Three-body forces in matter and nuclei

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Three-body forces from matter to nuclei
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"Three-body force status and needs"

Status:

Some results based on chiral NN interaction ($N^3LO$, E&M) + chiral 3NF

• Strong regulator/scheme dependence of chiral 3NF

• 3NF (a NNLO correction) pivotal for basic nuclear structure (magicity of $^{48}Ca$, drip line in oxygen...)

• Poor saturation of nuclear matter with chiral interactions

Needs:

• Consistently optimized (order by order) chiral interaction model

• Chiral interaction model with acceptable saturation properties

• Exploration of chiral interaction model at NNLO ($NNLO_{opt}$ etc)
Coupled-cluster, Green’s function, in-medium SRG methods ...

Wave-function based methods do not scale well with increasing mass number $A$. Increase in computing power (Moore’s law) is not commensurate with the scaling of this problem.

- Number of single-particle states: $N = (\text{const} \times R \lambda)^3$ for cutoff $\lambda$ and radius $R \sim A^{1/3}$.

- Hamiltonian has dimension: $D = (N \text{ choose } A) \approx (\text{const}^3 \times A \lambda^3 \text{ choose } A)$

Extrapolations (address $\text{const}$), RG (address $\lambda$), importance truncations (address $D$), alleviate but do not solve the scaling problem.

- Reducing $\lambda$ very useful ($\lambda \geq k_F$)

  Induced a-body forces non-negligible at cutoffs $\lambda \approx \left(\frac{4\pi^4 \rho}{3(a - 1)}\right)^{1/3}$

  Induced 3NF (4NF) non-negligible for $\lambda \approx 2.4 \text{ fm}^{-1}$ ($\lambda \approx 2.0 \text{ fm}^{-1}$)

- Significant components in wave function have size $\kappa \sim D^{-1/2}$
Coupled-cluster method (in CCSD approximation)

[Recent review: Hagen, TP, Hjorth-Jensen, Dean, arXiv:1312.7872]

Ansatz:

\[ |\Psi\rangle = e^T |\Phi\rangle \]

\[ T = T_1 + T_2 + \ldots \]

\[ T_1 = \sum_{ia} t_i a_d a_i \]

\[ T_2 = \sum_{ijab} t_{ij} a_d a_i a_j a_i \]

- Scales gently (polynomial) with increasing problem size \( o^2 u^4 \).
- Truncation is the only approximation.
- Size extensive (error scales with \( A \)).
- Most efficient for doubly magic nuclei.

Correlations are *exponentiated* 1p-1h and 2p-2h excitations. Part of np-nh excitations included!

Coupled cluster equations

\[ E = \langle \Phi | \overline{H} | \Phi \rangle \]

\[ 0 = \langle \Phi | T_i | \Phi \rangle \]

\[ 0 = \langle \Phi | T_{ij} | \Phi \rangle \]

\[ \overline{H} = e^{-T} He^T = \left( He^T \right)_c = \left( H + HT_1 + HT_2 + \frac{1}{2} HT_1^2 + \ldots \right)_c \]

Alternative view: CCSD generates similarity transformed Hamiltonian with no 1p-1h and no 2p-2h excitations.
Frame work of nuclear coupled cluster

Based on a reference state (closed subshell in j-coupled formulation)

Normal-ordered Hamiltonian w.r.t. reference

Decouples reference state (and its 2p-2h excitations) from remaining Hilbert space

CCSD: effective two-body Hamiltonian, CCSDT: effective three-body Hamiltonian

Imaginary time-evolution of CCSD technically similar to SRG evolution toward non-Hermitian Hamiltonian

Gamow basis for description of weakly bound and unbound nuclei

Practical solution of center-of-mass problem for intrinsic Hamiltonian

Excited states (and neighboring nuclei) from equations of motion approach

Permits user to employ “bare” interactions from chiral EFT
Gamow shell model for open quantum systems


Computational tool: coupled-cluster method
[Coester (1958); Coester & Kümmel (1960); Kümmel, Lührmann & Zabolitzky (1978); Bishop (1991); (... many others ...); Hagen, TP, Dean, & Hjorth-Jensen arXiv:1312.7872]
Is $^{54}\text{Ca}$ a magic nucleus?

Magic nuclei determine the structure of entire regions of the nuclear chart.

$^{40}\text{Ca}$ in our bones

Calcium isotopes from chiral interactions

[Hagen, Hjorth-Jensen, Jansen, Machleidt, TP, Phys. Rev. Lett. 109, 032502 (2012).]

S\(_{n}(^{52}\text{Ca}) = 5.98\text{MeV}\)

(Sn\(_{n}(^{52}\text{Ca}) = 5.98\text{MeV}\)

(Gallant et al PRL 2012)

S\(_{n}(^{54}\text{Ca}) = 3.84\text{MeV}\)

(Wienholtz Nature 2013)

In-medium effective 3NF: \(k_F=0.95\text{ fm}^{-1}\), \(c_E=0.735\), \(c_D=-0.2\)

[Holt, Kaiser, Weise 2009; Hebeler and Schwenk 2010]
Shell structure of $^{52,54}$Ca

Indicators of shell closure:
- Separation energy
- $2^+$ excited state
- $4^+/2^+$ ratio

suggest that $^{54}$Ca has a “soft” (sub-)shell closure similar to that of $^{52}$Ca


<table>
<thead>
<tr>
<th></th>
<th>$^{48}$Ca</th>
<th></th>
<th>$^{52}$Ca</th>
<th></th>
<th>$^{54}$Ca</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$2^+$</td>
<td>$4^+$</td>
<td>$4^+/2^+$</td>
<td>$2^+$</td>
<td>$4^+$</td>
</tr>
<tr>
<td>CC</td>
<td>3.58</td>
<td>4.20</td>
<td>1.17</td>
<td>2.19</td>
<td>3.95</td>
</tr>
</tbody>
</table>
1. Our prediction for excited $5/2^-$ and $1/2^-$ states in $^{53}\text{Ca}$ seen at RIKEN
2. Inversion of $9/2^+$ and $5/2^+$ states in neutron rich calcium isotopes
3. Harmonic oscillator gives the naïve shell model order

Continuum coupling crucial for level ordering
Chiral interaction $\text{NNLO}_{\text{opt}}$


\[ \text{LO } (Q/\Lambda_{\chi})^0 \]
\[ \text{NLO } (Q/\Lambda_{\chi})^2 \]
\[ \text{NNLO } (Q/\Lambda_{\chi})^3 \]

\begin{itemize}
  \item \textbf{2N Force}
  \item \textbf{3N Force}
\end{itemize}

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

Adjusted parameters
\[ \tilde{C}_{1S_0}^{pp}, \tilde{C}_{1S_0}^{nn}, \tilde{C}_{1S_0}^{np}, \tilde{C}_{3S_1} \\
C_{1S_0}, C_{3P_0}, C_{1P_1}, C_{3P_1}, C_{3S_1}, C_{3S_1-3D_1}, C_{3P_2} \\
c_1, c_3, c_4, (c_D, c_E) \]

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

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

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 $L \geq 2$)

<table>
<thead>
<tr>
<th>$\pi N$ LEC</th>
<th>$\pi N$-scattering</th>
<th>NN-PWA</th>
<th>NNLO</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>

Phase shifts of \( \text{NNLO}_{\text{opt}} \)
Oxygen isotopes (NN only)

Drip line in oxygen from NN alone (Oxygen isotopes not included in optimization)
Calcium isotopes (NN only)

Doubly magic $^{48}$Ca from NN alone
Nucleonic matter

• Use plane-wave basis with generalized boundary conditions (Bloch waves)
• 😊 Basis respects momentum conservation
• 😊 CCD (no singles) for closed-shell references
• 😊 Three-nucleon forces much simpler to implement than in shell-model basis
• 😞 Shell effects dominate finite-size corrections

Related studies with chiral interactions: Soma & Bozek (2008); Epelbaum, Krebs, Lee, & Meissner (2009); Hebeler & Schwenk (2010); Hebeler, Bogner, Furnstahl, Nogga, & Schwenk (2011); Holt, Kaiser, & Weise (2012); Carbone, Polls, & Rios (2013); Gezerlis, Tews, Epelbaum, Gandolfi, Hebeler, Nogga, & Schwenk (2013); ...
Mitigate shell oscillations

“Twist averaged” boundary conditions: average over all possible phases of Bloch waves. Exactly removes finite size effects for free Fermi gas.


Discrete momenta are

\[ k_{n_i} = \frac{(2\pi n_i + \theta_i)}{L}, \quad n_i = 0, \pm 1, \ldots, \pm n_{\text{max}} \]
Nuclear matter (NN only)

\[ SCGF = \text{Self-consistent Green’s function at } T=5 \text{ MeV} \] [A. Carbone, A. Polls, and A. Rios, Phys. Rev. C 88, 044302 (2013)].
Neutron matter is perturbative (NN only)
Nuclear matter less perturbative (NN only)

Overbinding and saturation at too high densities

NNLO$_{\text{opt}}$, $n_{\text{max}} = 4$, $A = 132$
Three nucleon force

**Local form of 3NF** [Navratil, Few Body Syst. 41, 117 (2007)], i.e. cutoff is in the momentum transfer based on [Epelbaum et al., Phys. Rev. C 66, 064001 (2002)].

Fit to $A=3,4$ binding energies and triton half life (Gazit, Navratil, & Quaglioni)

$c_D=0.389$, $c_E=0.39$
Inclusion of three-nucleon forces

3NFs in momentum space still require considerable computer time but less human time.

Normal-ordered (w.r.t. HF vacuum) Hamiltonian

\[
H_N = \sum_{pq} \langle k_p | f | k_q \rangle a_p^\dagger a_q + \frac{1}{4} \sum_{pqrs} \langle k_p k_q | v | k_r k_s \rangle a_p^\dagger a_q^\dagger a_s a_r \\
+ \frac{1}{36} \sum_{pqrstu} \langle k_p k_q k_r | w | k_s k_t k_u \rangle a_p^\dagger a_q^\dagger a_r^\dagger a_u a_t a_s. \tag{10}
\]

Normal-ordered 1-body interaction (contains information about NN force and 3NF)

\[
\langle k_p | f | k_q \rangle = \langle k_p | t | k_q \rangle + \sum_i \langle k_p k_i | V_{NN} | k_q k_i \rangle \\
+ \frac{1}{2} \sum_{ij} \langle k_p k_i k_j | V_{3NF} | k_q k_i k_j \rangle,
\]

Normal-ordered 2-body interaction (contains information of 3NF)

\[
\langle k_p k_q | v | k_r k_s \rangle = \langle k_p k_q | V_{NN} | k_r k_s \rangle \\
+ \sum_i \langle k_p k_q k_i | V_{3NF} | k_i k_r k_s \rangle
\]

“Residual” 3NF (enters leading triples correction)

\[
\langle k_p k_q k_r | w | k_s k_t k_u \rangle = \langle k_p k_q k_r | V_{3NF} | k_s k_t k_u \rangle
\]
Nucleonic matter with $\text{NNLO}_{\text{opt}}$ and 3NFs

[Hagen et al., PRC 89 014319 (2013)]

- 3NFs with different regulators and cutoffs act repulsively in neutron matter
- $\text{N2LO}_{\text{opt}} + 3\text{NFs}$ do not reproduce saturation density and binding energy of nuclear matter
- Strong dependence on regulator and cutoff in nuclear matter
Where actually does the cutoff cut off?

$k_f = 1.3 \text{fm}^{-1}$
For NNLO$_{opt}$ no combination of $c_D$, $c_E$ simultaneously satisfies light nuclei and nuclear matter.

5% error bands for saturation $k_f$, $E/N$ and binding energy of $^3$H

$max$ Variation of $c_D$ and $c_E$ not sufficient to simultaneously bind light nuclei and nuclear matter
Coupled-cluster effective interactions for the shell model


- Start from chiral NN(N3LO_{EM}) + 3NF(N2LO) interactions
- Solve for A+1 and A+2 using CC. Project A+1 and A+2 CC wave functions onto the s-d model space using Lee-Suzuki similarity transformation.
- Diagonalize the effective Hamiltonian in the valence space.

Comparison between coupled-cluster effective interaction (CCEI) and “exact” coupled-cluster calculation with inclusion of perturbative triples (Λ-CCSD(T)).

\[
\begin{align*}
\text{Q} & \quad p_{3/2} \\
\text{Q} & \quad f_{7/2} \\
\text{P} & \quad d_{3/2} \\
\text{P} & \quad s_{1/2} \\
\text{P} & \quad d_{5/2} \\
\text{Q} & \quad p_{1/2} \\
\text{Q} & \quad p_{3/2} \\
\text{Q} & \quad s_{1/2}
\end{align*}
\]

\( E(\text{MeV}) \)

- Experiment
- Λ-CCSD(T), \( n_{\text{max}} = 12, E_{3\text{max}} = 14 \)
- CCEI, \( n_{\text{max}} = 12, E_{3\text{max}} = 12 \)

\( \text{NN(n3lo)+3NF(400), } \lambda_{\text{SRG}} = 2.0 \text{fm}^{-1} \)
Coupled-cluster effective interactions for the shell model: Oxygen isotopes
Coupled-cluster effective interactions for the shell model: Carbon isotopes
Convergence in finite oscillator spaces

Calculations are performed in finite oscillator spaces. **How can one reliably extrapolate to infinity?** What is the equivalent of Lüscher’s formula for the harmonic oscillator basis [Lüscher, Comm. Math. Phys. 104, 177 (1986)]?

Convergence in momentum space (UV) and in position space (IR) needed [Stetcu *et al.*, PLB (2007); Hagen *et al.*, PRC (2010); Jurgenson *et al.*, PRC (2011); Coon *et al.*, PRC (2012)]

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

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

Nucleus needs to “fit” into basis:
- Nuclear radius \( R < L \)
- cutoff of interaction \( \Lambda < \Lambda_{UV} \)
Hard wall at $L_2$ is in the spirit of EFT

The difference between the HO basis and a box of size $L_2$ cannot be resolved at low momentum.

$$(\pi/L_2)^2$$ is the lowest eigenvalue of the operator $p^2$. 

$$L_2 = \sqrt{2\left(\mathcal{N} + \frac{3}{2} + 2\right)b}$$

Fourier transforms differ only at large momentum.
IR corrections to bound-state energies

Simple view: A node in the wave function

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

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

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

Model-independent approach based on S-matrix theory

\[ e^{-2k_L L} = [s_0(i k_L)]^{-1} \]


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

only observables enter

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

(with \( \beta \equiv 2k_\infty L \))

Energy extrapolation explains findings by [Coon et al, Phys. Rev. C 86, 054002 (2012)]
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, $k_\infty$ from energy fit

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

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

$\beta \equiv 2k_\infty L$

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![Graphs showing energy and neutron radii](image)
Summary

• Coupled cluster method efficient tool for many nuclei of interest

• Optimization of chiral interaction NNLO_{opt}
  • acceptable $\chi^2 \approx 1$ per degree of freedom for lab energies < 125 MeV
  • NN interactions alone reproduce some essential features in isotopes of oxygen and calcium

• Nucleonic matter in momentum space with NNLO_{opt}
  • Finite size corrections under control
  • Neutron matter is perturbative – nuclear matter somewhat less
  • Variation of $c_D$ and $c_E$ not sufficient to fit light nuclei and matter
  • 3NF with local regulator not without problems (large triples correction)

• Infrared extrapolations based on well-understood box size $L_2$