Ab-initio structure and the role of three-nucleon forces in nucleonic matter

Gaute Hagen (ORNL)

Lecture 3, TALENT school
Outline

• Nuclei across the chart and status of ab initio calculations with three-nucleon forces (3NFs)
• Chiral effective field theory – Why 3NFs?
  – SRG evolution of chiral interactions
• Role of 3NFs on spectra of light nuclei
• Role of 3NFs on weak decays and quenching of axial coupling in nuclei
• The oxygen dripline and 3NFs
• Evolution of shell structure in neutron calcium isotopes
• The problem of saturation and overbinding in nuclei from chiral interactions
  – Simultaneous Optimization of chiral forces with input from nuclei selected nuclei up to A ~ 25
  – Accurate binding energies and radii from a chiral interaction (NNLO$_{sat}$)
• Impact of 3NFs in infinite nucleonic matter
Nuclei across the chart

118 chemical elements (94 naturally found on Earth)
288 stable (primordial) isotopes

Thousands of short-lived isotopes – many with interesting properties

large isospin magnifies unknown physics
clustering behavior
novel evolution in structure

Shape transitions in Sm

45Fe 2-proton decay

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45Fe 2-proton decay
Reach of realistic *ab initio* calculations
(realistic meaning that binding energies are within 5% of experimental values)

Explosion of many-body methods
(Coupled clusters, Green’s function Monte Carlo, In-Medium SRG, Lattice EFT, No-Core Shell Model, Self-Consistent Green’s Function, ... )
Effective theories provide us with model independent approaches to atomic nuclei.

Key: Separation of scales

Chiral symmetry is broken

Pion is Nambu-Goldstone boson

Tool: Chiral effective field theory

Fig.: Bertsch, Dean, Nazarewicz, SciDAC review (2007)
Three–nucleon forces – Why?

- Nucleons are not point particles (i.e. not elementary).
- We neglected some internal degrees of freedom (e.g. Δ-resonance, “polarization effects”, …), and unconstrained high-momentum modes.

**Example from celestial mechanics:**
Earth-Moon system: point masses and modified two-body interaction

**Other tidal effects cannot be included in the two-body interaction!** Three-body force unavoidable for point masses.

The question is not: Do three-body forces enter the description?
The (only) question is: How large are three-body forces?
Three-body forces cont’d

Figure 23: Eliminating degrees of freedom leads to three-body forces. 
(taken from Bogner, Furnstahl, Schwenk, arXiv:0912.3688)

Leading three-nucleon force
1. Long-ranged two-pion term (Fujita & Miyazawa …)
2. Intermediate-ranged one-pion term
3. Short-ranged three-nucleon contact

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Green’s function Monte Carlo computations
Demonstration that light nuclei can be built from scratch

Argonne $v_{18}$ with Illinois-7 GFMC Calculations

- IL7: 4 parameters fit to 23 states
- 600 keV rms error, 51 states
- ~60 isobaric analogs also computed

As cutoff $\Lambda$ is varied, motion along “Tjon line”.

Addition of $\Lambda$-dependent three-nucleon force yields (almost) agreement with experiment. **Q: What’s missing?**

**A:** The complete description of $^4$He would require four-nucleon forces!
### Nuclear forces from chiral effective field theory

[Weinberg; van Kolck; Epelbaum *et al*.; Entem & Machleidt; …]

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<th>NN</th>
<th>3N</th>
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<td>LO $\mathcal{O} \left( Q^0 \over A^0 \right)$</td>
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- developing higher orders and higher rank (3NF, 4NF) [Epelbaum 2006; Bernard *et al* 2007; Krebs *et al* 2012; Hebeler *et al* 2015; …]

- implemented in continuum and on lattice [Borasoy *et al* 2007]

- local / non-local formulations [Gezerlis *et al* 2013]

- propagation of uncertainties on horizon [Navarro Perez 2014]

- different optimization protocols [Ekström *et al* 2013]

Much improved understanding and handling via renormalization group transformations [Bogner *et al* 2003; Bogner *et al* 2007]
Similarity renormalization group (SRG) transformation


Main idea: decouple low from high momenta via a (unitary) similarity transformation

Unitary transformation

$$\hat{H}(s) = U(s) \hat{H} U^\dagger(s) = U(s) \left( \hat{T} + \hat{V} \right) U^\dagger(s)$$

Evolution equation

$$\frac{d\hat{H}(s)}{ds} = [\eta(s), \hat{H}(s)]$$

with

$$\eta(s) \equiv \frac{dU(s)}{ds} U^\dagger(s) = -\eta^\dagger(s)$$

Choice of unitary transformation through (one does not need to construct U explicitly).

$$\eta(s) = \begin{bmatrix} \hat{T}, \hat{H}(s) \end{bmatrix}$$

yields scale-dependent potential that becomes more and more diagonal

$$\hat{H}(s) = \hat{T} + \hat{V}(s)$$

Note: Baker-Campbell-Hausdorff expansion implies that SRG of 2-body force generates many-body forces

$$e^{-\eta} \hat{H} e^\eta = \hat{H} + [\hat{H}, \eta] + \frac{1}{2!} \left[ [\hat{H}, \eta], \eta \right] + \ldots$$
SRG evolution of a chiral potential

(use cutoff $\lambda \equiv s^{-1/4}$ as evolution variable)

$^1S_0$ from N$^3$LO (500 MeV) of Entem/Machleidt

$^3S_1$ from N$^3$LO (500 MeV) of Entem/Machleidt

Fig.: Bogner & Furnstahl. See http://www.physics.ohio-state.edu/~ntg/srg
Understanding SRGs

Question: Which statement is correct?

1. The SRG is a unitary transformation, and no information is lost.
2. The SRG is only accurate up to the cutoff.
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2. The SRG is only accurate up to the cutoff.

When performing the SRG, up to A-body forces are created in an A-body system (“no free lunch theorem”). In practice, one hopes (with view to the chiral power counting) that the computation of 2-body and 3-body forces might be sufficient.

Q: How can we check in practice, that keeping 2-body and 3-body forces is sufficient?

1. Perform a computation with and without SRG an compare.
2. Check how results in the A-body system depend on the cutoff/evolution parameter
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Of course: Any observable other than the Hamiltonian also needs to be transformed.
Solution of $^3$H and $^4$He with induced and initial 3NF

Q: What is the effect of (omitted) 4NF and forces of even higher rank?

A: In $^4$He, (short ranged) 4NF yield about 200 keV (see energies at small momentum)
Note: This is consistent with deviation from experiment!

Second quantized normal–ordered Hamiltonian:

\[ H_N = \sum_{pq} \langle k_p | f | k_q \rangle \cdot a_p^\dagger a_q \cdot \]

\[ + \frac{1}{4} \sum_{pqrs} \langle k_p k_q | v | k_r k_s \rangle \cdot a_p^\dagger a_q^\dagger a_s a_r \cdot \]

\[ + \frac{1}{36} \sum_{pqrsstu} \langle k_p k_q k_r | w | k_s k_t k_u \rangle \cdot a_p^\dagger a_q^\dagger a_r^\dagger a_u a_t a_s \cdot \]

Note: all two-body matrix elements are here assumed to be anti-symmetric
Second quantized normal-ordered Hamiltonian:

The vacuum energy:

\[ E_0 = \langle \Phi_0 | H | \Phi_0 \rangle \]

\[ = \sum_i \langle k_i | f | k_i \rangle + \frac{1}{2} \sum_{i,j} \langle k_i k_j | v | k_i k_j \rangle \]

\[ + \frac{1}{6} \sum_{i,j,k} \langle k_i k_j k_l | w | k_i k_j k_l \rangle \]

The normal-ordered one-body part is given by:

\[ \langle k_p | f | k_q \rangle = \langle k_p | t | k_q \rangle + \sum_i \langle k_p k_i | V_{NN} | k_q k_i \rangle \]

\[ + \frac{1}{2} \sum_{i,j} \langle k_p k_i k_j | V_{3NF} | k_q k_i k_j \rangle . \]

The normal-ordered two-body part is given by:

\[ \langle k_p k_q | v | k_r k_s \rangle = \langle k_p k_q | V_{NN} | k_r k_s \rangle \]

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

The normal-ordered three-body part is given by:

\[ \langle k_p k_q k_r | w | k_s k_t k_u \rangle = \langle k_p k_q k_r | V_{3NF} | k_s k_t k_u \rangle \]
Normal–ordered Hamiltonian at the two–body level (approximation)

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

Can we neglect the residual three-body term of the normal ordered Hamiltonian?
If so, we can re-use all the formalism developed for two-nucleon forces!
What’s the role of three-nucleon forces?

Contributions to binding of $^4$He. [Hagen, Papenbrock, Dean, Schwenk, Nogga, Wloch, Piecuch, PRC 76, 034302 (2007)]

Contributions to binding of $^4$He, $^{16}$O, and $^{40}$Ca. R. Roth et al, Phys Rev. Lett. 109, 052501 (2012)

Residual normal-ordered 3N term can safely be neglected in finite nuclei with forces from chiral EFT
Figure 5. States dominated by $p$-shell configurations for $^{10}$B, $^{11}$B, $^{12}$C, and $^{13}$C calculated at $N_{\text{max}} = 6$ using $\hbar \Omega = 15$ MeV (14 MeV for $^{10}$B). Most of the eigenstates are isospin $T=0$ or 1/2; the isospin label is explicitly shown only for states with $T=1$ or 3/2. The excitation energy scales are in MeV.

Anomalous Long Lifetime of Carbon-14

Anomalous long lifetime of Carbon-14 (used in carbon dating) explained by ab-initio CI calculations using NN and NNN forces. Three-nucleon forces yield suppression of transition matrix element.

Quenching of Gamow–Teller strength in nuclei

The Ikeda sum-rule

\[ S^N(GT) = S^N(GT^-) - S^N(GT^+) = 3(N - Z) \]

**Long-standing problem:** Experimental beta-decay strengths quenched compared to theoretical results.

\[ Q = \frac{S_{GT}(\omega_{top}) - S_{GT}(\omega_{top}^+)}{3(N - Z)} \]

Surprisingly large quenching \( Q \) (50%) obtained from \((p,n)\) experiments. The excitation energies were just above the giant Gamow-Teller resonance \( \sim 10-15\text{MeV} \) (Gaarde 1983).

- Measurement of GT strengths to high energies (Sasano et al 2009, Yako et al 2005), suggests a much smaller quenching \( Q = 0.88-0.92 \)

- Renormalizations of the Gamow-Teller operator?
- Missing correlations in nuclear wave functions?
- Model-space truncations?

- What does two-body currents and three-nucleon forces add to this long-standing problem?
Optimization of chiral interactions currents at NNLO

c_D - c_E fit of A=3 binding energies and the \(^3\text{H}\) half life at NNLO for chiral cutoffs \(\Lambda = 450,500,550\) MeV
\([c_D, c_E] = [0.043, -0.501]\)
Coupled cluster calculations of odd–odd nuclei

Diagonalize $\overline{H} = e^{-T} H_N e^T$ via a novel equation-of-motion technique:

$$R \equiv \sum_{ia} r^{a\dagger}_{i} p^a_{a} n_i + \frac{1}{4} \sum_{ijab} r^{ab\dagger}_{ij} p^a_{a} N^\dagger_{b} N^\dagger_{j} n_i$$

- Compute spectra of daughter nuclei as beta decays of mother nuclei
- Level densities in daughter nuclei increase slightly with 3NF
- Predict several states in neutron rich Fluorine
Quenching of Gamow–Teller strength in nuclei


Gamow-Teller matrix element:

\[ \hat{O}_{\text{GT}} = \hat{O}_{\text{GT}}^{(1)} + \hat{O}_{\text{GT}}^{(2)} = g_A^{-1} \sqrt{3\pi E_1^A} \]

The Gamow-Teller strength functions:

\[ S_- = \langle \Lambda | \hat{O}_\text{GT}^\dag \cdot \hat{O}_\text{GT} | \text{HF} \rangle \]
\[ S_+ = \langle \Lambda | \hat{O}_\text{GT} \cdot \hat{O}_\text{GT}^\dag | \text{HF} \rangle \]

- Quenching of the Ikeda sum rule in \(^{14}\text{C}\) and \(^{22,24}\text{O}\) for different cutoffs. \(q = 0.92...0.96\)
- Grey area is region which reproduce triton half-life
- The quenching \(q^2\) is about 8-16% and agrees with estimates in \(^{90}\text{Zr}\)
Anomalous life–time of $^{14}$C revisited


The life time of $^{14}$C depends in a complicated way on 3NFs, 2BCs and the energy of the first excited $1^+$ state in $^{14}$N.

- 3NFs decrease the transition matrix element significantly
- 2BC counter the effect of 3NFs to some degree.
- Note that 2BCs increases the strength to the first $1^+$ state in $^{14}$N but overall quenches the Ikeda sum rule.

$E_{1^+}^A$ varies between $5 \times 10^{-3}$ to $2 \times 10^{-2}$ which is more than one order of magnitude larger than the empirical value $\approx 6 \times 10^{-4}$ extracted from the 5700 a half life of $^{14}$C.
Computation of the Hoyle state

The Hoyle state (postulated in 1954) explains the abundance of $^{12}\text{C}$ in stars.

Nuclear Lattice Effective Field Theory Collaboration


**Is $^{28}$O a bound nucleus?**

### Experimental situation
- “Last” stable oxygen isotope $^{24}$O
- $^{25,26}$O unstable (Hoffman et al. 2008, Lunderberg et al. 2012)
- $^{28}$O not seen in experiments
- $^{31}$F exists (adding on proton shifts drip line by 6 neutrons!?)


Continuum shell model with HBUSD interaction predict $^{28}$O unbound. A. Volya and V. Zelevinsky PRL (2005)
Benchmarking different ab-initio methods in the oxygen chain

Calculations based on chiral NN and 3NF forces. Continuum not taken into account

Evolution of shell structure in neutron rich Calcium

1949 Nobel Prize 1963

Nuclear Shell Structure

N/Z

• How do shell closures and magic numbers evolve towards the dripline?
• What are the underlying mechanisms and how do we identify new shell structure?

Magic nuclei determine the structure of entire regions of the nuclear chart
Including the effects of 3NFs (approximation!)
[J.W. Holt, Kaiser, Weise, PRC 79, 054331 (2009); Hebeler & Schwenk, PRC 82, 014314 (2010)]

3NFs as in-medium effective two-nucleon forces
Integration of Fermi sea of symmetric nuclear matter: $k_F$

**Parameters:** For Calcium we use $k_F = 0.95$ fm$^{-1}$, $c_E = 0.735$, $c_D = -0.2$ from binding energy of $^{40}$Ca and $^{48}$Ca (The parameters $c_D$, $c_E$ differ from values proposed for light nuclei)
Neutron rich calcium isotopes


Gallant et al., PRL 2012
Wienholtz Nature 2013

Erler et al., Nature 486, 509 (2012)
Spectra and shell evolution in Calcium isotopes

RIKEN [Steppenbeck, Nature 502, 207 (2013)]

Will be measured at RIKEN?
1. Our prediction for excited $5/2^-$ and $1/2^-$ states in $^{53}$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

Chiral NN + 3NFs overbind and give to small radii in medium mass and heavy nuclei

S. Binder et al. PLB 736 (2014) 119-123
Chiral NN + 3NFs and the problem of saturation


Significant overbinding is found in calcium and nickel isotopes using chiral NN and 3NFs


Energy differences such as two-neutron separation energies are better reproduced
Accurate nuclear binding energies and radii from a chiral interaction

Our solution: simultaneous optimization of NN and 3NFs with input from selected nuclei up to $A \sim 25$ (NNLO$_{sat}$). A. Ekström et al, Phys. Rev. C 91, 051301(R) (2015)
Simultaneous optimization of NN and 3NFs

Traditional approach:
- Fit interactions nucleon by nucleon
- Fit to NN scattering data up to \( \sim 350 \text{MeV} \)
- \( c_E \) and \( c_D \) fit to \( A=3,4 \)

Our approach:
- Simultaneous optimization of NN and 3NFs
- Fit to few-body data and BEs/radii in nuclei with \( A \sim 25 \)

Not new: GFMC with AV18 and Illinois-7 are fit to 23 levels in nuclei with \( A < 10 \)
Charge densities of $^{40,48}\text{Ca}$ with NNLO$_{\text{sat}}$

Effects of 3NFs in neutron matter and neutron star structure

Auxiliary Field Diffusion Quantum Monte Carlo calculations of neutron matter and equation of state with Argonne and Urbana/Illinois NN + NNN forces. Constraining the maximum mass and radius of neutron stars and the nuclear symmetry energy

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Gandolfi, Carlson, Reddy, PRC 85, 032801 (2012)

adapted from
Steiner, Gandolfi, PRL 108, 081102 (2012)
Benchmark calculations of neutron matter

Comparison with continuum coupled-cluster method [Baardsen et al., PRC (2013)]

Comparison with auxiliary field diffusion Monte Carlo and Minnesota potential
Role of particle–hole excitations in nucleonic matter

Particle-hole and non-linear terms in CCD are small in pure neutron matter.
MBPT2/CCD$_{\text{ladd}}$/CCD results agree within 500keV/A. Indicates that PNM is perturbative.
Particle-hole and non-linear terms play a larger role in symmetric nuclear matter.
CCD$_{\text{ladd}}$ and CCD results differ by up to 1.5MeV/A around saturation density.
Three nucleon force (3NF) and regulator dependence


Nonlocal form of 3NF [Epelbaum et al. PRC (2002)]: Cutoff is in Jacobi momenta
Λ=500 MeV: $c_D=-2$, $c_E=-0.791$ (from $A=3$ binding energies)

Local form of 3NF [Navratil, Few Body Syst. (2007)]: Cutoff is in the momentum transfer
Λ=500 MeV: $c_D=-0.39$, $c_E=-0.389$ (from $A=3,4$ binding and $^3$H $\tau_{1/2}$ (Gazit, Navratil, & Quaglioni)
Λ=400 MeV: $c_D=-0.39$, $c_E=-0.27$ (adjusted to $^4$He)
Neutron matter is perturbative (small differences between MBPT2 and coupled clusters)
3NFs act repulsively in neutron matter and NNLO\textsubscript{opt}
Error bands from variation of cutoffs and level of sophistication in treating 3NFs
Symmetric nuclear matter

Nuclear matter is not perturbative (larger differences between MBPT2 and coupled clusters)

3NFs act repulsively in nuclear matter and NNLO$_{\text{opt}}$

Regularization scheme dependence of 3NF; sensitivity to sophistication in treatment of 3NFs
Understanding the 3NF at NNLO

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

נשים $c_D$ and $c_E$ not sufficient to simultaneously bind light nuclei and nuclear matter

Cutoff dependent fraction of residual 3NF contribution to MBPT2 energy per particle in SNM around saturation density.

Local regulators converge slower than non-local regulators
Question: Your favorite physics friend comes to you and suggests to determine the effects of the three-body force on the structure of your favorite nucleus. You reply

1. Let’s do this. This will put us on the fast track to Stockholm.

2. This is difficult to disentangle. But it can be done in a three-body system such as $^3\text{H}$.

3. Which interaction are you looking at?

4. Answers 2 & 3 are correct.
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The size and form of three-body forces depends on the cutoff, and the chosen renormalization scheme. Different schemes (“implementations of the EFT at order $n$”) yield predictions that expected to agree within the error estimate $(Q/\Lambda)^{n+1}$. Only the sum of interactions can be probed.