$O: unbound w.r.t. decay into alpha particles [Contessi et al. 2017].
  2. Lattice Nuclei (at $m_\pi \sim 806$ MeV)
    • $^{16}$O: unbound w.r.t. decay into alpha particles. [Barnea et al. 2015; Contessi et al. 2017].

• In this work,
  • NLO calculation of physical and lattice $^{16}$O, $^{40}$Ca nuclei.
  • NLO terms added non-perturbatively. [Lensky et al. 2016].
Fast $E_3$ convergence at specific oscillator frequency

<table>
<thead>
<tr>
<th>$h\omega$</th>
<th>$\Lambda$</th>
<th>$^{16}\text{O}$</th>
<th>$^{40}\text{Ca}$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>$N = E_3 = 12$</td>
<td>$N = E_3 = 14$</td>
</tr>
<tr>
<td>10</td>
<td>328.59</td>
<td>136.8</td>
<td>136.2</td>
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<tr>
<td>22</td>
<td>487.38</td>
<td>143.1</td>
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<tr>
<td>40</td>
<td>657.19</td>
<td>144.7</td>
<td>146.2</td>
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</tbody>
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Physical Nuclei :

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<tr>
<td>40</td>
<td>866.97</td>
<td>547.8</td>
<td>546.0</td>
</tr>
</tbody>
</table>

Lattice Nuclei :

- At $h\omega = 22$ MeV, fastest $E_3$ convergence (highlighted in yellow).

- Open question / Speculation : Frequency close to that of Gaussian centre of mass wave function?
IR Extrapolations

\[ \frac{\hbar^2 k_{\text{sep}}^2}{2m} = B_t - B_d \]

\[ E(N_{\text{max}}) = E_{\infty} + a e^{-2k_{\infty}L} \]

[Phys. Rev. C 86, 054002]

\[ S = \frac{\hbar^2 k_{\infty}^2}{2m} \]

\( k_{\infty} \) is the separation energy of the lowest breakup channel.

[ With C. Forssén ]

<table>
<thead>
<tr>
<th>( k_{\text{sep}} )</th>
<th>( k_{\infty} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.56 fm(^{-1})</td>
<td>0.55 fm(^{-1})</td>
</tr>
</tbody>
</table>
Regulated Interaction

Note: x- and y-axis represent momentum in fm\(^{-1}\). Regulated by HO space, \(N_{\text{max}} = 8\), \(hw = 22\), \(l = 0\).

\[
V_{ct}^{(0)}(1S_0) = \tilde{C}_{1S_0}, \quad V_{ct}^{(0)}(3S_1) = \tilde{C}_{3S_1}, \quad V_{3NF}^{ct} = c_E \sum_{j \neq i} \vec{\tau}_i \cdot \vec{\tau}_j. \quad V_{ct}^{(2)}(3S_1) = C_{3S_1}(p^2 + p'^2), \quad V_{ct}^{(2)}(1S_0) = C_{1S_0}(p^2 + p'^2).
\]

Large Cutoffs

- Physical range of the potential $R$ is inversely proportional to UV cutoff, at higher cutoffs the effective range cannot be reproduced.

- When adding higher order terms non-perturbatively, higher-order effects can become uncontrolled if interaction is too short-ranged. [Lesnky et al.(arXiv:1605.03898 [nucl-th])].
Small Cutoffs

- From free Fermi-gas model, $E/A = (3/5)E_F$. This leads to a Fermi momentum $k_F \sim \Lambda_{UV}$ at small cutoffs for heavier nuclei.

- Similar behavior is seen in the case of lattice nuclei.

Reasoning:
Interaction not equipped to scatter nucleons on/close to fermi-sphere to momentum states outside of the fermi-sphere. This causes over-binding.
Same UV cut-off, different basis size

- Everything so far, cutoff variation at same N and different oscillator frequency.

- Results for A≤4 nuclei at same cutoff in different model space size.

- Binding energy does not show any N dependence.

<table>
<thead>
<tr>
<th>$E_{3_{\text{max}}} = N$ (triangular)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>LO</strong></td>
</tr>
<tr>
<td>$N$</td>
</tr>
<tr>
<td>-----</td>
</tr>
<tr>
<td>6</td>
</tr>
<tr>
<td>8</td>
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<tr>
<td>10</td>
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<table>
<thead>
<tr>
<th><strong>NLO</strong></th>
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<tbody>
<tr>
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<td>6</td>
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<tr>
<td>8</td>
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<tr>
<td>10</td>
</tr>
</tbody>
</table>

$\Lambda_{\text{UV}} \sim 490$ MeV
Regulator: Finite Harmonic Oscillator Basis

Basis parameters:-

\((N, \omega) \rightarrow (\Lambda_{UV}, L)\)

Key Idea:

By construction, interaction is regulated to live within the phase space covered by finite HO basis. No further regulator employed.

\[ L \approx \sqrt{2N \frac{\hbar}{m\omega}} \]

\[ \Lambda_{UV} \approx \sqrt{2N \frac{m\omega}{\hbar}} \]

Phase space covered by Oscillator basis with \((N_{\text{max}}, \omega)\) or \((\Lambda_{UV}, L)\)

**How small can the basis be?**

Basis parameters:-(\(N_{\text{max}}, \omega\) → (\(\Lambda_{\text{UV}}, L\))

- nucleus needs to fit into phase space:
  - \(L > R_{\text{nucl}}\)

- interaction needs to be captured:
  - \(\Lambda_{\text{UV}} > \Lambda_{\text{int}}\)

\[ L \approx \sqrt{2N_{\text{max}} \frac{\hbar}{m\omega}} \]

\[ \Lambda_{\text{UV}} \approx \sqrt{2N_{\text{max}} \frac{m\omega}{\hbar}} \]

phase space covered by Oscillator basis with (\(N_{\text{max}}, \omega\)) or (\(\Lambda_{\text{UV}}, L\))

S. Binder, T. Papenbrock
Key Idea:

- Same example as before: \( V(k', k) = g(k)g(k') = C_0 \)
- Blue curve gives the IR improved interaction potential

We demand correct low energy behavior of the potential by giving away the agreement of matrix elements at highest discrete momentum eigenvalue.
$^4$He: NCSM vs CCSD

- Shows that singles - doubles CC calculation is a good approximation, even with three nucleon force included.

- Binding energy results for $^4$He at NLO from both the methods is similar.

<table>
<thead>
<tr>
<th>$\hbar \omega$</th>
<th>$\Lambda$</th>
<th>$E_{\text{NCSM}}(^4\text{He})$</th>
<th>$E_{\text{CCSD}}(^4\text{He})$</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>232.35</td>
<td>27.5</td>
<td>27.5</td>
</tr>
<tr>
<td>10</td>
<td>328.59</td>
<td>27.3</td>
<td>27.2</td>
</tr>
<tr>
<td>22</td>
<td>487.39</td>
<td>29.3</td>
<td>29.0</td>
</tr>
</tbody>
</table>
Key Idea: 

\[ |k, l> = \sum_{n=0}^{\infty} <n, l|k, l> |n, l> = \sum_{n=0}^{\infty} \tilde{\psi}_{n, l}(k)|n, l> \quad \Rightarrow \quad |\phi_{\mu, l}> = c_{\mu, l} \sum_{n=0}^{N_{\text{max}}} \tilde{\psi}_{n, l}(k_{\mu, l})|n, l> \]

- Quantifying truncation errors in effective field theory: Furnstahl et al. (2015)
References

- Inverse scattering J-matrix approach to nucleus-nucleus scattering and the shell model: Shirokov et al. (2009)
- Ultraviolet extrapolations in finite oscillator bases: S. Konig et al. (2014)
- Systematic expansion for infrared oscillator basis extrapolations: R.J. Furnstahl (2014)
- Corrections to nuclear energies and radii in finite oscillator spaces: R.J. Furnstahl et al. (2012)
- Universal Properties of infrared oscillator basis extrapolations: S.N. More et al. (2013)
- The potential of effective field theory in NN scattering (1997): SR Beane et al.
- Local three nucleon interaction form chiral effective field theory: P. Navratil (2007)
- Three-nucleon forces from Chiral Effective field theory: Epelbaum et al. (2002)