Toward model-independent calculations of atomic nuclei

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SciDAC
Scientific Discovery through Advanced Computing

Computational Challenges in Nuclear and Many-Body Physics
Nordita, September 18, 2014

NUCLEI
Nuclear Computational Low-Energy Initiative

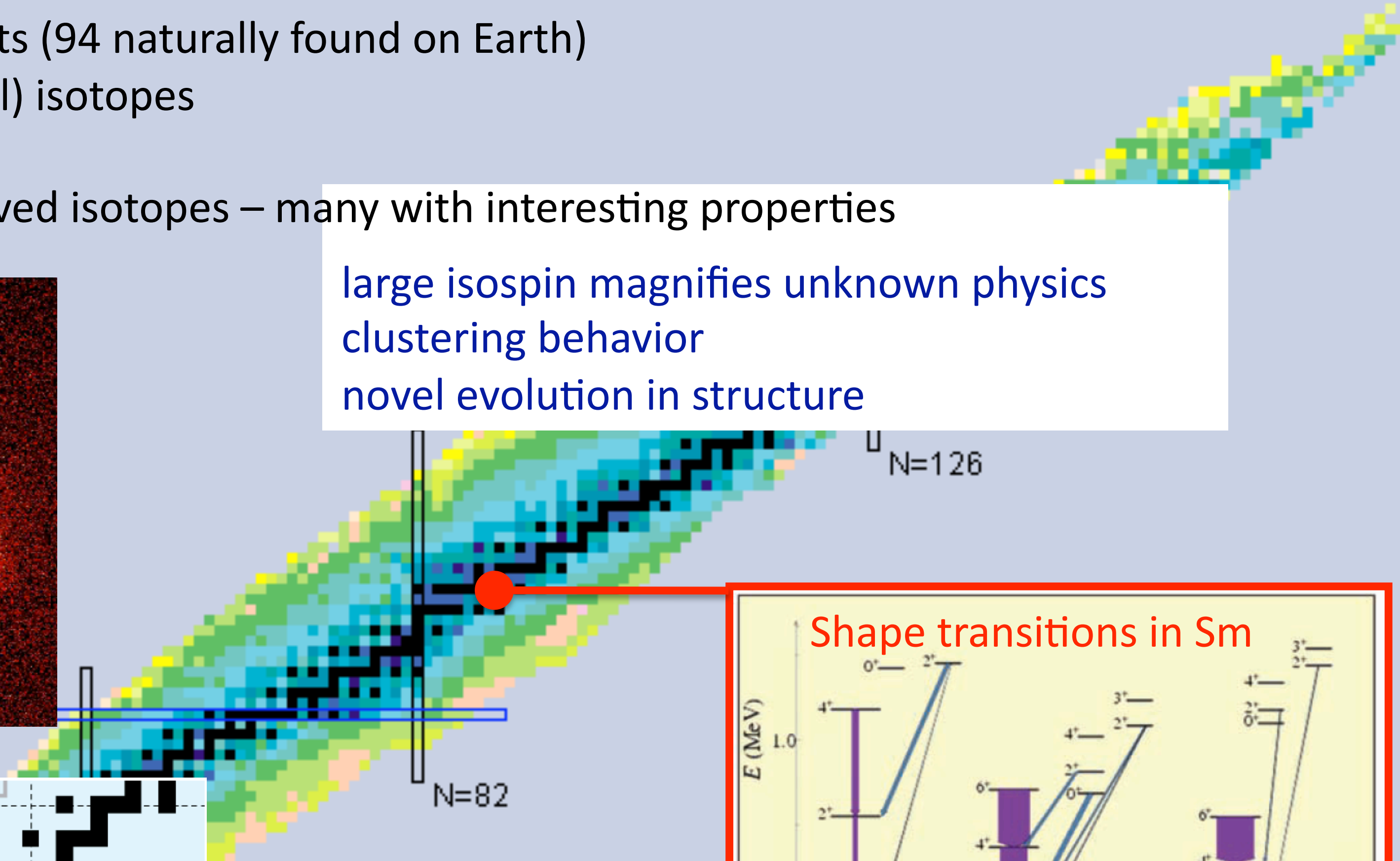
Research partly funded by the US Department of Energy

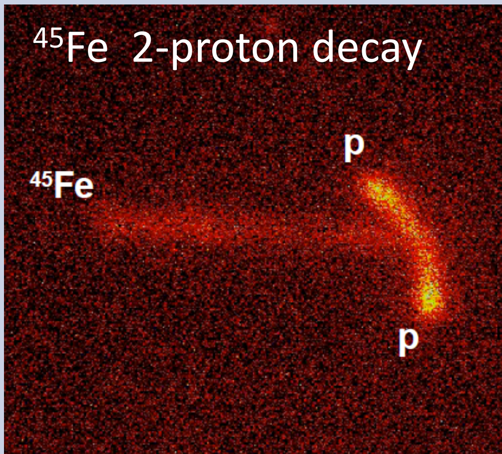
Nuclei across the chart

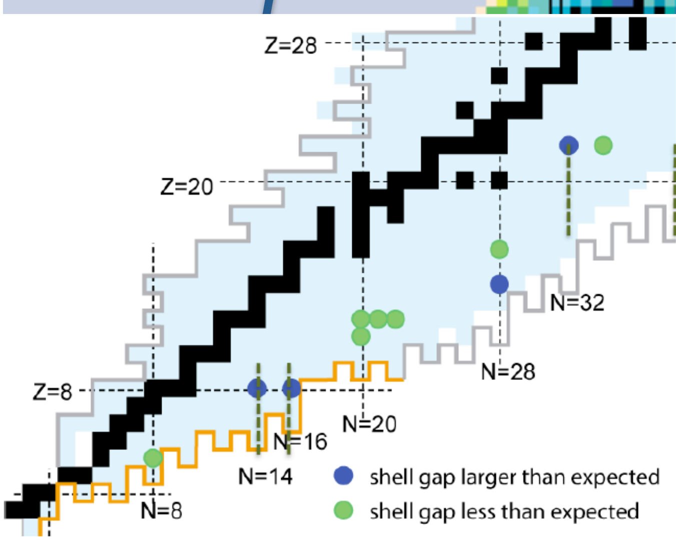
118 chemical elements (94 naturally found on Earth)
288 stable (primordial) isotopes

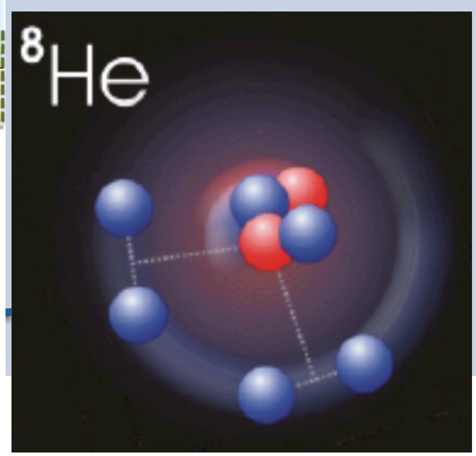
Thousands of short-lived isotopes – many with interesting properties

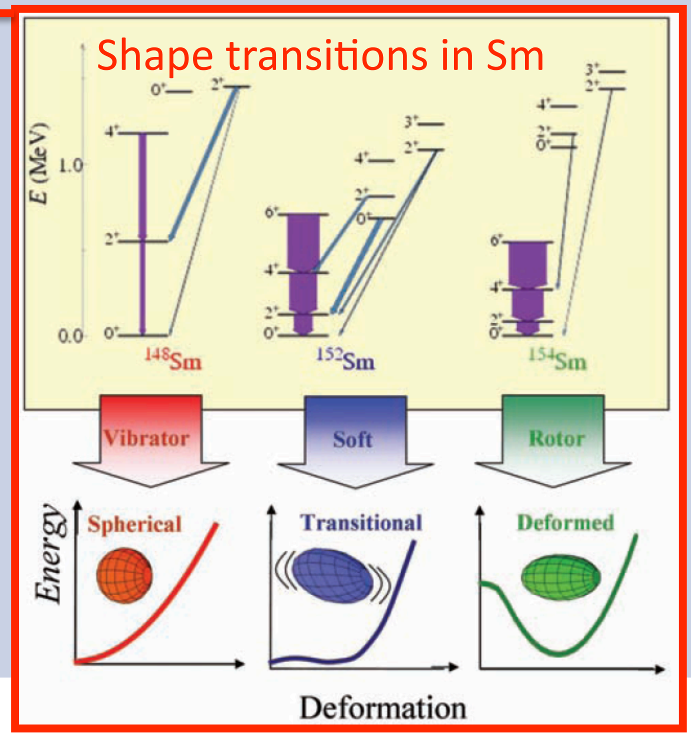
large isospin magnifies unknown physics
clustering behavior
novel evolution in structure



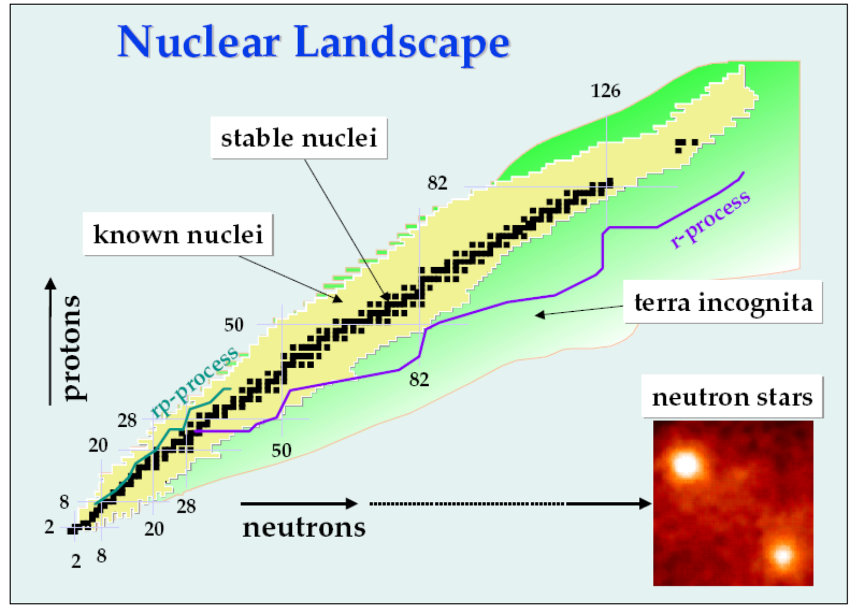








Science questions



Basic science questions in the physics of nuclei:

1. What binds nucleons into stable nuclei and rare isotopes?
2. What are the limits of nuclear binding?
3. What is the origin of simple modes in complex systems?

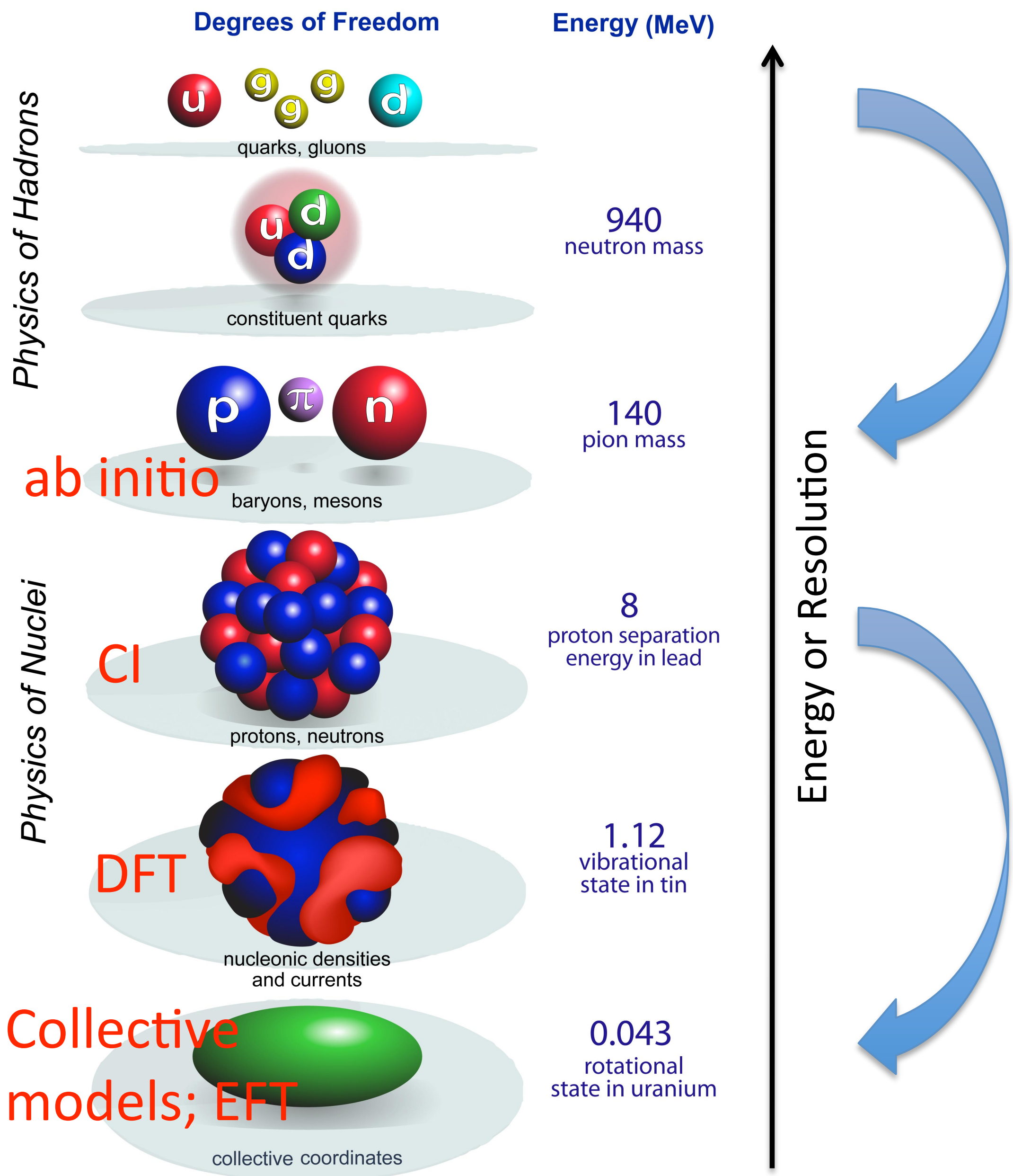
Basic science questions in nuclear astrophysics:

4. How are the elements from iron to uranium made?
5. What is the fate of massive stars?
6. What is the mass of the neutrino, and what is its nature (Dirac / Majorana fermion)?

Understanding of rare isotopes central to addressing four of these questions (1, 2, 4, 5).

Rare isotopes also relevant for medical applications (imaging and therapy), and energy production

Energy scales and relevant degrees of freedom



Chiral symmetry is broken

Pion is Nambu-Goldstone boson

Tool: Chiral effective field theory

Emergent breaking of rotational symmetry

No Nambu-Goldstone boson; rotations are zero mode

Tool: effective field theory

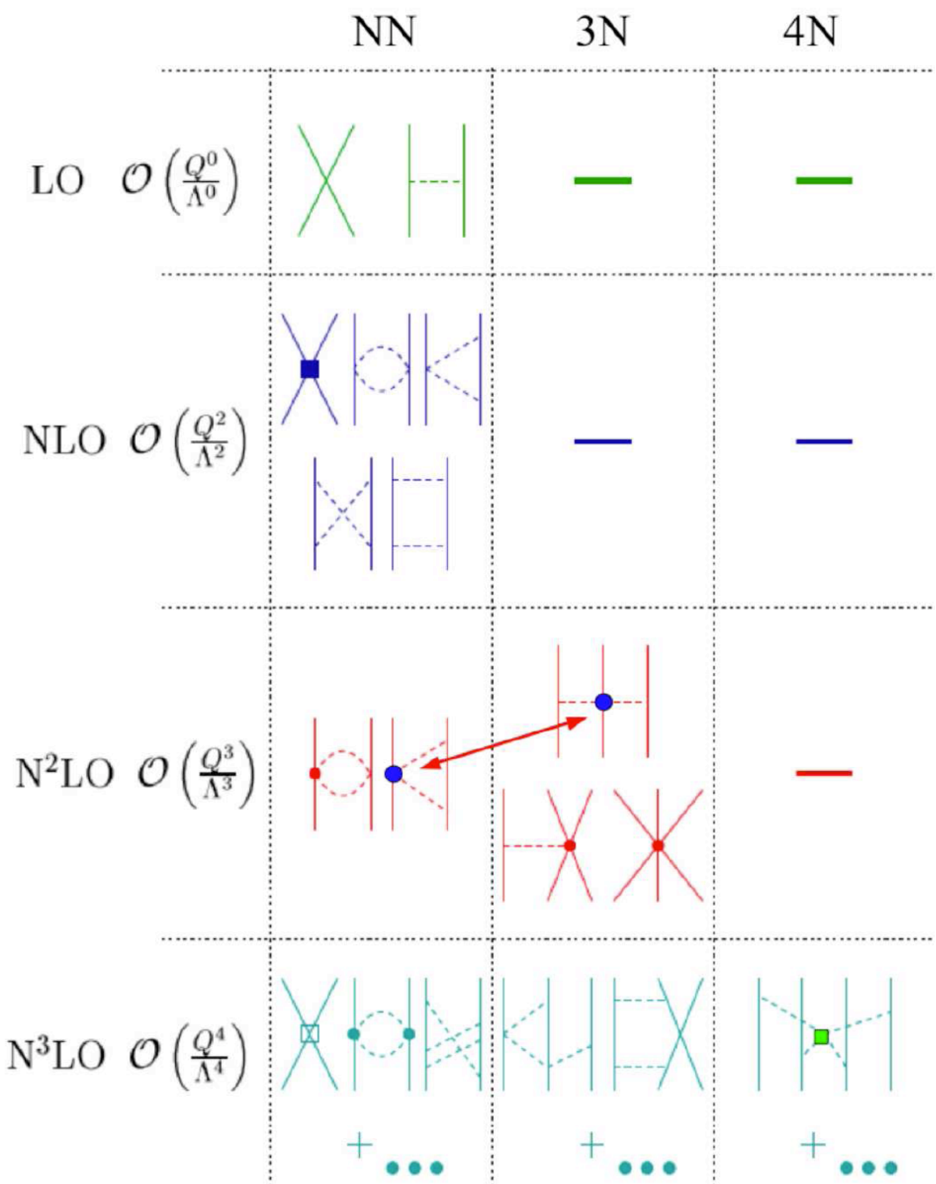
Effective theories provide us with model independent approaches to atomic nuclei

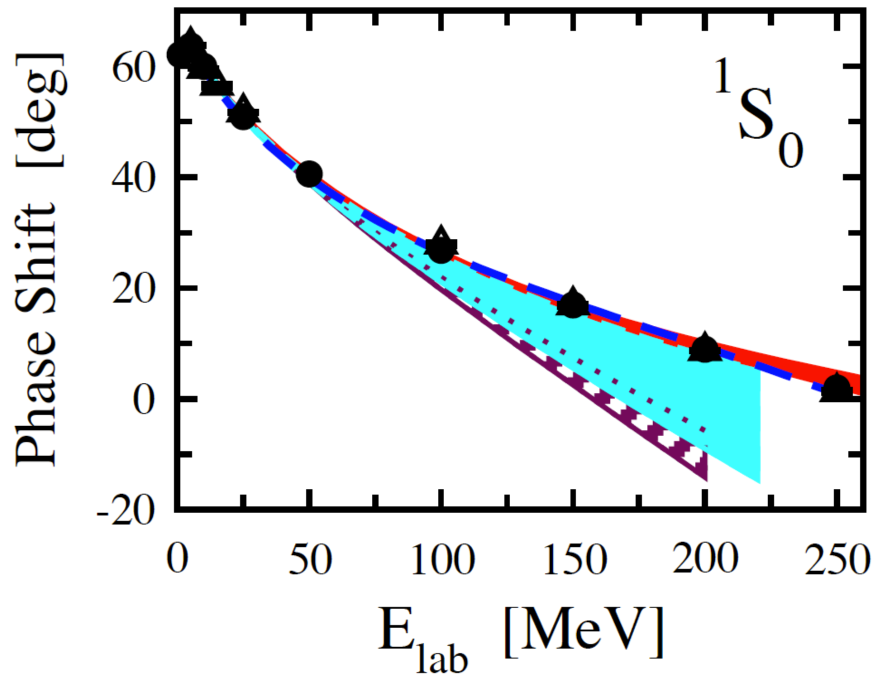
Key: Separation of scales

Fig.: Bertsch, Dean, Nazarewicz, SciDAC review (2007)

Nuclear forces from chiral effective field theory

[Weinberg; van Kolck; Epelbaum, Gloeckle, Meissner; Entem & Machleidt; …]



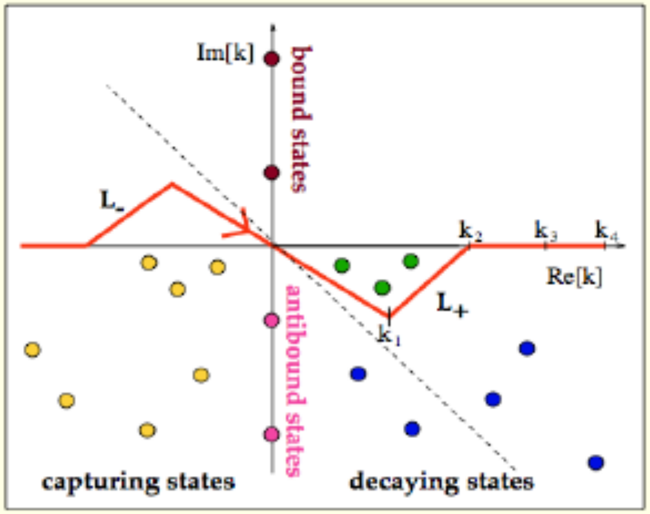


[Epelbaum, Hammer, Meissner RMP 81, 1773 (2009)]

Low energy constants from fit of NN data, A=3,4 nuclei, or light nuclei.

Gamow Shell Model (2002)

Gamow shell model for open quantum systems

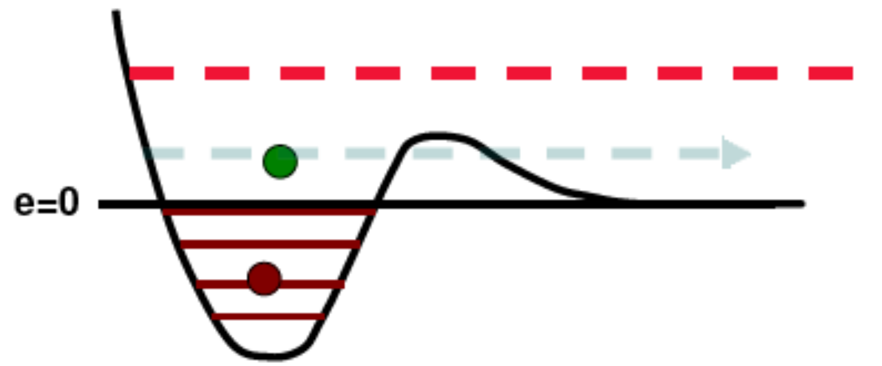


$$\sum_{n=b,r} |u_n\rangle\langle\tilde{u}_n| + \frac{1}{\pi}\int_{L_+} |u(k)\rangle\langle u(k^*)|\, dk = 1$$

particular case: Newton completeness relation

$$\sum_{n=b} |u_n\rangle\langle\tilde{u}_n| + \frac{1}{\pi}\int_{R} |u(k)\rangle\langle u(k^*)|\, dk = 1$$

(N. Michel *et al*, PRL 89 (2002) 042502)



complex-symmetric eigenvalue problem for hermitian hamiltonian

Review: Michel et al., J. Phys. G **36**, 013101 (2009)

Computational tool: coupled-cluster method

[Coester (1958); Coester & Kümmel (1960); (… many others …); Bartlett & Musial (2007); Hagen, TP, Dean, & Hjorth-Jensen (2014)]

Coupled-cluster method (in CCSD approximation)

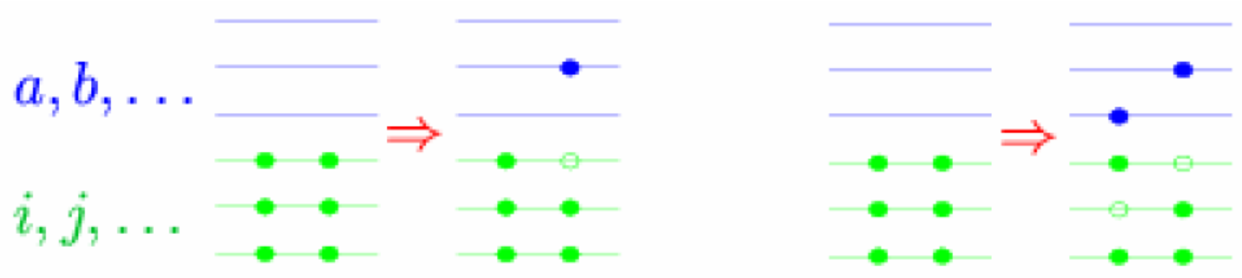
[Hagen, TP, Hjorth-Jensen, Dean, Rep. Prog. Phys. 77, 096302 (2014); arXiv:1312.7872]

Ansatz:

$$
\begin{aligned}
|\Psi\rangle &= e^{T}|\Phi\rangle \\
T &= T_1 + T_2 + \ldots \\
T_1 &= \sum_{ia} t_i^a a_a^\dagger a_i \\
T_2 &= \sum_{ijab} t_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i
\end{aligned}
$$

- ☺ Scales gently (polynomial) with increasing problem size o^2u^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!

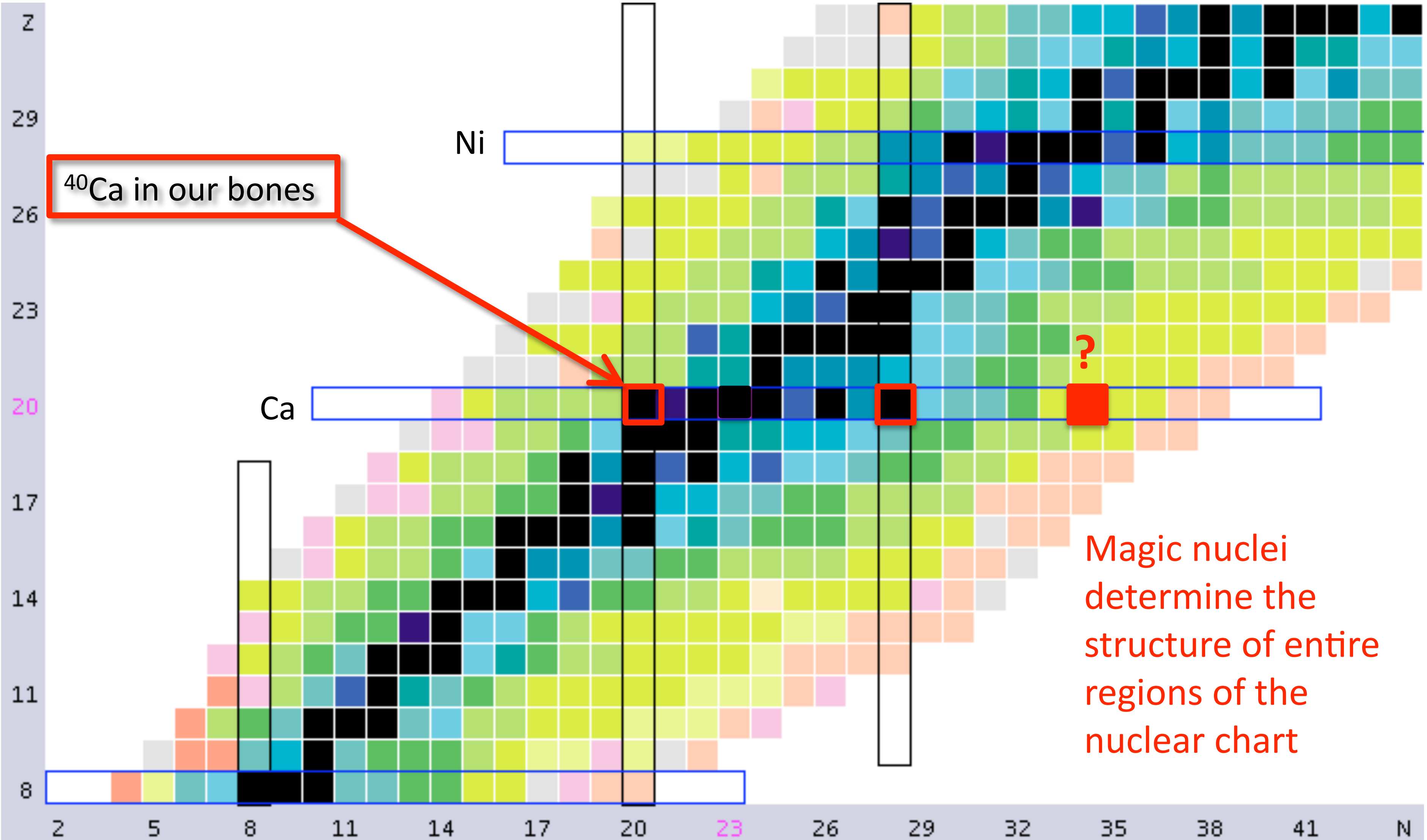


Coupled cluster equations

$$
\begin{aligned}
E &= \langle\Phi|\overline{H}|\Phi\rangle \\
0 &= \langle\Phi_i^a|\overline{H}|\Phi\rangle \\
0 &= \langle\Phi_{ij}^{ab}|\overline{H}|\Phi\rangle \\
\overline{H} &\equiv e^{-T}He^{T} = \left(He^{T}\right)_c = \left(H + HT_1 + HT_2 + \frac{1}{2}HT_1^2 + \ldots\right)_c
\end{aligned}
$$

Alternative view: CCSD generates similarity transformed Hamiltonian with no 1p-1h and no 2p-2h excitations.

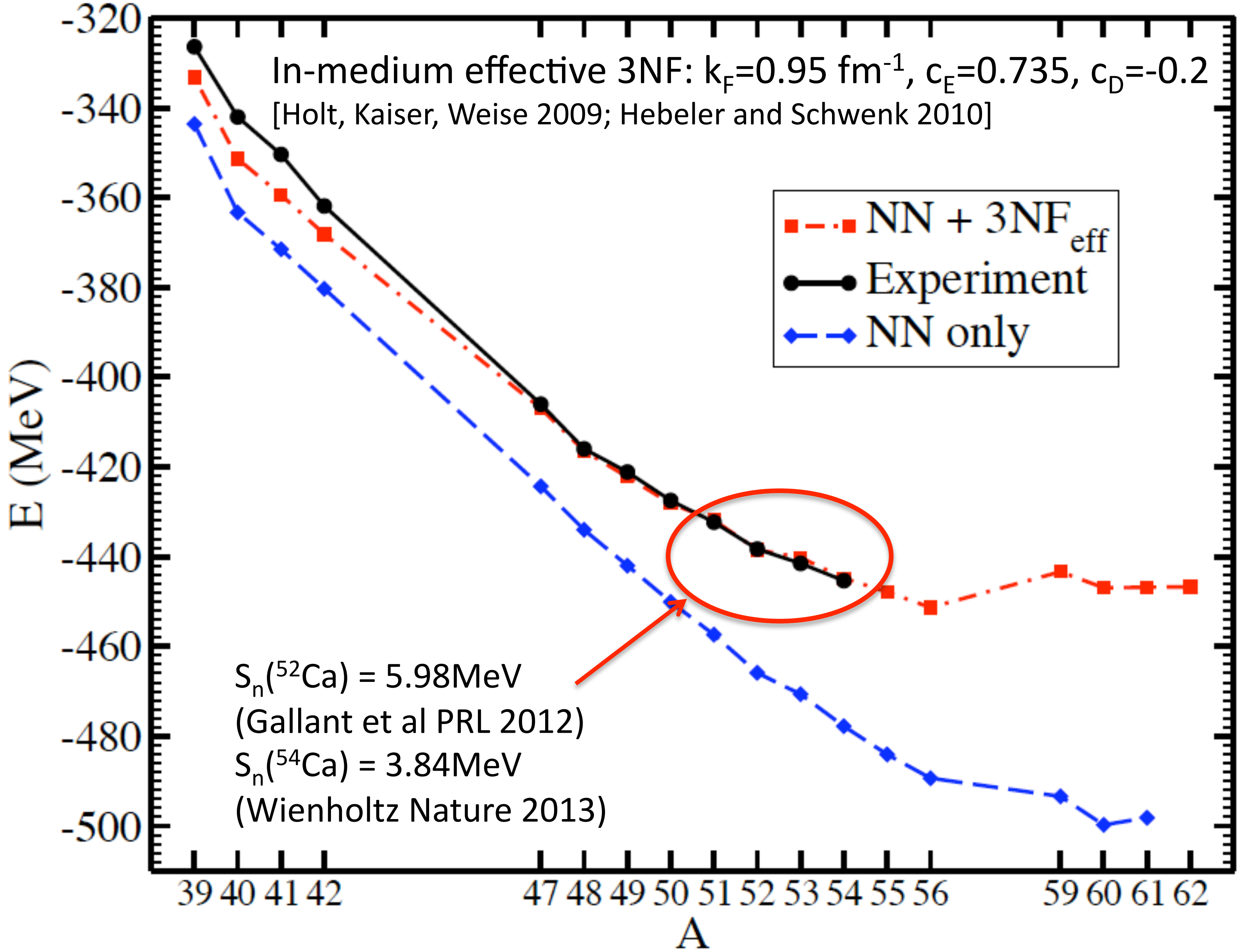
Is ^{54}Ca a magic nucleus?



Ca: Huck et al, PRC (1985); Ti: R. Janssens et al, PLB (2002); Cr: Prisciandaro et al, PRC (2001)

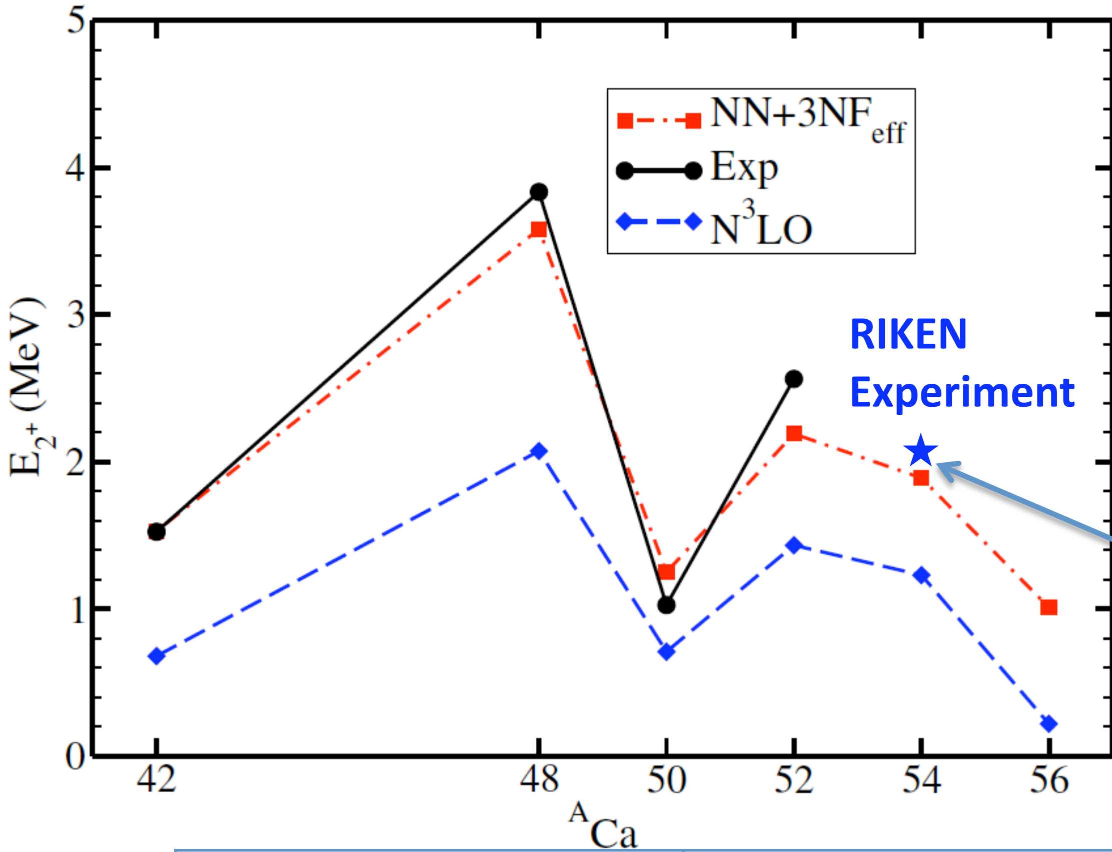
Calcium isotopes from chiral interactions

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



Shell structure of ^{52,54}Ca

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



Indicators of shell closure:

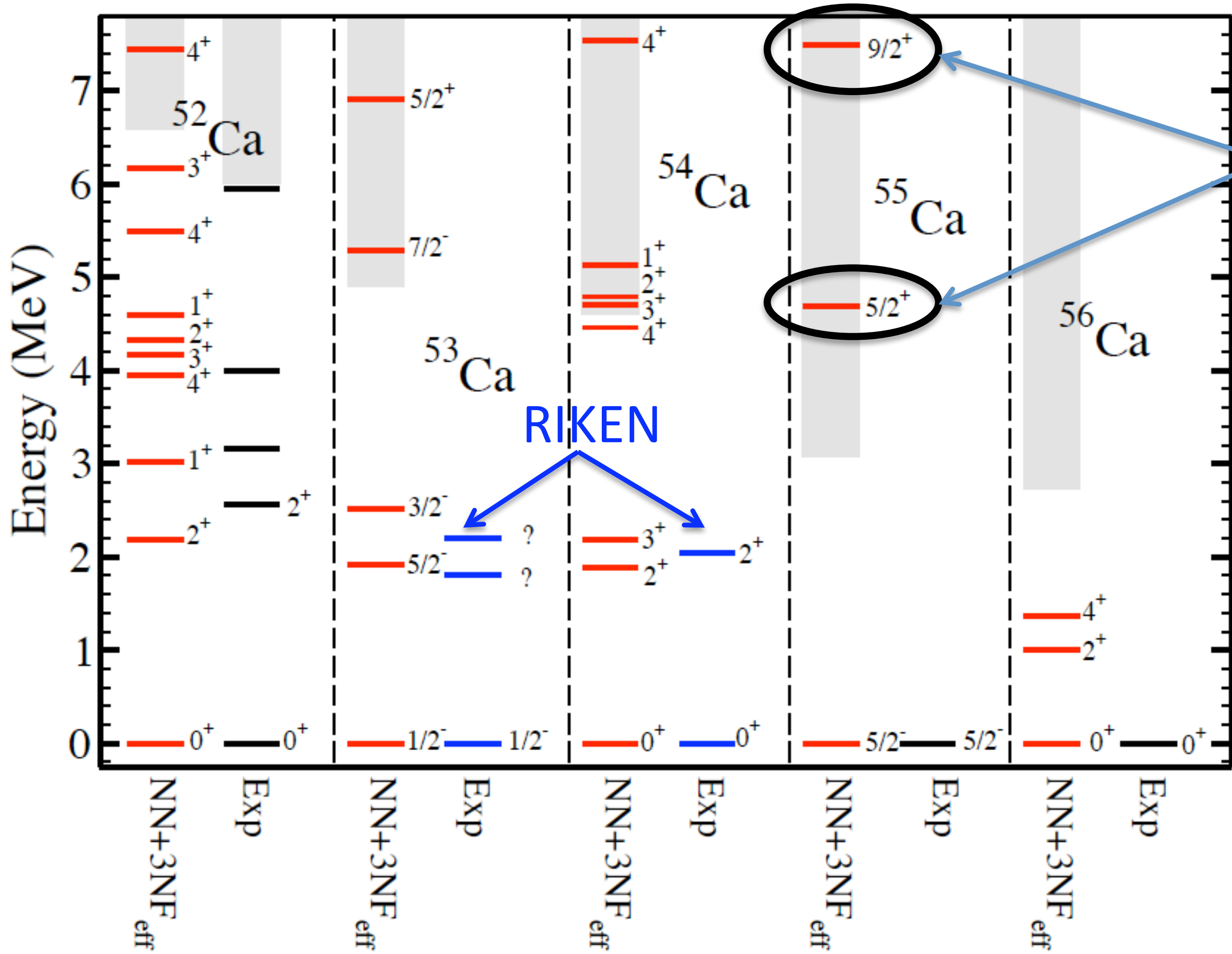
- Separation energy
- 2^+ excited state
- $4^+/2^+$ ratio

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

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

	^{48}Ca			^{52}Ca			^{54}Ca		
	2^+	4^+	$4^+/2^+$	2^+	4^+	$4^+/2^+$	2^+	4^+	$4^+/2^+$
CC	3.58	4.20	1.17	2.19	3.95	1.80	1.89	4.46	2.36
Exp	3.83	4.50	1.17	2.56	?	?	?	?	?

Spectra and shell evolution in Calcium isotopes



1. Our prediction for excited $5/2^-$ and $½^-$ 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

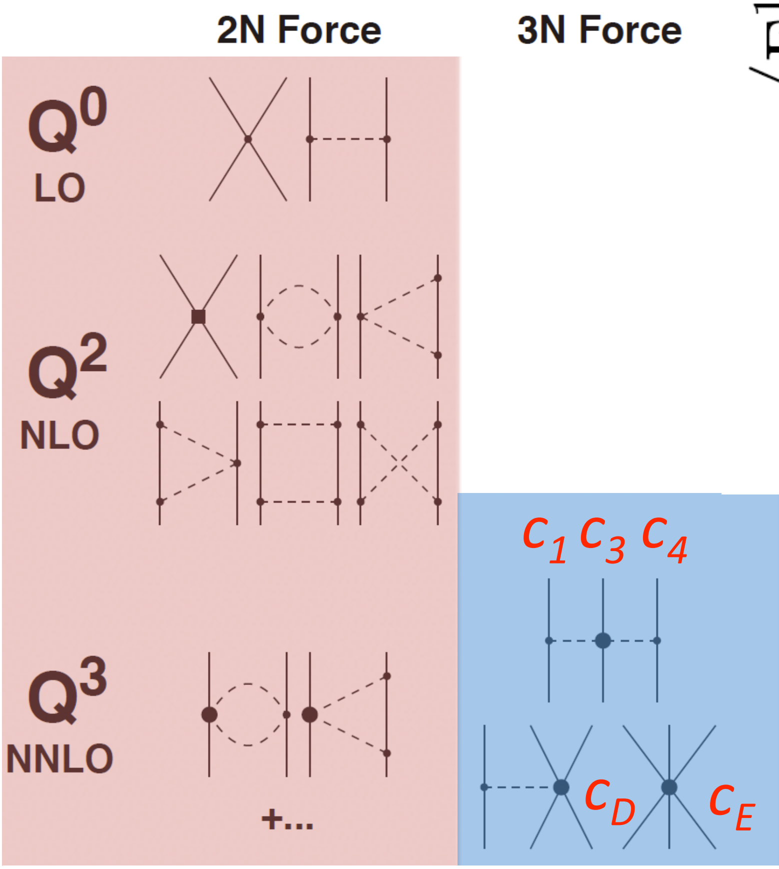
Continuum coupling relevant for level ordering

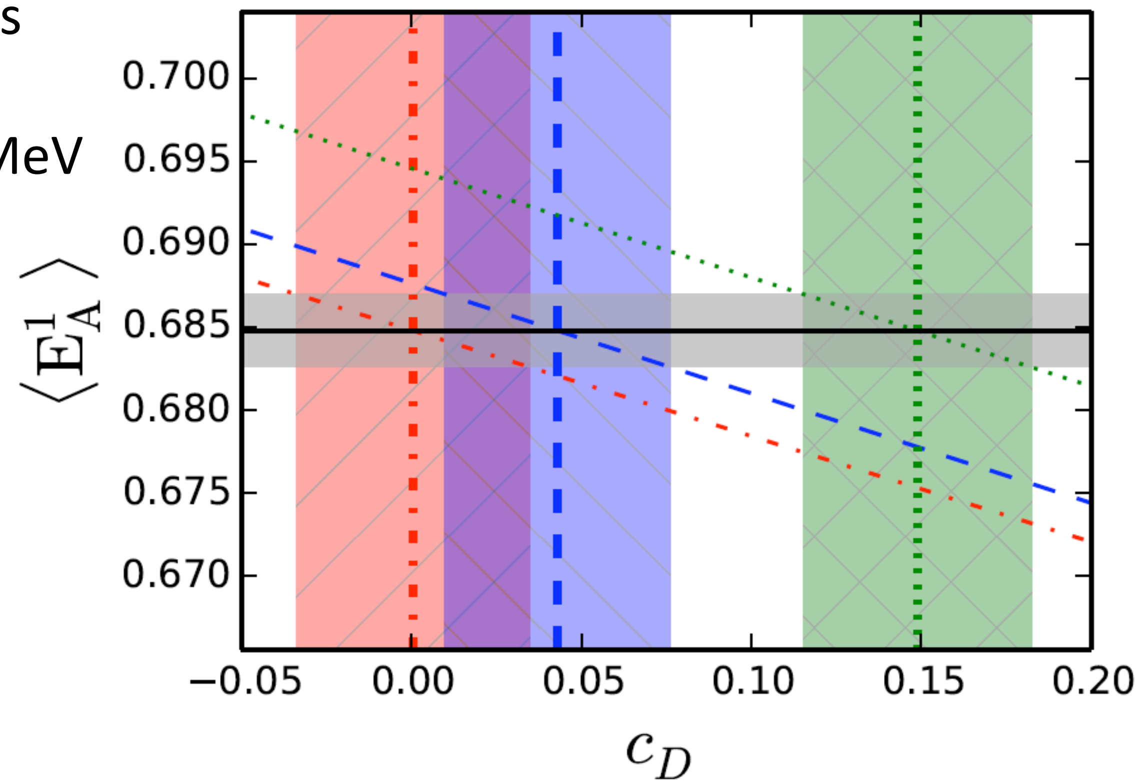
Three-nucleon forces and two-body currents in β decay

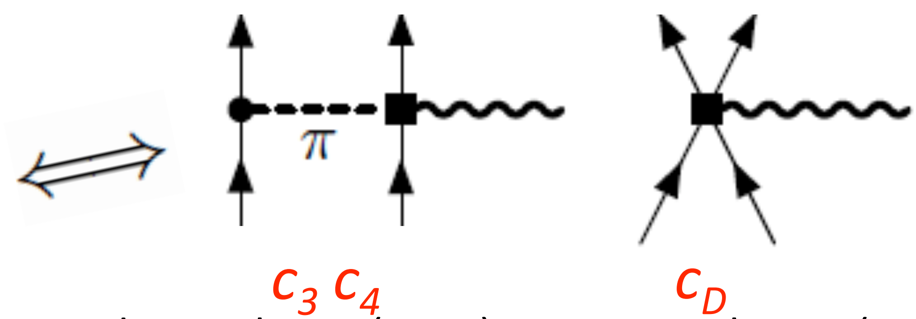
Ekström, Jansen, Wendt, Hagen, TP, Bacca, Carlsson, Gazit, arXiv:1406.4696

c_D, c_E fit to A=3 binding energies and the ^{3}H half life at NNLO for chiral cutoffs Λ = 450,500,550 MeV

[c_D, c_E] = [0.043, -0.501]





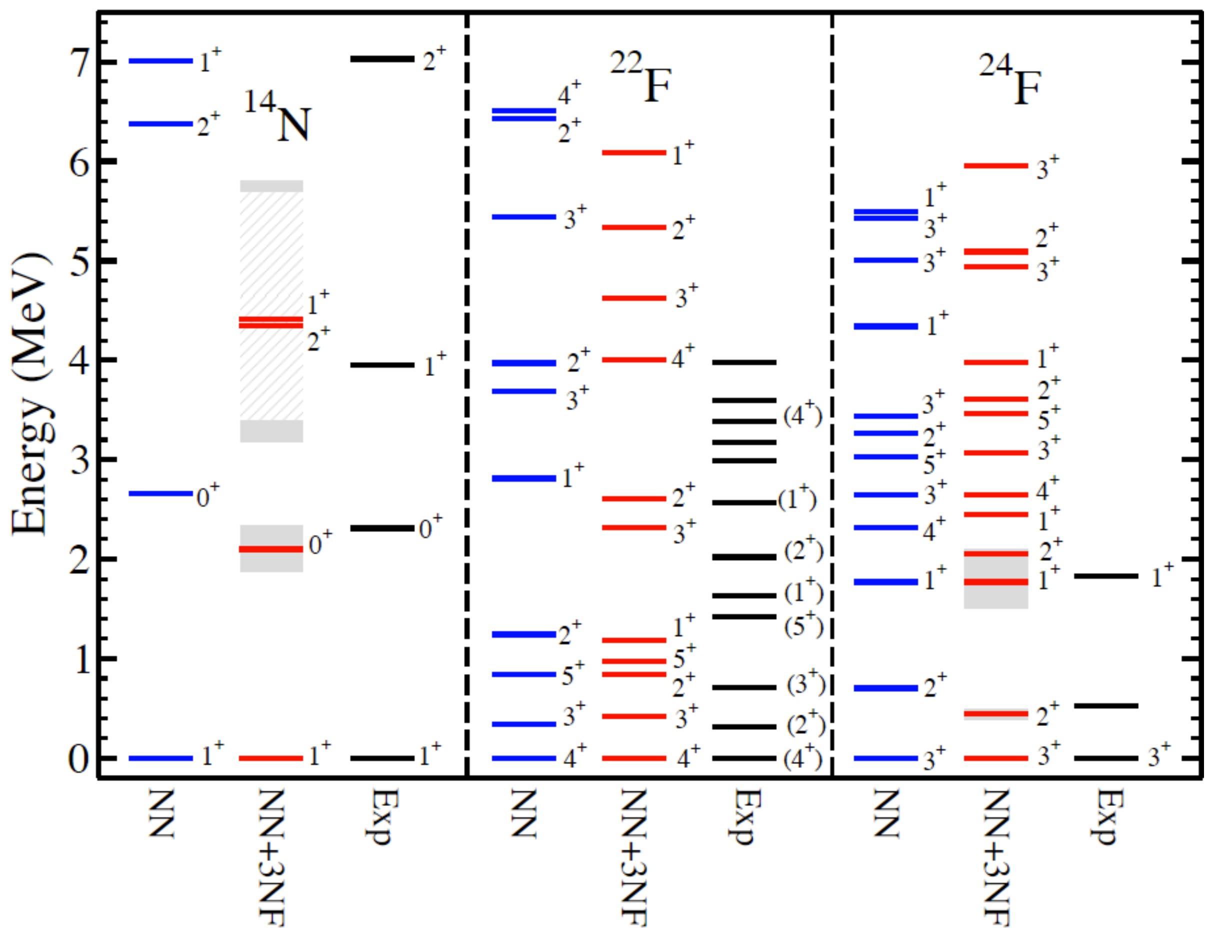


Menendez et al, PRL (2011); Lovato et al., PRL (2014); Pastore et al, PRC (2013)

Isospin breaking equation-of-motion technique for odd-odd nuclei

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

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



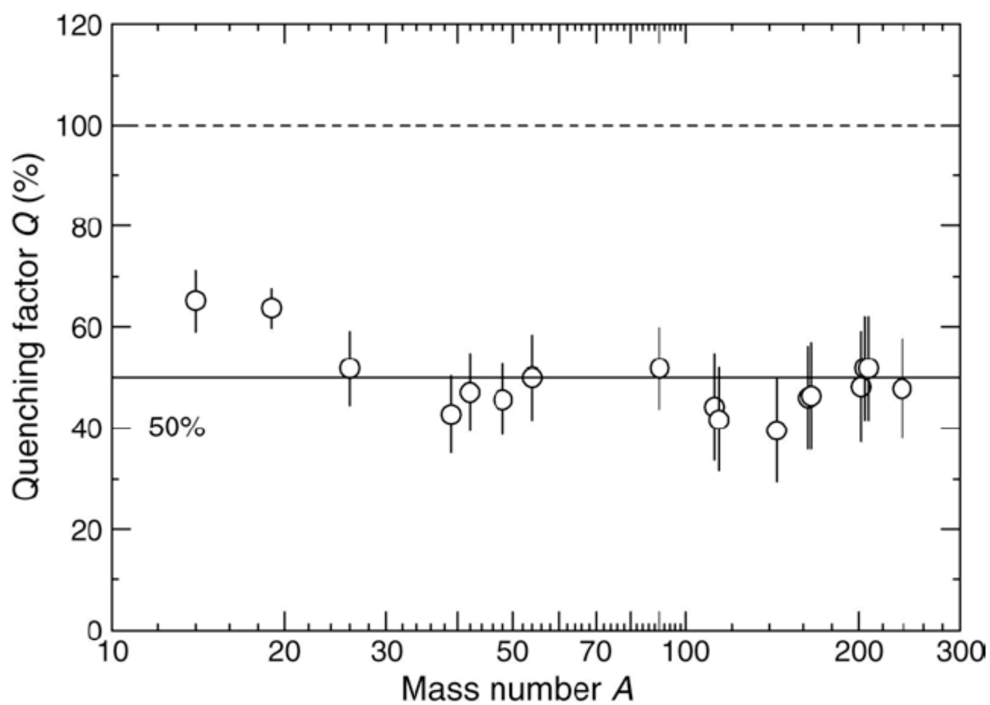
- Compute spectra of daughter nuclei as beta decays of mother nuclei
- Level densities in daughter nuclei increase slightly with 3NF
- Predictions for neutron rich fluorine
- Few error bars from cutoff variation
- (BE too small for ^{14}C, $^{22,24}O$)
- Gray bands: cut-off sensitivity

Quenching of Gamow-Teller strength in nuclei

The Ikeda sum-rule for στ⁻ operator $S^{\mathrm{N}}(\mathrm{GT}) = S^{\mathrm{N}}(\mathrm{GT}^{-}) - S^{\mathrm{N}}(\mathrm{GT}^{+}) = 3(N-Z)$

Measurement of Gamow-Teller strengths suggest a quenching *Q* of the Ikeda sum-rule

$$Q = \frac{S^{-}_{\mathrm{GT}}(\omega^{-}_{\mathrm{top}}) - S^{+}_{\mathrm{GT}}(\omega^{+}_{\mathrm{top}})}{3(N-Z)}$$



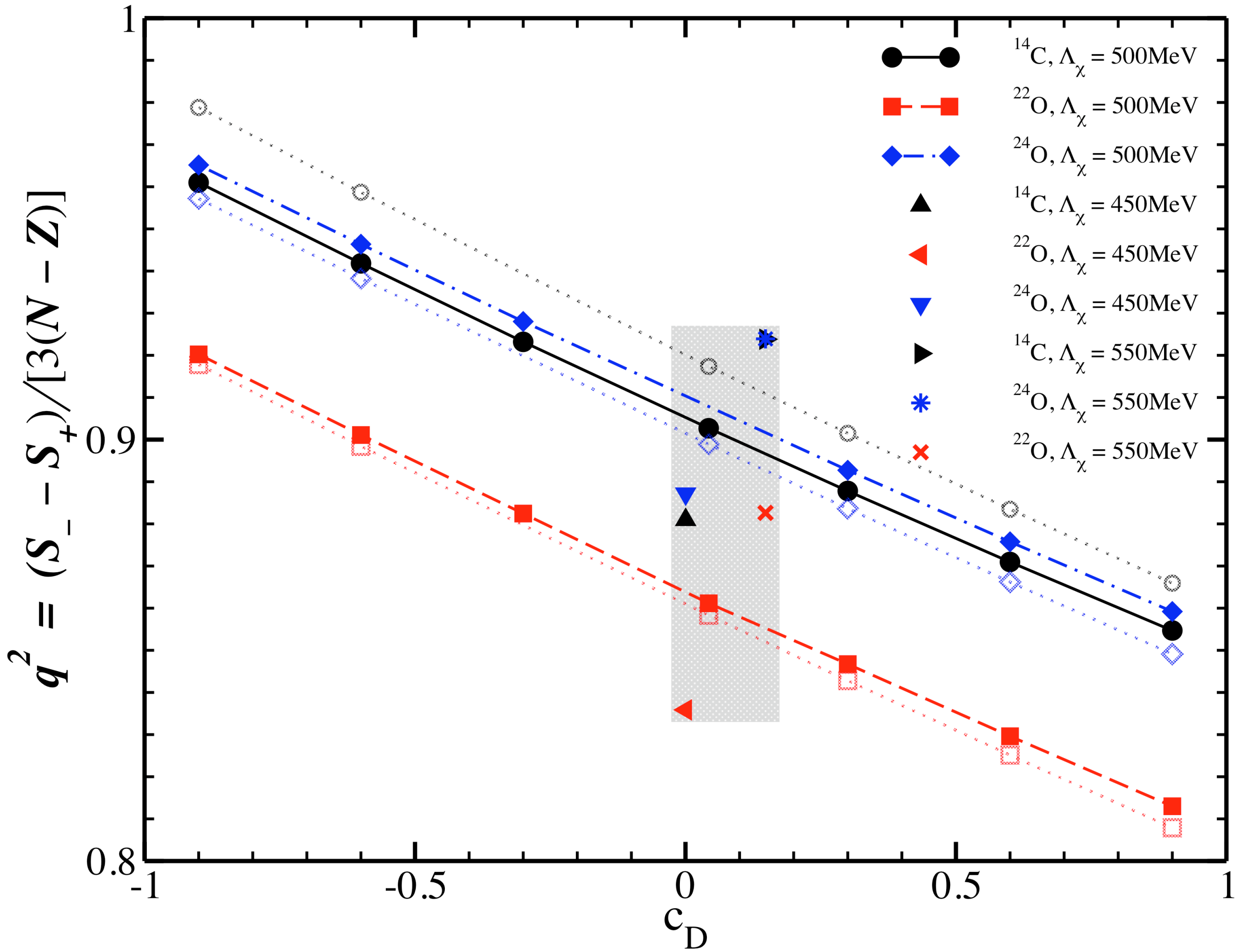
Surprisingly large quenching *Q* (50%) obtained from (*p*,*n*) experiments. The excitation energies were just above the giant Gamow-Teller resonance ~10-15MeV [Gaarde 1983].

- Measurements of GT strengths to high energies [Sasano et al 2009, Yako et al 2005] suggest 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 do two-body currents and three-nucleon forces add to this long-standing problem?

Quenching of Gamow-Teller strength in nuclei

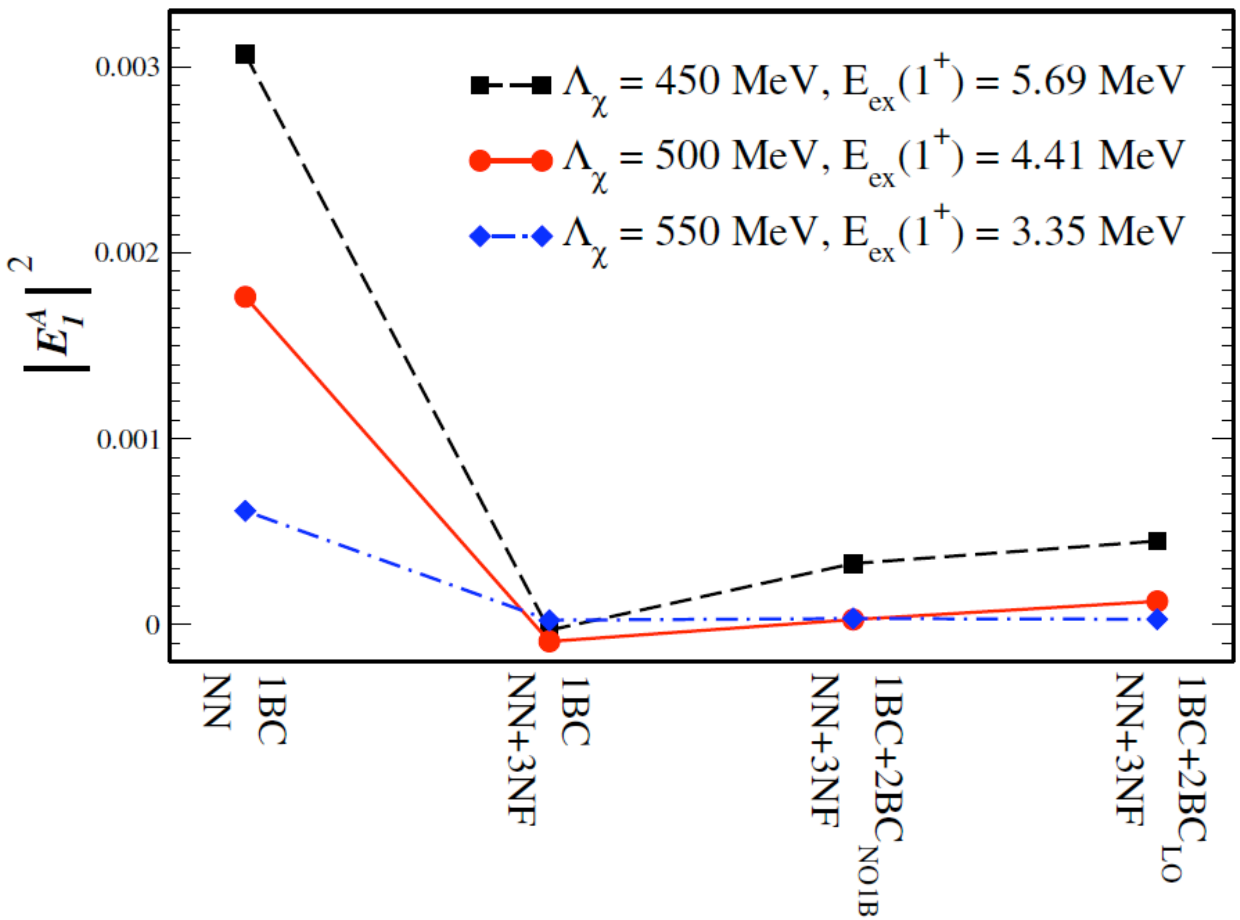


- Quenching of the Ikeda sum rule in ^{14}C and $^{22,24}O$ for different cutoffs
- Gray area reproduces triton half-life
- Quenching factor $q^2 \approx 0.84\text{-}0.92$.
- Significant GT strength above 10 MeV

Ekström, Jansen, Wendt, Hagen, TP, Bacca, Carlsson, Gazit, arXiv:1406.4696

Anomalous life-time (5700 years) of ^{14}C revisited

3NF main contributor to long half life: J. W. Holt et al., PRL (2008); Maris et al, PRL (2011)



Life time of ^{14}C depends on 3NFs, 2BCs and the energy of the first excited 1^+ state in ^{14}N.

- 3NFs decrease the transition matrix element significantly [Maris et al 2011]
- 2BC counter the effect of 3NFs to some degree.
- The transition matrix decreases with decreasing energy of the first excited 1^+ state in ^{14}N.

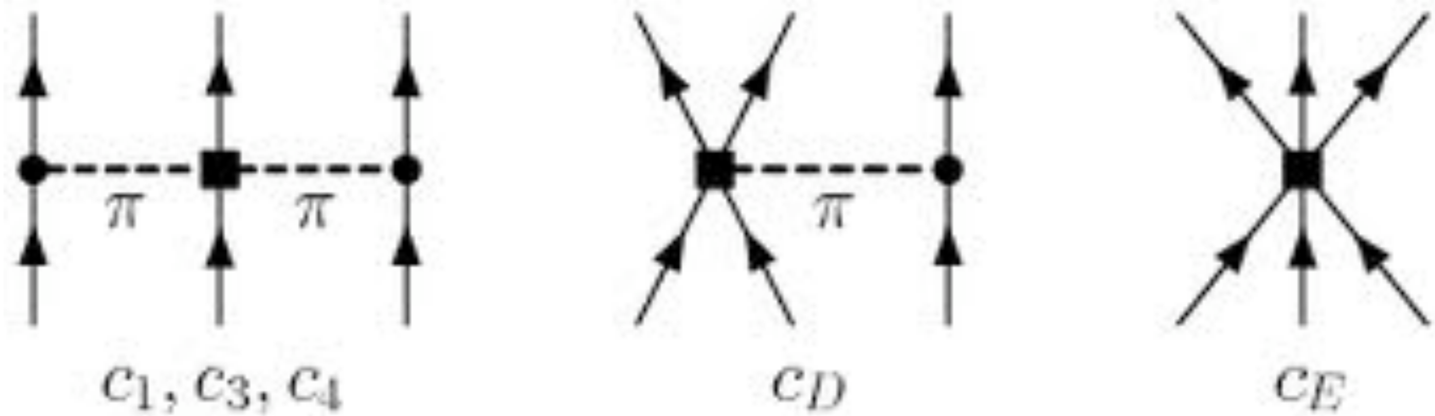
E_1^A varies between 5×10^{-3} to 2×10^{-2} which is more orders of magnitude larger than the empirical value ~6×10^{-6} extracted from the 5700 years half life of ^{14}C

Ekström, Jansen, Wendt, Hagen, TP, Bacca, Carlsson, Gazit, arXiv:1406.4696

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

$$H_N = \sum_{pq} \langle \mathbf{k}_p | f | \mathbf{k}_q \rangle \, a_p^\dagger a_q + \frac{1}{4} \sum_{pqrs} \langle \mathbf{k}_p \mathbf{k}_q | v | \mathbf{k}_r \mathbf{k}_s \rangle \, a_p^\dagger a_q^\dagger a_s a_r$$
$$+ \frac{1}{36} \sum_{pqrstu} \langle \mathbf{k}_p \mathbf{k}_q \mathbf{k}_r | w | \mathbf{k}_s \mathbf{k}_t \mathbf{k}_u \rangle \, a_p^\dagger a_q^\dagger a_r^\dagger a_u a_t a_s . \qquad (10)$$

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

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

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

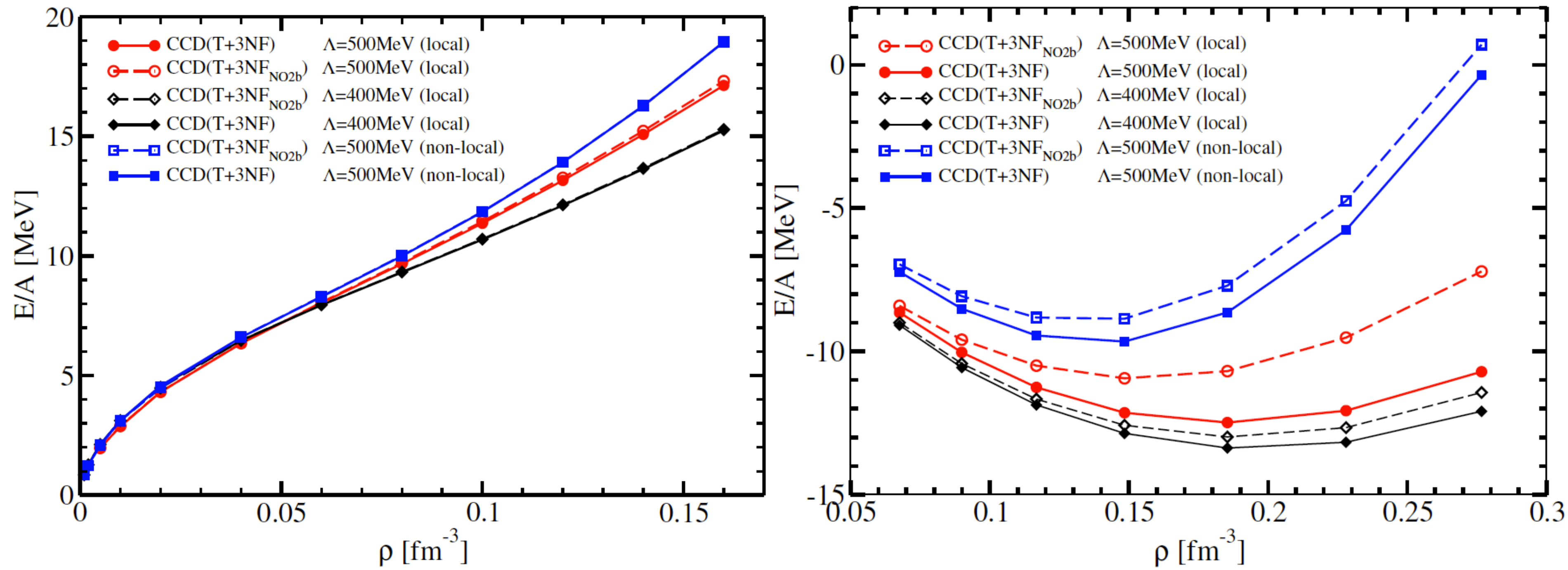
$$\langle \mathbf{k}_p \mathbf{k}_q | v | \mathbf{k}_r \mathbf{k}_s \rangle = \langle \mathbf{k}_p \mathbf{k}_q | V_{\mathrm{N}N} | \mathbf{k}_r \mathbf{k}_s \rangle$$
$$+ \sum_i \langle \mathbf{k}_p \mathbf{k}_q \mathbf{k}_i | V_{3\mathrm{NF}} | \mathbf{k}_i \mathbf{k}_r \mathbf{k}_s \rangle$$

“Residual” 3NF (enters leading triples correction)

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

Nucleonic matter with $NNLO_{opt}$ and 3NFs

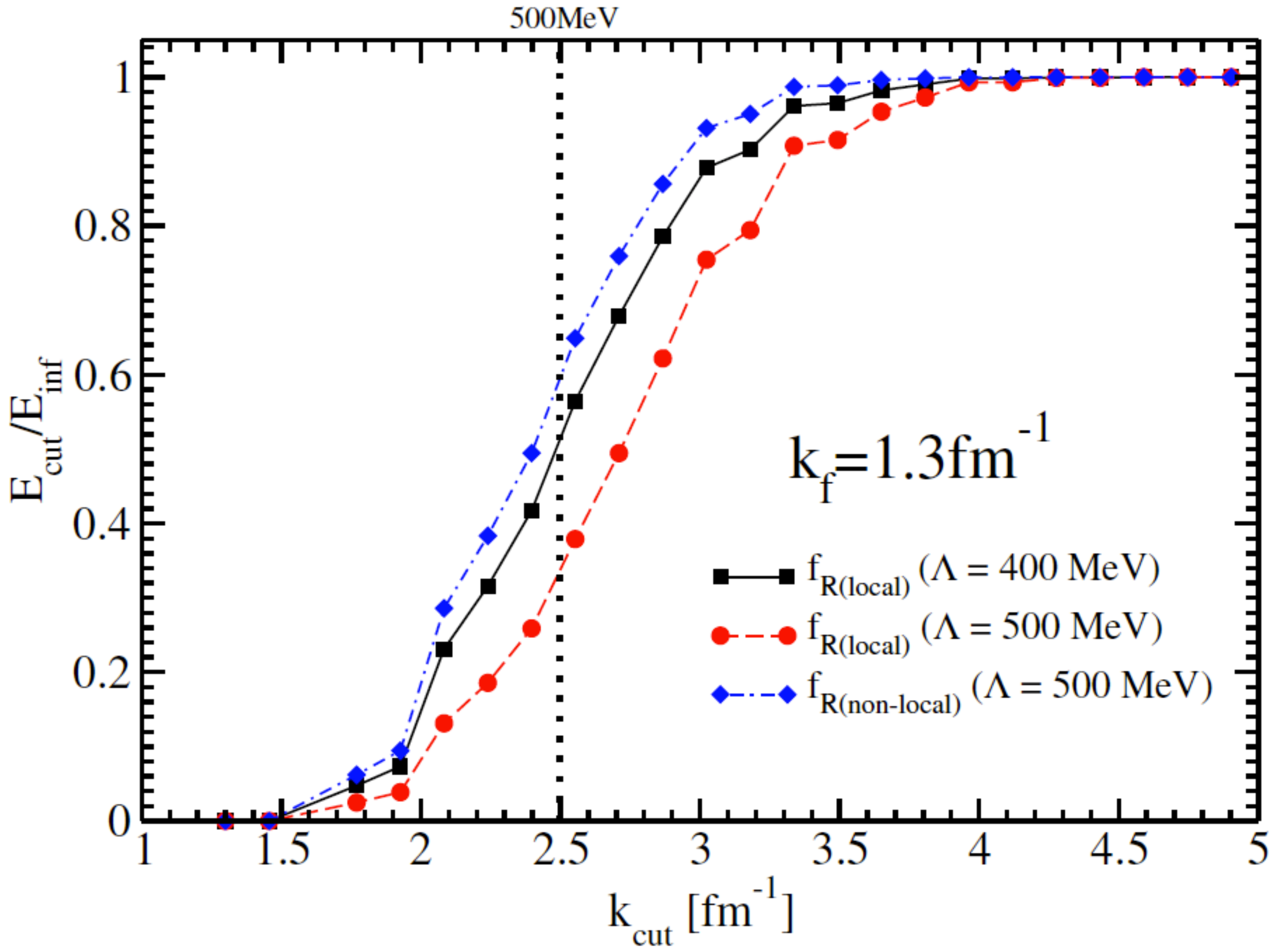
[Hagen, TP, Ekström, Wendt, Baardsen, Gandolfi, Hjorth-Jensen, Horowitz, PRC 89 014319 (2013)]



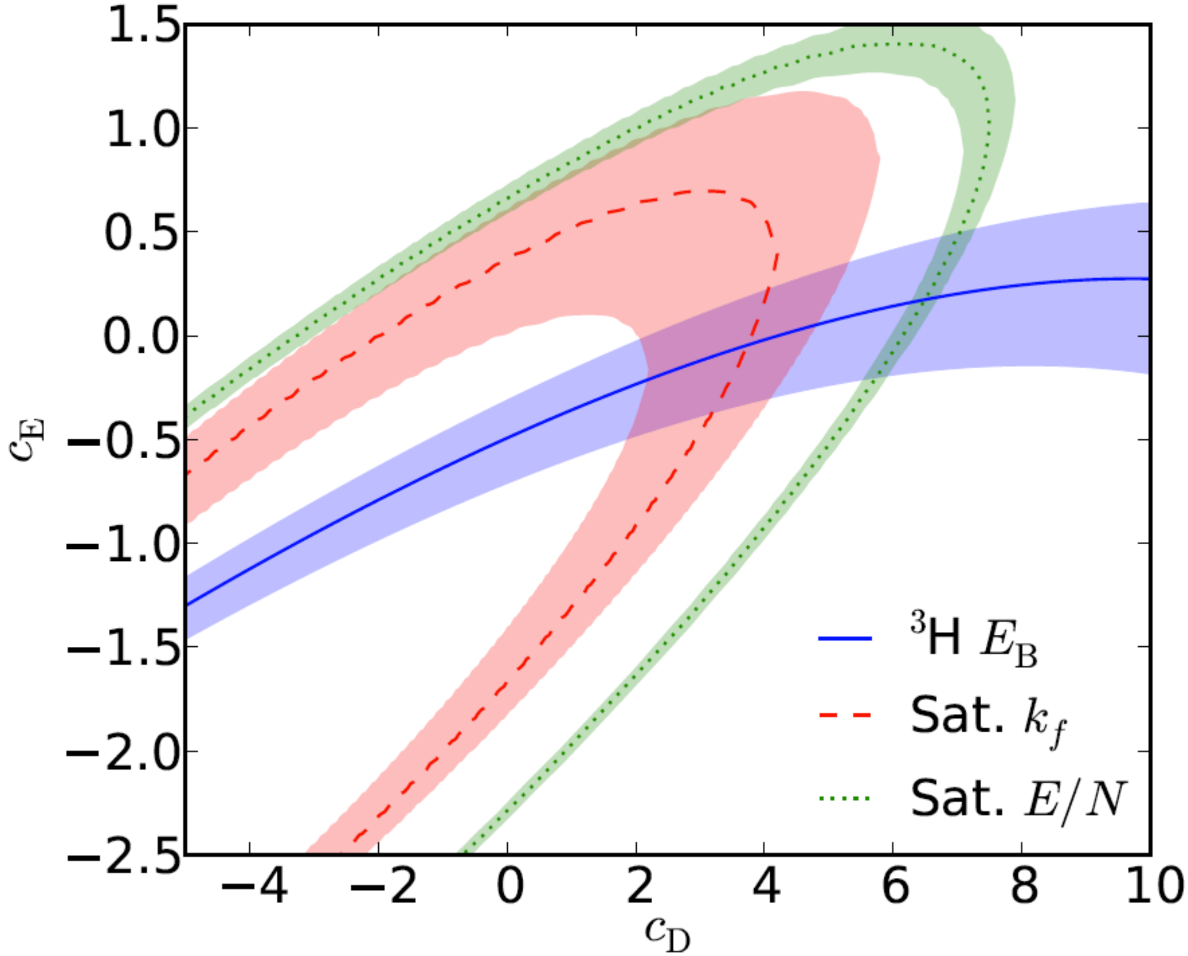
- 3NFs with different regulators and cutoffs act repulsively in neutron matter
- $N2LO_{opt}$ + 3NFs do not reproduce saturation density and binding energy of nuclear matter
- Strong dependence on regulator and cutoff in nuclear matter

… Light nuclei and neutron matter not very sensitive to saturation point.

Where actually does the cutoff cut off?



For NNLO$_{opt}$ no combination of c_D, c_E simultaneously satisfies light nuclei and nuclear matter



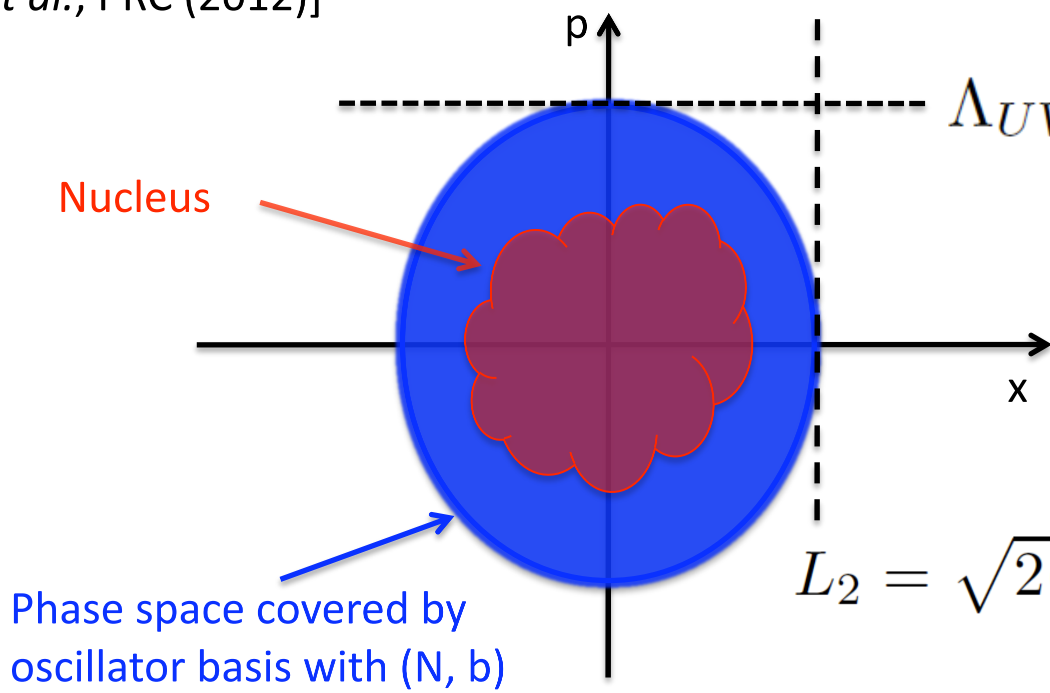
5% error bands for saturation k_f, E/N and binding energy of ^{3}H

☹ Variation of c_D and c_E not sufficient to simultaneously bind light nuclei and nuclear matter

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)]



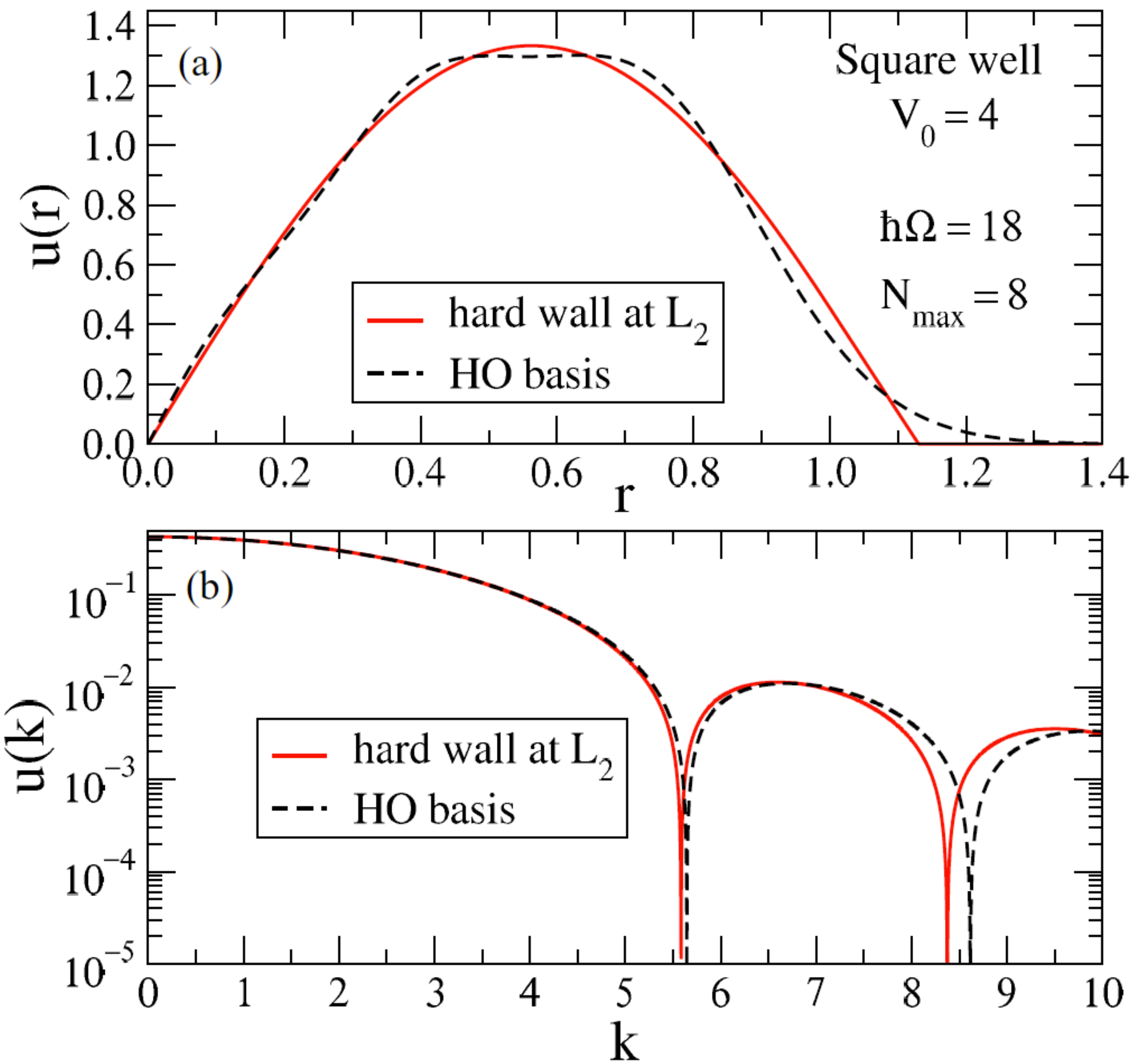
$$\Lambda_{UV} \equiv \sqrt{2(N+3/2)}\hbar/b$$

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

Nucleus needs to "fit" into basis:

- Nuclear radius R < L
- cutoff of interaction $\Lambda < \Lambda_{UV}$

For long wave lengths, a finite HO basis resembles a spherical box



ground wave functions in position space

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

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

Fourier transforms differ only at large momentum

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

IR corrections to bound-state energies

Simple view: A node in the wave function

$$u_E(r) \xrightarrow{r \gg R} A_E(e^{-k_E r} + \alpha_E e^{+k_E r})$$

At r=L yields computable corrections to observables.

Final results [Furnstahl, Hagen, TP, Phys. Rev. C 86, 031301 (2012); More, Ekström, Furnstahl, Hagen, TP, Phys. Rev. C 87, 044326 (2013); Furnstahl, More, TP, Phys. Rev. C 89, 044301 (2014)]

ANC^2 Binding momentum

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

only observables enter

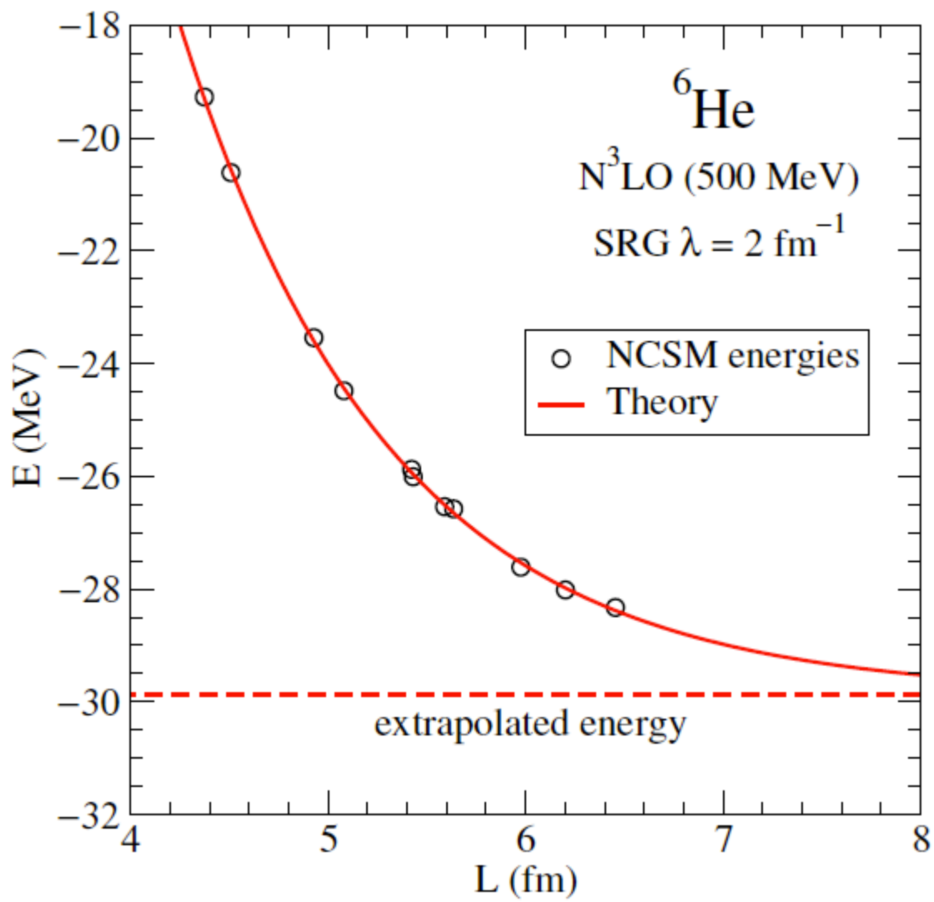
$$\langle r^2 \rangle_L \approx \langle r^2 \rangle_\infty [1 - (c_0 \beta^3 + c_1 \beta) e^{-\beta}] \qquad (\text{with } \beta \equiv 2k_\infty L)$$

Energy extrapolation explains findings by [Coon et al, Phys. Rev. C 86, 054002 (2012)]

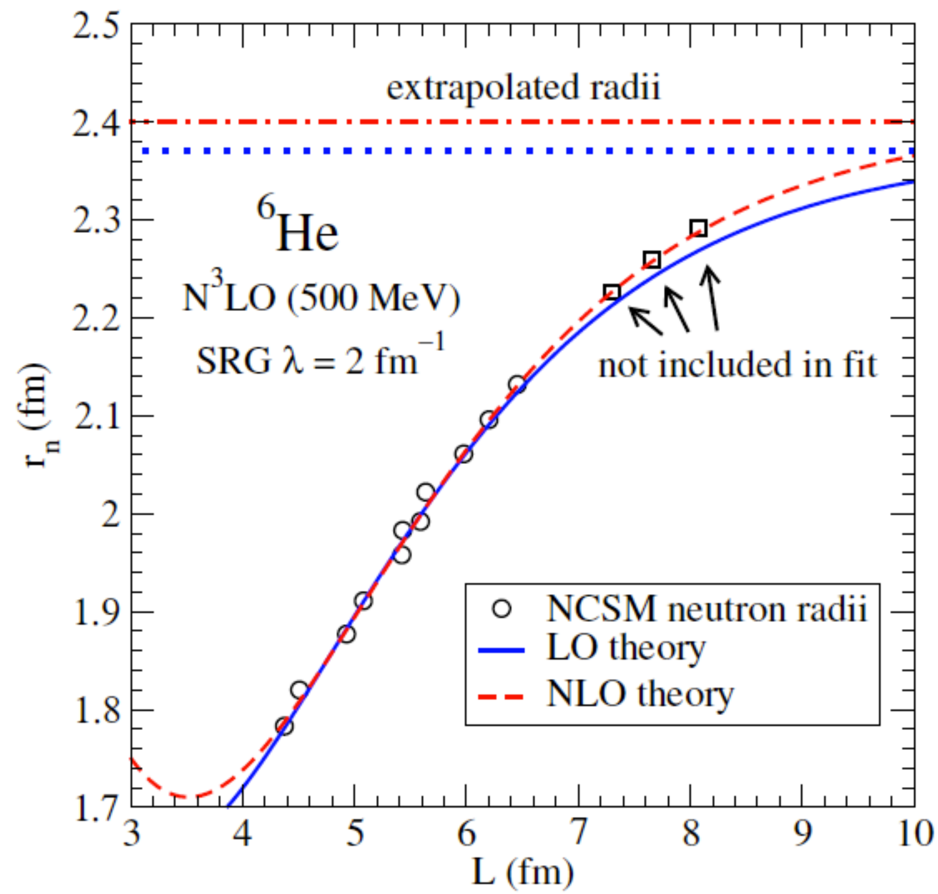
Corrections due to finite Hilbert spaces

- 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_∞ from energy fit

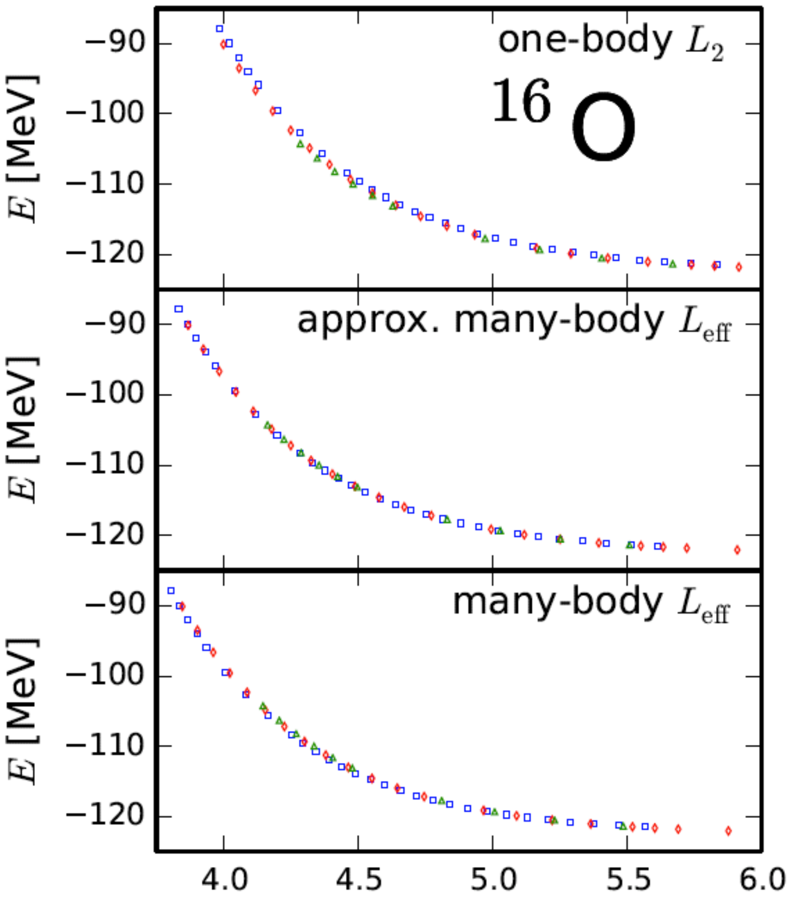
$$E_L = E_\infty + a_0 e^{-2k_\infty L}$$



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



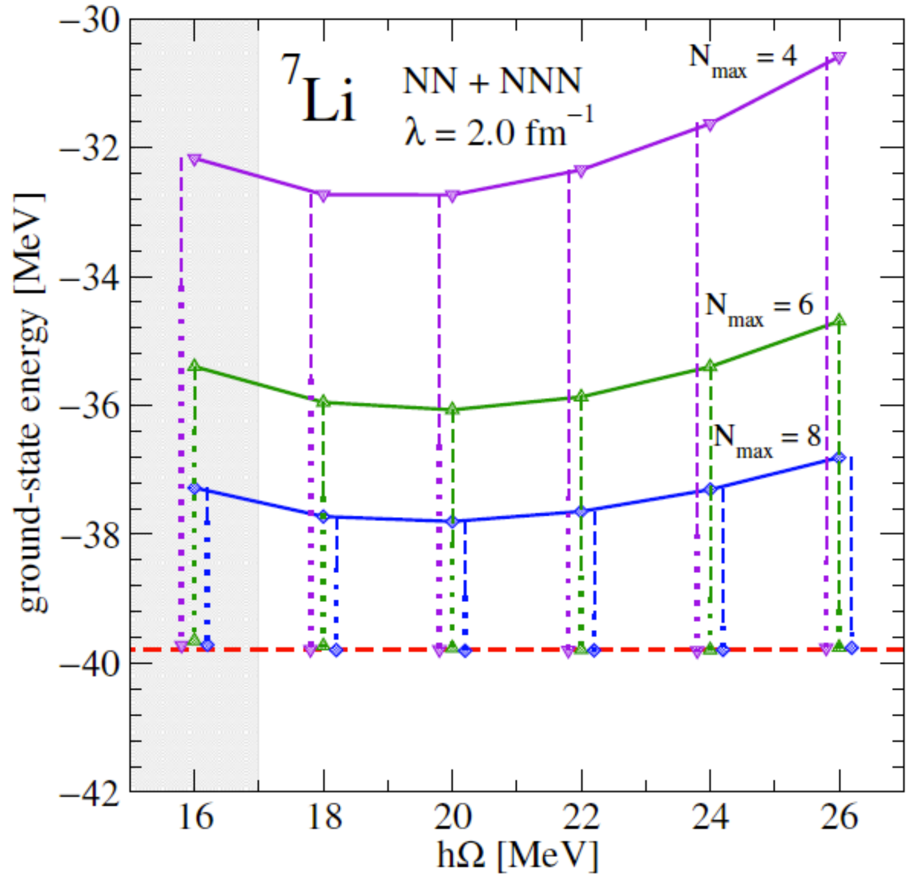
L_{eff} for many-fermion system
Furnstahl, Hagen, Wendt, TP (2014)



$$\sum_{nl} \nu_{nl} \kappa_{ln}^2 = \sum_{nl} \nu_{nl} \left(\frac{a_{l,n}}{L_{\rm eff}} \right)^2$$

K^2 = eigenvalue of squared momentum operator; $a_{l,n}$: n^{th} zero of spherical Bessel function $j_l(a_{l,n})=0$

Combind IR/UV extrapolations for SRG interactions [Jurgenson et al., PRC 2013]



$$E(\Lambda_{UV}, L) \approx E_\infty + B_0 e^{-2\Lambda_{UV}^2/B_1^2} + B_2 e^{-2k_\infty L}$$

Summary

- Coupled cluster method efficient tool for many nuclei of interest; with predictive power also for rare isotopes
- 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
- Role of 3NFs and 2BC in beta decay
  - quenching of Ikeda sum rule (~ 10% level)
  - 2BC slightly counter effects of 3NFs in ^{14}C beta decay
- Infrared extrapolations based on mapping of HO basis ←→ spherical box at long wave lengths; well-understood box size L_2; equivalent of Lüscher's formula for HO