Nuclear/Neutron Matter and Pairing in Nuclei with 3NF

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(presented by Dick Furnstahl)

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“Improved nuclear matter calculations from chiral low-momentum interactions”

- Evolve $\Lambda$ down with RG (to $\Lambda \approx 2\text{ fm}^{-1}$ for ordinary nuclei)
  - NN interactions fully, NNN interactions approximately
- Fit two 3NF constants to triton binding and $^4\text{He}$ radius
  $\implies$ predict nuclear matter


Use effective $V_{3N}$ in MBPT

![Graph showing binding energy and radius as functions of $k_F$.](image)
Chiral 3NF drives saturation for low-momentum interactions

Uncertainties due to:
- RG scheme dependence ($V_{\text{low }k}$ vs. SRG)
- interaction dependence (EM vs. EGM chiral N$^3$LO)
- $c_i$ coupling uncertainties (long-range 2–pion 3NF)

Comparable to cutoff dependence (includes many-body)
Application to neutron matter and neutron stars

- Significantly reduced cutoff dependence at 2nd order
- Energy sensitive to long-range 3NF $c_3$ variations

Equation of state of pure neutron matter

$$E_{NN+3N,\text{eff}}^{(1)}$$

$$2.0 < \Lambda_{3N} < 2.5 \text{ fm}^{-1}$$

Energy/nucleon [MeV]

0 5 10 15 20

$\rho$ [fm$^{-3}$]

0 0.05 0.10 0.15

KH and A. Schwenk PRC 82, 014314 (2010)
Application to neutron matter and neutron stars

- Significantly reduced cutoff dependence at 2nd order
- Energy sensitive to long-range 3NF $c_3$ variations
- Good agreement with other approaches (different NN)
Neutron star radii

Problem:
Solution of TOV equation requires EOS up to very high densities.

Radius of a typical NS (M~1.4 M⊙) theoretically not well constrained.

But:
Radius of NS is relatively insensitive to high density region.

\[ \log_{10} \rho \text{ [g/cm}^3] \]

\[ \log_{10} P \text{ [dyne/cm}^2] \]

\[ \rho_1 \quad \rho_2 \]

\[ \Gamma_1 \quad \Gamma_2 \]

\[ P \text{ [10}^{33}\text{dyne/cm}^2] \]

\[ \rho \text{ [} \rho_0 \text{]} \]

KH, Lattimer, Pethick, Schwenk, PRL 05, 161102 (2010)

- Significantly reduced cutoff dependence at 2nd order
- Energy sensitive to long-range 3NF \( c_3 \) variations
- Good agreement with other approaches (different NN)
- Piecewise EOS \( \rightarrow \) Constrain neutron star radius
- Also: spin-singlet and spin-triplet \( (^3P_2–^3F_2) \) pairing gaps
Theoretical and experimental neutron/proton three-point mass differences along isotopic/isotonic chains

First order in chiral low-momentum NN and 3N interactions with $\Lambda/\Lambda_{3NF} = 1.8/2.0$ fm$^{-1}$

NN+3N gaps systematically lower by about 30% than NN
*Chiral three-nucleon forces and pairing in nuclei*


- Uncertainties: 100–200 keV for NN; 100–250 keV for 3N
- Short-range higher-order NN and 3N; long-range 3N \( c_i \)'s
- 3N needed for quantitative pairing gaps
- 1st-order low-momentum leaves 30% for higher orders

Next: normal self-energy and higher-order contributions to pairing kernel consistently based on low-momentum NN+3N

- Apply non-empirical pairing EDF to deformed nuclei
Hierarchy of many-body contributions

- Binding energy results from cancellations of much larger kinetic and potential energy contributions
- Chiral hierarchy of many-body terms preserved for considered density range
- Cutoff dependence of natural size, consistent with chiral expansion parameter $\sim 1/3$

When 3NF is fit to few-body properties, no apparent problem with 3NF growth (but 4NF probably significant)

What about consistently evolved 3NF?
When 3NF is fit to few-body properties, no apparent problem with 3NF growth (but 4NF probably significant)
Hierarchy of many-body forces at low resolution

- Binding energy results from cancellations of much larger kinetic and potential energy contributions.
- Chiral hierarchy of many-body terms preserved for considered density range.
- Cutoff dependence of natural size, consistent with chiral expansion parameter \( \sim 1/3 \).

When 3NF is fit to few-body properties, no apparent problem with 3NF growth (but 4NF probably significant).

What about consistently evolved 3NF?
“Evolving nuclear many-body forces with the SRG”

- Look at ground-state matrix elements of KE, NN, 3N, 4N

- Clear hierarchy, but also strong cancellations at NN level
- What about the $A$ dependence?
“Evolving nuclear many-body forces with the SRG”

- Look at running of $^4$He and $^6$Li energy with $\lambda$

- Manifest induced 4NF but same whether initial 3NF or not

- What about the $A$ dependence? No problem up to $^6$Li
“Similarity-transformed chiral NN+3N interactions for the ab initio description of 12-C and 16-O”

R. Roth, J. Langhammer, A. Calci, S. Binder, P. Navrátil, arXiv:1105.3173v1

- SRG evolved in HO basis \textit{à la} Jurgenson thesis
- Importance-truncated NCSM $\implies$ larger $N_{\text{max}}$
- Here: $E_{\text{gs}}$ vs. $N_{\text{max}}$
- NN-only is not unitary
- NN+3N-induced and NN+3N-full are unitary
- Induced 4NF small
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- SRG evolved in HO basis
- Importance-truncated NCSM $\Rightarrow$ larger $N_{\text{max}}$
- Here: $E_{gs}$ vs. $N_{\text{max}}$
- NN-only is not unitary
- NN+3N-induced is still unitary
- NN+3N-full spreads $\Rightarrow$ significant 4NF (confirmed by Jurgenson)
- Small spread for spectrum
Coupled cluster NN-only results: (from G. Hagen et al.)

- $^{16}$O 7.7 MeV 2.3 fm$^{-1}$
- $^{40}$Ca 8.6 MeV 2.8 fm$^{-1}$
- $^{48}$Ca 8.3 MeV 2.9 fm$^{-1}$
Coupled cluster NN-only results: (from G. Hagen et al.)

\[ \begin{align*}
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\end{array}
\]
Questions under investigation in Year 5

- Impact of 3NF (including uncertainties on observables) on
  - neutron star physics
  - pairing
  - DME input for functionals
  - NCSM p-shell nuclei

- How best to fine-tune for functionals?

- RG evolutions of NN and 3NF and other operators
  - Evolved vs. fitted 3NF
  - Ranges and nature of induced interactions from evolution
  - Alternative SRG generators to control many-body operators
  - Renew project for evolving 3NF in momentum space
Options for SRG evolution of 3NF

- Transform an initial hamiltonian, $H = T + V$:

  $$H_s = U_s H U_s^{\dagger} \equiv T + V_s \quad \text{with} \quad U_s^{\dagger} U_s = U_s U_s^{\dagger} = 1$$

  where $s$ is the flow parameter. Flow equation:

  $$\frac{dH_s}{ds} = \frac{dV_s}{ds} = [[G_s, H_s], H_s]$$

  $G_s$ determines flow $\Longrightarrow$ many choices ($T, H_d, H_{bd}, \ldots$)

- Harmonic oscillator basis (E.D. Jurgenson et al.)
  - Evolve full $H_s$ in $A = 3$ and subtract $V_{12}$ evolved in $A = 2$
  - Closely tied to NCSM technology
  - Possible convergence issues; inconvenient for infinite matter

- Momentum basis (K. Hebeler [also L. Platter])
  - Separate $dV_{123}/ds$ evolution to avoid spectator issues
  - Similar technology to solving Faddeev equations
  - Immediate matrix elements for infinite matter MBPT
  - More varied generators easier to implement
Solving SRG equations for $A=3$

- SRG flow equation $\frac{dH_s}{ds} = [[G_s, H_s], H_s]$, e.g., $G_s = T_{\text{rel}}$
  - Insert complete sets of $A = 3$ basis states
  - $A$-body operators fixed in $A$-particle subspace

- What about spectator nucleons and their delta functions?
  - Direct solution in discrete (harmonic oscillator) basis
  - Or, decoupling of $3N$ part in momentum space

$$
\frac{dV_s}{ds} = \frac{dV_{12}}{ds} + \frac{dV_{13}}{ds} + \frac{dV_{23}}{ds} + \frac{dV_{123}}{ds} = [[T_{\text{rel}}, V_s], H_s],
$$

$$
\implies \frac{dV_{123}}{ds} = [[T_{12}, V_{12}], (T_3 + V_{13} + V_{23} + V_{123})] + \{123 \to 132\}
+ \{123 \to 231\} + [[T_{\text{rel}}, V_{123}], H_s]
$$

- No “multi-valued” two-body interactions (dependence on excitation energy of unlinked spectators)

- Tricky part: right side in 3-body Jacobi partial waves
  - need $\langle pq\alpha | V_{13} | p' q' \alpha' \rangle_{23} = \langle pq\alpha | P_{123}^{-1} V_{23} P_{123} | p' q' \alpha' \rangle_{23}$, etc.
Sample term in Jacobi partial wave basis $|pq\alpha\rangle$

\[
\begin{align*}
\langle pq\alpha | [[T_{13}, V_{13}], V_{123}] | p' q' \alpha' \rangle_{23} &= \int dq'' dq''^2 \int_{-1}^{1} dx \int_{-1}^{1} dy \left[ \frac{p^2 - p_2^2(q_{(2)}^*, q'', y)}{4m} + \frac{13}{16} \frac{q^2 - q''^2}{m} \right] \frac{1}{4} \frac{q_{(2)}^2}{p|q_{(2)}^* + qx/2|} \\
&\quad \times \sum_{\bar{\alpha}} F_{\alpha \bar{\alpha}}(p, q, q'', x, y) \langle p_2^2(q_{(2)}^*, q'', y)q'' \bar{\alpha}| V_{123} | p' q' \alpha' \rangle \\
- \int dq'' dq''^2 \int_{-1}^{1} dx \int_{-1}^{1} dy \left[ \frac{p_1^2(q'', q_{(1)}^*, x)}{4m} - p''^2 \right] + \frac{13}{16} \frac{q''^2 - q''^2}{m} \frac{1}{4} \frac{q_{(1)}^2}{p' |q_{(1)}^* + q'y/2|} \\
&\quad \times \sum_{\bar{\alpha}} \langle pq\alpha | V_{123} | p_1(q'', q_{(1)}^*, x)q'' \alpha_1 \rangle \tilde{F}_{\bar{\alpha} \alpha'}(p', q', q'', x, y) \\
\end{align*}
\]

with

\[
\begin{align*}
q_{(1)}^* &= \pm \sqrt{p'^2 + \frac{1}{4} q''^2 (y^2 - 1)} - \frac{1}{2} q'y, \quad p_2(q_{(1)}^*, q', y) = p' \\
q_{(2)}^* &= \pm \sqrt{p^2 + \frac{1}{4} q^2 (x^2 - 1)} - \frac{1}{2} qx, \quad p_1(q, q_{(2)}^*, x) = p \\
\end{align*}
\]

The $F$ functions are sums of geometric factors ($G$ coefficients as defined in Glöckle’s book) times NN matrix elements.
A = 3 Faddeev code written from scratch (NN-only so far)
  - Extend to include 3NF
Right side of SRG differential equations for $V_{123}$ evolution
  - Expressions recently derived
  - Coded but not fully tested (uses OpenMP $\Rightarrow$ add MPI)
  - Improve efficiency (suggestions?)
Computational issues
  - Many coupled first-order differential equations:

$$|p \ q \ \alpha\rangle \quad \Rightarrow \quad (# \ p \ points) \times (# \ q \ points) \times (\alpha \ partial \ wave \ sum)$$

with $15 \leq p \leq 40$, $10 \leq q \leq 25$, $5 \leq \alpha \leq 34$

- At each step in $s$, right side matrix elements each have up to 4 internal loops besides 6 external loops over $p, p', q, q', \alpha, \alpha'$
Test using Faddeev code and against 3NF HO evolution
Apply to HF (and beyond) for infinite matter
Extra slides
Diagrams for SRG \( \iff \) Disconnected cancels

\[
V_s^{(2)} = \begin{array}{c}
\times
\end{array} \quad [T, V_s^{(2)}] = \begin{array}{c}
\times
\end{array} \quad [[T, V_s^{(2)}], T] = \begin{array}{c}
\times
\end{array}
\]

\[
V_s^{(3)} = \begin{array}{c}
\times
\end{array} \quad [T, V_s^{(3)}] = \begin{array}{c}
\times
\end{array} \quad [[T, V_s^{(3)}], T] = \begin{array}{c}
\times
\end{array}
\]

\[
\frac{dV_s^{(2)}(a, b)}{ds} = a \begin{array}{c}
\times
\end{array} b + a \begin{array}{c}
\circ
\end{array} c \begin{array}{c}
\times
\end{array} b - a \begin{array}{c}
\circ
\end{array} c \begin{array}{c}
\times
\end{array} b
\]

\[
= -(\epsilon_a - \epsilon_b)^2 V_s^{(2)}(a, b) + \sum_c [(\epsilon_a - \epsilon_c) - (\epsilon_c - \epsilon_b)] V_s^{(2)}(a, c) V_s^{(2)}(c, b)
\]

\[
\frac{dV_s^{(3)}}{ds} = \begin{array}{c}
\times
\end{array} + \begin{array}{c}
\circ
\end{array} \begin{array}{c}
\times
\end{array} + \begin{array}{c}
\circ
\end{array} \begin{array}{c}
\times
\end{array} + \begin{array}{c}
\circ
\end{array} \begin{array}{c}
\times
\end{array} + \cdots
\]
$V_3$ analysis in $A = 3$

$$
\frac{d}{d\lambda} \langle \psi_\lambda^{(3)} | V_3 | \psi_\lambda^{(3)} \rangle = \langle \psi_\lambda^{(3)} | [\bar{V}_2, V_2]_c - [\bar{V}_3, V_3] | \psi_\lambda^{(3)} \rangle
$$

- Majority evolution dominated by $[\bar{V}_2, V_2]$, $(\bar{V} \equiv [T, V])$
- Hierarchy of contributions

- $\hbar \Omega = 20$ MeV
- $N_{A3\text{max}} = 32$

Ground-State Energy [MeV]

<table>
<thead>
<tr>
<th>$\lambda$ [fm$^{-1}$]</th>
<th>NN-only</th>
<th>NN + NNN-induced</th>
<th>NN + NNN</th>
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<tr>
<td>1</td>
<td>7.8</td>
<td>8.2</td>
<td>8.6</td>
</tr>
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<td>8.6</td>
</tr>
<tr>
<td>20</td>
<td>7.8</td>
<td>8.2</td>
<td>8.6</td>
</tr>
</tbody>
</table>

g.s. Expectation Value

<table>
<thead>
<tr>
<th>$\lambda$ [fm$^{-1}$]</th>
<th>d$&lt;V_3&gt;/d\lambda$</th>
<th>$&lt;[[T,V_2],V_2]&gt;_c$</th>
<th>$&lt;[[T,V_3],V_3]&gt;$</th>
</tr>
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<tbody>
<tr>
<td>1</td>
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<td>0.7</td>
</tr>
</tbody>
</table>

$\lambda$ [fm$^{-1}$]
$V_4$ analysis in $A = 4$

$$\frac{d}{d\lambda} \langle \psi^{(4)}_\lambda | V_4 | \psi^{(4)}_\lambda \rangle = \langle \psi^{(4)}_\lambda | [\bar{V}_2, V_3]_c + [\bar{V}_3, V_2]_c + [\bar{V}_3, V_3]_c - [\bar{V}_3, V_4] | \psi^{(4)}_\lambda \rangle$$

- No $[\bar{V}_2, V_2] \implies$ Induced 4-body is relatively suppressed
- Initial hierarchy of few-body forces is maintained (?)