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

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#### 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<sub>sat</sub>)
- 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



## Reach of realistic ab initio calculations

(realistic meaning that binding energies are within 5% of experimental values)



### Energy scales and relevant degrees of freedom



Chiral symmetry is broken Pion is Nambu-Goldstone boson Tool: Chiral effective field theory

Effective theories provide us with model independent approaches to atomic nuclei

Key: Separation of scales

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.  $\Delta$ -resonance, "polarization effects", ...), and unconstrained high-momentum modes.



The question is not: Do three-body forces enter the description? **The (only) question is: How large are three-body forces?**  Other tidal effects cannot be included in the two-body interaction! Three-body force unavoidable for point masses.



## **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-poin term
- 3. Short-ranged three-nucleon contact

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### **Green's function Monte Carlo computations**

Demonstration that light nuclei can be build from scratch



Energy (MeV)

## Non-uniqueness of three-nucleon forces



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 <sup>4</sup>He would require four-nucleon forces!

## Nuclear forces from chiral effective field theory

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



- 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

Glazek, & Wilson, PRD 48 (1993) 5863; 49 (1994) 4214; Wegner, Ann. Phys. 3 (1994) 77; Perry, Bogner, & Furnstahl (2007)

**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** 

$$\frac{d\hat{H}(s)}{ds} = \left[\eta(s), \hat{H}(s)\right] \quad \text{with} \quad \eta(s) \equiv \frac{dU(s)}{ds} U^{\dagger}(s) = -\eta^{\dagger}(s)$$

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

$$\eta(s) = \left[\widehat{T}, \widehat{H}(s)\right]$$

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

$$e^{-\eta}\hat{H}e^{\eta} = \hat{H} + \left[\hat{H},\eta\right] + \frac{1}{2!}\left[\left[\hat{H},\eta\right],\eta\right] + \dots$$

## SRG evolution of a chiral potential

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



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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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.
- 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 <sup>3</sup>H and <sup>4</sup>He with induced and initial 3NF



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

A: In <sup>4</sup>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:

$$\begin{split} H_N &= \sum_{pq} \langle \mathbf{k}_p | f | \mathbf{k}_q \rangle : a_p^{\dagger} a_q : \\ &+ \frac{1}{4} \sum_{pqrs} \langle \mathbf{k}_p \mathbf{k}_q | v | \mathbf{k}_r \mathbf{k}_s \rangle : a_p^{\dagger} a_q^{\dagger} a_s a_r : \\ &+ \frac{1}{36} \sum_{pqrstu} \langle \mathbf{k}_p \mathbf{k}_q \mathbf{k}_r | w | \mathbf{k}_s \mathbf{k}_t \mathbf{k}_u \rangle : a_p^{\dagger} a_q^{\dagger} a_r^{\dagger} a_u a_t a_s : \end{split}$$

Note: all two-body matrix elements are here assumed to be anti-symmetric

#### Second quantized normal-ordered Hamiltonian:

The vacuum energy:

$$E_{0} = \langle \Phi_{0} | H | \Phi_{0} \rangle$$
  
=  $\sum_{i} \langle \mathbf{k}_{i} | f | \mathbf{k}_{i} \rangle + \frac{1}{2} \sum_{i,j} \langle \mathbf{k}_{i} \mathbf{k}_{j} | v | \mathbf{k}_{i} \mathbf{k}_{j} \rangle$   
+  $\frac{1}{6} \sum_{ijk} \langle \mathbf{k}_{i} \mathbf{k}_{j} \mathbf{k}_{l} | w | \mathbf{k}_{i} \mathbf{k}_{j} \mathbf{k}_{l} \rangle$ 

The normal-ordered one-body part is given by

$$\begin{aligned} \langle \mathbf{k}_p | f | \mathbf{k}_q \rangle &= \langle \mathbf{k}_p | t | \mathbf{k}_q \rangle + \sum_i \langle \mathbf{k}_p \mathbf{k}_i | V_{\mathrm{NN}} | \mathbf{k}_q \mathbf{k}_i \rangle \\ &+ \frac{1}{2} \sum_{ij} \langle \mathbf{k}_p \mathbf{k}_i \mathbf{k}_j | V_{\mathrm{3NF}} | \mathbf{k}_q \mathbf{k}_i \mathbf{k}_j \rangle \,. \end{aligned}$$

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

$$\langle \mathbf{k}_{p} \mathbf{k}_{q} | v | \mathbf{k}_{r} \mathbf{k}_{s} \rangle = \langle \mathbf{k}_{p} \mathbf{k}_{q} | V_{NN} | \mathbf{k}_{r} \mathbf{k}_{s} \rangle$$

$$+ \sum_{i} \langle \mathbf{k}_{p} \mathbf{k}_{q} \mathbf{k}_{i} | V_{3NF} | \mathbf{k}_{i} \mathbf{k}_{r} \mathbf{k}_{s} \rangle$$

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

$$\langle \mathbf{k}_p \mathbf{k}_q \mathbf{k}_r | w | \mathbf{k}_s \mathbf{k}_t \mathbf{k}_u \rangle = \langle \mathbf{k}_p \mathbf{k}_q \mathbf{k}_r | V_{3NF} | \mathbf{k}_s \mathbf{k}_t \mathbf{k}_u \rangle$$

## Normal-ordered Hamiltonian at the two-body level (approximation)

$$\begin{split} H_N &= \sum_{pq} \langle \mathbf{k}_p | f | \mathbf{k}_q \rangle : a_p^{\dagger} a_q : \\ &+ \frac{1}{4} \sum_{pqrs} \langle \mathbf{k}_p \mathbf{k}_q | v | \mathbf{k}_r \mathbf{k}_s \rangle : a_p^{\dagger} a_q^{\dagger} a_s a_r : \\ &+ \frac{1}{36} \sum_{pqrstu} \langle \mathbf{k}_p \mathbf{k}_q \mathbf{k}_r | w | \mathbf{k}_s \mathbf{k}_t \mathbf{k}_u \rangle : a_p^{\dagger} a_q^{\dagger} a_r^{\dagger} a_u a_t a_s : \end{split}$$

Can we neglect the residual three-body term of the normal ordered Hamiltonian? If so, we can re-use all the formalism developed for twonucleon forces!

### What's the role of three-nucleon forces?



Residual normal-ordered 3N term can safely be neglected in finite nuclei with forces from chiral EFT

Contributions to binding of <sup>4</sup>He. [Hagen, Papenbrock, Dean, Schwenk, Nogga, Wloch, Piecuch, PRC 76, 034302 (2007)]

Contributions to binding of <sup>4</sup>He, <sup>16</sup>O, and <sup>40</sup>Ca. R. Roth et al, Phys Rev. Lett. 109, 052501 (2012)



# Light nuclei from chiral NN and 3NFs with no-core shell model



Figure 5. States dominated by *p*-shell configurations for <sup>10</sup>B, <sup>11</sup>B, <sup>12</sup>C, and <sup>13</sup>C calculated at  $N_{\text{max}} = 6$  using  $\hbar \Omega = 15$  MeV (14 MeV for <sup>10</sup>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.

P. Navratil et al., Phys. Rev. Lett. 99, 042501 (2007), nucl-th/0701038. Review: Navratil, Quaglioni, Stetcu, Barrett, J. Phys. G 36, 083101 (2009); arXiv:0904.0463.

#### **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.



z	120 0.40 MeV P	130 8.58 MS €p: 100.00% €: 100.00%	140 70.620 S €: 100.00%	150 122.24 S €: 100.00%	160 STABLE 99.757%	170 STABLE 0.038%	180 STABLE 0.205%	190 26.88 S β-: 100.00%	200 13.51 S β-: 100.00%
7	11N 0.83 MeV P: 100.00%	12N 11.000 MS €: 100.00%	13N 9.965 M €: 100.00%	14N STABLE 99.636%	15N STABLE 0.364%	16N 7.13 S β-: 100.00% β-α: 1.2E-3%	17N 4.173 S β-: 100.00% β-n: 95.1%	18N 620 MS β-: 100.00% β-α: 12.20%	19N 336 MS β-: 100.00% β-n: 41.80%
6	10C 19.308 S €: 100.00%	11C 20.334 M € 100.00%	12C STABLE 98.93%	13C STABLE 1.07%	14C 5700 Υ β-: 100.00%	15C 2.449 S β-: 100.00%	16C 0.747 S β-: 100.00% β-n: 99.00%	17C 193 MS β-: 100.00% β-n: 32.00%	18C 92 MS β-: 100.00% β-n: 31.50%
5	9B 0.54 KeV 2a: 100.00% P: 100.00%	10B STABLE 19.9%	11B STABLE 80.1%	12B 20.20 MS β-: 100.00% B3A: 1.58%	13B 17.33 MS β-: 100.00%	14B 12.5 MS β-: 100.00%	15B 9.93 MS β-: 100.00% β-n: 93.60%	16B <190 PS N	17B 5.08 MS β-: 100.00% β-n: 63.00%
4	8Be 5.57 eV α: 100.00%	9Be STABLE 100.%	10Be 1.387E+6 Υ β-:100.00%	11Be 13.81 S β-: 100.00% β-α: 3.1%	12Be 21.49 MS β-:100.00% β-n≤ 1.00%	13Be 2.7E-21 S N	14Be 4.35 MS β-: 100.00% β-n: 81.00%	15Be <200 NS N	16Be <200 NS 2N
	4	5	6	7	8	9	10	11	N



shell Maris, Vary, Navrátil, Ormand, Nam, Dean, Phys. Rev. Lett. 106, 202502 (2011)

#### 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.



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

What does two-body currents and three-nucleon forces add to this long-standing problem?

#### **Optimization of chiral interactions currents at NNLO**

A. Ekström, G. Jansen, K. Wendt et al, PRL 113 262504 (2014)



#### **Coupled cluster calculations of odd-odd nuclei**

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

$$R \equiv \sum_{ia} r_i^a p_a^{\dagger} n_i + \frac{1}{4} \sum_{ijab} r_{ij}^{ab} p_a^{\dagger} N_b^{\dagger} N_j n_i$$



- 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

A. Ekström, G. Jansen, K. Wendt et al, PRL 113 262504 (2014)

Gamow-Teller matrix element:

 $\hat{O}_{\rm GT} \equiv \hat{O}_{\rm GT}^{(1)} + \hat{O}_{\rm GT}^{(2)} \equiv g_4^{-1} \sqrt{3\pi} E_1^A$ 

The Gamow-Teller strength functions:

$$S_{-} = \langle \Lambda | \overline{\hat{O}_{\text{GT}}^{\dagger}} \cdot \overline{\hat{O}_{\text{GT}}} | \text{HF} \rangle$$
$$S_{+} = \langle \Lambda | \overline{\hat{O}_{\text{GT}}} \cdot \overline{\hat{O}_{\text{GT}}^{\dagger}} | \text{HF} \rangle$$



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

## Anomalous life-time of <sup>14</sup>C revisited

A. Ekström, G. Jansen, K. Wendt et al, PRL 113 262504 (2014)



 $E_1^A$  varies between 5x10<sup>-3</sup> to 2x10<sup>-2</sup> which is more than one order of magnitude larger than the empirical value ~6x10<sup>-4</sup> extracted from the 5700 a half life of <sup>14</sup>C The life time of <sup>14</sup>C depends in a complicated way on 3NFs, 2BCs and the energy of the first excited 1<sup>+</sup> state in <sup>14</sup>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<sup>+</sup> state in <sup>14</sup>N but overall quenches the Ikeda sum rule.

## **Computation of the Hoyle state**

The Hoyle state (postulated in 1954) explains the abundance of <sup>12</sup>C in stars.

Nuclear Lattice Effective Field Theory Collaboration



Epelbaum, Krebs, Lee, Meißner, Phys. Rev. Lett. 106, 192501 (2011)



Epelbaum, Krebs, Lähde, Lee, Meißner, Phys. Rev. Lett. 109, 252501 (2012)

## Is <sup>28</sup>O a bound nucleus?

<sup>23</sup>Ne

22F

21O

<sup>20</sup>N

19C

<sup>22</sup>Ne

21F

20O

19N

18C

<sup>24</sup>Ne

23F

22O

21N

20C

#### **Experimental situation**

- "Last" stable oxygen isotope <sup>24</sup>O
- <sup>25,26</sup>O unstable (Hoffman et al 2008, Lunderberg et al 2012)
- <sup>28</sup>O not seen in experiments
- <sup>31</sup>F exists (adding on proton shifts drip line by 6 neutrons!?)





Continuum shell model with HBUSD interaction predict <sup>28</sup>O unbound. A. Volya and V. Zelevinsky PRL (2005)

Shell model (sd shell) with monopole corrections based on threenucleon force predicts 2<sup>nd</sup> O as last stable isotope of oxygen. [Otsuka, Suzuki, Holt, Schwenk, Akaishi, PRL (2010), arXiv:0908.2607]



Hebeler, Holt, Menendez, Schwenk, Ann. Rev. Nucl. Part. Sci. in press (2015)

### **Evolution of shell structure in neutron rich Calcium**



How do shell closures and magic numbers evolve towards the dripline?

 What are the underlying mechanisms and how do we identify new shell structure?



#### **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<sub>F</sub>

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

## **Neutron rich calcium isotopes**

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



#### Spectra and shell evolution in Calcium isotopes



#### Spectra and shell evolution in Calcium isotopes



Continuum coupling crucial for level ordering

#### 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

H. Hergert et al Phys. Rev. C 90, 041302 (2014)



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



## 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<sub>sat</sub>). 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 ~350MeV
- cE and cD 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 ~ 25

Not new: GFMC with AV18 and Illinois-7 are fit to 23 levels in nuclei with A <10

## Charge density and negative parity states of <sup>16</sup>O



A. Ekström, G. Jansen, K. Wendt et al, PRC 91, 051301 2015

## Charge densities of <sup>40,48</sup>Ca with NNLO<sub>sat</sub>



# 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



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<sub>ladd</sub>/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<sub>ladd</sub> and CCD results differ by up to 1.5MeV/A around saturation density.

# Three nucleon force (3NF) and regulator dependence

van Kolck, Phys. Rev. C 49, 2934 (1994); Epelbaum et al., Phys. Rev. C 66, 064001 (2002)



**Nonlocal form of 3NF** [Epelbaum et al. PRC (2002)]: Cutoff is in Jacobi momenta  $\Lambda$ =500 MeV: c<sub>D</sub>=-2, c<sub>E</sub>=-0.791 (from A=3 binding energies)

**Local form of 3NF** [Navratil, Few Body Syst. (2007)]: Cutoff is in the momentum transfer  $\Lambda$ =500 MeV:  $c_D$ =-0.39,  $c_E$ =-0.389 (from A=3,4 binding and <sup>3</sup>H  $\tau_{1/2}$  (Gazit, Navratil, & Quaglioni)  $\Lambda$ =400 MeV:  $c_D$ =-0.39,  $c_E$ =-0.27 (adjusted to <sup>4</sup>He)

## **Neutron matter**



Neutron matter is perturbative (small differences between MBPT2 and coupled clusters 3NFs act repulsively in neutron matter and NNLO<sub>opt</sub> 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<sub>opt</sub>

<sup>(C)</sup> Regularization scheme dependence of 3NF; sensitivity to sophistication in treatment of 3NFs

## **Understanding the 3NF at NNLO**



5% error bands for saturation  $k_{\rm f}$  , E/N and binding energy of  $^3{\rm H}$ 

 $\textcircledinom{O}{O}$  Variation of  $c_D$  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 nonlocal regulators

## Nuclear matter from chiral NN and 3NFs



Nuclear matter saturation curves for NNLO<sub>sat</sub> and other interactions. Hagen et al (2014); Carbone et al (2013); Coraggio et al 2014; Hebeler *et al* PRC 2011. 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.
- This is difficult to disentangle. But it can be done in a three-body system such as <sup>3</sup>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**.