Advances in nuclear structure calculations: extrapolations in finite model spaces and optimized chiral interactions at NNLO

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Convergence in finite oscillator spaces

Calculations are performed in finite oscillator spaces. How can one reliably extrapolate to infinity?

Convergence in momentum space (UV) and in position space (IR) needed

\[ \Lambda_{UV} \equiv \sqrt{2(N + 3/2)\hbar/b} \]

Phase space covered by oscillator basis with \((N, b)\)

Nucleus needs to “fit” into basis:
- Nuclear radius \(R < L\)
- cutoff of interaction \(\Lambda < \Lambda_{UV}\)
What is the infrared cutoff in the HO basis?
(Question asked by Bira van Kolck at INT workshop in spring 2009. Bira’s answer: \(1/b\) [Stetcu, Barrett, van Kolck, Phys. Lett. B 653, 358 (2007); nucl-th0609023])

Very precise answer [More, Ekström, Furnstahl, Hagen, TP, 2013] based on length scale

\[ L_2 = \sqrt{2(N + 3/2 + 2)b} \]

1. At low energies, the HO basis looks like a “box” of radius \(L_2\).
2. \(\pi/L_2\) is the infrared cutoff.
3. Knowledge can be used for theoretically founded extrapolations in HO basis, computations of phase shifts in HO basis ...

Spectrum of the operator $p^2$ in the HO basis

- At low momentum, number of states increases linearly with increasing momentum.
- Spectrum looks like that of the momentum operator in a box.

The number of s-wave eigenstates with $p^2 < k^2$ is given by the expression:

$$M(k) = \frac{bk}{2\pi} \sqrt{2N + 3 - b^2 k^2} + \frac{N + 3/2}{\pi} \arcsin \frac{bk}{\sqrt{2N + 3}}$$
Eigenfunctions of $p^2$ with lowest eigenvalues in oscillator basis

Eigenfunctions look like those from a box of size $L_2$. 

- $\sin(\pi x/L_2)$
- $\sin(2\pi x/L_2)$
Squared infrared cutoff is the lowest eigenvalue of $p^2$

The lowest eigenvalue $\kappa_{\text{min}}$ can be computed analytically for $N \gg 1$. **Result:** $\pi/L_2$

Note: $N \gg 1$ does not imply impractically large model spaces

<table>
<thead>
<tr>
<th>$N$</th>
<th>$\kappa_{\text{min}}$</th>
<th>$\pi/L_2$</th>
<th>$\pi/L_0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1.2247</td>
<td>1.1874</td>
<td>1.8138</td>
</tr>
<tr>
<td>2</td>
<td>0.9586 <strong>highlighted</strong></td>
<td>0.9472</td>
<td>1.1874</td>
</tr>
<tr>
<td>4</td>
<td>0.8163</td>
<td>0.8112</td>
<td>0.9472</td>
</tr>
<tr>
<td>6</td>
<td>0.7236</td>
<td>0.7207</td>
<td>0.8112</td>
</tr>
<tr>
<td>8</td>
<td>0.6568</td>
<td>0.6551</td>
<td>0.7207</td>
</tr>
<tr>
<td>10</td>
<td>0.6058</td>
<td>0.6046</td>
<td>0.6551</td>
</tr>
<tr>
<td>12</td>
<td>0.5651</td>
<td>0.5642</td>
<td>0.6046</td>
</tr>
<tr>
<td><strong>14</strong></td>
<td><strong>highlighted</strong></td>
<td><strong>highlighted</strong></td>
<td><strong>highlighted</strong></td>
</tr>
<tr>
<td>16</td>
<td>0.5035</td>
<td>0.5031</td>
<td>0.5310</td>
</tr>
<tr>
<td>18</td>
<td>0.4795</td>
<td>0.4791</td>
<td>0.5031</td>
</tr>
<tr>
<td>20</td>
<td>0.4585</td>
<td>0.4582</td>
<td>0.4791</td>
</tr>
</tbody>
</table>

$L_i \equiv \sqrt{2(N + 3/2 + i)b}$

1% deviation at $N > 2$

0.1% deviation at $N > 14$

$\pi/L_2$ is very precise value of the IR cutoff
IR corrections to bound-state energies

**Simple view:*** A node in the wave function

\[ u_E(r) \xrightarrow{r \gg R} A_E (e^{-k_E r} + \alpha_E e^{+k_E r}) \]

at \( r = L_2 \) requires \( \alpha_E = -\exp(-2k_EL_2) \). This yields a (kinetic) energy correction

\[ E_L = E_\infty + a_0 e^{-2k_\infty L} \]

**Model-independent approach** based on linear energy method [D. Djajaputra & B. R. Cooper, Eur. J. Phys. 21, 261 (2000)] yields energy correction

\[ \Delta E_L \approx -u_\infty(L) \left( \frac{du_E(L)}{dE} \bigg|_{E_\infty} \right)^{-1} \]


\[ \Delta E_L = \frac{\hbar^2 k_\infty \gamma_\infty^2}{\mu} e^{-2k_\infty L} + O(e^{-4k_\infty L}) \]

\[ \langle r^2 \rangle_L \approx \langle r^2 \rangle_\infty \left[ 1 - (c_0 \beta^3 + c_1 \beta)e^{-\beta} \right] \quad (\text{with } \beta \equiv 2k_\infty L) \]

Triton binding energy from SRG interactions: only observables enter into the IR extrapolation
Phase shifts computed directly in the HO basis

1. Compute states in channel \( l \) with positive energies \( E_i \) and momentum \( p_i \) in HO basis at fixed \( N \)
2. In a box, the \( i^{th} \) state determines the box size \( L_i = L(p_i) \) at that energy via 
   \[ j_l(p_i L_i / \hbar) = 0 \]
3. Compute phase shift from usual formula:
   \[ \tan \delta_l(k_i) = \frac{j_l(k_i L(\hbar k_i))}{\eta_l(k_i L(\hbar k_i))} \]
4. Repeat for several \( \hbar \Omega \)

![Graph showing phase shift vs. \( E_{Lab} \)]

Different sets of points from different \( \hbar \Omega \)
Alternative approaches based on [Busch et al 1998] employ a harmonic potential and use $\hbar \omega \to 0$ for finite-range interactions.

How well can one distinguish $L_2$ in practice?

FIG. 2: (color online) Ground-state energies versus $L_0$ (top), $L'_0$ (middle), and $L_2$ (bottom) for a Gaussian potential well Eq. (5) with $V_0 = 5$ and $R = 1$. The crosses are the energies from HO basis truncation. The energies obtained by numerically solving the Schrödinger equation with a Dirichlet boundary condition at $L$ lie on the solid line. The horizontal dotted lines mark the exact energy $E_\infty = -1.27$. Deuteron ($N^3$LO E&M)
Corrections for shallow bound states

\[
(\Delta E_L)_{\text{mod}} = \frac{\hbar^2 k_\infty \gamma^2}{\mu} e^{-2k_\infty L} \frac{e^{-2k_\infty L}}{(1 - \gamma^2 L e^{-2k_\infty L})}
\]

\[
\Delta E_L = \frac{\hbar^2 k_\infty \gamma^2}{\mu} e^{-2k_\infty L} + \mathcal{O}(e^{-4k_\infty L})
\]
Corrections due to finite Hilbert spaces

- UV practically converged (because $\lambda < \Lambda_{UV}$)
- IR convergence is slower due to exponential decay of wave function
- Dirichlet boundary condition at $x=L$ in position space

\[ E_L = E_\infty + a_0 e^{-2k_\infty L} \]

\[ \langle r^2 \rangle_L \approx \langle r^2 \rangle_\infty [1 - (c_0 \beta^3 + c_1 \beta)e^{-\beta}] \]

\[ \beta \equiv 2k_\infty L \]

---

**Graphs:**

- **N$^3$LO (500 MeV)**
- **SRG $\lambda = 2$ fm$^{-1}$**

**6He**

- NCSM energies
  - **Red Line** Theory

**Extrapolated energy**

**Not included in fit**
Empirical approach: combined UV and IR fits for SRG interactions

At lower $\hbar \Omega$:
- IR converged
- extrapolate UV

At higher $\hbar \Omega$:
- UV converged
- extrapolate IR
Empirical approach: combined UV and IR fits for SRG interactions

\[ E(\Lambda_{UV}, L) \approx E_\infty + A_0 e^{-2\Lambda_{UV}^2/A_1^2} + A_2 e^{-2k_\infty L} \]


Figures from [Jurgenson, Maris, Furnstahl, Navratil, Ormand, Vary arXiv:1302.5473]
Recipe

1. Perform calculations at sufficiently large values of ħΩ (these have small or no UV corrections)

2. Plot results (energies, radii) vs. L₂ (UV converged results are expected to fall onto a single line)

3. Perform fit to extrapolation formulas and read off asymptotic value

4. General: Compute IR and UV cutoffs from diagonalization of p²
Summary

• Much improved understanding of IR properties of HO basis
• At low momenta, HO basis behaves as a box of size $L^2$
• $\pi/L^2$ is the IR cutoff
• Computation of phase shifts directly from the positive energy states in HO basis
• Energy extrapolation law expressed solely in terms of observables
• Corrections for shallow bound states worked out

Outlook: IR properties in *any localized* basis
• Diagonalize operator $p^2$ in a given model space $\rightarrow$ IR and UV cutoffs, and $L$ for this model space.
• Be in the UV-converged regime.
• Plot energies and radii as a function of $L$, and extrapolate.
Optimization of chiral interaction an NNLO

Andreas Ekström, Baarsden, Forssen, Hagen, Hjorth-Jensen, Jansen, Machleidt, Nazarewicz, TP, Sarich, Wild, arXiv:1303.4674

2N Force

LO
\((Q/\Lambda_\chi)^0\)

\[\times\]

NLO
\((Q/\Lambda_\chi)^2\)

\[\times\]

NNLO
\((Q/\Lambda_\chi)^3\)

3N Force

Kept fixed
\(m_{\pi^+}, m_{\pi^-}, m_{\pi^0}, m_n, m_p, g_A, f_\pi, \Lambda_{LS}, \Lambda_\chi\)

Adjusted parameters
\(\tilde{C}_1^{pp}, \tilde{C}_1^{nn}, \tilde{C}_1^{np}, \tilde{C}_3^{S_1}, C_1^{S_0}, C_3^{p_0}, C_1^{p_1}, C_3^{p_1}, C_3^{S_1}, C_3^{S_1-3D_1}, C_3^{p_2}, c_1, c_3, c_4, (c_D, c_E)\)

Weinberg; van Kolck; Epelbaum, Glöckle & Meißner; Entem & Machleidt; Krebs; ...
Optimization to phase shifts; $\chi^2$ from data

$$f(\vec{x}) = \sum_{q=1}^{N_q} \left( \frac{\delta_{\text{NNLO}}(\vec{x}) - \delta_{\text{Nijm93}}}{\omega_q} \right)^2$$

Weights for contacts scale as $Q^3$; for pion-nucleon couplings from Nijmegen analysis

Pion nucleon couplings determined from fits to peripheral D, F, G partial waves (NNLO contacts do not contribute for $L\geq2$)

<table>
<thead>
<tr>
<th>$\pi N$ LEC</th>
<th>$\pi N$-scattering$^1$</th>
<th>NN-PWA$^2$</th>
<th>NNLO$^3$</th>
<th>N3LO</th>
<th>POUNDerS</th>
</tr>
</thead>
<tbody>
<tr>
<td>$c_1$ [GeV$^{-1}$]</td>
<td>-0.81±0.15</td>
<td>-0.76±0.07</td>
<td>-0.81</td>
<td>-0.81</td>
<td>-0.9186</td>
</tr>
<tr>
<td>$c_3$ [GeV$^{-1}$]</td>
<td>-4.69±1.34</td>
<td>-4.78±0.10</td>
<td>-3.40</td>
<td>-3.20</td>
<td>-3.8887</td>
</tr>
<tr>
<td>$c_4$ [GeV$^{-1}$]</td>
<td>+3.40±0.04</td>
<td>+3.96 ±0.22</td>
<td>+3.40</td>
<td>+5.40</td>
<td>+4.3103</td>
</tr>
</tbody>
</table>

\(\chi^2/\text{datum}, \ np \ scattering \ data \ (1999 \ database)\)

The previous picture...

<table>
<thead>
<tr>
<th>(T_{\text{lab}} ) bin (MeV)</th>
<th>N3LO</th>
<th>NNLO(^1)</th>
<th>NLO(^1)</th>
<th>AV18</th>
</tr>
</thead>
<tbody>
<tr>
<td>0-100</td>
<td>1.06</td>
<td>1.71</td>
<td>5.20</td>
<td>0.95</td>
</tr>
<tr>
<td>100-190</td>
<td>1.08</td>
<td>12.9</td>
<td>49.3</td>
<td>1.10</td>
</tr>
<tr>
<td>190-290</td>
<td>1.15</td>
<td>19.2</td>
<td>68.3</td>
<td>1.11</td>
</tr>
<tr>
<td><strong>0-290</strong></td>
<td><strong>1.10</strong></td>
<td><strong>10.1</strong></td>
<td><strong>36.2</strong></td>
<td><strong>1.04</strong></td>
</tr>
</tbody>
</table>


... changes with POUNDerS

<table>
<thead>
<tr>
<th>(T_{\text{lab}} ) bin (MeV)</th>
<th>POUNDerS-NNLO(500)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0-35</td>
<td>0.85</td>
</tr>
<tr>
<td>35-125</td>
<td>1.17</td>
</tr>
<tr>
<td>125-183</td>
<td>1.87</td>
</tr>
<tr>
<td>183-290</td>
<td>6.09</td>
</tr>
<tr>
<td><strong>0-290</strong></td>
<td><strong>2.95</strong></td>
</tr>
</tbody>
</table>
\( \chi^2 / \text{datum}, \ pp \text{ scattering data (1999 database)} \)

### The previous picture...

<table>
<thead>
<tr>
<th>( T_{\text{lab}} ) bin (MeV)</th>
<th>N3LO</th>
<th>NNLO(^1)</th>
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<tbody>
<tr>
<td>0-100</td>
<td>1.05</td>
<td>6.66</td>
<td>57.8</td>
<td>0.96</td>
</tr>
<tr>
<td>100-190</td>
<td>1.50</td>
<td>28.3</td>
<td>62.0</td>
<td>1.31</td>
</tr>
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<td>190-290</td>
<td>1.93</td>
<td>66.8</td>
<td>111.6</td>
<td>1.82</td>
</tr>
<tr>
<td><strong>0-290</strong></td>
<td><strong>1.50</strong></td>
<td><strong>35.4</strong></td>
<td><strong>80.1</strong></td>
<td><strong>1.38</strong></td>
</tr>
</tbody>
</table>


### ... changes with POUNDerS

<table>
<thead>
<tr>
<th>( T_{\text{lab}} ) bin (MeV)</th>
<th>POUNDerS-NNLO(500)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0-35</td>
<td>1.11</td>
</tr>
<tr>
<td>35-125</td>
<td>1.56</td>
</tr>
<tr>
<td>125-183</td>
<td>23.95 (4.35(^a))</td>
</tr>
<tr>
<td>183-290</td>
<td>29.26</td>
</tr>
<tr>
<td><strong>0-290</strong></td>
<td><strong>17.10 (14.03)(^2)</strong></td>
</tr>
</tbody>
</table>

\(^2\) Total (0-290) MeV \( pp \) \( \chi^2 / \text{datum} \) when excluding two low-uncertainty data sets.
Optimization with POUNDerS

Graphs show phase shifts and mixing parameters for different states:

- $^1S_0$
- $^3P_0$
- $^3S_1$
- $^3D_1$
- $^3P_1$
- $^3D_2$
- $^1P_1$
- $^3F_2$
- $^1D_2$
- $^3P_2$

Parameters are plotted against lab energy (MeV).
Differential cross sections at 90 MeV

A. Ekström et al (2012), unpublished
Differential cross sections at 144 MeV

A. Ekström et al (2012), unpublished
## Nucleon-nucleon properties

<table>
<thead>
<tr>
<th></th>
<th>$N^3LO_{EM}$</th>
<th>NNLO$_{opt}$</th>
<th>Exp.</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a^C_{pp}$</td>
<td>-7.8188</td>
<td>-7.8174</td>
<td>-7.8196(26)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>-7.8149(29)</td>
</tr>
<tr>
<td>$r^C_{pp}$</td>
<td>2.795</td>
<td>2.755</td>
<td>2.790(14)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>2.769(14)</td>
</tr>
<tr>
<td>$a^N_{pp}$</td>
<td>-17.083</td>
<td>-17.825</td>
<td>-18.95(40)</td>
</tr>
<tr>
<td>$r^N_{pp}$</td>
<td>2.876</td>
<td>2.817</td>
<td>2.75(11)</td>
</tr>
<tr>
<td>$a_{nn}$</td>
<td>-18.900</td>
<td>-18.889</td>
<td>-23.740(20)</td>
</tr>
<tr>
<td>$r_{nn}$</td>
<td>2.838</td>
<td>2.797</td>
<td>2.77(5)</td>
</tr>
<tr>
<td>$a_{np}$</td>
<td>-23.732</td>
<td>-23.749</td>
<td>-23.740(20)</td>
</tr>
<tr>
<td>$r_{np}$</td>
<td>2.725</td>
<td>2.684</td>
<td>2.77(5)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>$B_D$ (MeV)</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$r_D$ (fm)</td>
<td>1.975</td>
<td>1.967</td>
<td>1.97535(85)</td>
</tr>
<tr>
<td>$Q_D$ (fm$^2$)</td>
<td>0.275</td>
<td>0.272</td>
<td>0.2859(3)</td>
</tr>
<tr>
<td>$P_D$ (%)</td>
<td>4.51</td>
<td>4.05</td>
<td></td>
</tr>
</tbody>
</table>
The graph shows the total energy $E_{\text{NCSM}}$ (MeV) as a function of $N_{\text{max}}$ for $^3\text{H}$, with the following key features:

- **POUNDerS-NNLO (NN+NNN)** represented by green circles.
- **POUNDerS-NNLO (NN)** represented by red squares.
- **N3LO (NN)** represented by blue diamonds.
- The dashed black line represents experimental data.

The parameters $c_D = 0.50$ and $c_E = -0.210$ are indicated on the horizontal axis.
$^4$He, NNLO (POUNDerS)

![Graph showing the energy $E_{NCSM}$ vs. $hw$ for different $N$ values: N = 6, N = 12, N = 20, and the experimental data.](image-url)
$E_{\text{NCSM}}$ (MeV)

$N_{\text{max}}$

$c_D = 0.50$ and $c_E = -0.210$

- POUNDerS-NNLO (NN)
- POUNDerS-NNLO (NN+NNN)
- N3LO (NN)
- Experiment
Three nucleon force


TABLE IV. Ground-state energies (in MeV) and point proton radii (in fm) for $^3$H, $^3$He, and $^4$He using the NNLO$_{opt}$ with and without the NNLO 3NF interaction for $c_D = -0.20$ and $c_E = -0.36$.

<table>
<thead>
<tr>
<th></th>
<th>$E(^3\text{H})$</th>
<th>$E(^3\text{He})$</th>
<th>$E(^4\text{He})$</th>
<th>$r_p(^4\text{He})$</th>
</tr>
</thead>
<tbody>
<tr>
<td>NNLO</td>
<td>-8.249</td>
<td>-7.501</td>
<td>-27.759</td>
<td>1.43(8)</td>
</tr>
<tr>
<td>Experiment</td>
<td>-8.482</td>
<td>-7.717</td>
<td>-28.296</td>
<td>1.467(13)</td>
</tr>
</tbody>
</table>

→ See Gustav Jansen’s talk this afternoon
Neutron matter with optimized chiral interactions at NNLO

\[ \frac{E}{N} \text{ (MeV)} \]


Pauli-operator from [Suzuki et al. (2000)]; Coupled cluster (and Bruckner HF)
Summary

• Optimization of chiral interaction at NNLO
• acceptable $\chi^2 \approx 1$ per degree of freedom for lab energies $\lesssim 125$ MeV
• NN interactions alone reproduce essential features in isotopes of oxygen and calcium $\rightarrow$ Gustav Jansen’s talk this afternoon