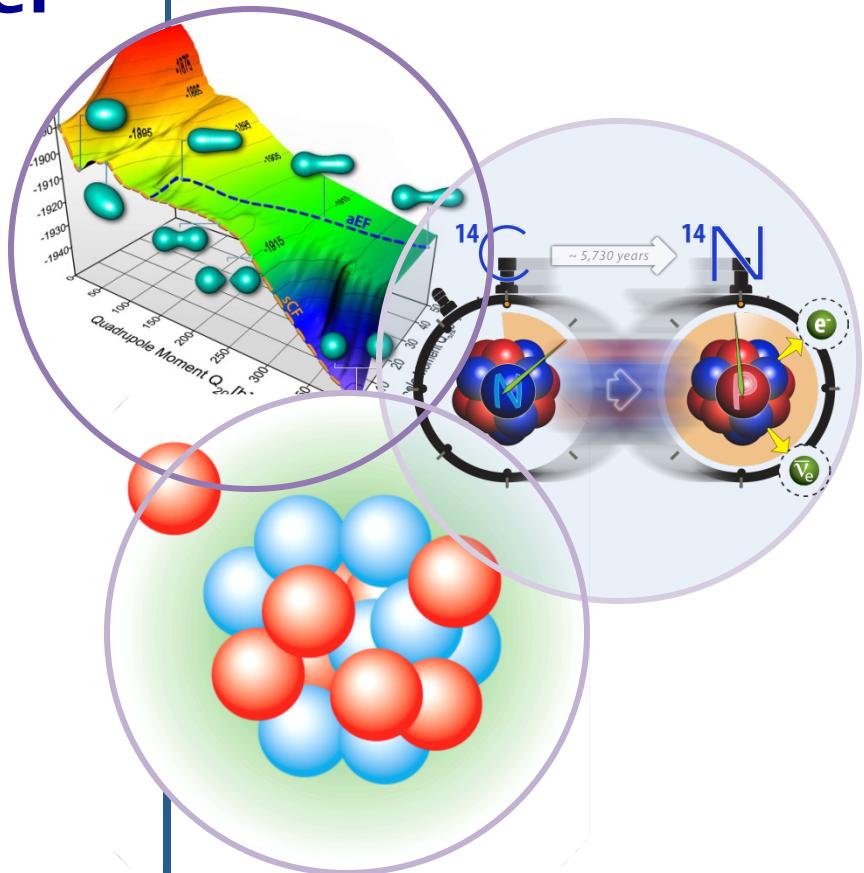


Ab-initio structure and the role of three-nucleon forces in nucleonic matter

Gaute Hagen (ORNL)



Lecture 3, TALENT school

Outline

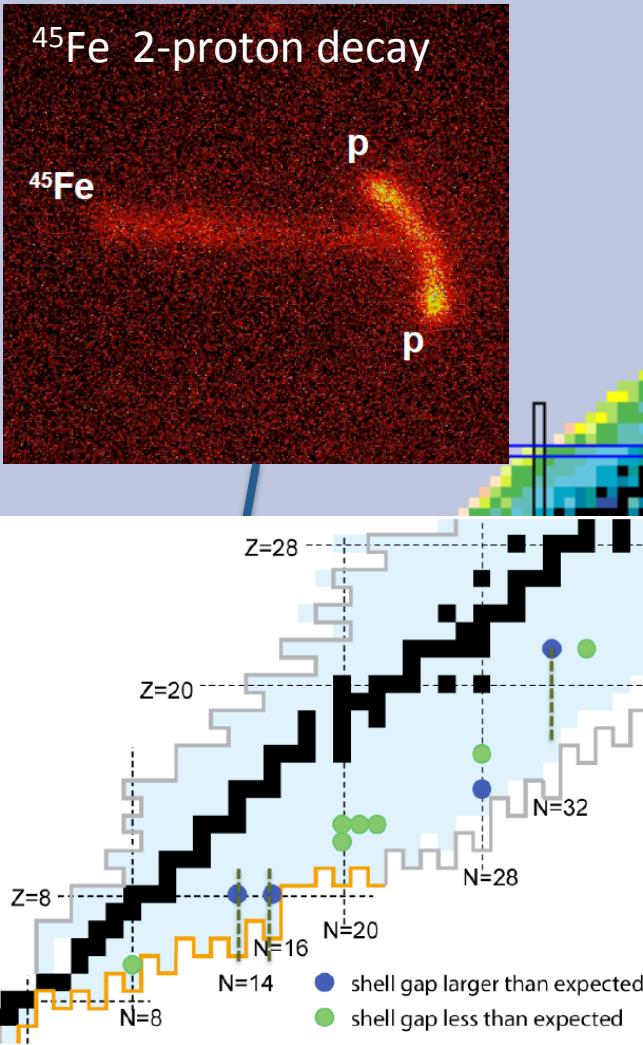
- Nuclei across the chart and status of *ab initio* calculations with three-nucleon forces (3NFs)
- Chiral effective field theory – Why 3NFs?
 - SRG evolution of chiral interactions
- Role of 3NFs on spectra of light nuclei
- Role of 3NFs on weak decays and quenching of axial coupling in nuclei
- The 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 $A \sim 25$
 - Accurate binding energies and radii from a chiral interaction (NNLO_{sat})
- Impact of 3NFs in infinite nucleonic matter

Nuclei across the chart

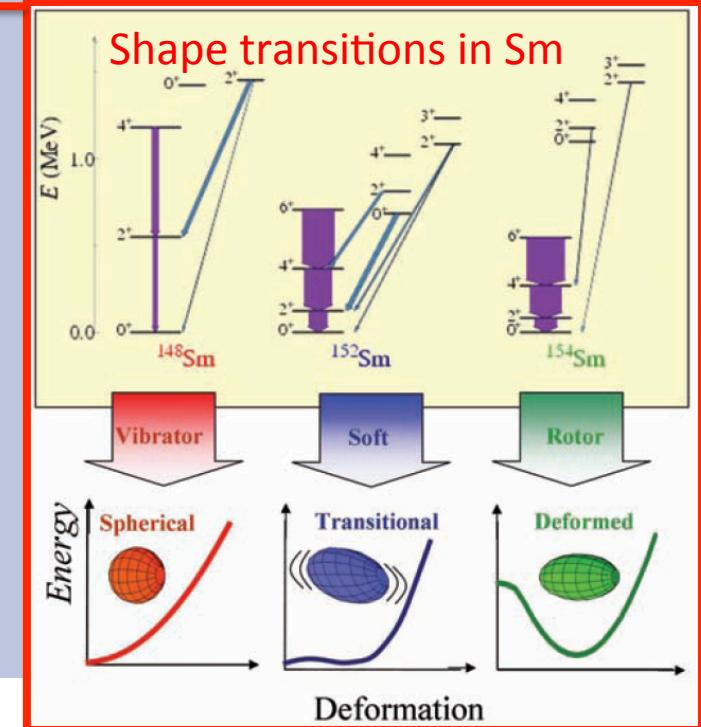
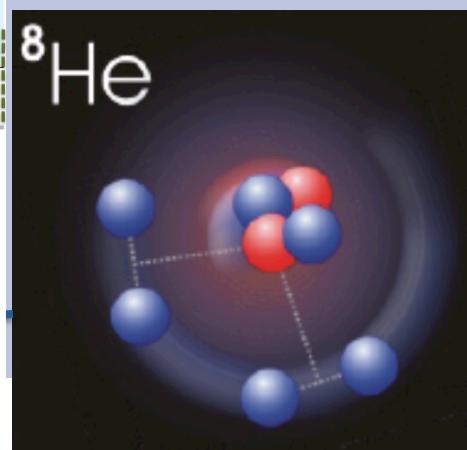
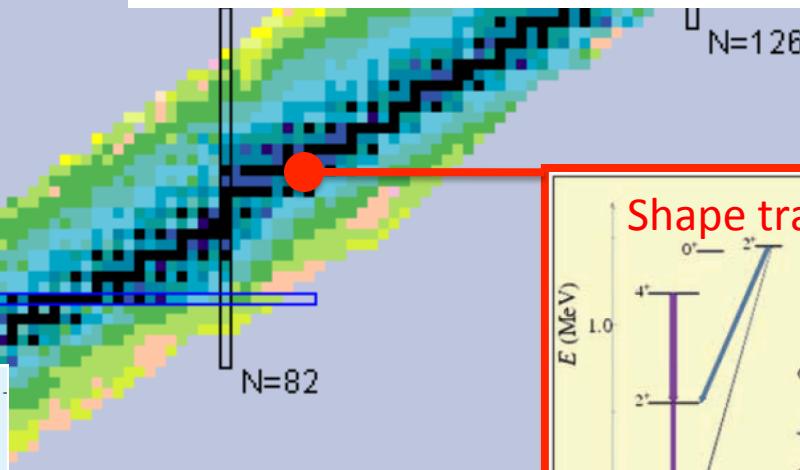
118 chemical elements (94 naturally found on Earth)
288 stable (primordial) isotopes



Thousands of short-lived isotopes – many with interesting properties

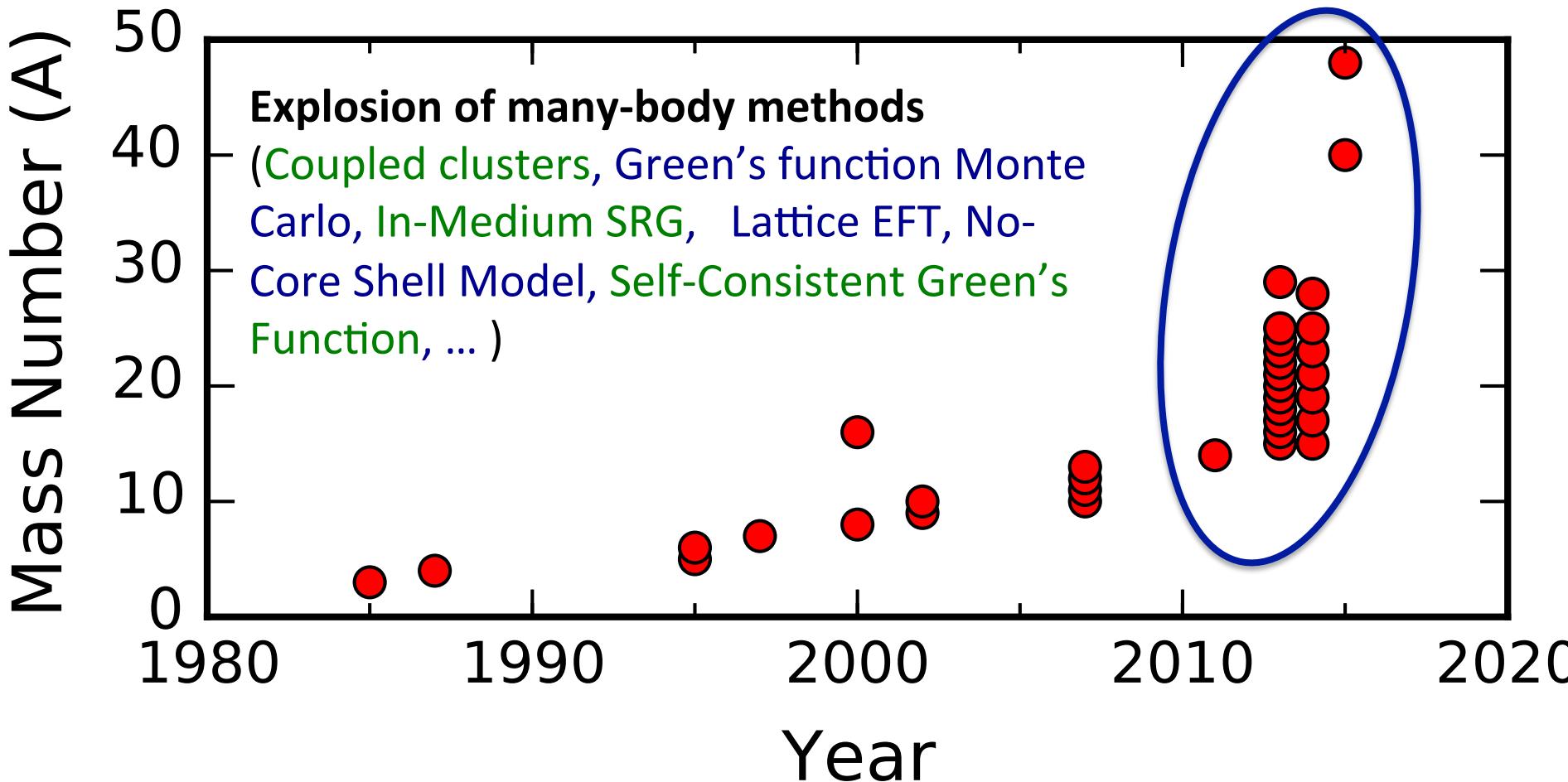


large isospin magnifies unknown physics
clustering behavior
novel evolution in structure



Reach of realistic *ab initio* calculations

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



Energy scales and relevant degrees of freedom

Physics of Hadrons

Degrees of Freedom



quarks, gluons

Energy (MeV)

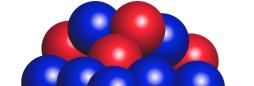
940
neutron mass

constituent quarks



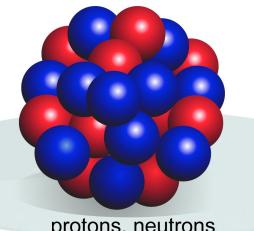
baryons, mesons

ab initio



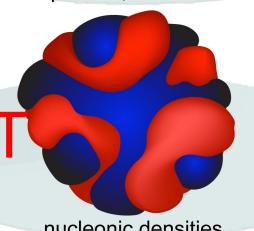
baryons, mesons

CI



protons, neutrons

DFT



nucleonic densities
and currents

collective
models

collective coordinates

Energy or Resolution



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

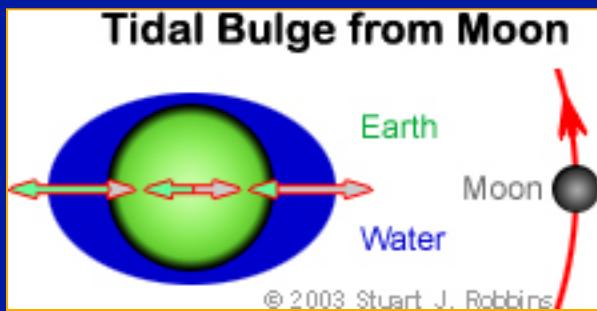
Three-nucleon forces – Why?



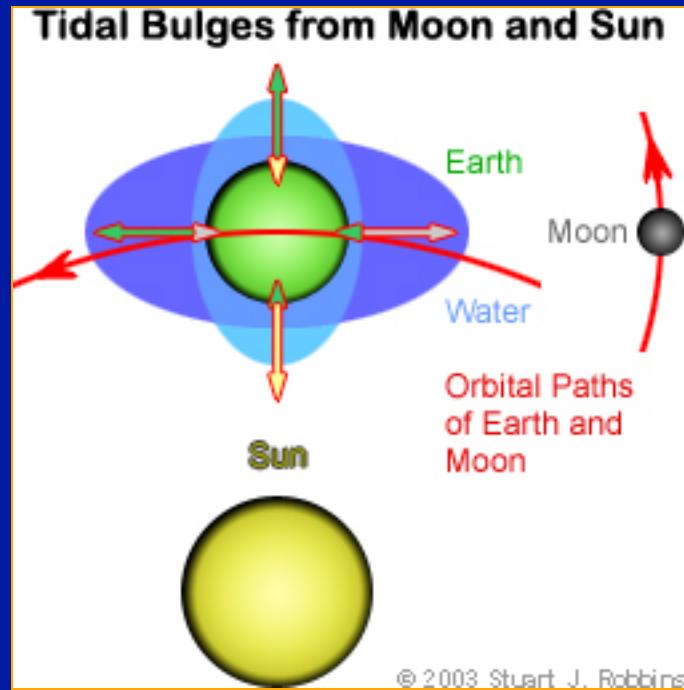
- Nucleons are not point particles (i.e. not elementary).
- We neglected some internal degrees of freedom (e.g. Δ -resonance, “polarization effects”, ...), and unconstrained high-momentum modes.

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

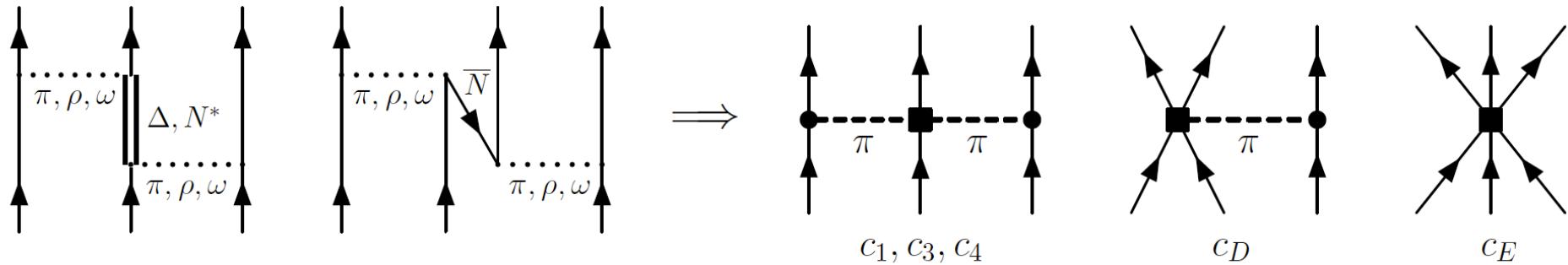


Figure 23: Eliminating degrees of freedom leads to three-body forces.
(taken from Bogner, Furnstahl, Schwenk, arXiv:0912.3688)

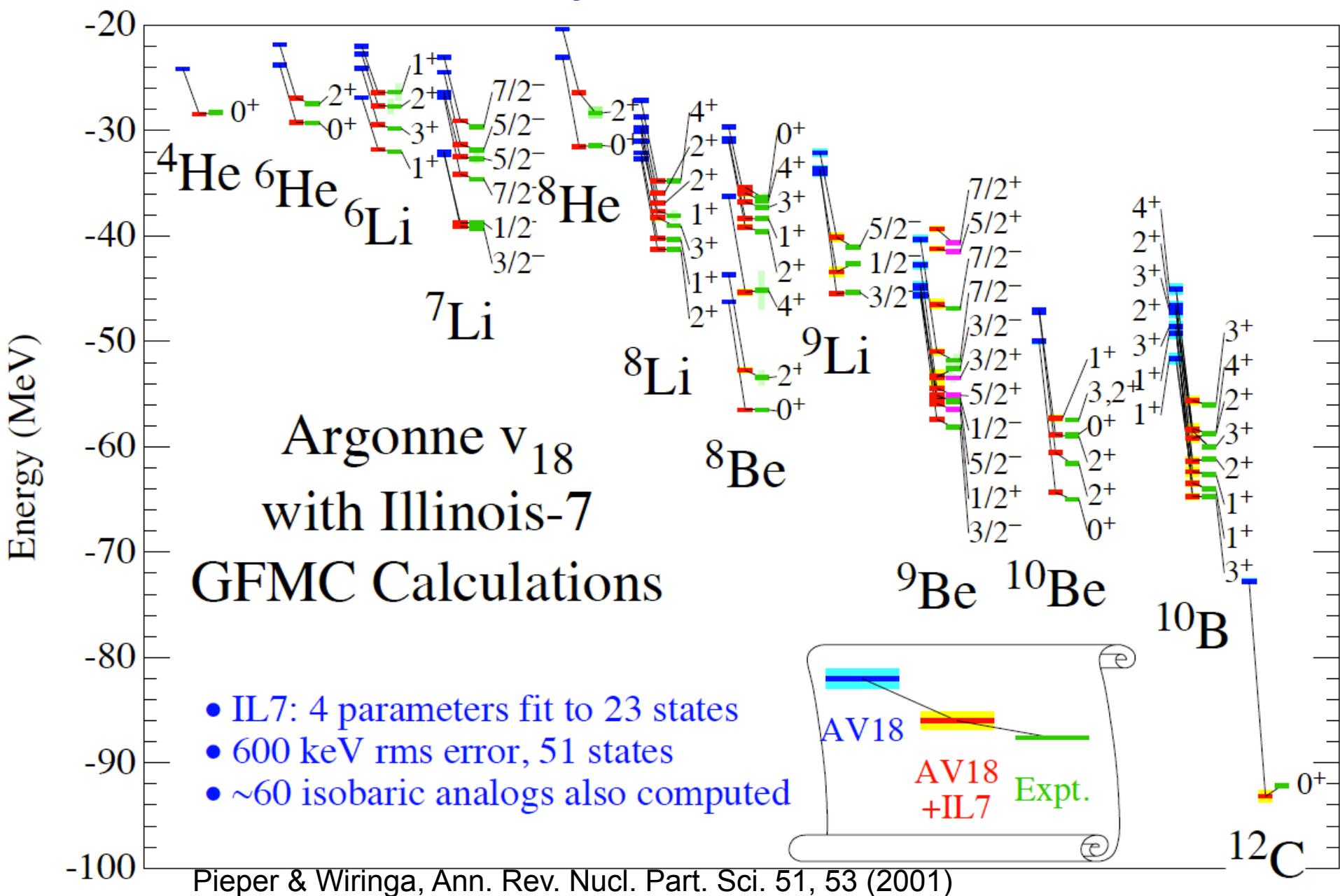
Leading three-nucleon force

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

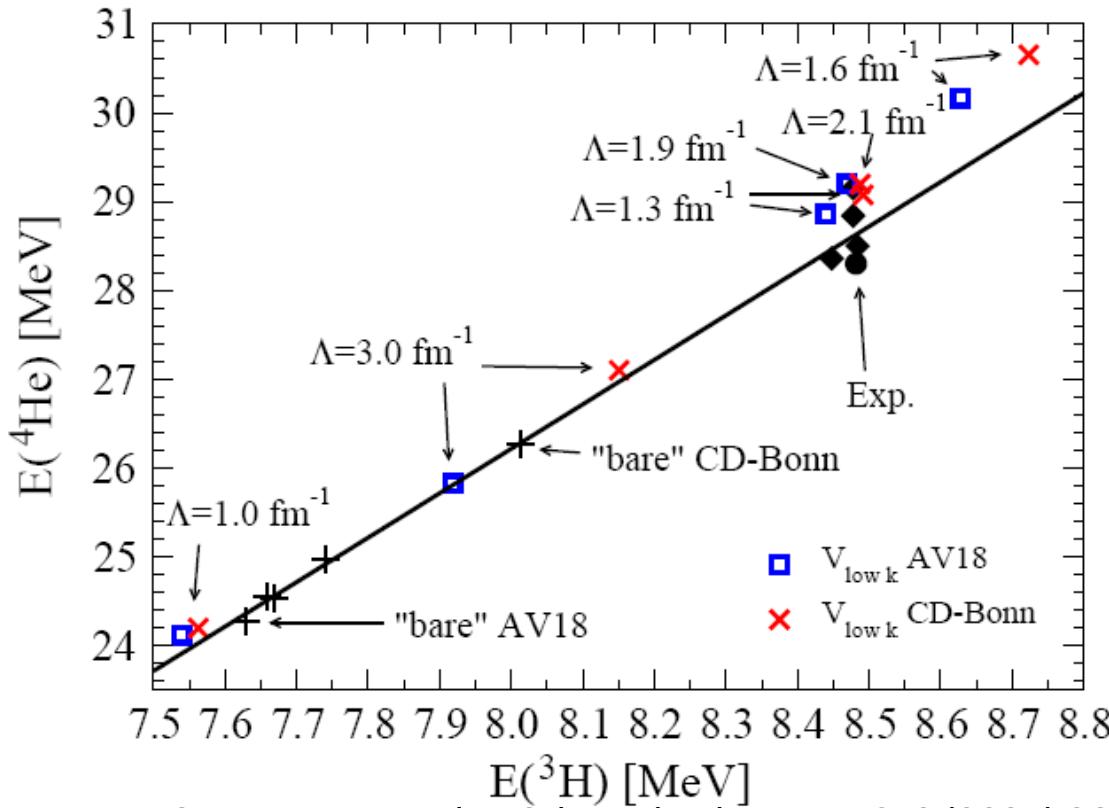
The question is not: Do three-body forces enter the description?
The (only) question is: How large are three-body forces?

Green's function Monte Carlo computations

Demonstration that light nuclei can be build from scratch



Non-uniqueness of three-nucleon forces



A. Nogga, S. K. Bogner, and A. Schwenk, Phys.Rev. C70 (2004) 061002

As cutoff Λ is varied, motion along “Tjon line”.

Addition of Λ -dependent three-nucleon force yields (almost) agreement with experiment. **Q: What's missing?**

A: The complete description of ^4He would require four-nucleon forces!

Nuclear forces from chiral effective field theory

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

	NN	3N	4N
LO $\mathcal{O}\left(\frac{Q^0}{\Lambda^0}\right)$			—
NLO $\mathcal{O}\left(\frac{Q^2}{\Lambda^2}\right)$		—	—
N ² LO $\mathcal{O}\left(\frac{Q^3}{\Lambda^3}\right)$		—	—
N ³ LO $\mathcal{O}\left(\frac{Q^4}{\Lambda^4}\right)$		+ ...	+ ...

- 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

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

Evolution equation

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

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

$$\eta(s) = [\hat{T}, \hat{H}(s)]$$

yields scale-dependent potential that becomes more and more diagonal

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

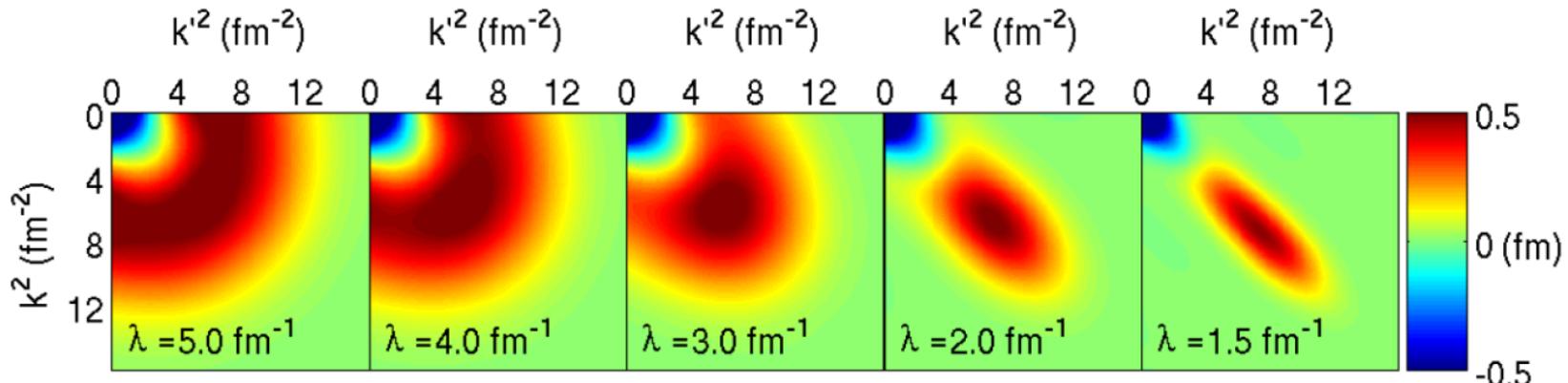
Note: Baker-Campbell-Hausdorff expansion implies that SRG of 2-body force generates many-body forces

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

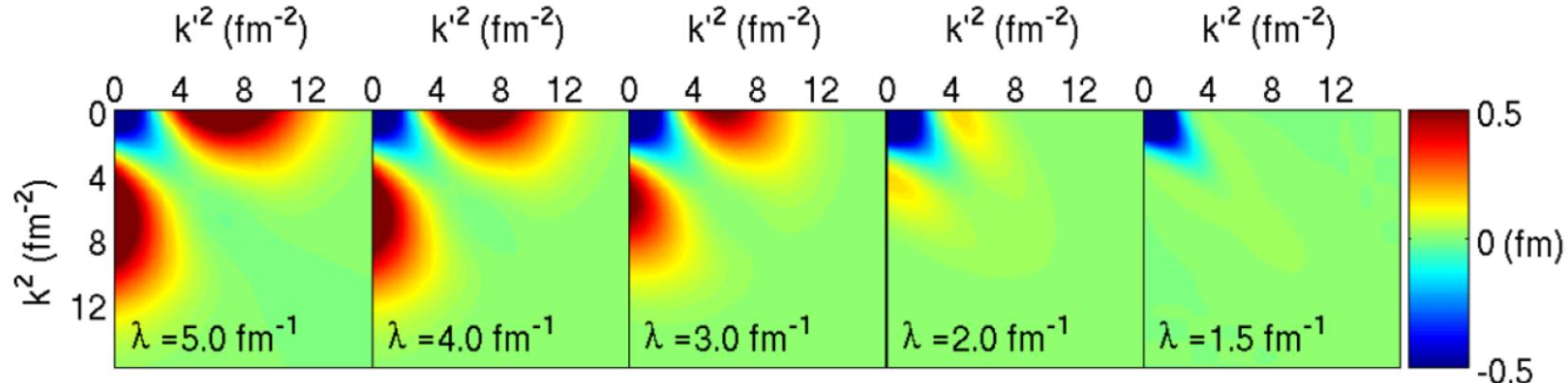
SRG evolution of a chiral potential

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

1S_0 from N³LO (500 MeV) of Entem/Machleidt



3S_1 from N³LO (500 MeV) of Entem/Machleidt



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 and compare.
2. Check how results in the A-body system depend on the cutoff/evolution parameter

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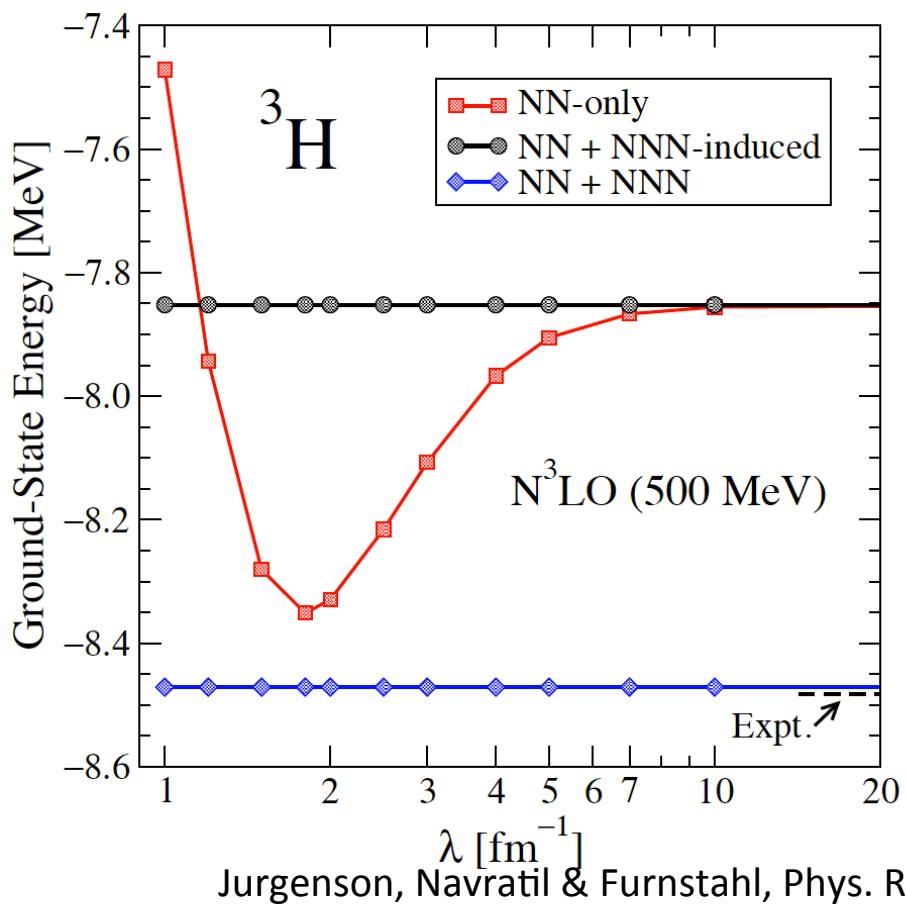
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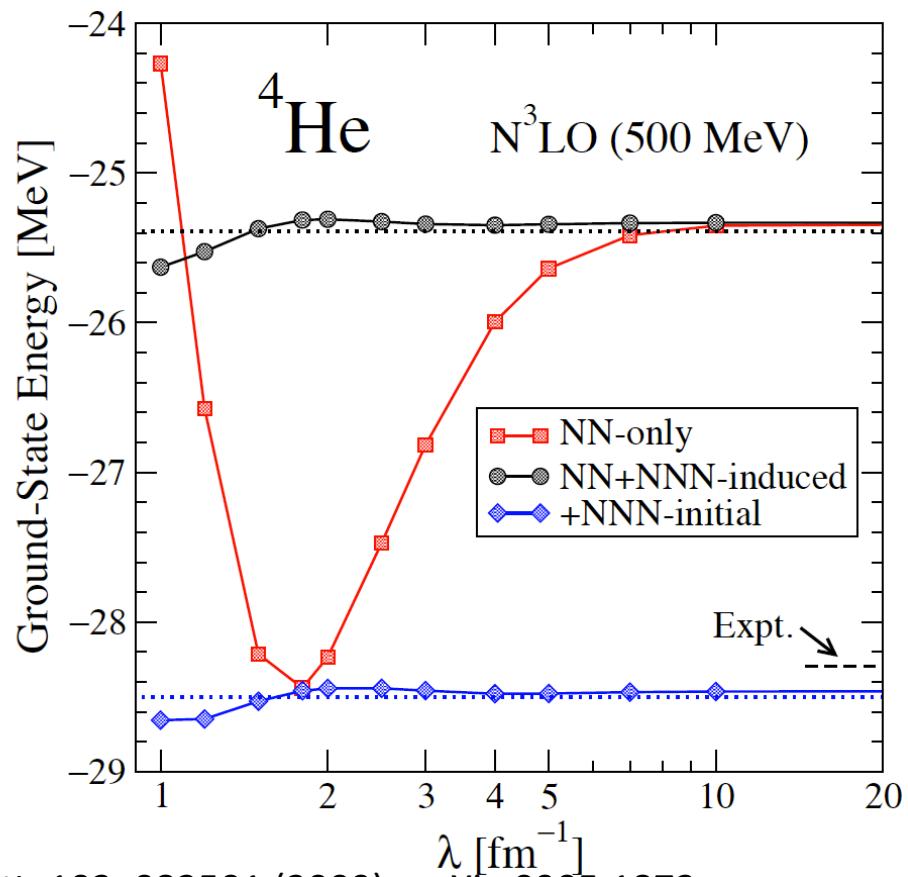
1. Perform a computation with and without SRG and compare.
2. Check how results in the A-body system depend on the cutoff/evolution parameter ✓

Of course: Any observable other than the Hamiltonian also needs to be transformed.

Solution of ^3H and ^4He with induced and initial 3NF



Jurgenson, Navratil & Furnstahl, Phys. Rev. Lett. 103, 082501 (2009), arXiv:0905.1873

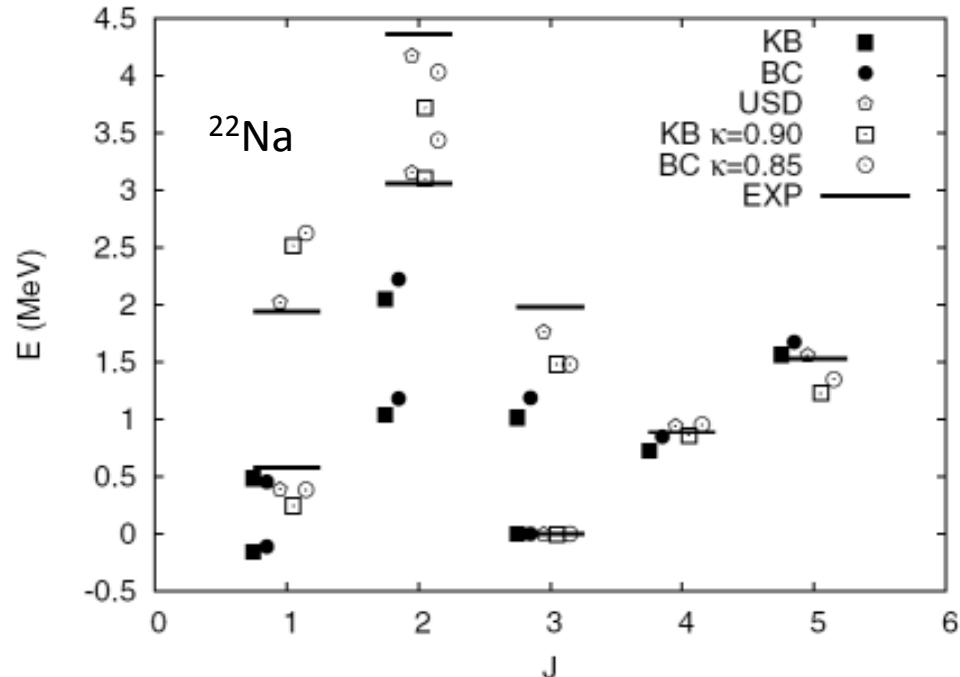


Q: What is the effect of (omitted) 4NF and forces of even higher rank?

A: In ^4He , (short ranged) 4NF yield about 200 keV (see energies at small momentum)

Note: This is consistent with deviation from experiment!

What's the role of three-nucleon forces?

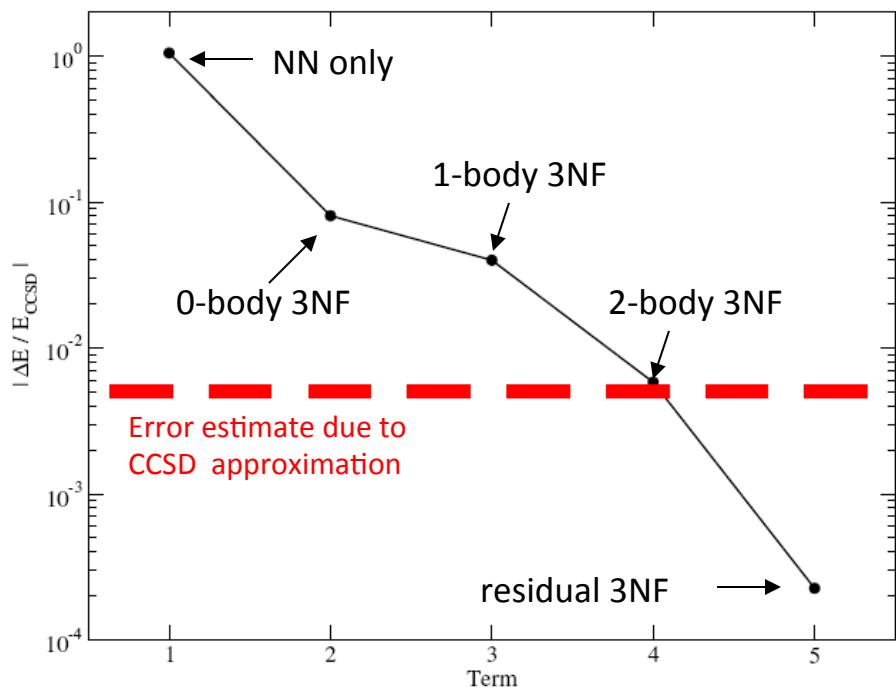


Contributions to binding of ^4He . [Hagen, TP, Dean, Schwenk, Nogga, Wloch, Piecuch, PRC 76, 034302 (2007); Roth et al, arXiv:1112.0287]

$$\begin{aligned} \hat{H}_3 = & \frac{1}{6} \sum_{ijk} \langle ijk | ijk \rangle + \frac{1}{2} \sum_{ijpq} \langle ijp | ijq \rangle \{ \hat{a}_p^\dagger \hat{a}_q \} \\ & + \frac{1}{4} \sum_{ipqrs} \langle ipq | irs \rangle \{ \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_s \hat{a}_r \} + \hat{h}_3, \end{aligned}$$



Monopole shifts from 3NF as density-dependent NN force.
[A.Zuker, PRL 90, 42502 (2003)]



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

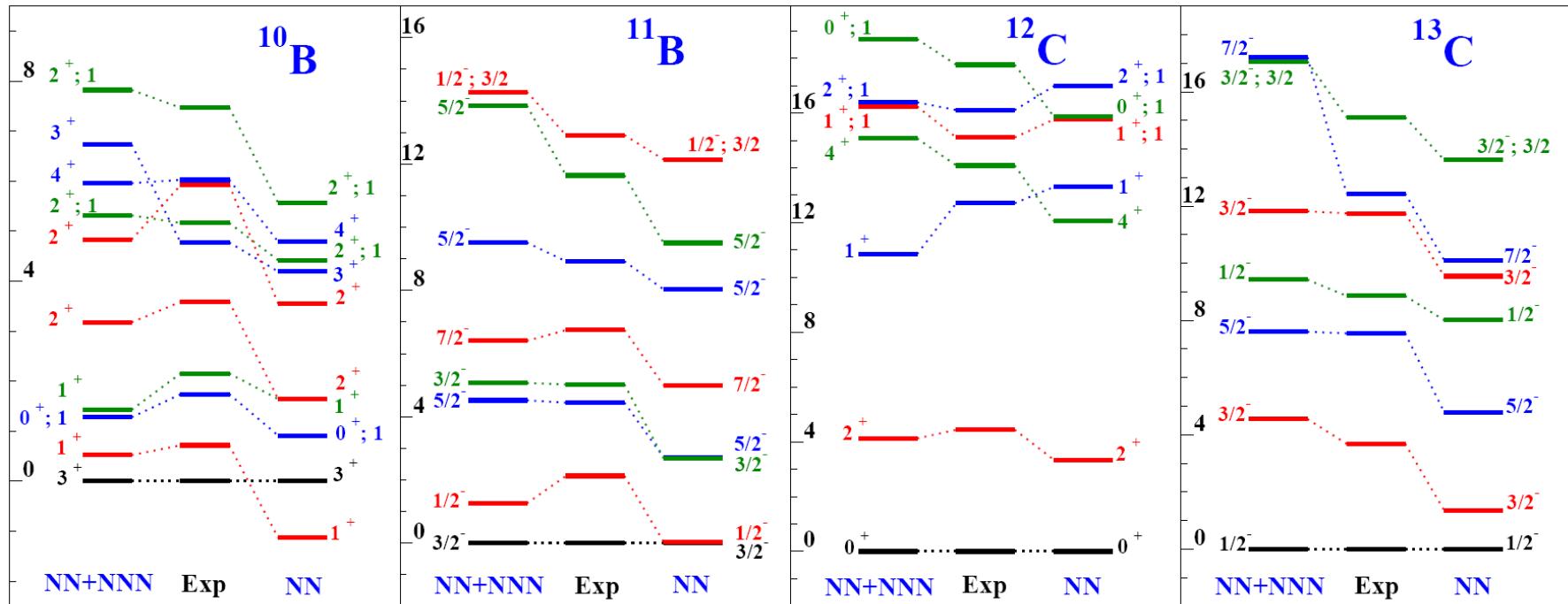


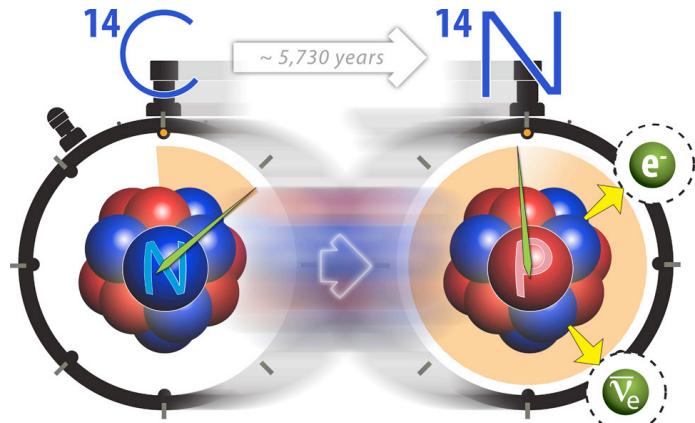
Figure 5. States dominated by p -shell configurations for ^{10}B , ^{11}B , ^{12}C , and ^{13}C calculated at $N_{\max} = 6$ using $\hbar\Omega = 15$ MeV (14 MeV for ^{10}B). Most of the eigenstates are isospin $T=0$ or $1/2$, the isospin label is explicitly shown only for states with $T=1$ or $3/2$. The excitation energy scales are in MeV.

P. Navratil et al., Phys. Rev. Lett. 99, 042501 (2007), nucl-th/0701038.

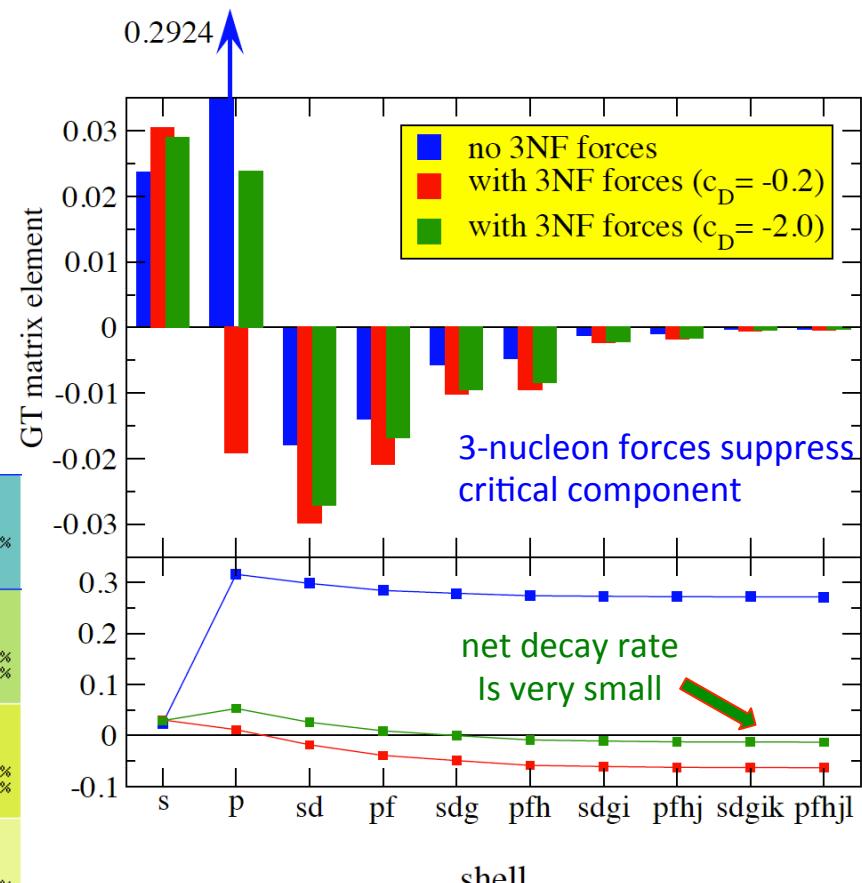
Review: Navratil, Quaglioni, Stetcu, Barrett, J. Phys. G 36, 083101 (2009); arXiv:0904.0463.

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 $\epsilon_p: 100.00\%$ $\epsilon: 100.00\%$	140 70.620 S $\epsilon: 100.00\%$	150 122.24 S $\epsilon: 100.00\%$	160 STABLE 99.757%	170 STABLE 0.038%	180 STABLE 0.205%	190 26.88 S $\beta^-: 100.00\%$	200 13.51 S $\beta^-: 100.00\%$
7	11N 0.83 MeV $P: 100.00\%$	12N 11.000 MS $\epsilon: 100.00\%$	13N 9.965 M $\epsilon: 100.00\%$	14N STABLE 99.636%	15N STABLE 0.364%	16N 7.18 S $\beta^-: 100.00\%$ $\beta^-n: 1.2E-3$	17N 4.173 S $\beta^-: 100.00\%$ $\beta^-n: 95.1\%$	18N 620 MS $\beta^-: 100.00\%$ $\beta^-n: 12.20\%$	19N 336 MS $\beta^-: 100.00\%$ $\beta^-n: 41.80\%$
6	10C 19.308 S $\epsilon: 100.00\%$	11C 20.334 M $\epsilon: 100.00\%$	12C STABLE 98.98%	13C STABLE 1.07%	14C 5700 Y $\beta^-: 100.00\%$	15C 2.449 S $\beta^-: 100.00\%$	16C 0.747 S $\beta^-: 100.00\%$ $\beta^-n: 99.00\%$	17C 193 MS $\beta^-: 100.00\%$ $\beta^-n: 32.00\%$	18C 92 MS $\beta^-: 100.00\%$ $\beta^-n: 31.50\%$
5	9B 0.54 KeV $2\alpha: 100.00\%$ $P: 100.00\%$	10B STABLE 19.9%	11B STABLE 80.1%	12B 20.20 MS $\beta^-: 100.00\%$ $\beta^-n: 1.58\%$	13B 17.33 MS $\beta^-: 100.00\%$	14B 12.5 MS $\beta^-: 100.00\%$	15B 9.93 MS $\beta^-: 100.00\%$ $\beta^-n: 93.60\%$	16B <190 PS N	17B 5.08 MS $\beta^-: 100.00\%$ $\beta^-n: 63.00\%$
4	8Be 5.57 eV $\alpha: 100.00\%$	9Be STABLE 100%	10Be 1.387E+6 Y $\beta^-: 100.00\%$	11Be 13.81 S $\beta^-: 100.00\%$ $\beta^-n: 3.1\%$	12Be 21.49 MS $\beta^-: 100.00\%$ $\beta^-n: 1.00\%$	13Be 2.7E-21 S N	14Be 4.35 MS $\beta^-: 100.00\%$ $\beta^-n: 81.00\%$	15Be <200 NS N	16Be <200 NS $2N$
	4	5	6	7	8	9	10	11	N



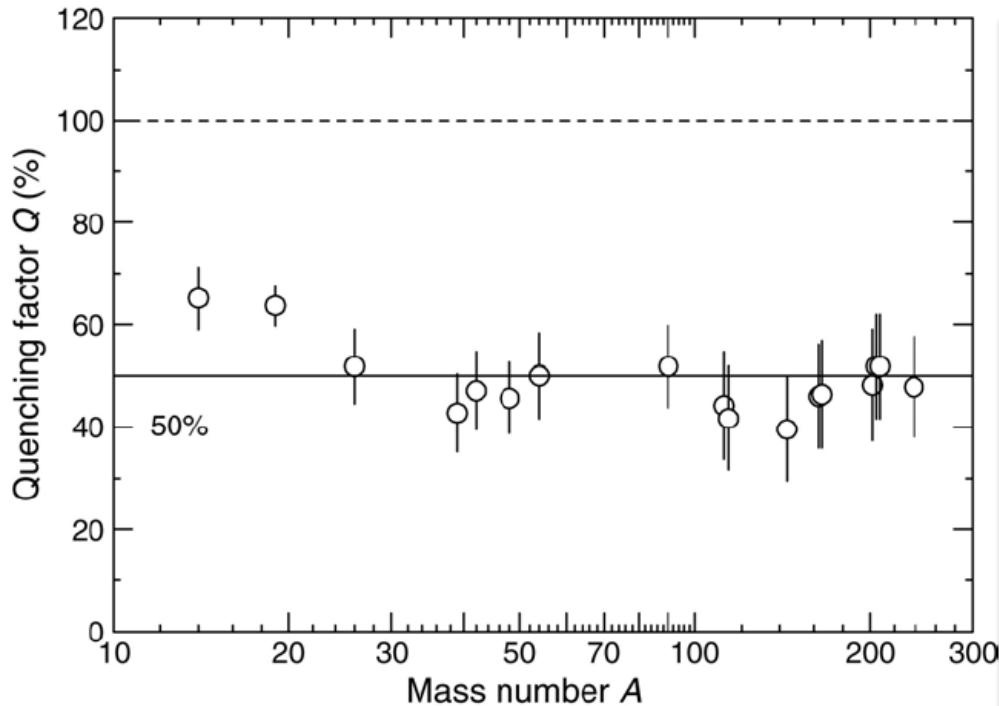
shell
Maris, Vary, Navrátil, Ormand, Nam, Dean,
Phys. Rev. Lett. 106, 202502 (2011)

Quenching of Gamow-Teller strength in nuclei

The Ikeda sum-rule $S^N(\text{GT}) = S^N(\text{GT}^-) - S^N(\text{GT}^+) = 3(N - Z)$

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

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



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

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



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

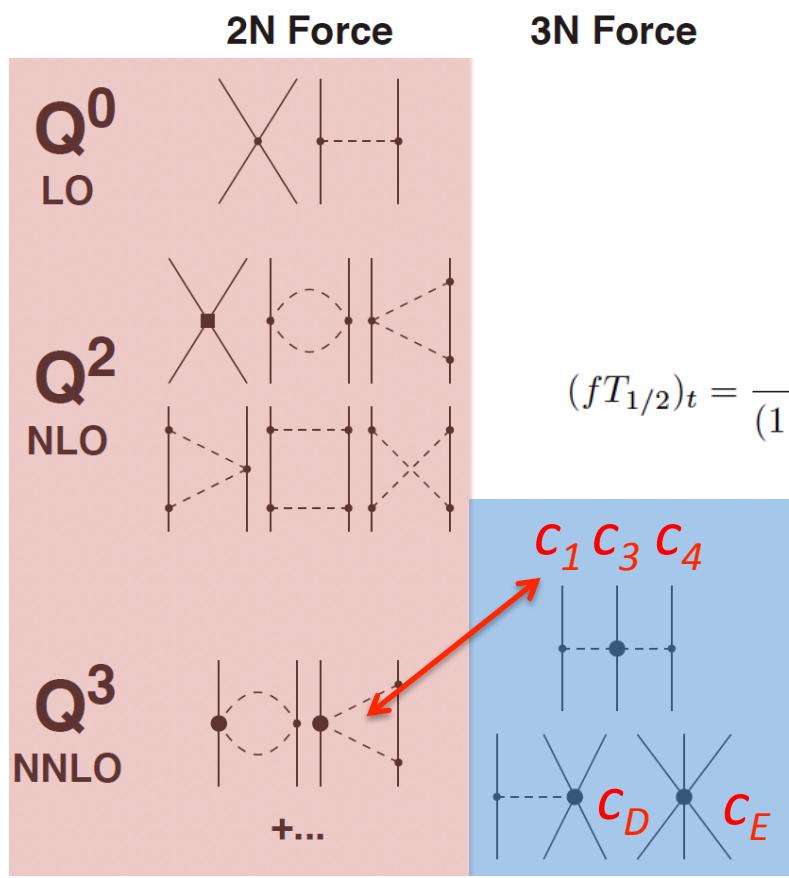


- **What does two-body currents and three-nucleon forces add to this long-standing problem?**

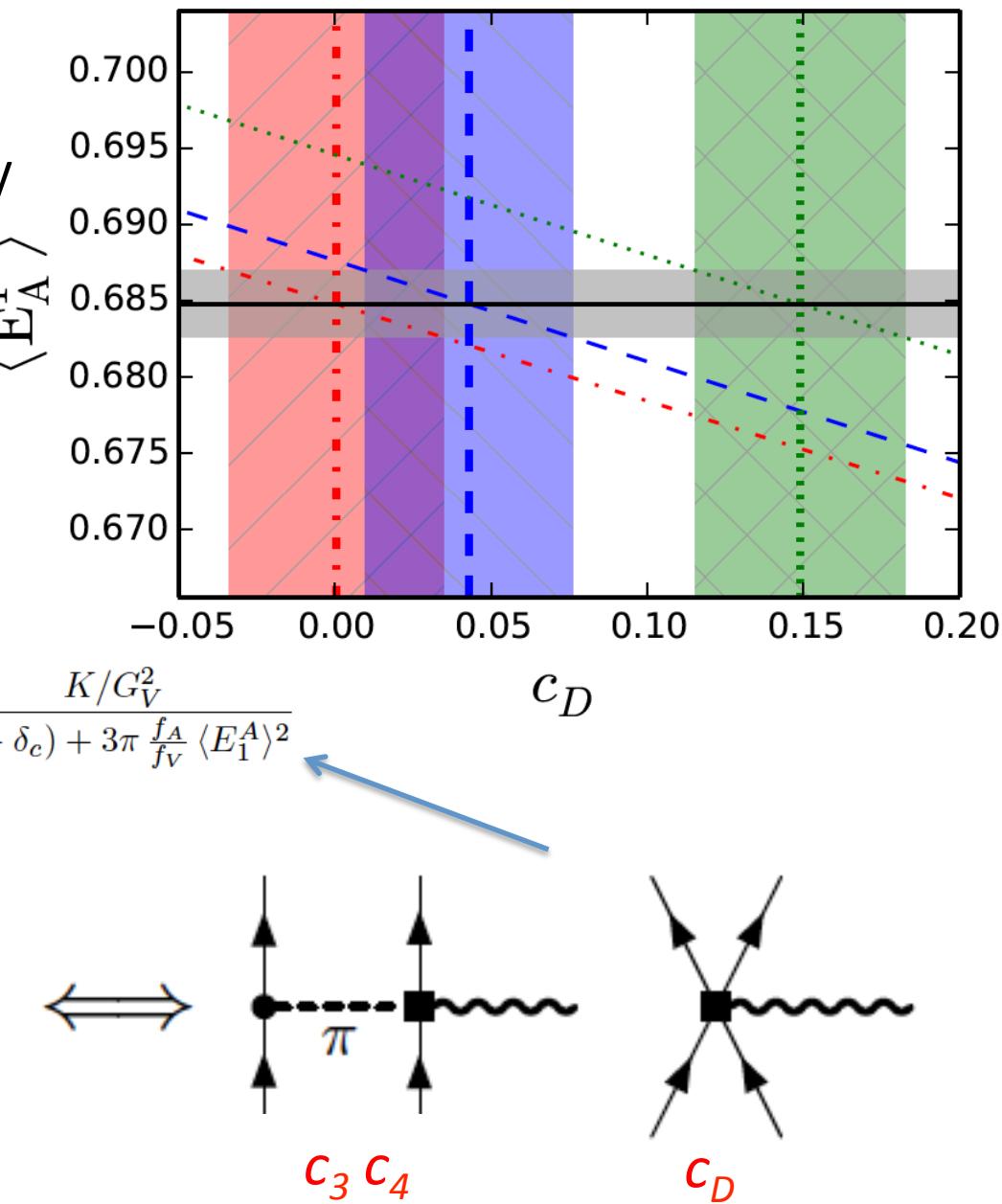
Optimization of chiral interactions currents at NNLO

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

$c_D - c_E$ fit of A=3 binding energies
and the ^3H half life at NNLO for
chiral cutoffs $\Lambda = 450, 500, 550$ MeV
 $[c_D, c_E] = [0.043, -0.501]$



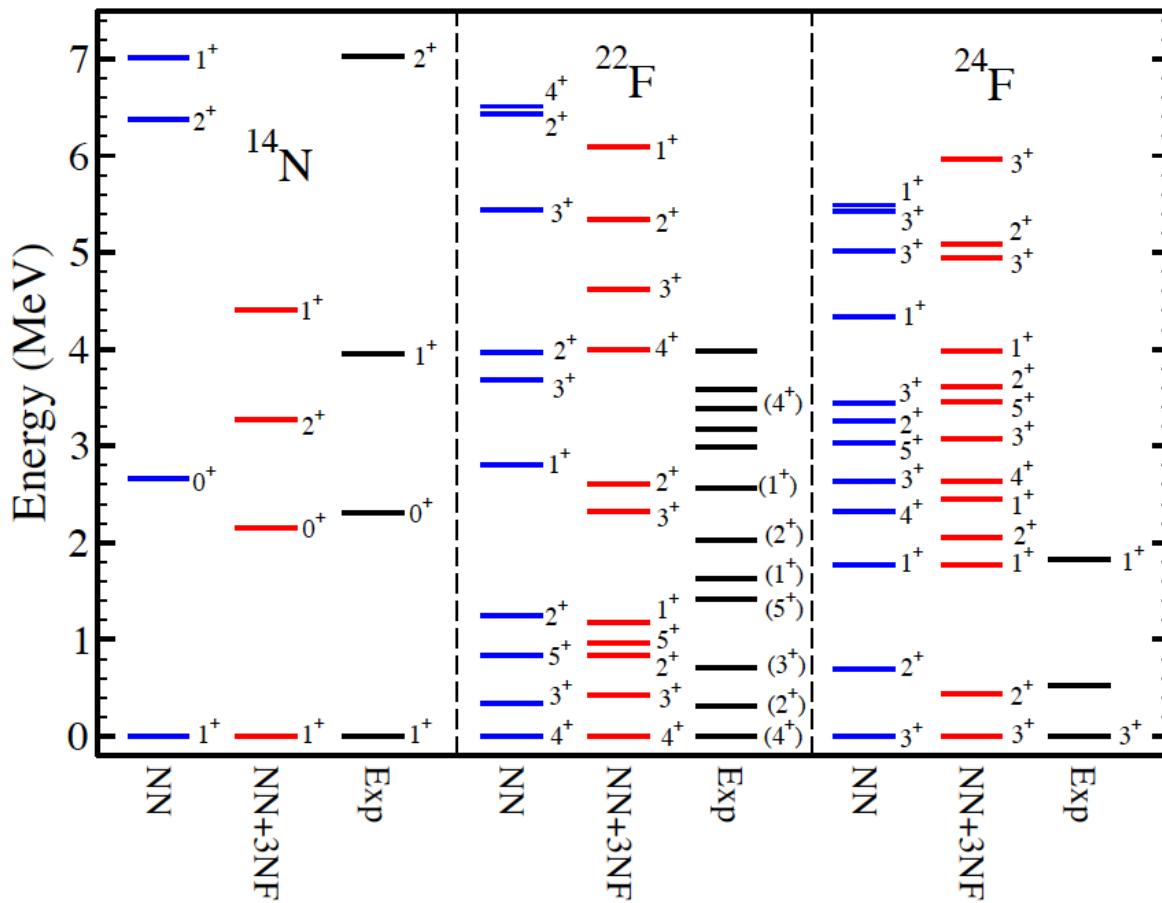
$$(fT_{1/2})_t = \frac{K/G_V^2}{(1 - \delta_c) + 3\pi \frac{f_A}{f_V} \langle E_1^A \rangle^2} c_D$$



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)

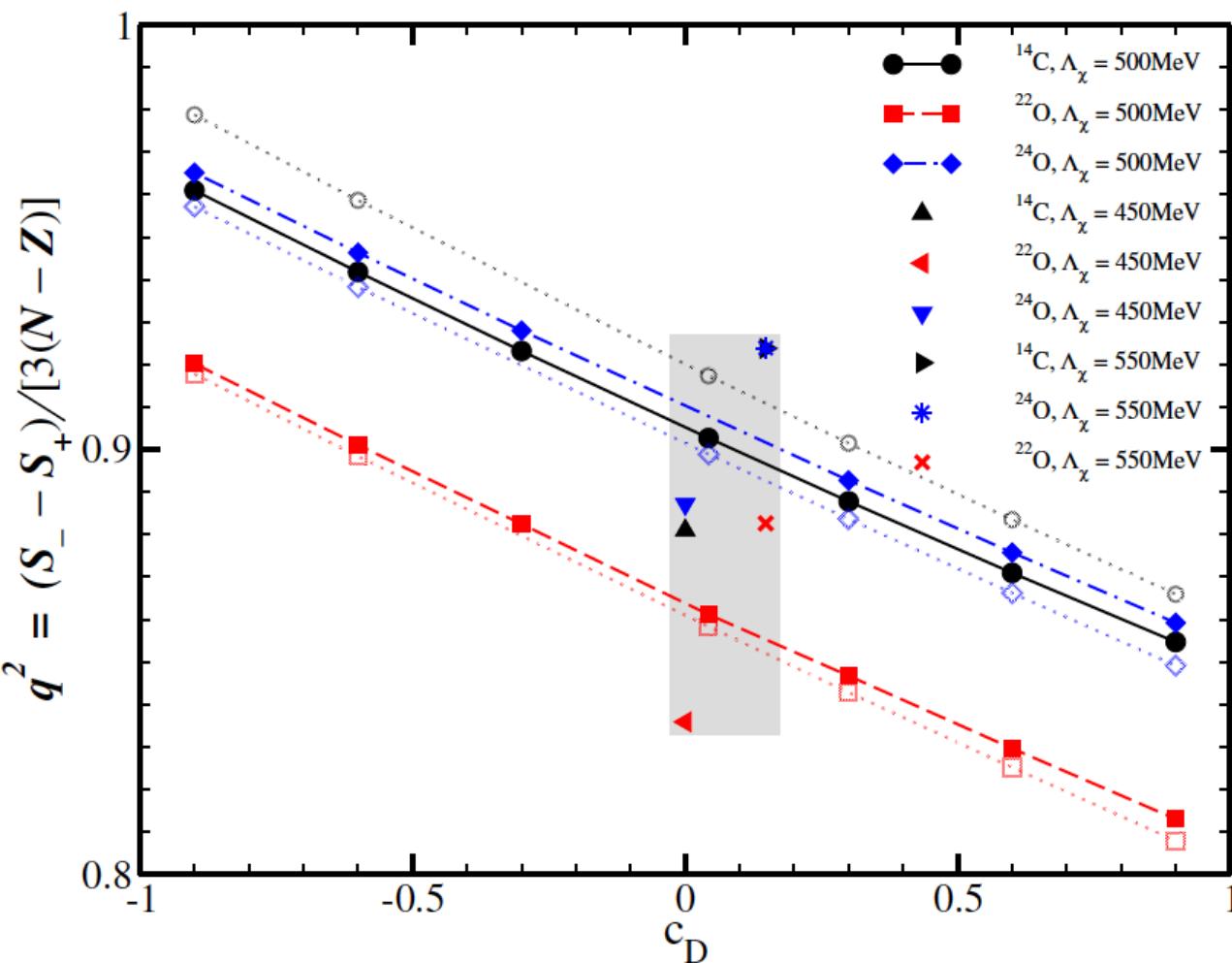
Gamow-Teller matrix element:

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

The Gamow-Teller strength functions:

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

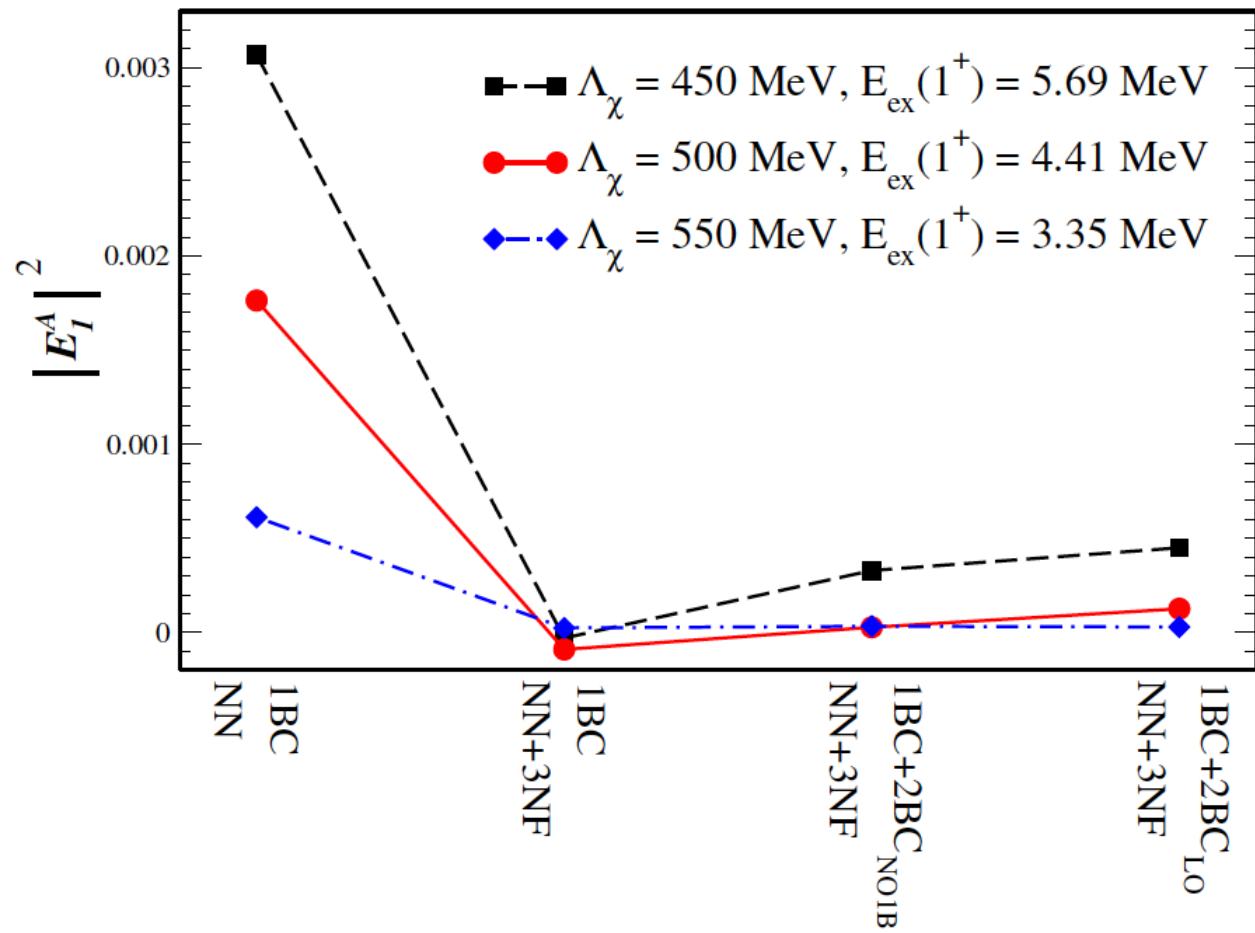
$$S_+ = \langle \Lambda | \overline{\hat{O}_{\text{GT}}} \cdot \overline{\hat{O}_{\text{GT}}^\dagger} | \text{HF} \rangle$$



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

Anomalous life-time of ^{14}C revisited

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



E_A^1 varies between 5×10^{-3} to 2×10^{-2} which is more than one order of magnitude larger than the empirical value $\sim 6 \times 10^{-4}$ extracted from the 5700 a half life of ^{14}C

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 .

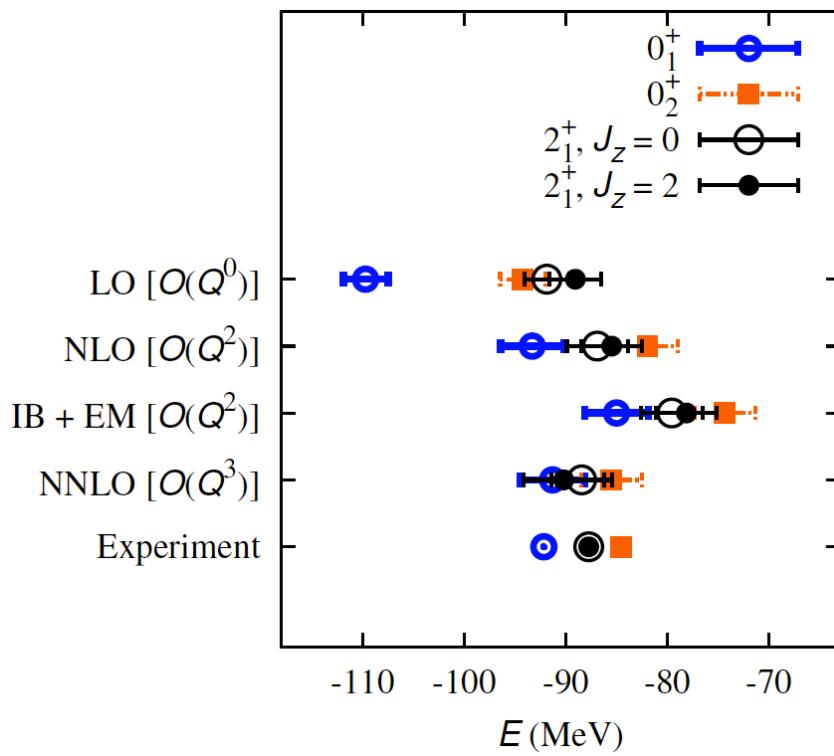


- 3NFs decrease the transition matrix element significantly
- 2BC counter the effect of 3NFs to some degree.
- Note that 2BCs increases the strength to the first 1^+ state in ^{14}N but overall quenches the Ikeda sum rule.

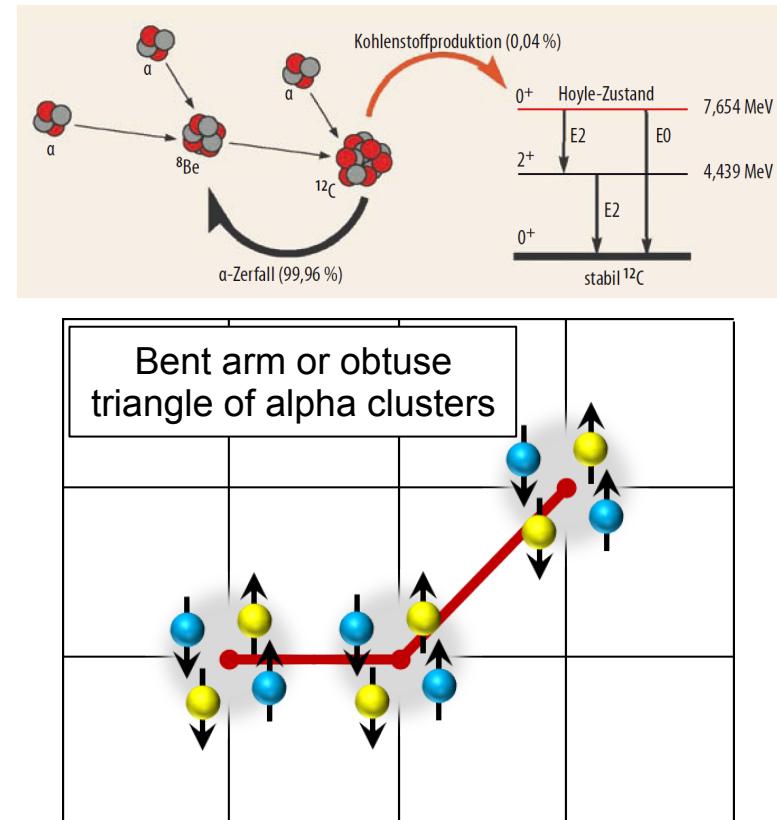
Computation of the Hoyle state

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

Nuclear Lattice Effective Field Theory Collaboration



Epelbaum, Krebs, Lee, Mei  ner,
Phys. Rev. Lett. 106, 192501 (2011)

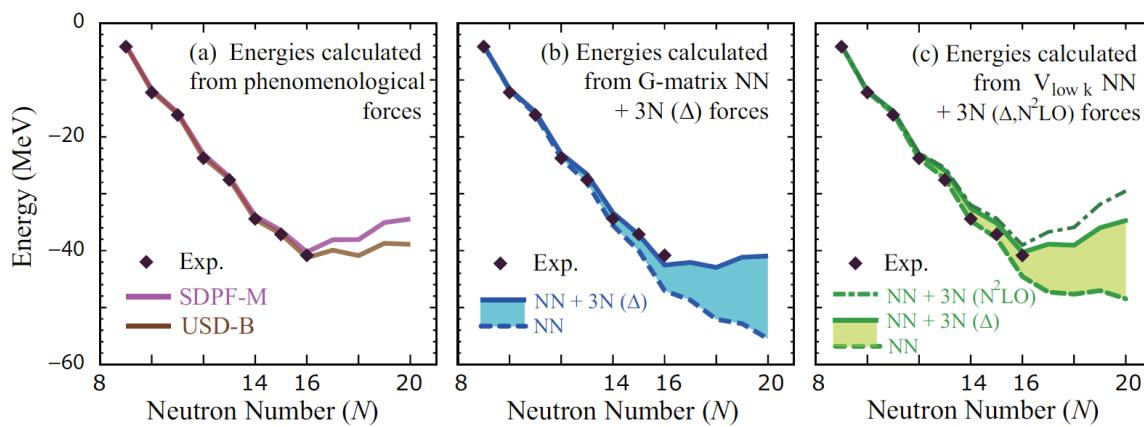
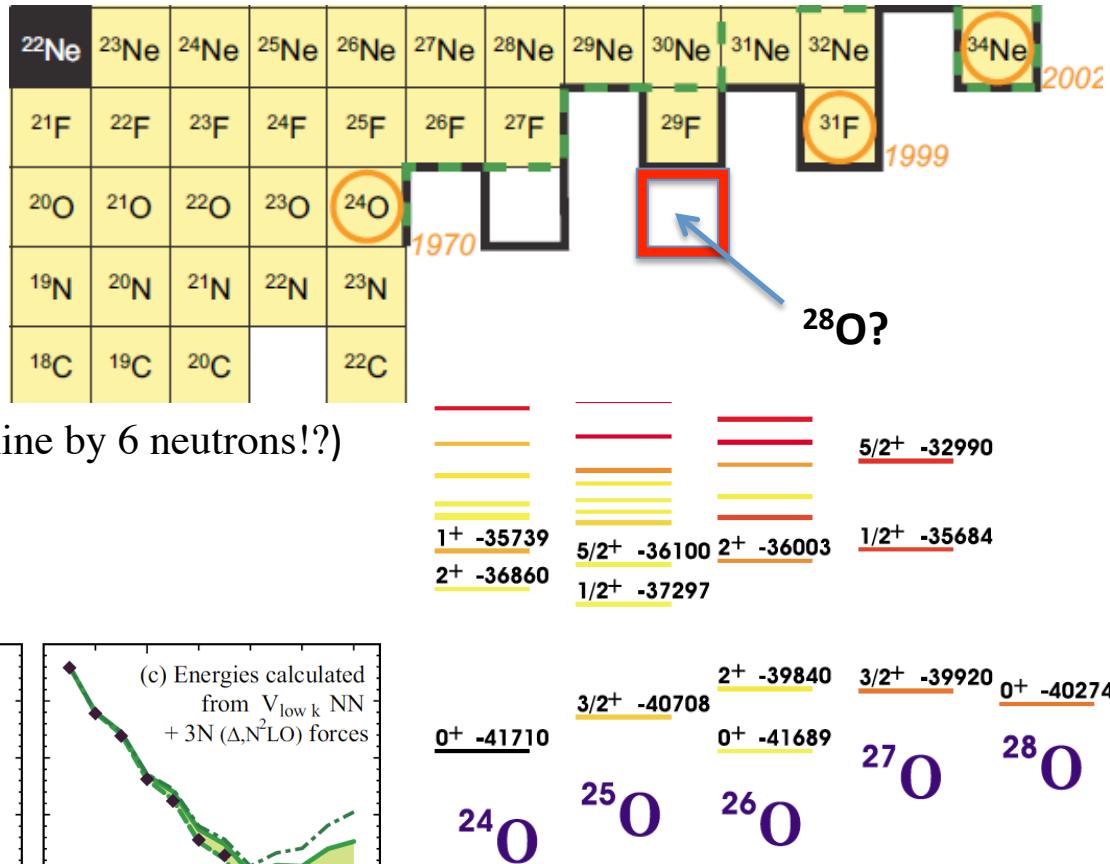


Epelbaum, Krebs, L  hde, Lee, Mei  ner,
Phys. Rev. Lett. 109, 252501 (2012)

Is ^{28}O a bound nucleus?

Experimental situation

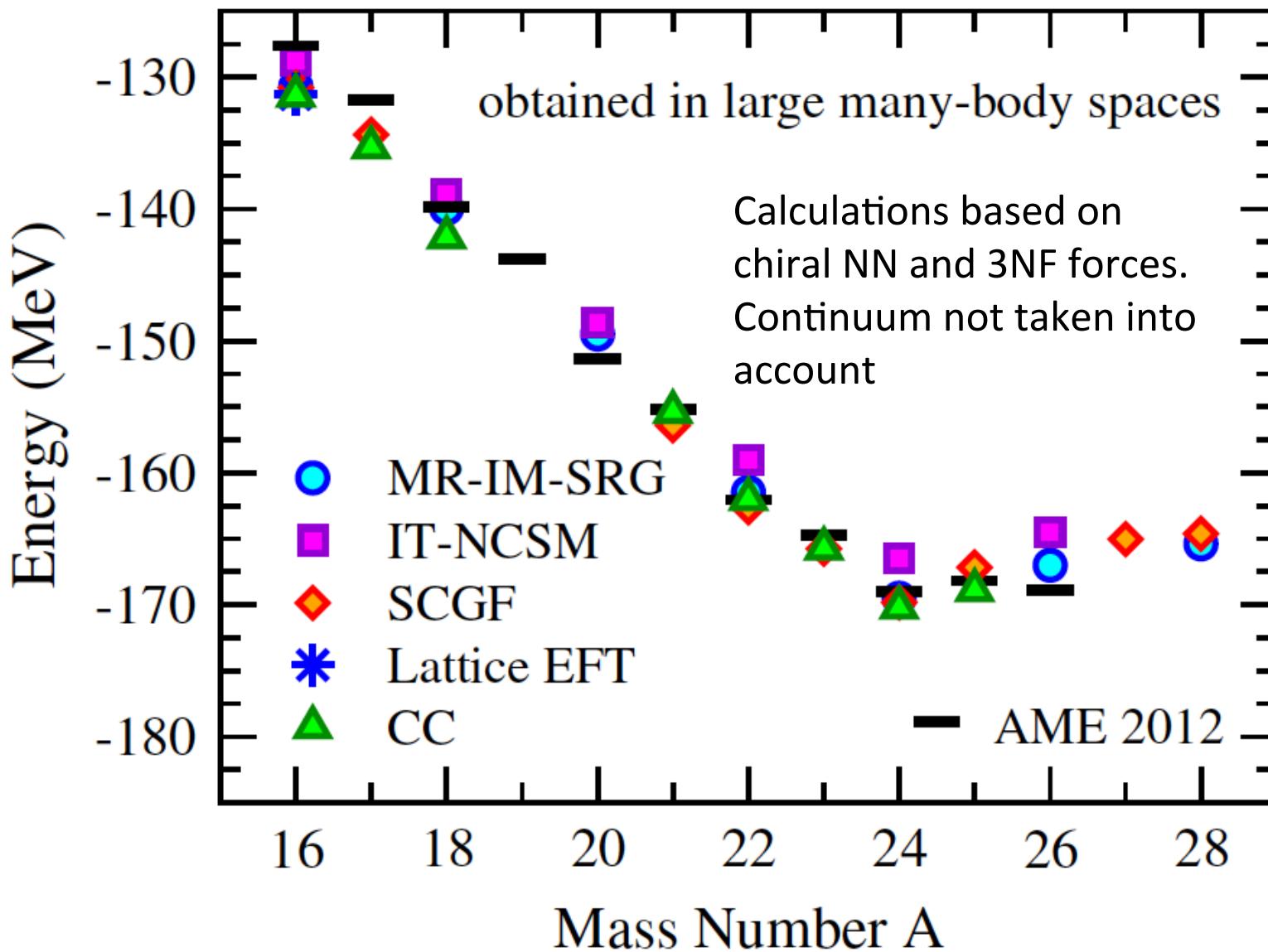
- “Last” stable oxygen isotope ^{24}O
- $^{25,26}\text{O}$ unstable (Hoffman et al 2008, Lunderberg et al 2012)
- ^{28}O not seen in experiments
- ^{31}F exists (adding on proton shifts drip line by 6 neutrons!?)



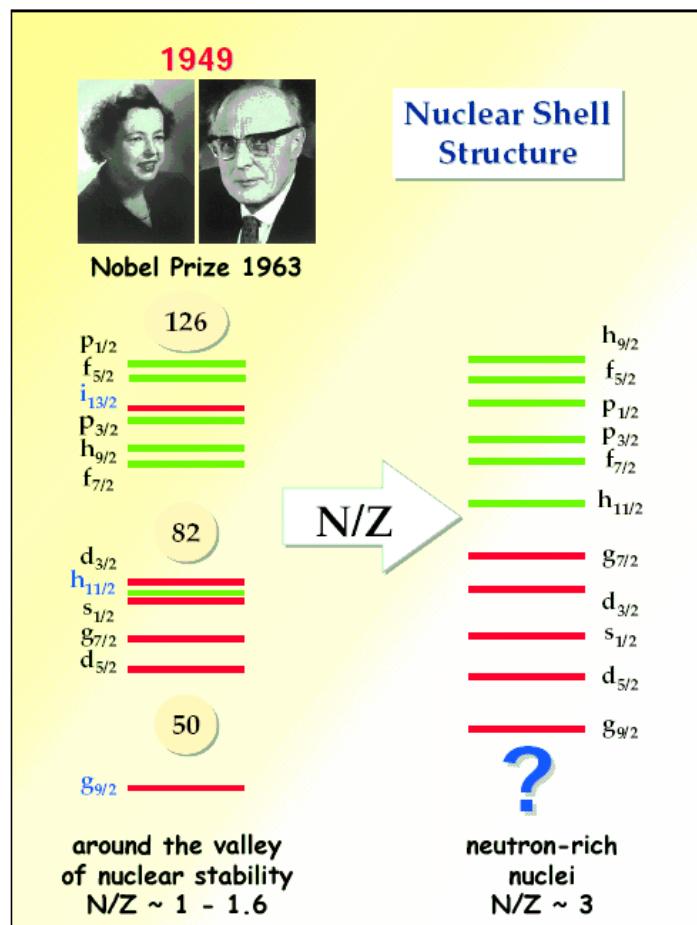
Shell model (sd shell) with monopole corrections based on three-nucleon force predicts $^{2\text{nd}}$ O as last stable isotope of oxygen. [Otsuka, Suzuki, Holt, Schwenk, Akaishi, PRL (2010), arXiv:0908.2607]

Continuum shell model with HBUSD interaction predict ^{28}O unbound. A. Volya and V. Zelevinsky PRL (2005)

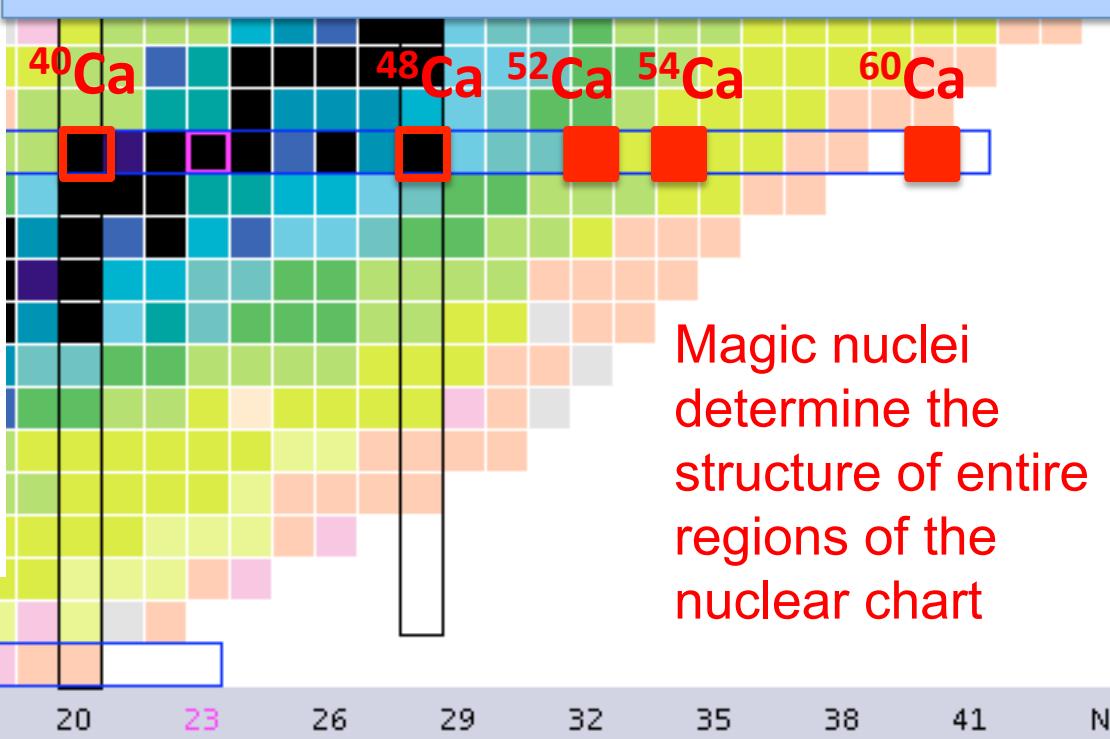
Benchmarking different ab-initio methods in the oxygen chain



Evolution of shell structure in neutron rich Calcium

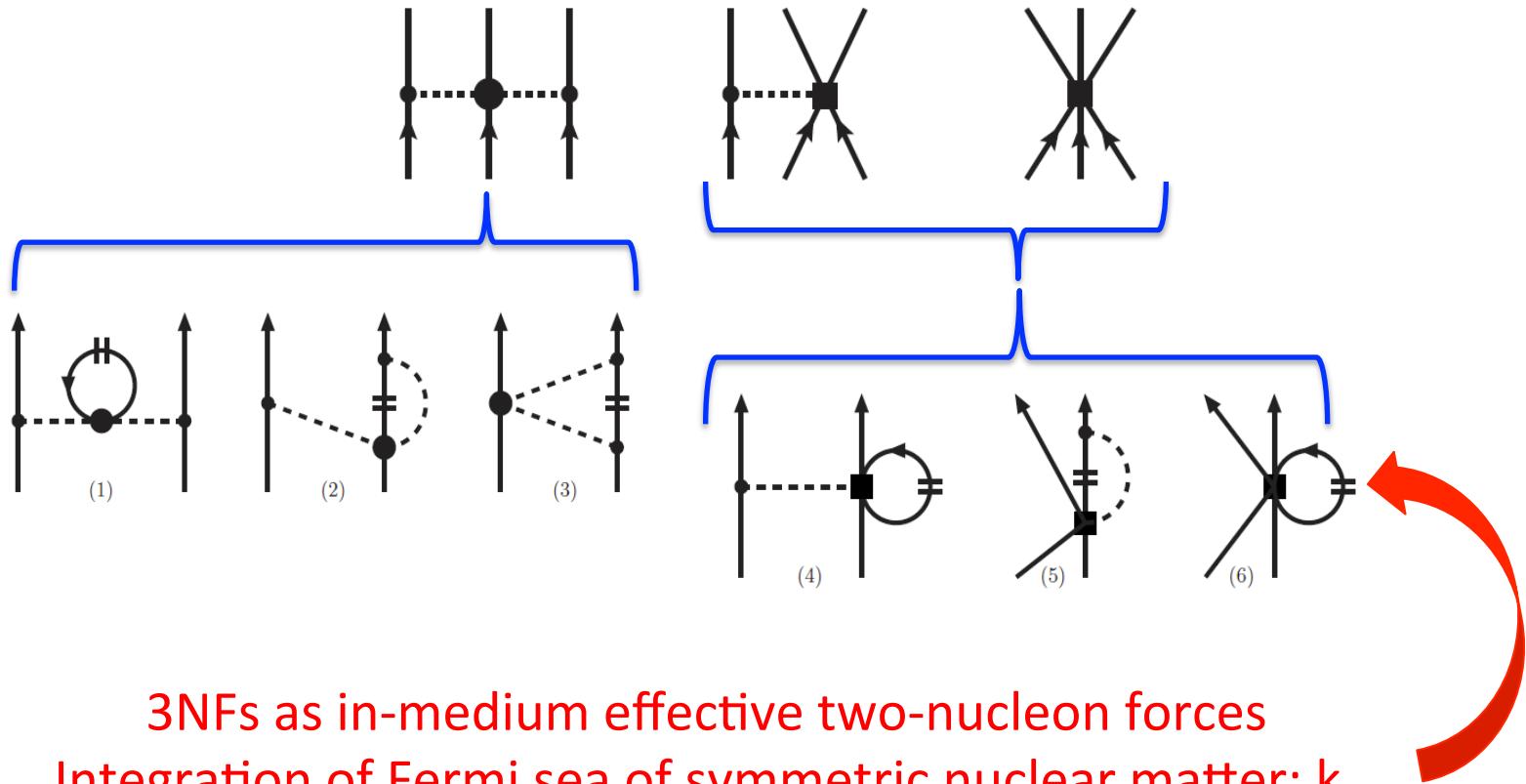


- How do shell closures and magic numbers evolve towards the dripline?
- What are the underlying mechanisms and how do we identify new shell structure?



Including the effects of 3NFs (approximation!)

[J.W. Holt, Kaiser, Weise, PRC 79, 054331 (2009); Hebeler & Schwenk, PRC 82, 014314 (2010)]



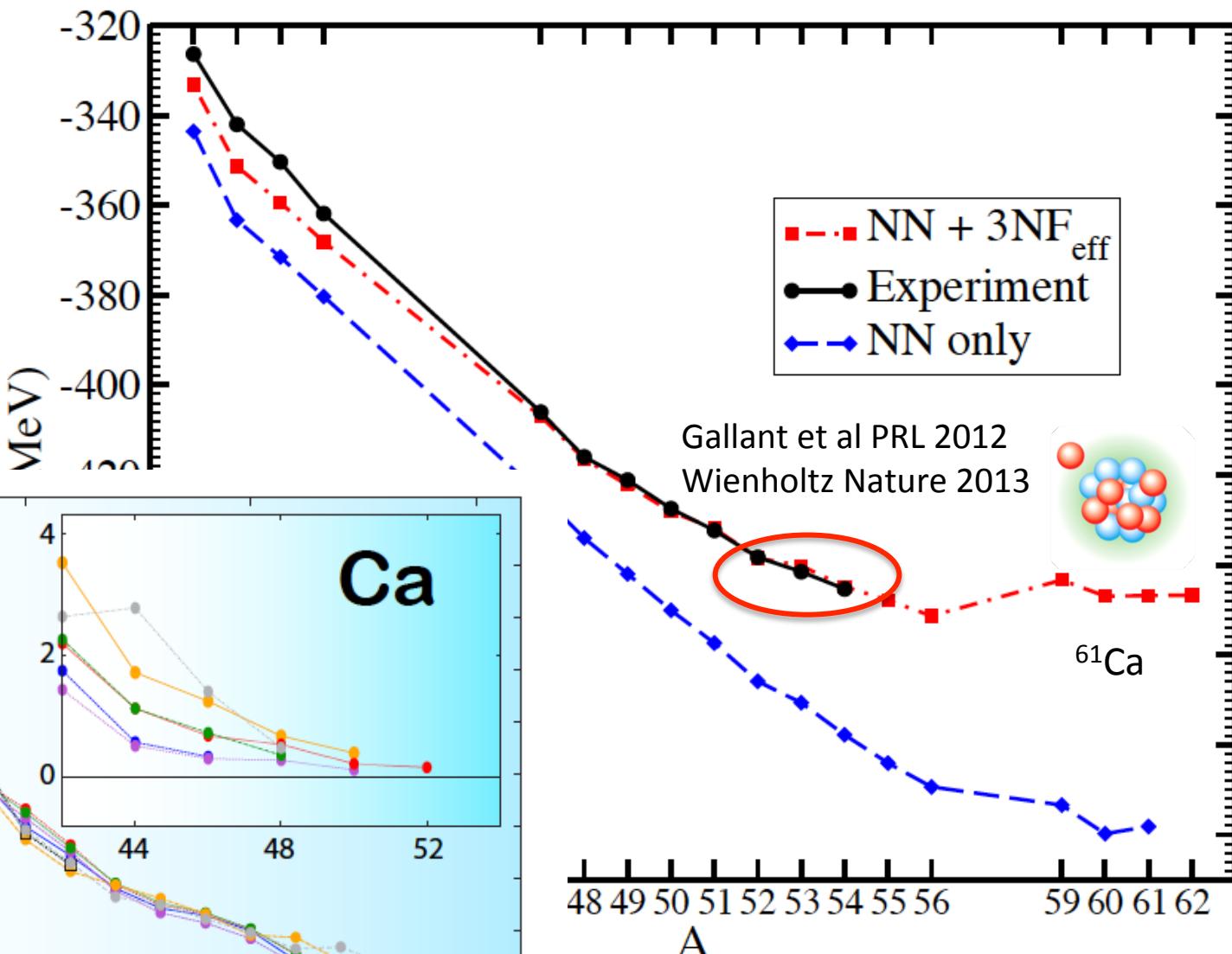
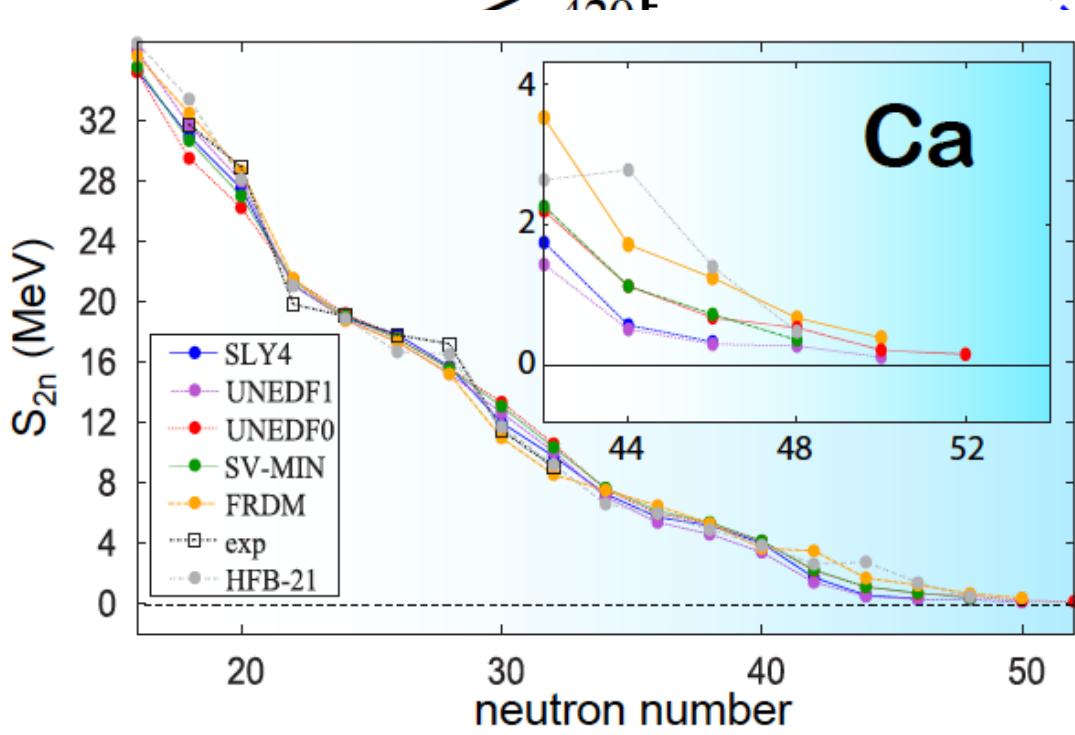
3NFs as in-medium effective two-nucleon forces
Integration of Fermi sea of symmetric nuclear matter: k_F

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

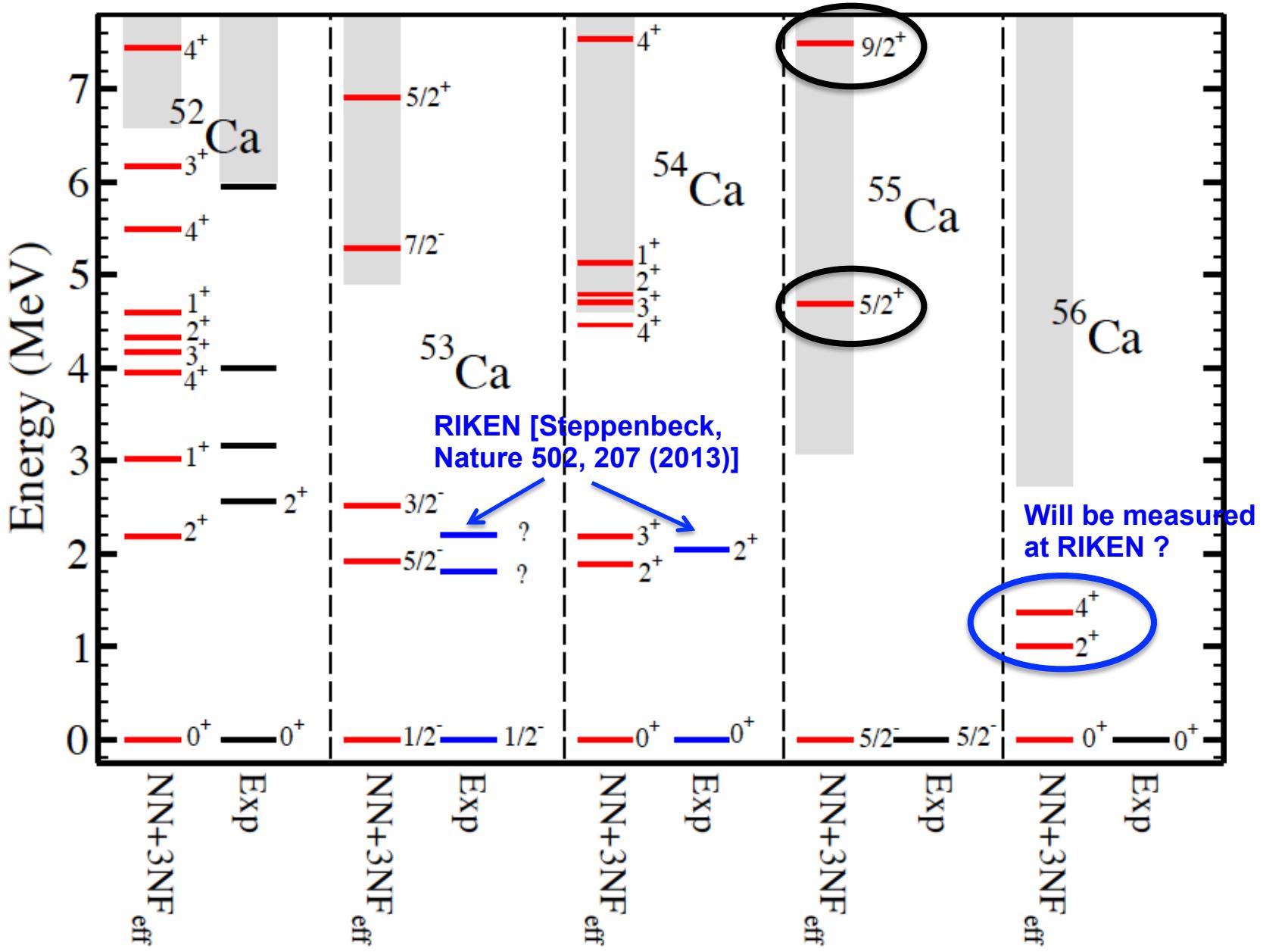
Neutron rich calcium isotopes

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

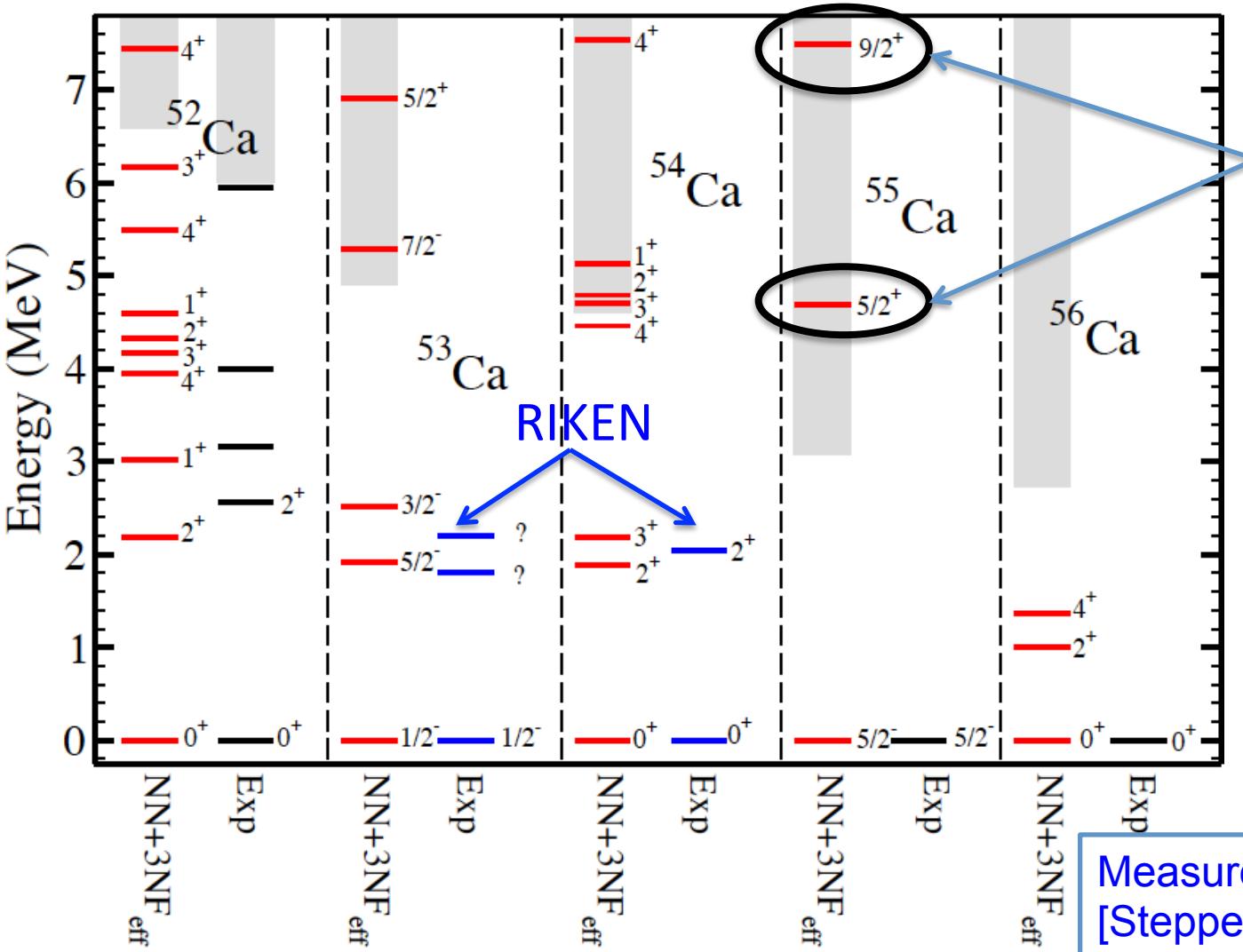
C Forssén et al
Phys. Scr. 014022 (2013)
Erler et al., Nature 486,
509 (2012)



Spectra and shell evolution in Calcium isotopes



Spectra and shell evolution in Calcium isotopes

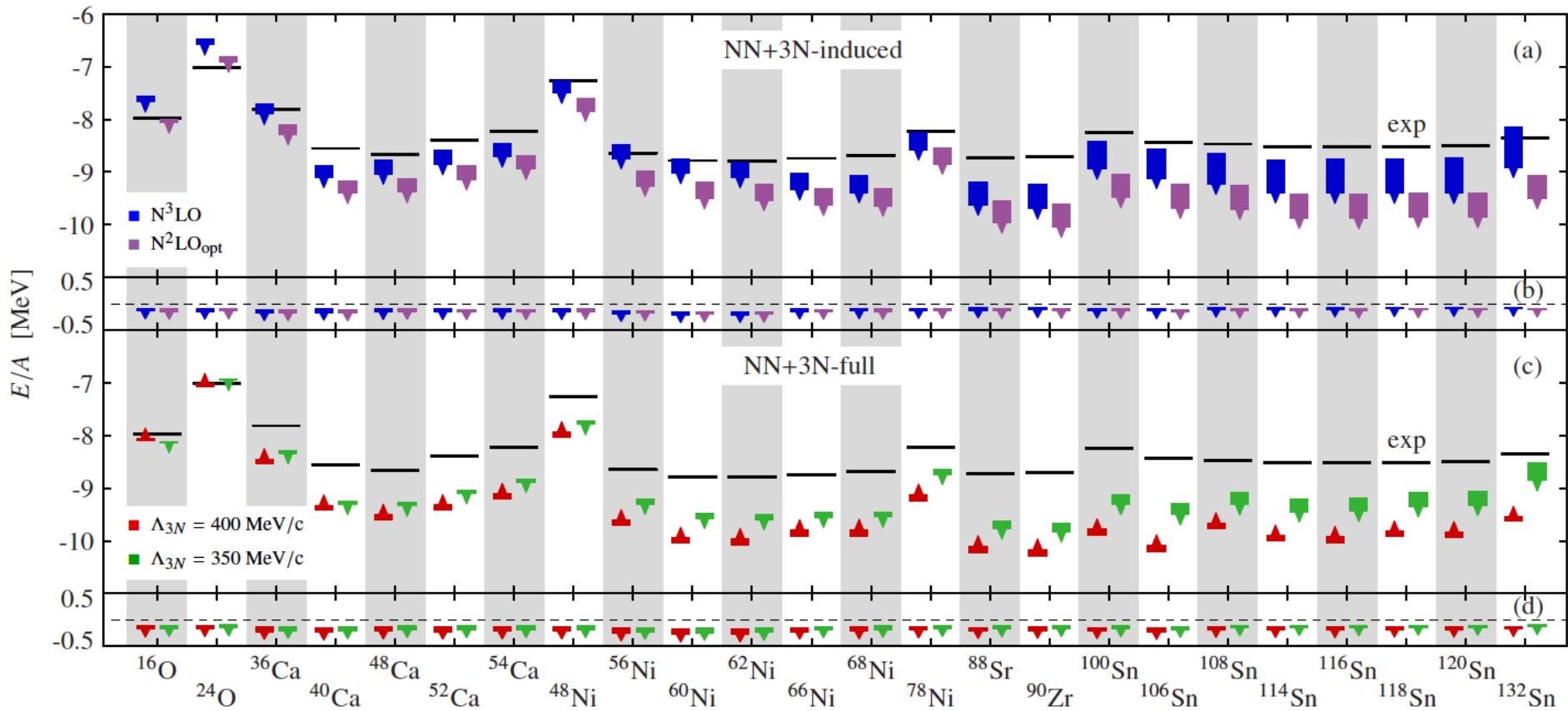


1. Our prediction for excited $5/2^-$ and $1/2^-$ states in ^{53}Ca seen at RIKEN
2. Inversion of $9/2^+$ and $5/2^+$ states in neutron rich calcium isotopes
3. Harmonic oscillator gives the naïve shell model order

Measurement at RIKEN
[Steppenbeck et al., J. Phys. G 2013; Nature 502, 207 (2013);] confirms our prediction.

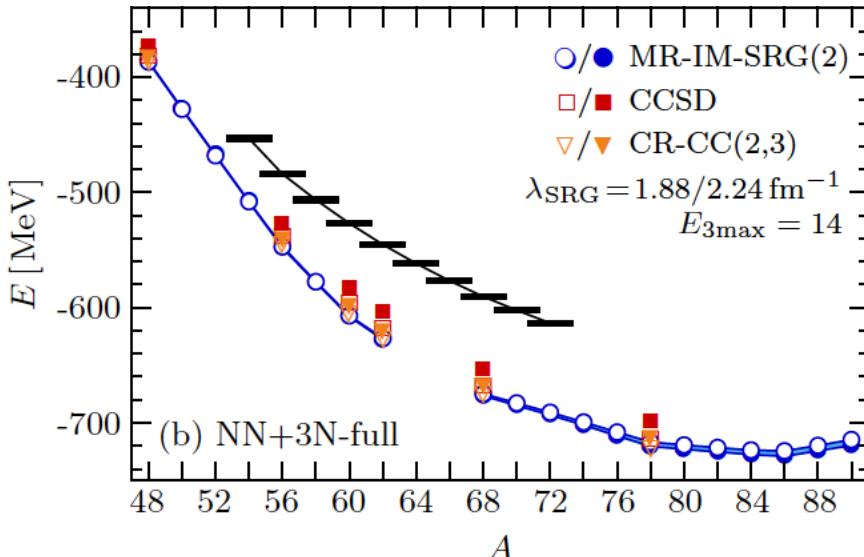
Continuum coupling crucial for level ordering

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

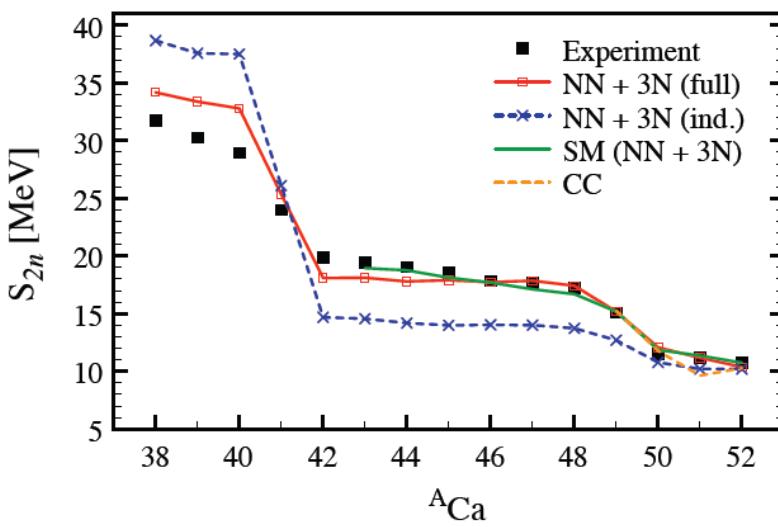


Chiral NN + 3NFs and the problem of saturation

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

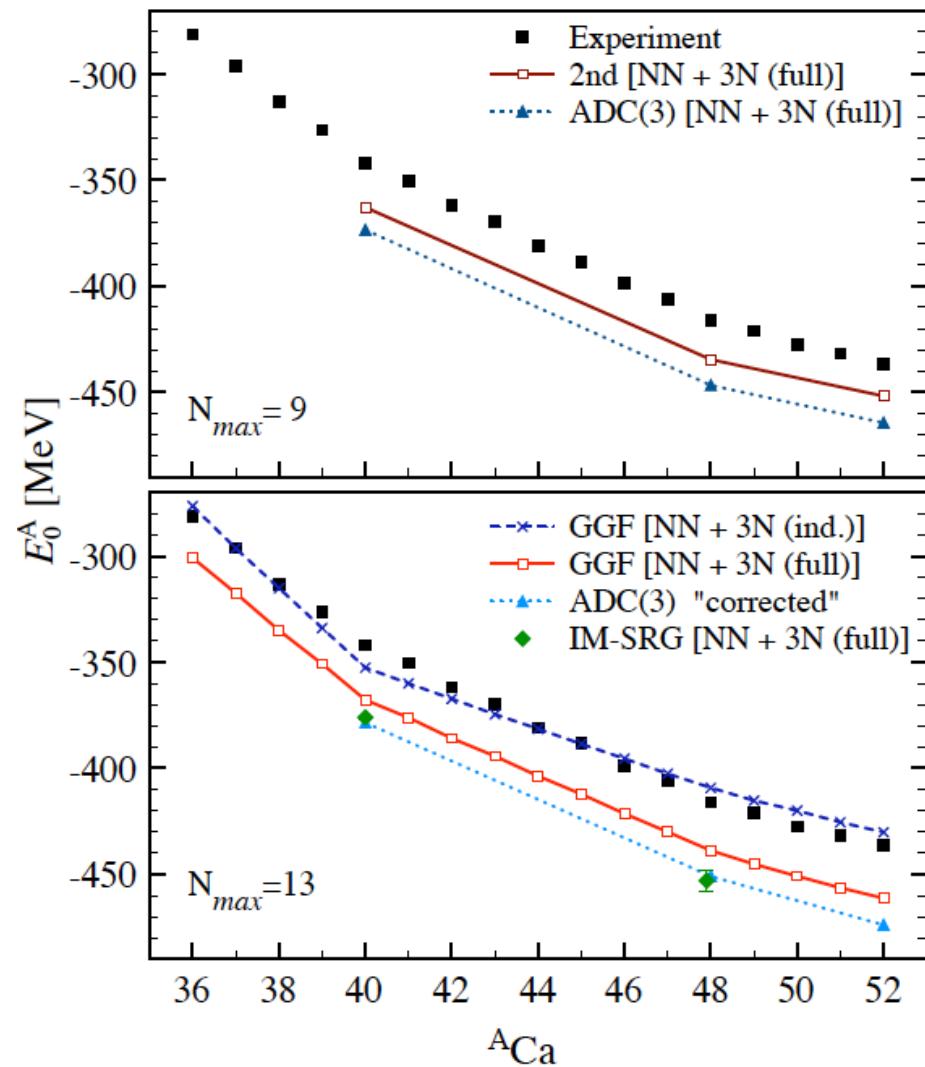


Energy differences such as two-neutron separation energies are better reproduced

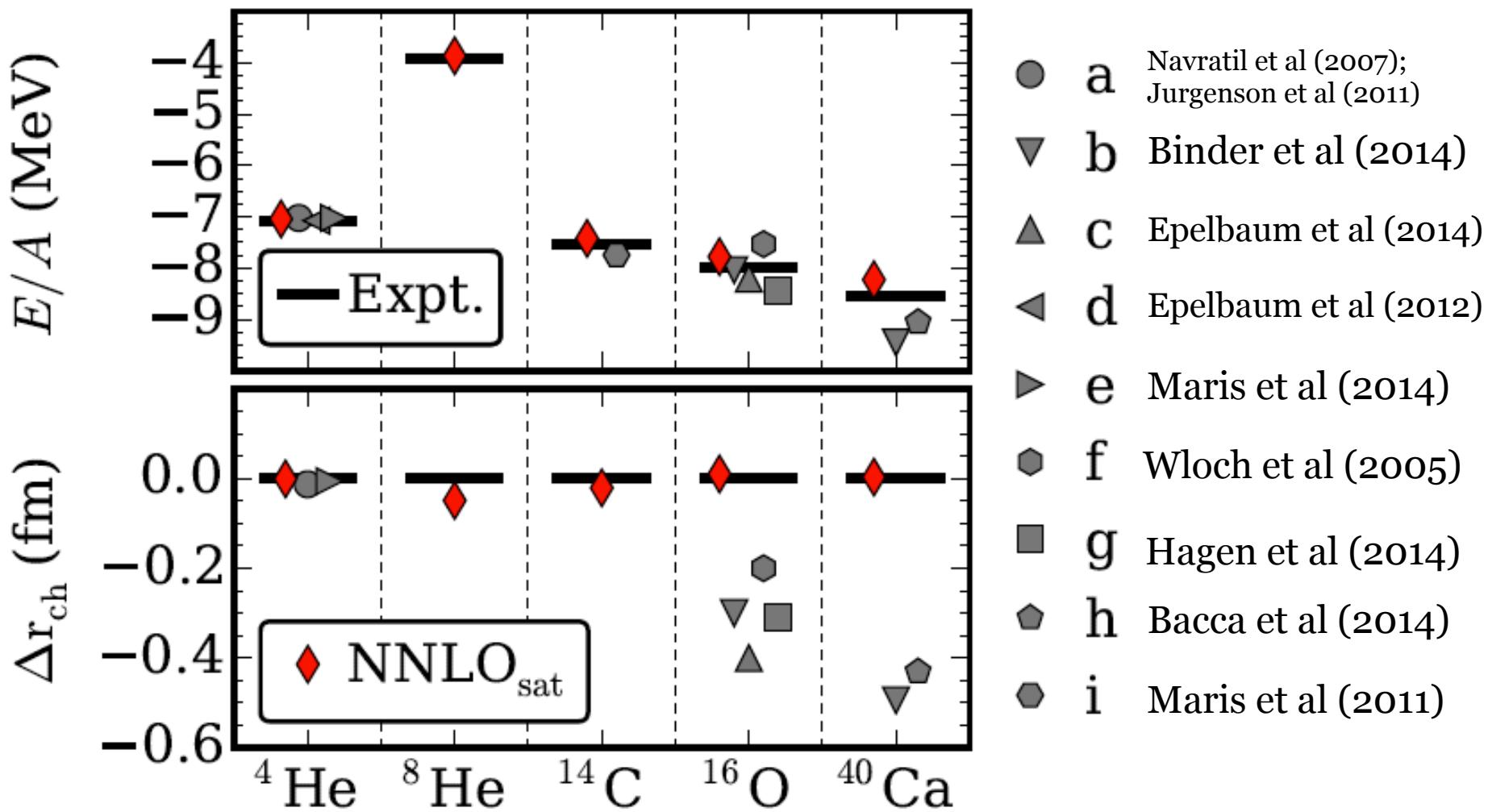


Significant overbinding is found in calcium and nickel isotopes using chiral NN and 3NFs

V. Soma et al Phys. Rev. C 89, 061301 (2014)

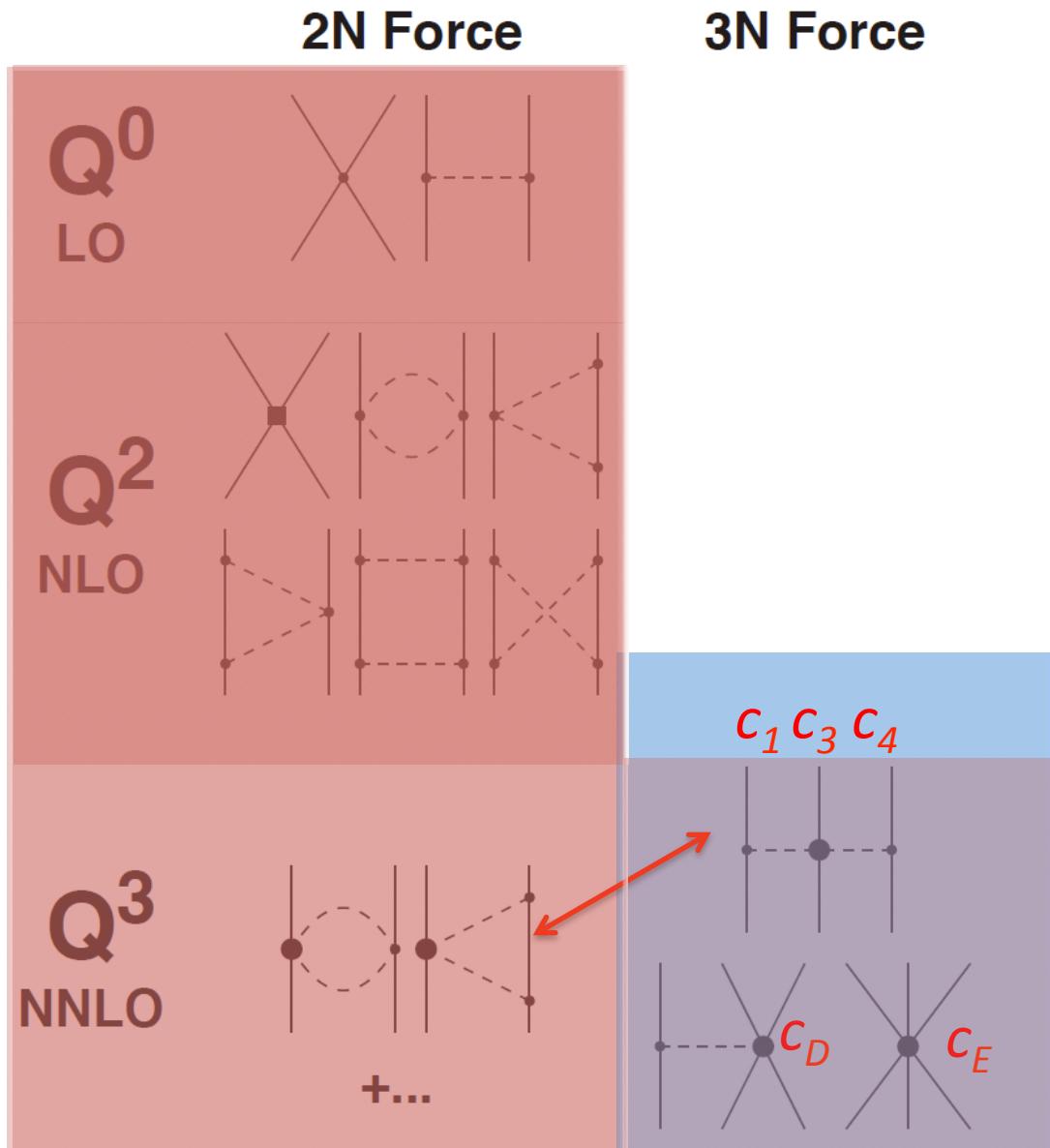


Accurate nuclear binding energies and radii from a chiral interaction



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:

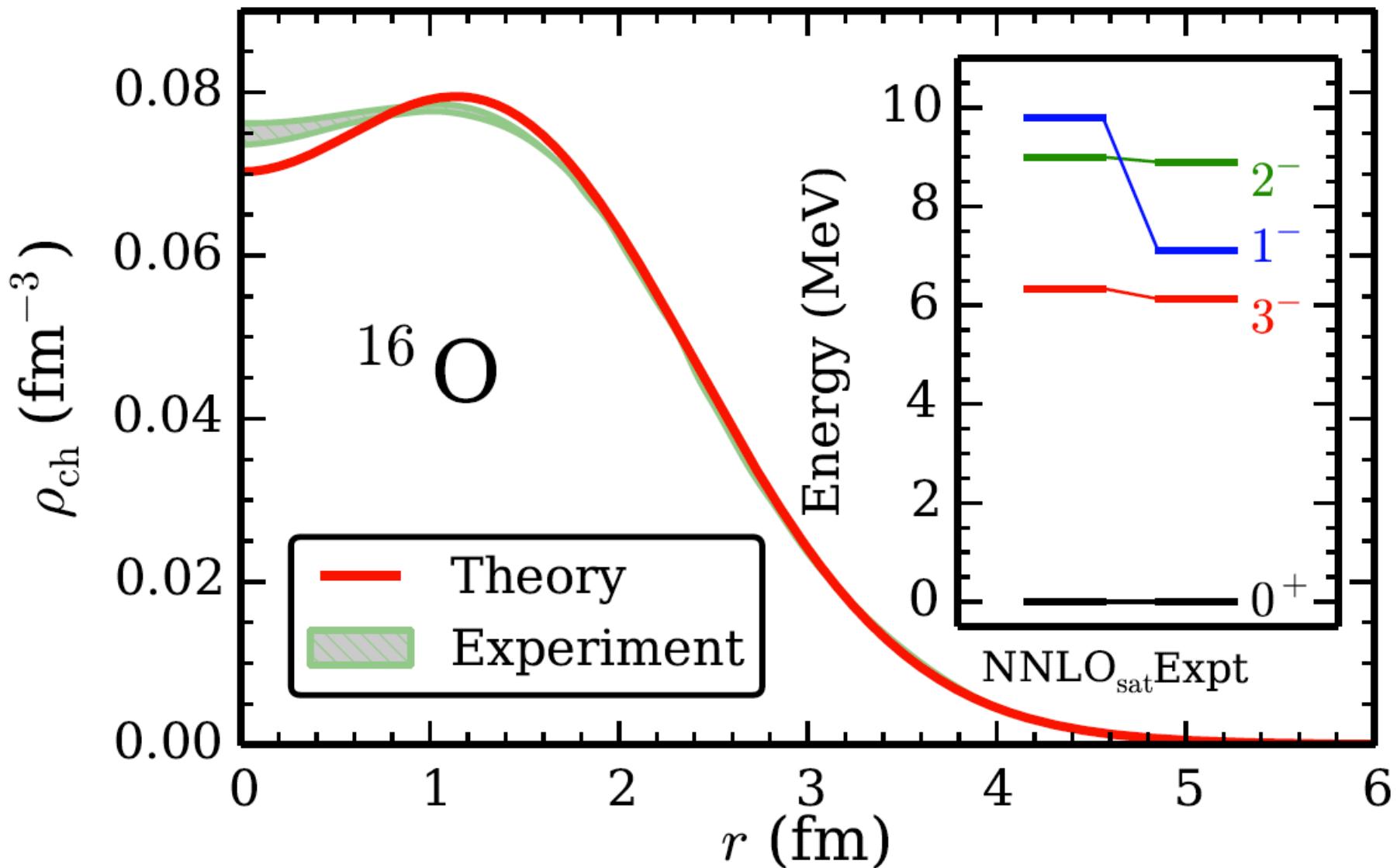
- Fit interactions nucleon by nucleon
- Fit to NN scattering data up to $\sim 350\text{MeV}$
- cE and cD fit to $A=3,4$

Our approach:

- Simultaneous optimization of NN and 3NFs
- Fit to few-body data and BEs/radii in nuclei with $A \sim 25$

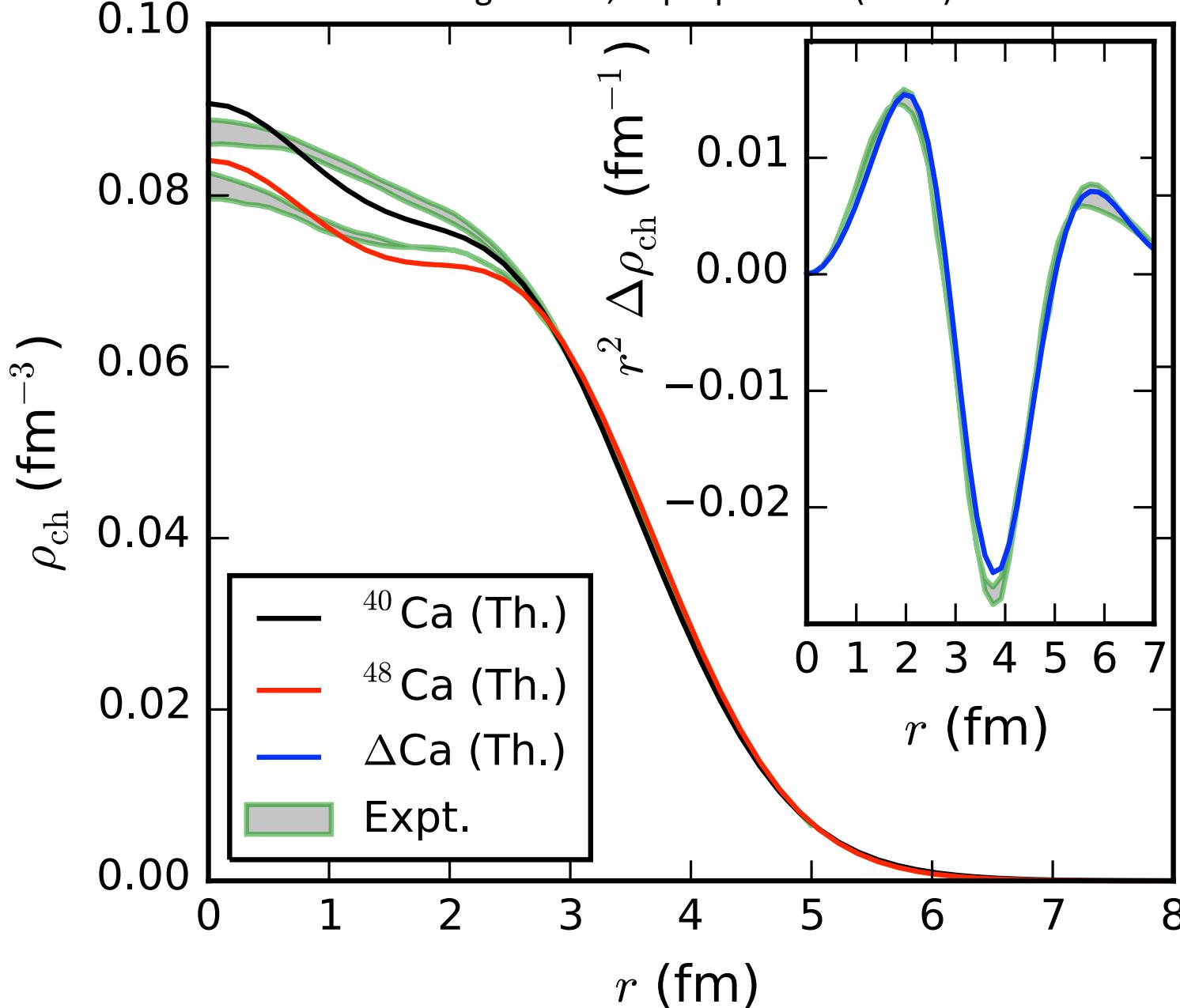
Not new: GFMC with AV18 and Illinois-7 are fit to 23 levels in nuclei with $A < 10$

Charge density and negative parity states of ^{16}O



Charge densities of $^{40,48}\text{Ca}$ with NNLO_{sat}

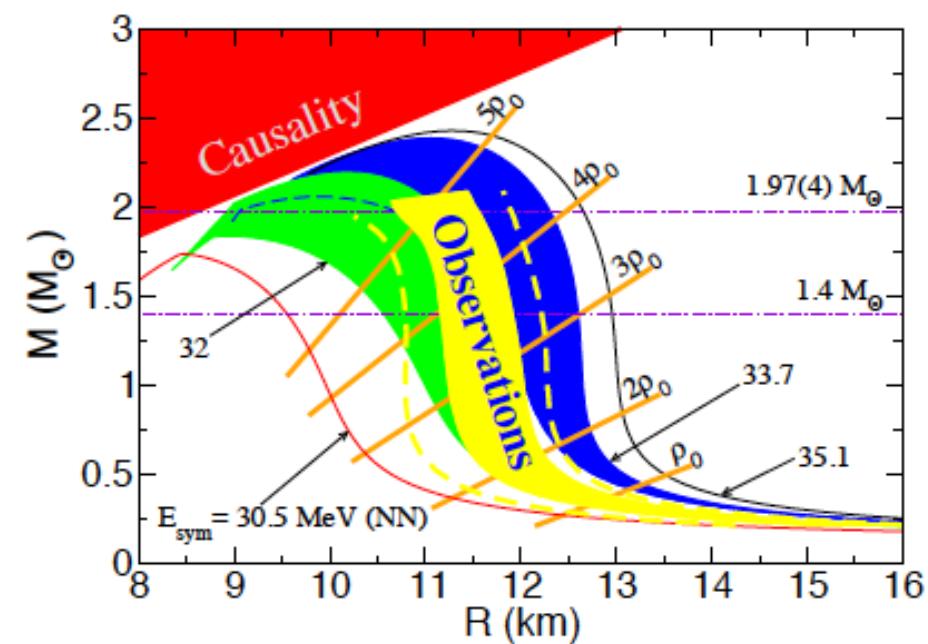
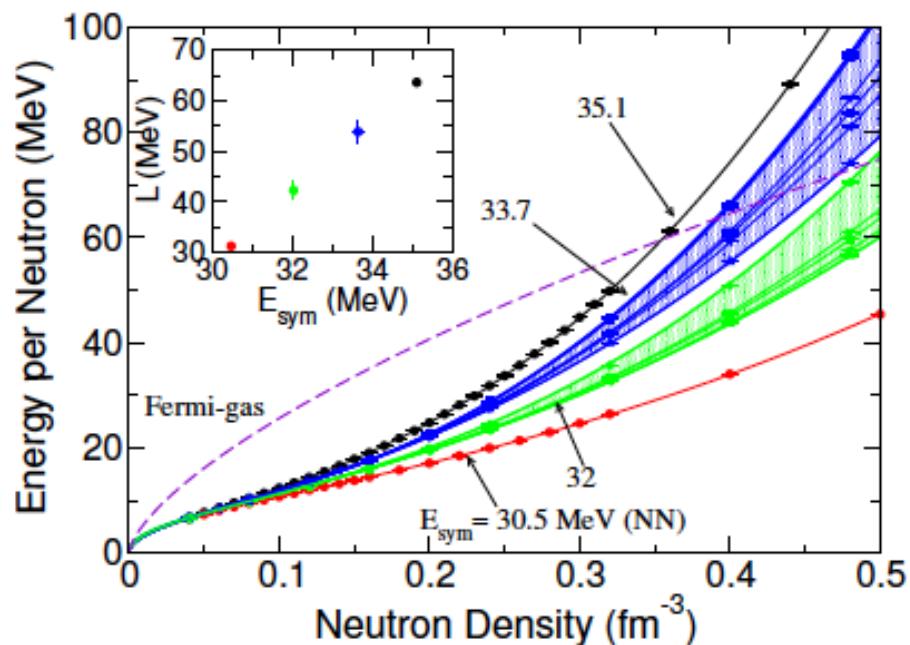
G. Hagen et al, in preparation (2015)



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.

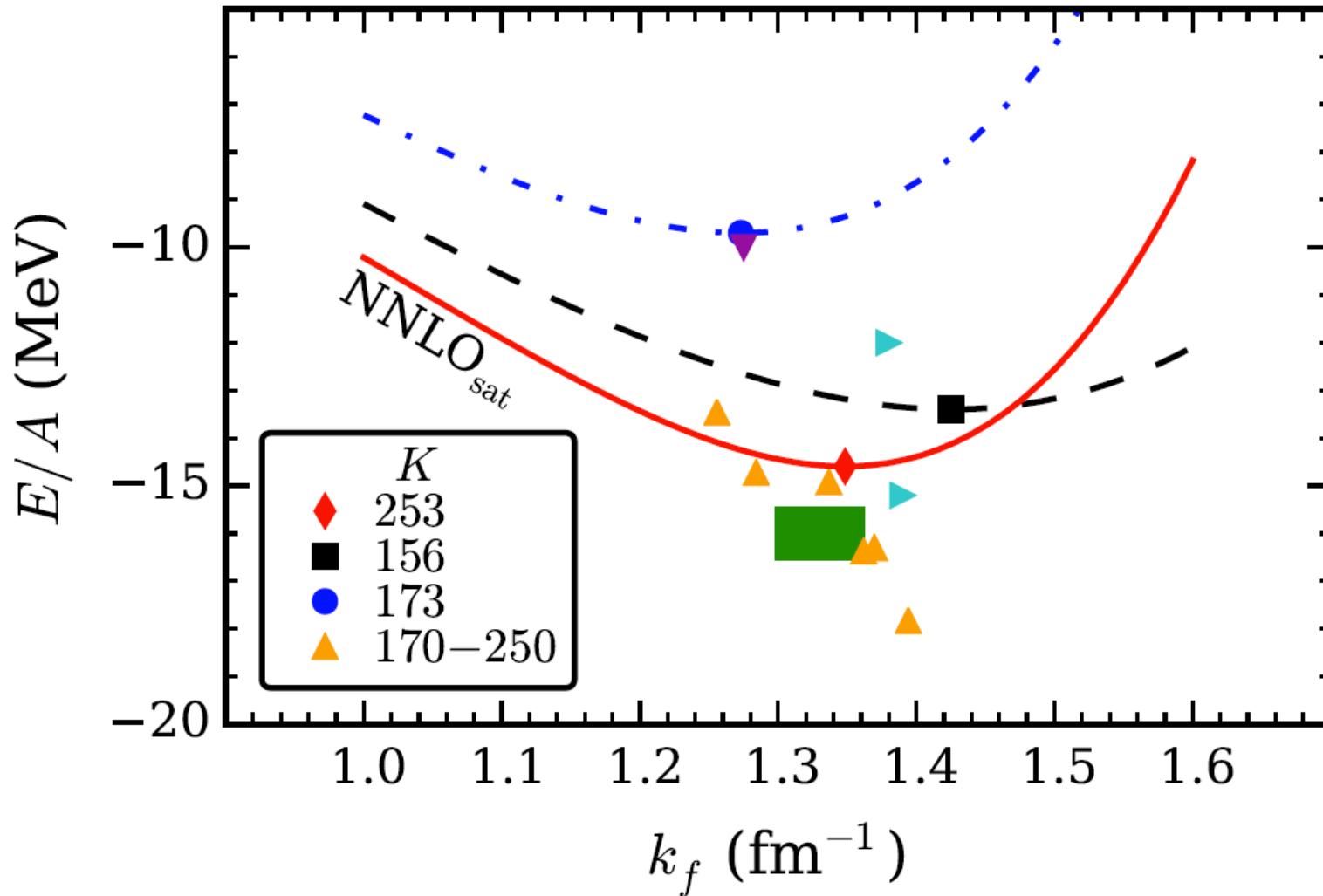
Constraining the maximum mass and radius of neutron stars and the nuclear symmetry energy



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

adapted from
Steiner, Gandolfi, PRL 108, 081102 (2012)

Nuclear matter from chiral NN and 3NFs



Nuclear matter saturation curves for NNLO_{sat} 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.
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.