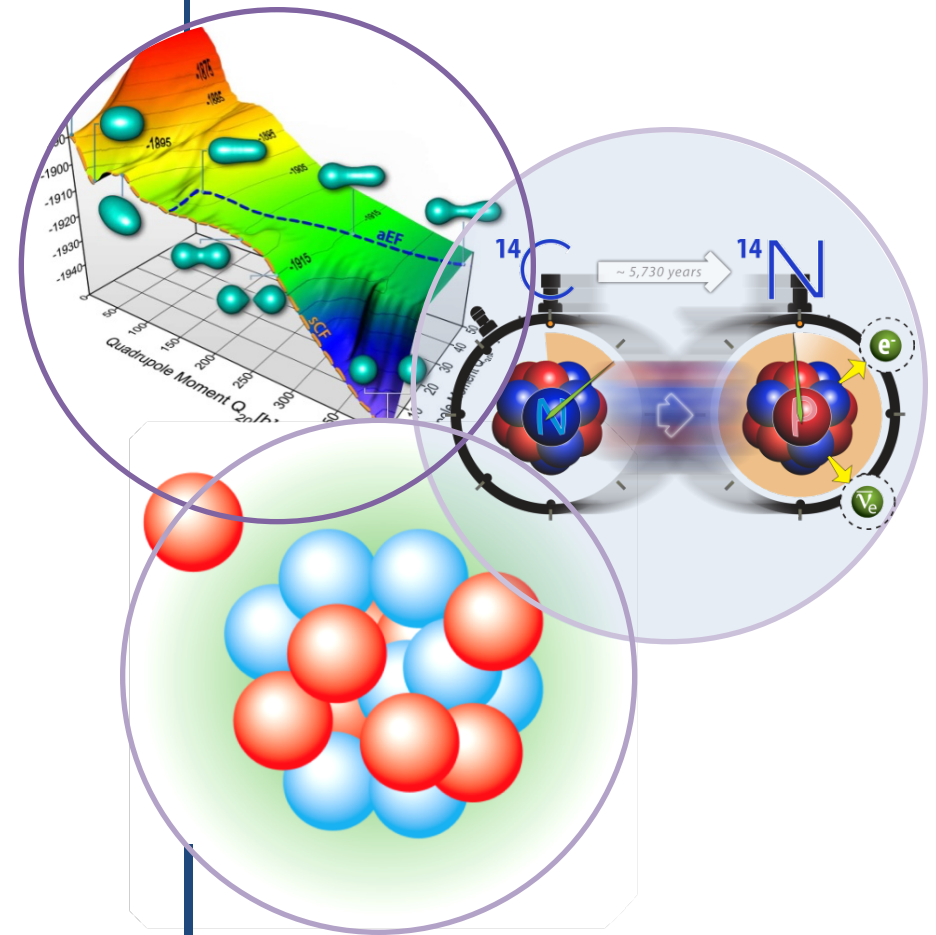


# Nuclear Structure Theory I

Interactions and currents from chiral effective field theory and renormalization group transformations

Gaute Hagen (ORNL)

ANL, EBSS, July 24<sup>th</sup>, 2017



# Contents of lectures

## Lecture 1: Nucleon-nucleon and three-nucleon interactions

- Phenomenological versus first principles approaches to nuclear structure.
- Nuclear interactions and currents from chiral effective field theory (EFT).
- Renormalization and effective interactions for the nuclear many-body problem.

## Lecture 2: Ab-initio approach to nuclear structure

- Brief introduction to ab-initio methods and nuclear structure, and status of the field.
- Coupled-cluster approaches to nuclear structure
- Role of three-nucleon forces in ab-initio nuclear structure calculations.

# Reading suggestions

[More is different](#), P. W. Anderson, *Science* **177**, 393 (1972)

[Elementary features of nuclear structure](#), B.R. Mottelson, in: H. Nifenecker, J.P. Blaizot, G. Bertsch, W. Weise, F. David (Eds.), *Trends in Nuclear Physics, 100 Years Later*, North-Holland, Amsterdam, 1998

## [Chiral effective field theory and nuclear forces](#)

- Machleidt & Entem, *Chiral effective field theory and nuclear forces*, *Phys. Rept.* 503, (2011); Machleidt, arXiv:0704.0807
- Epelbaum Hammer & Meißner, *Modern theory of nuclear forces*, *Rev. Mod. Phys.* **81**, 1773 (2009); arXiv:0811.1338
- P. Lepage, *How to Renormalize the Schrodinger Equation*, arXiv:nucl-th/9706029 (1997).

## [Low-momentum interactions and similarity transforms](#)

- Bogner, Furnstahl & Schwenk, *From low-momentum interactions to nuclear structure*, *Prog. Part. Nucl. Phys.* **65**, 94 (2010); arXiv:0912.3688

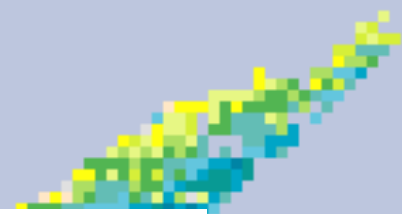
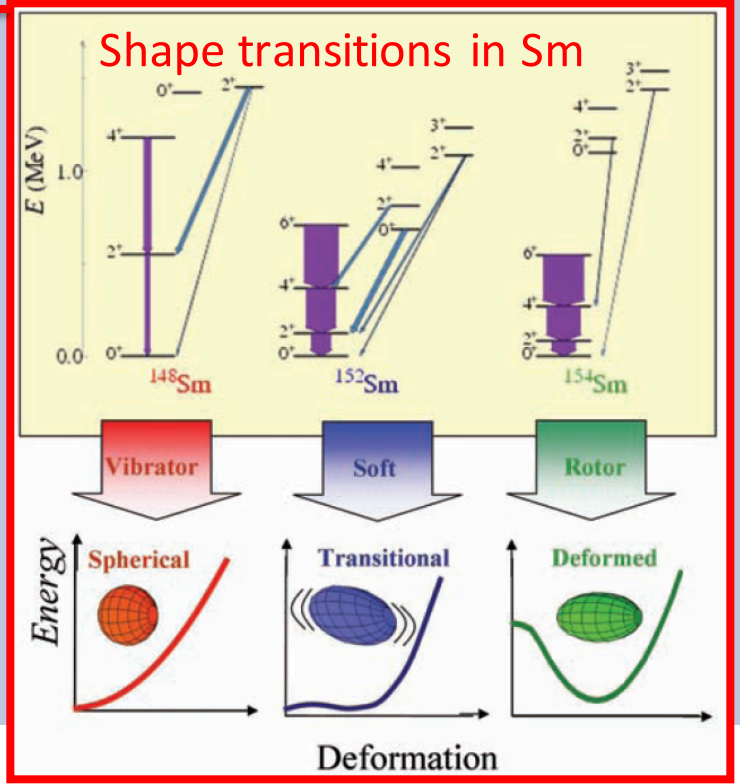
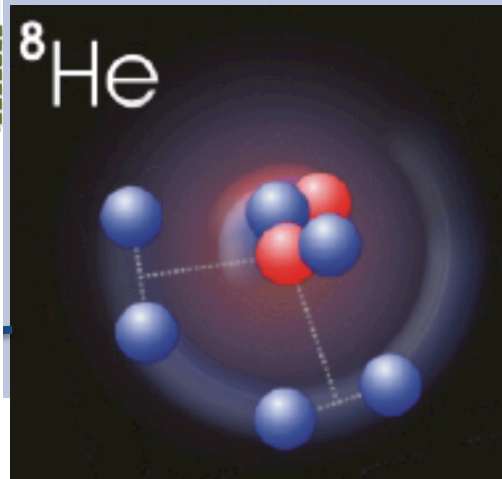
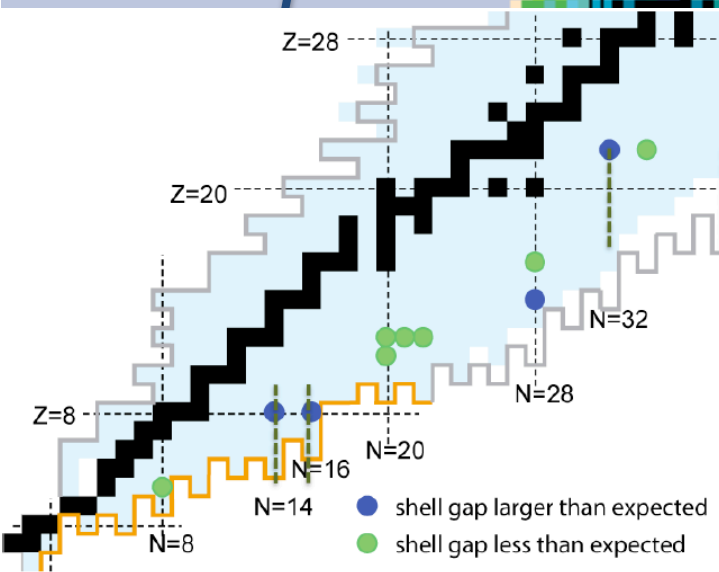
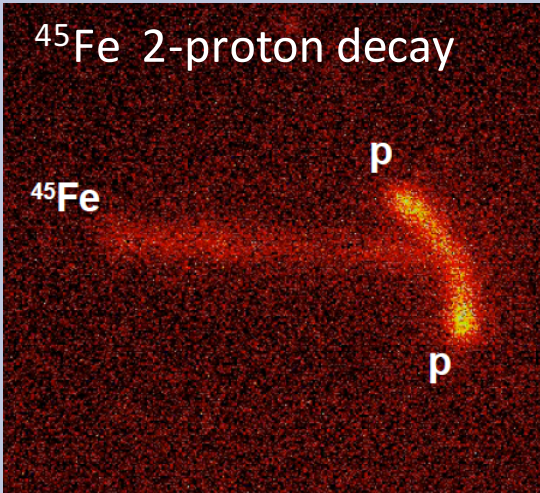
# Nuclei across the chart

118 chemical elements (94 naturally found on Earth)

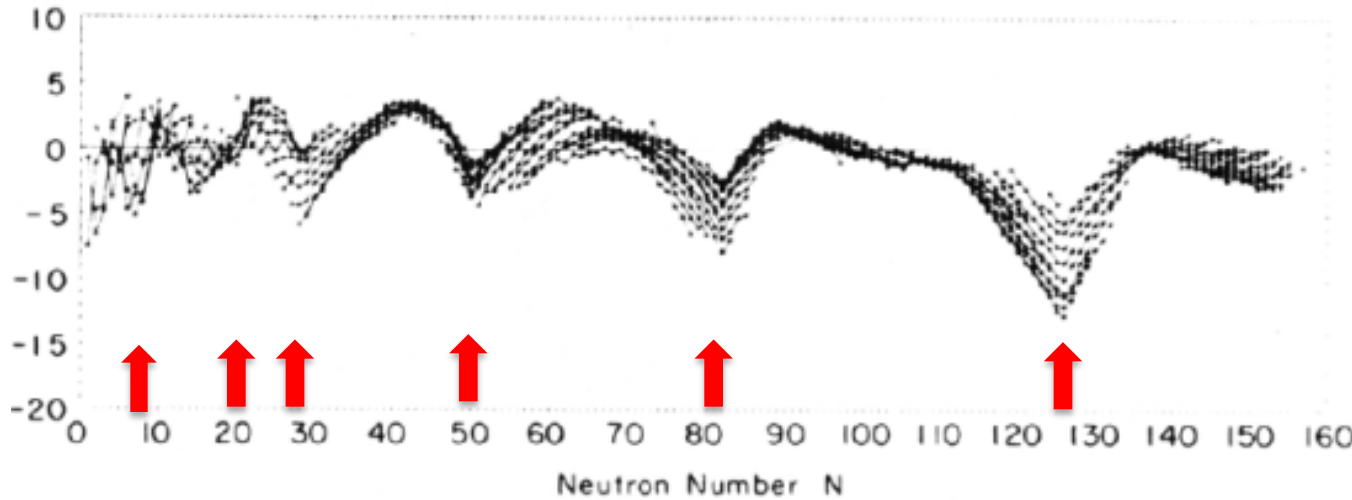
288 stable (primordial) isotopes

Thousands of short-lived isotopes – many with interesting properties

large isospin magnifies unknown physics  
clustering behavior  
novel evolution in structure



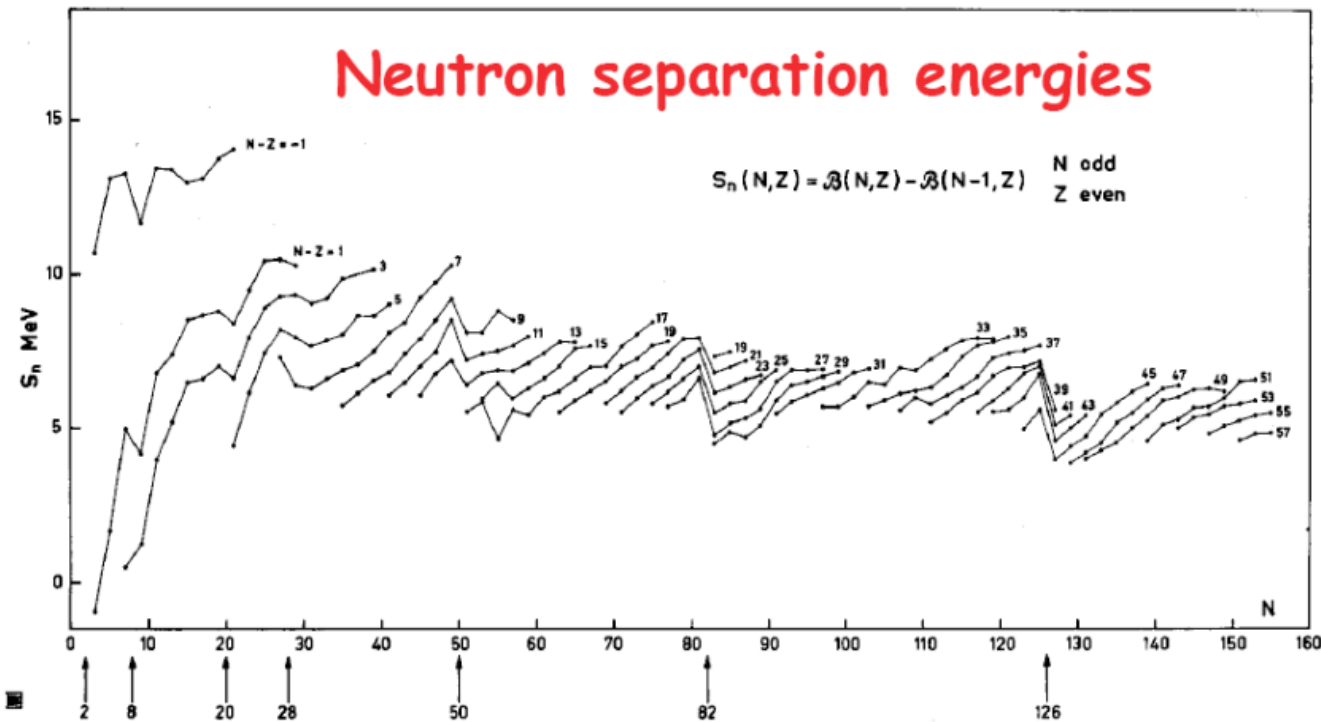
# Signatures of shell structure in nuclei



From W.D. Meyers and W.J. Swiatecki, Nucl. Phys. 81, 1 (1966).

Mass differences: Liquid drop – experiment. Minima at closed shells.

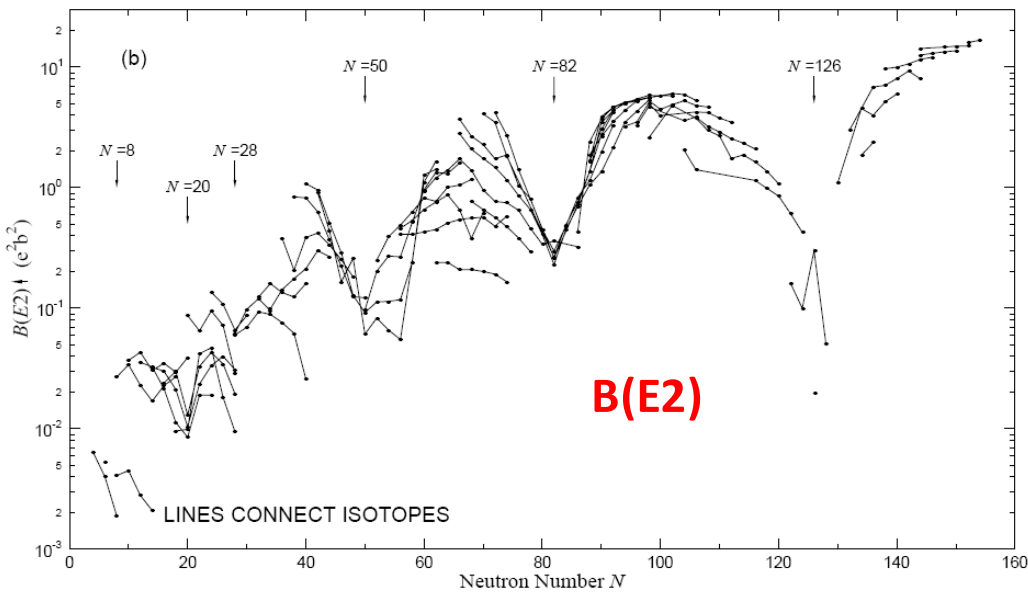
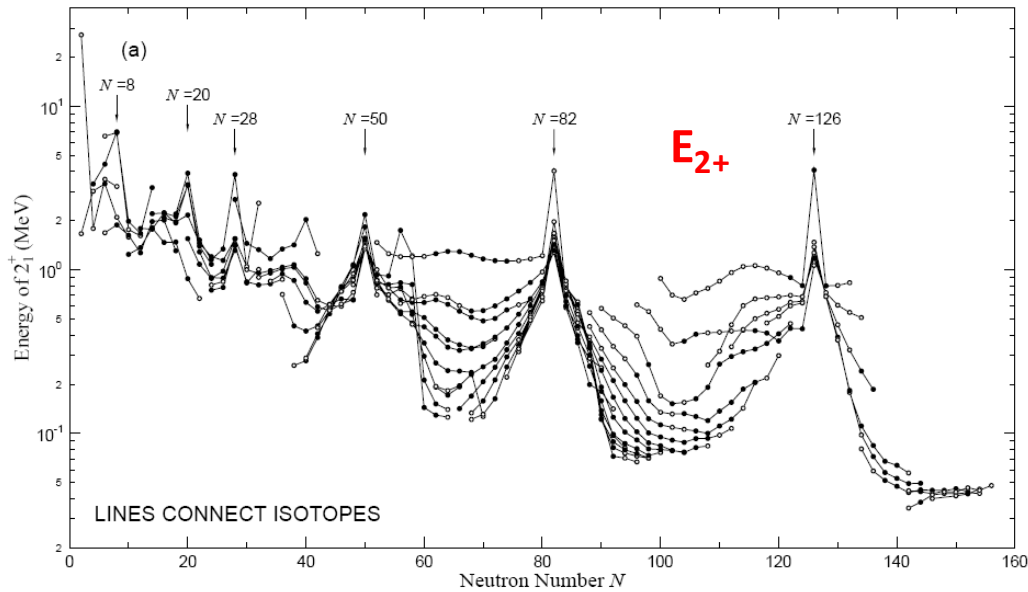
## Neutron separation energies



- Expensive to remove a neutron from a closed shell.
- Signature of magic shell closures for  $N=2, 8, 20, 28, 50, 82, 128$

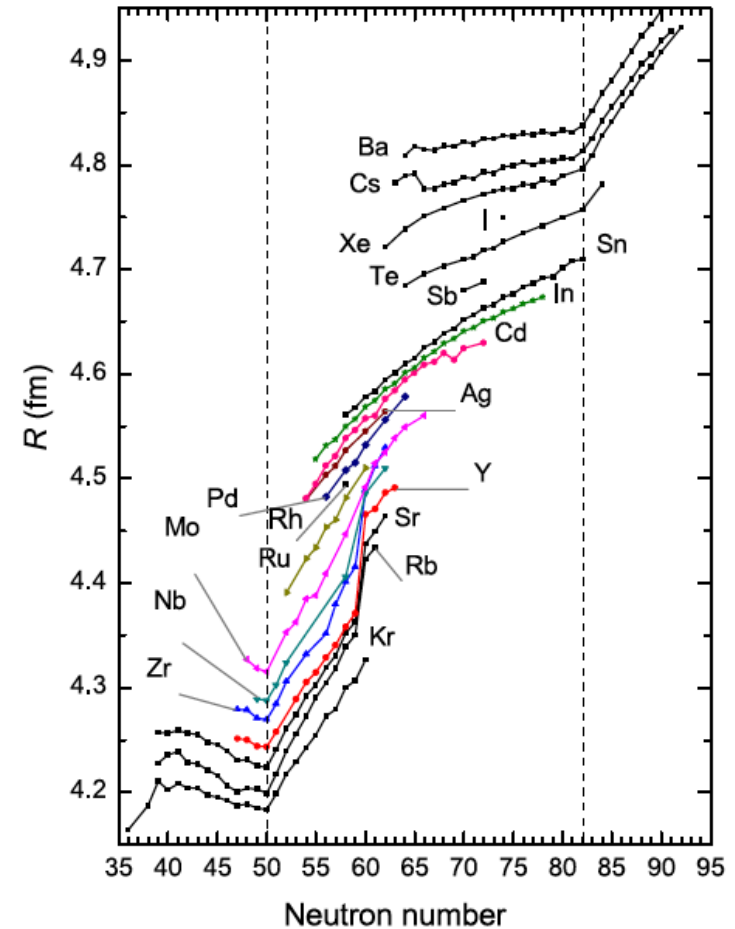
Bohr & Mottelson,  
Nuclear Structure.

# Signatures of shell structure in nuclei



## Nuclei with magic N :

- Large separation energies
- High-lying first  $2^+$  excited state
- Low  $B(E2)$  transition strength
- Kink/drop in charge radii



# Magic numbers: 2, 8, 20, 28, 50, 82...

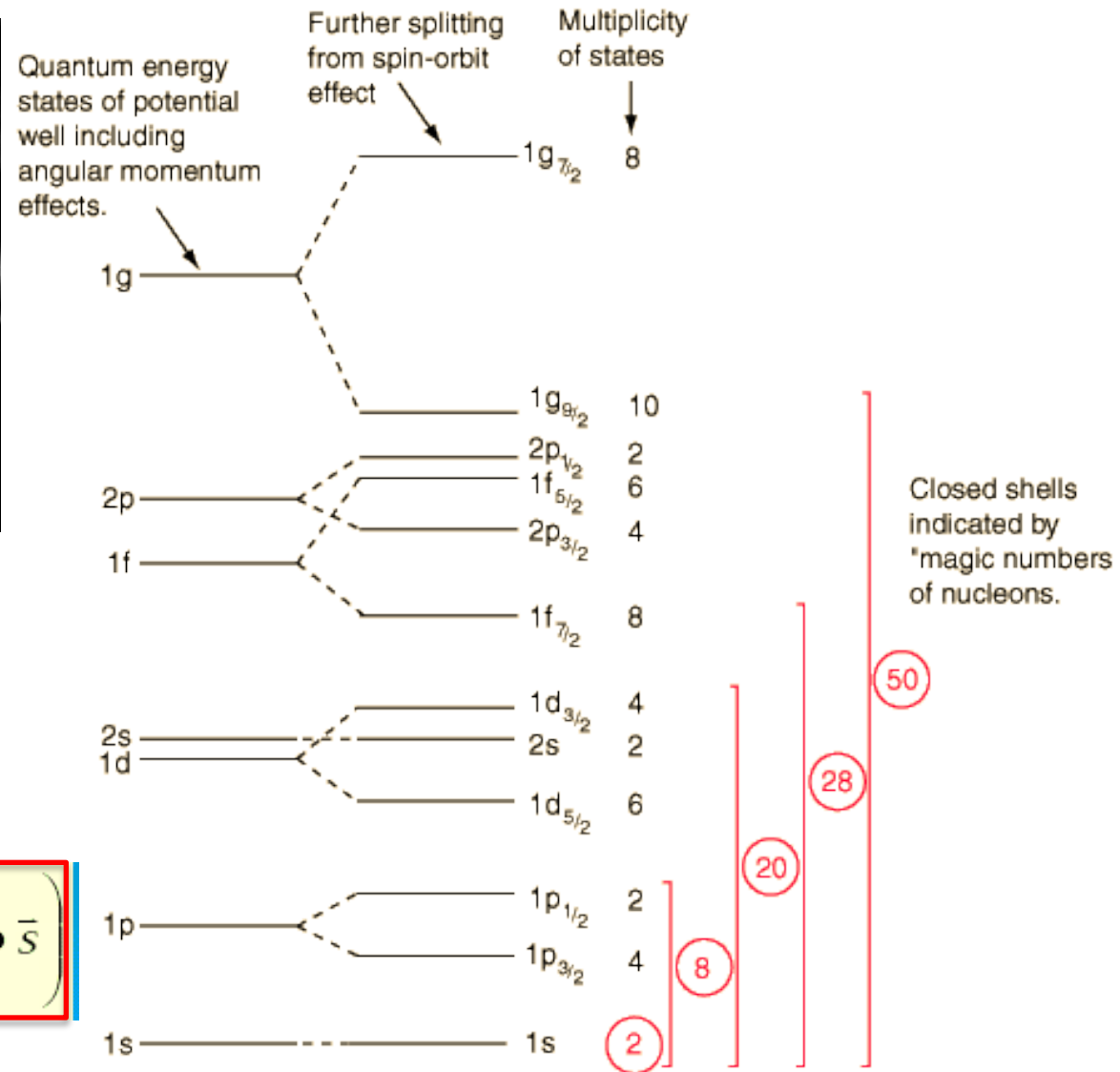
## Nobel Prize 1963



**Goeppert-Mayer Jensen**

Need spin-orbit force to explain magic numbers beyond 20.

$$H_{SM} = \sum_{i=1}^A \left( \frac{\hbar^2}{2M} \nabla^2 + \frac{m}{2} \omega^2 r^2 + \eta_l \bar{l}^2 + \zeta_{ls} \bar{l} \cdot \bar{s} \right)$$



# First principles versus phenomenological approach

**“The first, the basic approach, is to study the elementary particles, their properties and mutual interaction. Thus one hopes to obtain knowledge of the nuclear forces. If the forces are known, one should, in principle, be able to calculate deductively the properties of individual nuclei. Only after this has been accomplished can one say that one completely understands nuclear structure....The other approach is that of the experimentalist and consists in obtaining by direct experimentation as many data as possible for individual nuclei. One hopes in this way to find regularities and correlations which give a clue to the structure of the nucleus....The shell model, although proposed by theoreticians, really corresponds to the experimentalist’s approach.”**

***–M. Goepfert-Mayer, Nobel Lecture***



# No free lunch

Not well known



Well known

DFT



Shell model



Ab-initio



Interactions



EFT



QCD

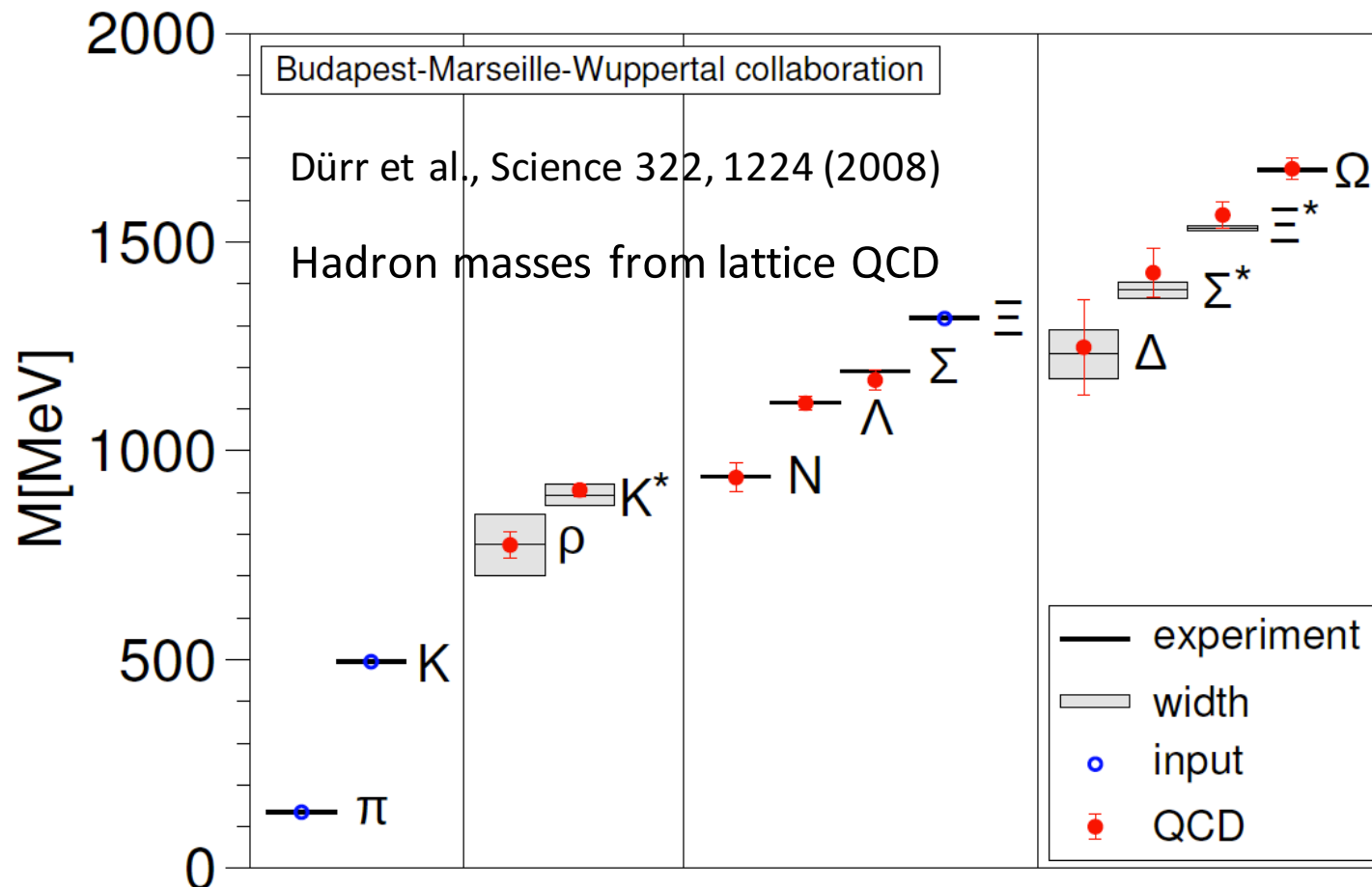
Easy to solve



Difficult to solve

These lectures presents several aspects of this duality.

# Quantum chromo dynamics – theory of the strong interaction



Most impressive progress

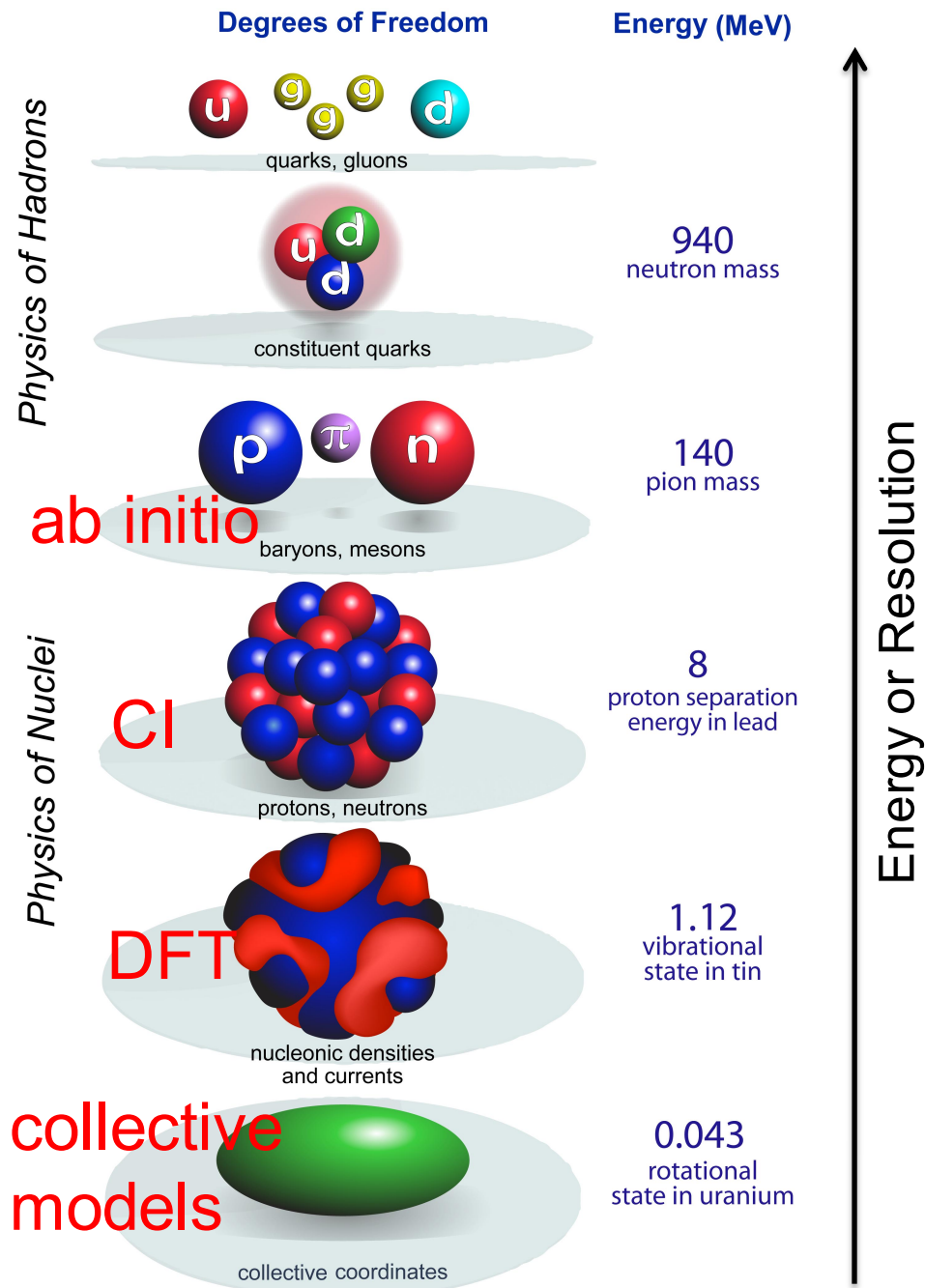
But: first-principle computation of nuclei from QCD are still far away ...

Worse: Looking at the QCD Lagrangian, it is not obvious what the low-energy QCD physics is.

Neither the spontaneous breaking of chiral symmetry nor the emergence of selfbound nuclei is obvious or predicted from QCD.

(The QED Lagrangian also does not tell us about emerging phenomena such as superconductivity or crystals.) We need another approach!

# Energy scales and relevant degrees of freedom



Effective theories provide us with model independent approaches to atomic nuclei

Key: Separation of scales

Weinberg's third law of Progress in theoretical Physics:

"You may use any degrees of freedom you like to describe a physical system, but if you use the wrong ones, you'll be sorry!"

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

# Construction of nuclear potentials via chiral EFT

Weinberg; Rho; Bedaque & van Kolck; Kaplan, Savage & Wise; Griesshammer; Hammer; Phillips; ...

1. Identify the **relevant degrees of freedom** for the resolution scale of atomic nuclei: **nucleons**.
2. Identify the **relevant symmetries** of low-energy QCD and investigate if and how they are broken
3. Construct the most general Lagrangian consistent with those symmetries and the symmetry breaking.
4. Design an **organizational scheme** that can distinguish between more and less important contributions: a low-momentum expansion: **power counting**
5. Guided by the expansion, calculate Feynman diagrams / potentials to the desired accuracy for the problem under consideration.

## Reviews/pedagogical texts:

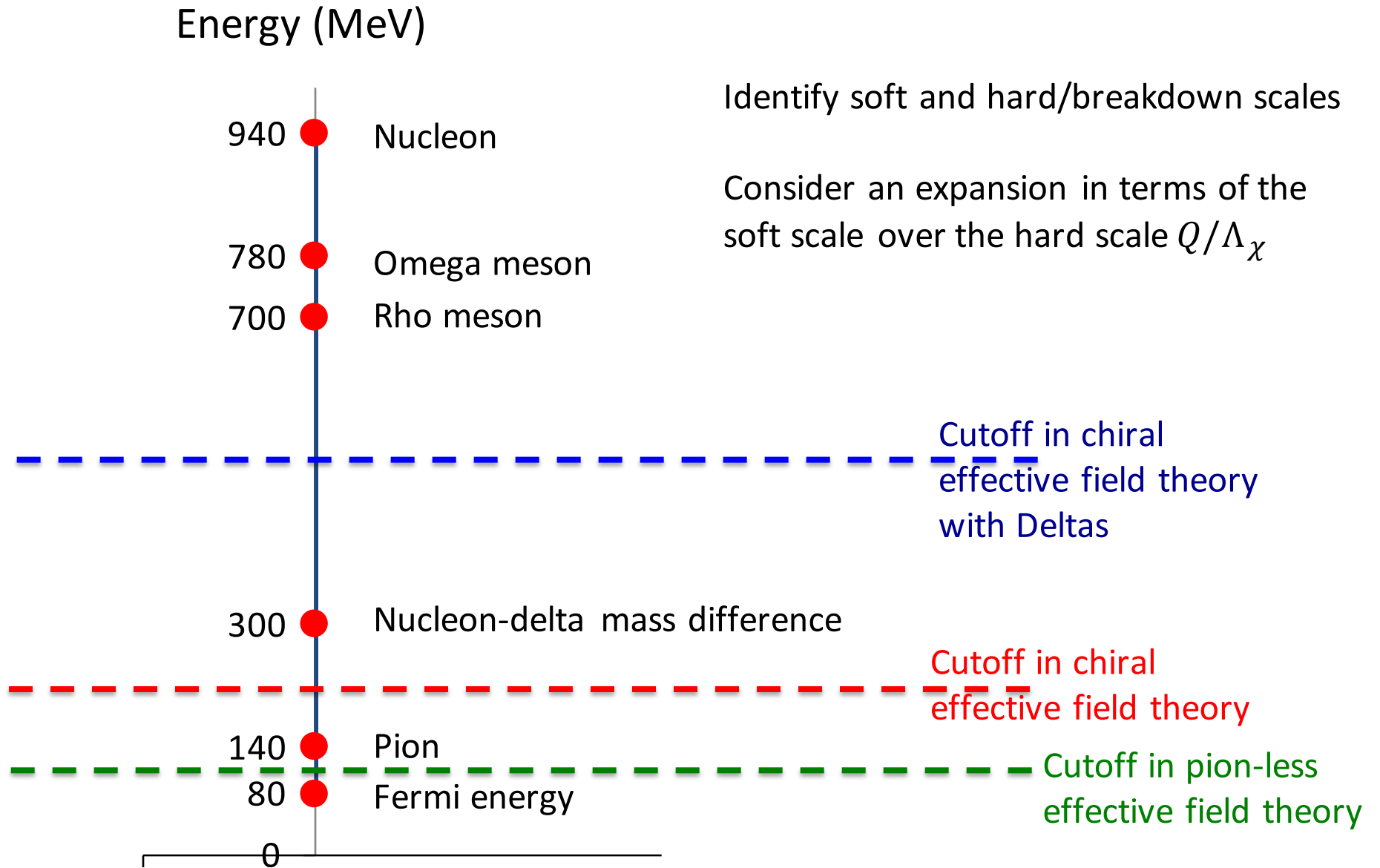
Bedaque and van Kolck, Ann. Rev. Nucl. Part. Sci. 52 (2002) 339, nucl-th/0205058.

Kirscher, arXiv:1506.00347.

Lepage, "How to renormalize the Schrödinger Equation?", nucl-th/9706029.

# Identify relevant degrees of freedom

– Separation of scale!



# Summary of scales

The separation of scale in pionless EFT is good for light nuclei (well explored) and possibly also for heavy nuclei (unexplored yet).

The separation of scale in pionful EFT (chiral EFT) is reasonable (most popular/most used and studied nuclear EFT ).

The separation of scale seems best in a chiral EFT with  $\Delta$  degrees of freedom (work under progress).

# Chiral effective field theory

After identifying the relevant degrees of freedom and breakdown scales, the next step is to build the most general effective Lagrangian consistent with (broken) symmetries of QCD. We expand the Lagrangian in powers of derivatives and pion masses, or more precisely in powers of  $Q/\Lambda_\chi$  here  $Q$  is small momentum or pion mass and  $\Lambda_\chi \sim 1$  GeV is the hard (breakdown) scale.

$$\mathcal{L} = \mathcal{L}_{\pi\pi} + \mathcal{L}_{\pi N} + \mathcal{L}_{NN} + \dots ,$$

$$V = V_{1\pi} + V_{2\pi} + V_{3\pi} + V_{4\pi} + \dots ,$$

Finally we organize the NN Lagrangian order-by-order in powers of  $Q/\Lambda_\chi$  (only even powers due to parity conservation)

$$\mathcal{L}_{NN} = \mathcal{L}_{NN}^{(0)} + \mathcal{L}_{NN}^{(2)} + \mathcal{L}_{NN}^{(4)} + \mathcal{L}_{NN}^{(6)} + \dots ,$$

The pion exchange contributions are organized in a similar low-momentum expansion:

$$V_{1\pi} = V_{1\pi}^{(0)} + V_{1\pi}^{(2)} + V_{1\pi}^{(3)} + V_{1\pi}^{(4)} + V_{1\pi}^{(5)} + V_{1\pi}^{(6)} + \dots$$

$$V_{2\pi} = V_{2\pi}^{(2)} + V_{2\pi}^{(3)} + V_{2\pi}^{(4)} + V_{2\pi}^{(5)} + V_{2\pi}^{(6)} + \dots$$

# Chiral effective field theory order by order



Nucleons: full lines  
Pions: dashed lines

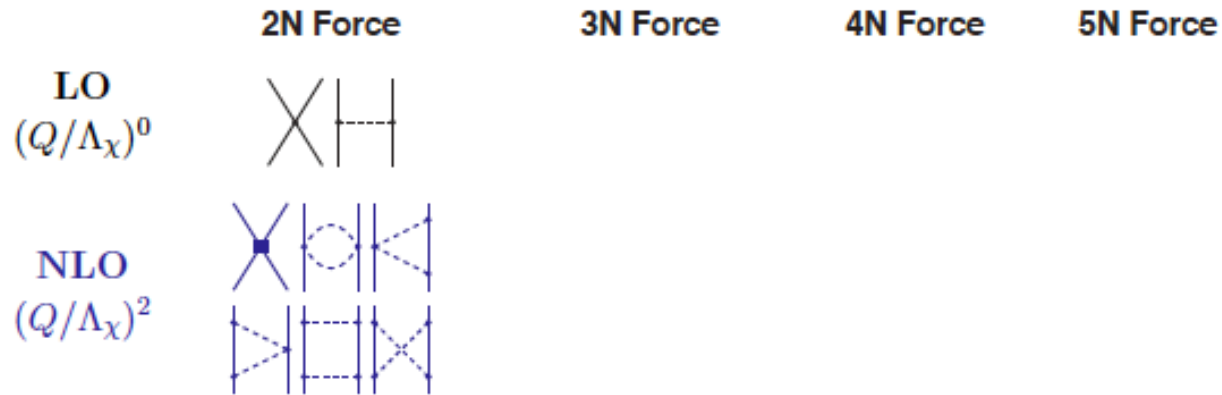
Features:

1. Systematic expansion of nucleon potential; small parameter  $(Q/\Lambda)$
2. Unresolved short-range physics encoded in contact interactions
3. Low-energy constants from fit to data
4. Hierarchy of forces  
 $NN \gg NNN \gg NNNN$

[from Machleidt:  
Physica Scripta 91 (2016) 083007  
arXiv:1608.05978]



# Chiral effective field theory order by order



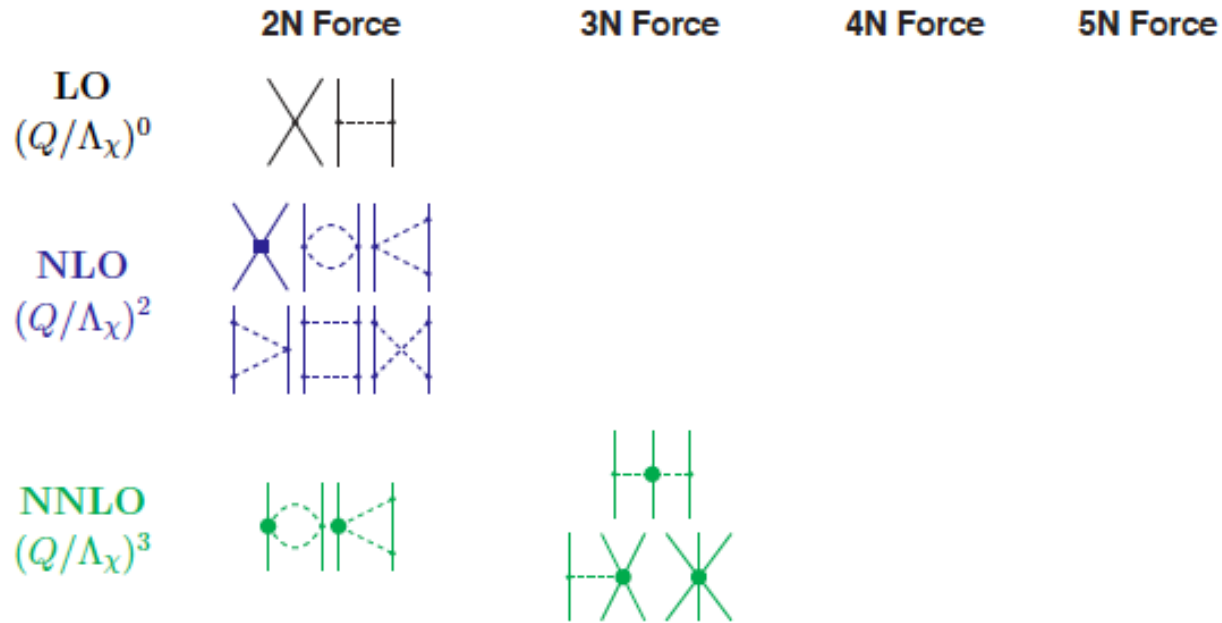
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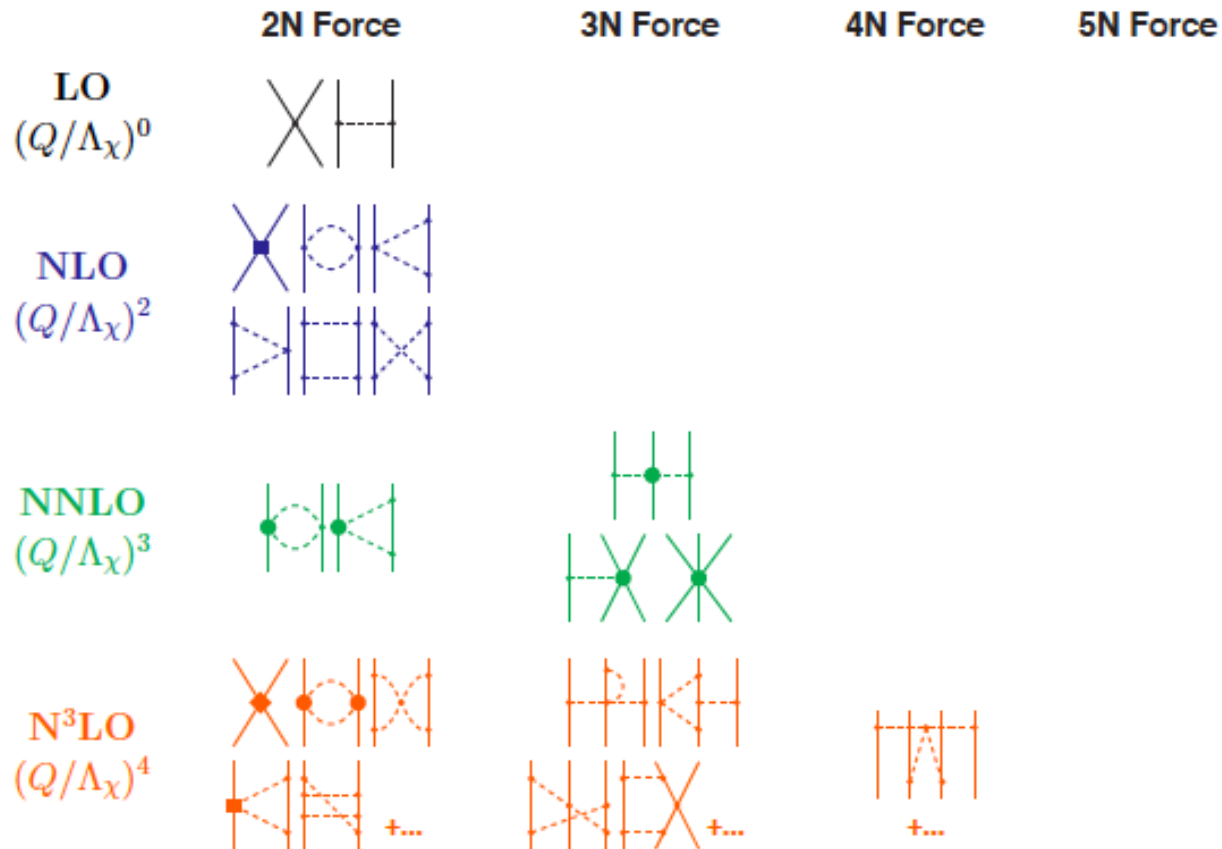
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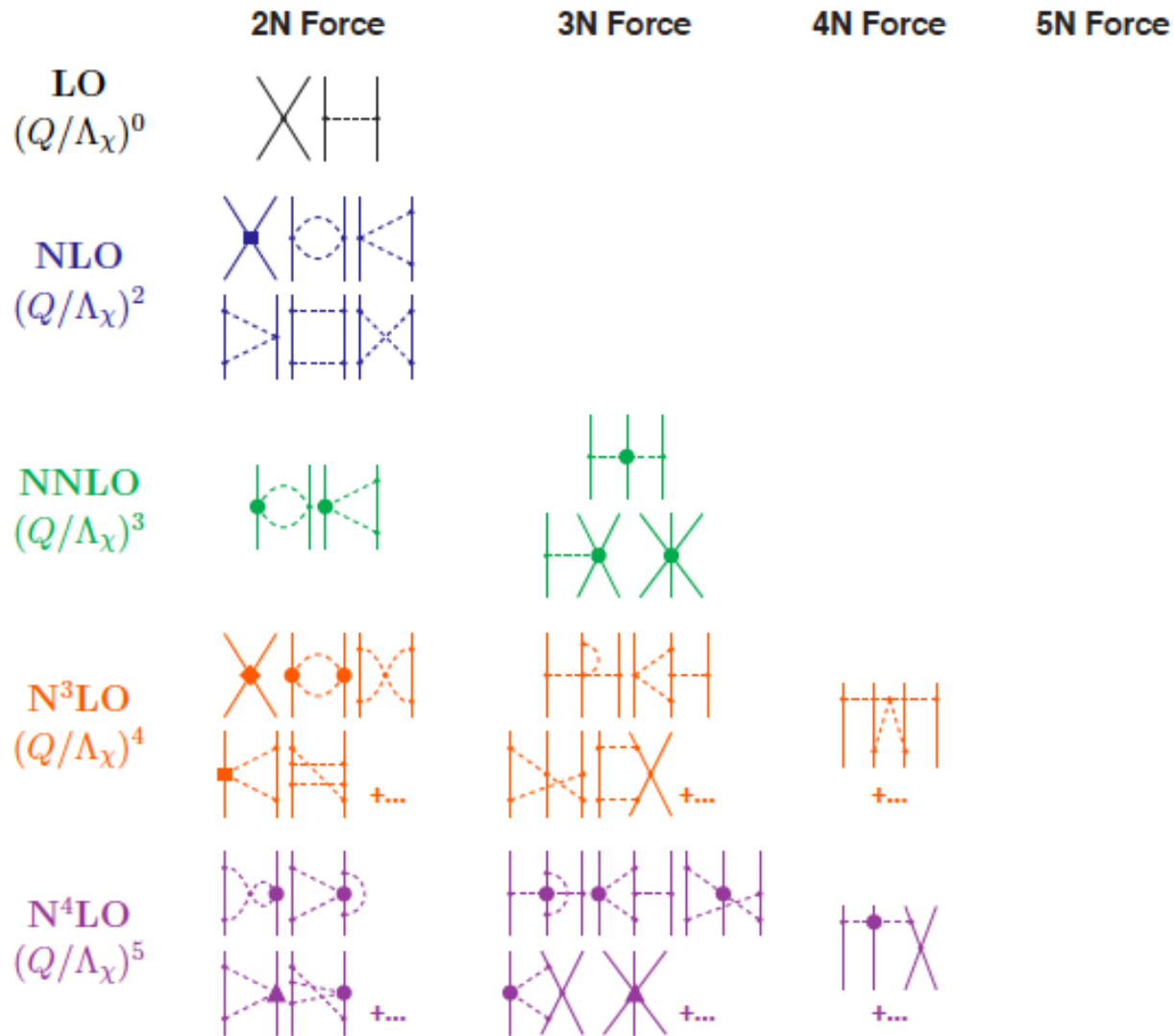
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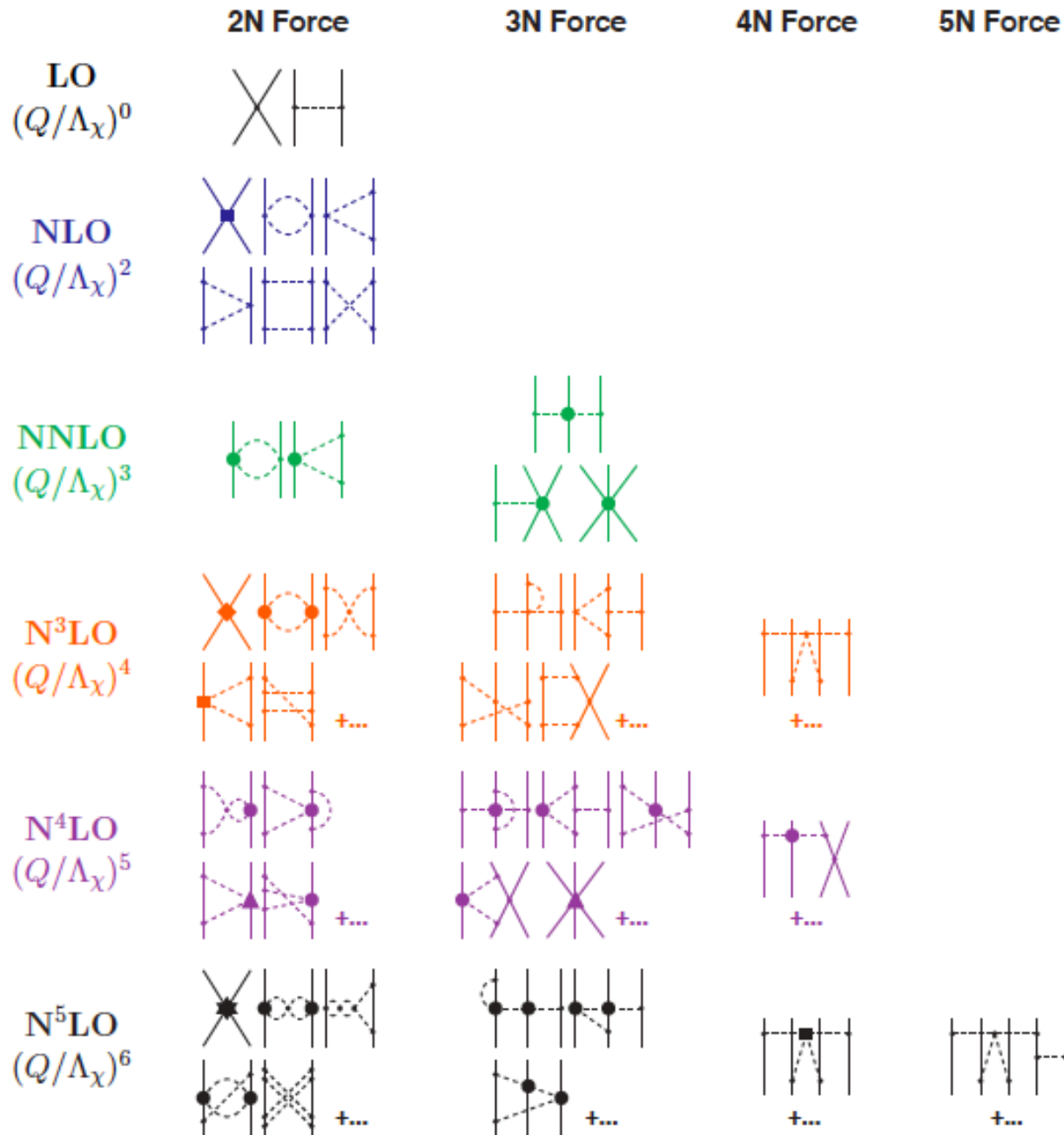
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[from Machleidt:  
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# Chiral nucleon–nucleon potential at leading order


One-pion exchange potential ( $p, p'$  are initial and final relative momenta)

$$V_{1\pi}(\vec{p}', \vec{p}) = -\frac{g_A^2}{4f_\pi^2} \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \frac{\vec{\sigma}_1 \cdot \vec{q} \vec{\sigma}_2 \cdot \vec{q}}{q^2 + m_\pi^2}$$

$$\vec{q} \equiv \vec{p}' - \vec{p}$$

Leading order contact term (encode unknown short-range physics)

$$V^{(0)}(\vec{p}', \vec{p}) = C_S + C_T \vec{\sigma}_1 \cdot \vec{\sigma}_2$$



Must determine low-energy constants (LECs) from data.

# How does the momentum cutoff $\Lambda$ enter the EFT?

1. The construction of the chiral potential involves solving the Lippmann-Schwinger equation (T-matrix).

$$\widehat{T}(\vec{p}', \vec{p}) = \widehat{V}(\vec{p}', \vec{p}) + \int d^3 p'' \widehat{V}(\vec{p}', \vec{p}'') \frac{M}{p^2 - p''^2 + i\epsilon} \widehat{T}(\vec{p}'', \vec{p})$$

2. In order to avoid infinities when iterating the T-matrix we need to regularize and introduce a cutoff ( $\Lambda$  is the cutoff in this equation)

$$\widehat{V}(\vec{p}', \vec{p}) \longmapsto \widehat{V}(\vec{p}', \vec{p}) e^{-(p'/\Lambda)^{2n}} e^{-(p/\Lambda)^{2n}}$$

3. As a result, the low-energy constants depend implicitly on the regularization scheme and the cutoff. The calculated observables should be independent of the employed cutoff to ensure the renormalization group invariance (RGI).
4. There are (infinitely) many different chiral potentials! Differences of potentials that employ different values for the cutoff or regulator must be of higher order.
5. Regularization schemes, and form of potentials that encode short-ranged physics (contact potential or potentials with a very short range) are at the potential builder's discretion. **This makes the approach model independent.**

# The nucleon–nucleon scattering problem

The nucleon-nucleon scattering problem is usually solved in a partial wave decomposition in the center of mass frame

The quantum numbers of the nucleon-nucleon system:

- Orbital angular momentum  $\mathbf{L} = 0, 1, 2, \dots \rightarrow S, P, D, \dots$  (even/odd = symmetric/antisymmetric)
- Total spin  $S = \frac{1}{2}(\sigma_1 + \sigma_2), S = 0, 1$  ( $S = 1$  antisymmetric,  $S = 0$  symmetric)
- Total angular momentum  $\mathbf{J} = \mathbf{L} + \mathbf{S}$ , conserved by rotational symmetry
- Total isospin  $T = \frac{1}{2}(\tau_1 + \tau_2), T = 0, 1$  ( $T = 1$  antisymmetric,  $T = 0$  symmetric)

We use the spectroscopic notation  $^{2S+1}L_J$  to specify the allowed NN scattering channels (from requirement that wave function is antisymmetric):

$^1S_0, ^3S_1, ^1P_1, ^3P_0, ^3P_1, ^3P_2, ^1D_2, ^3D_1, ^3D_2, ^3D_3, ^1F_3, ^3F_2, ^3F_3, ^3F_4,$

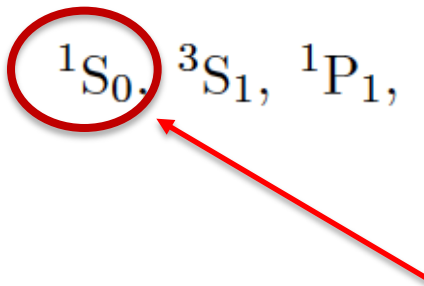
Note, the tensor force which enters at NLO couples partial waves, for example the deuteron with total  $J=1$  mixes  $^3S_1$  and  $^3D_1$  partial waves.



# The nucleon–nucleon scattering problem

If we consider very low-energy neutron-neutron scattering what is the allowed partial wave?

$^1S_0, ^3S_1, ^1P_1, ^3P_0, ^3P_1, ^3P_2, ^1D_2, ^3D_1, ^3D_2, ^3D_3, ^1F_3, ^3F_2, ^3F_3, ^3F_4,$



In very low-energy scattering we have s-waves and from requirement that wave function is antisymmetric we have  $T = 1, S = 0$  and  $L = 0$

What about the deuteron?

## How to determine the low-energy constants?

$$V_{1\pi}(\vec{p}', \vec{p}) = -\frac{g_A^2}{4f_\pi^2} \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \frac{\vec{\sigma}_1 \cdot \vec{q} \vec{\sigma}_2 \cdot \vec{q}}{q^2 + m_\pi^2}$$

$$V^{(0)}(\vec{p}', \vec{p}) = C_S + C_T \vec{\sigma}_1 \cdot \vec{\sigma}_2$$

Leading order acts only in S waves (low energy):

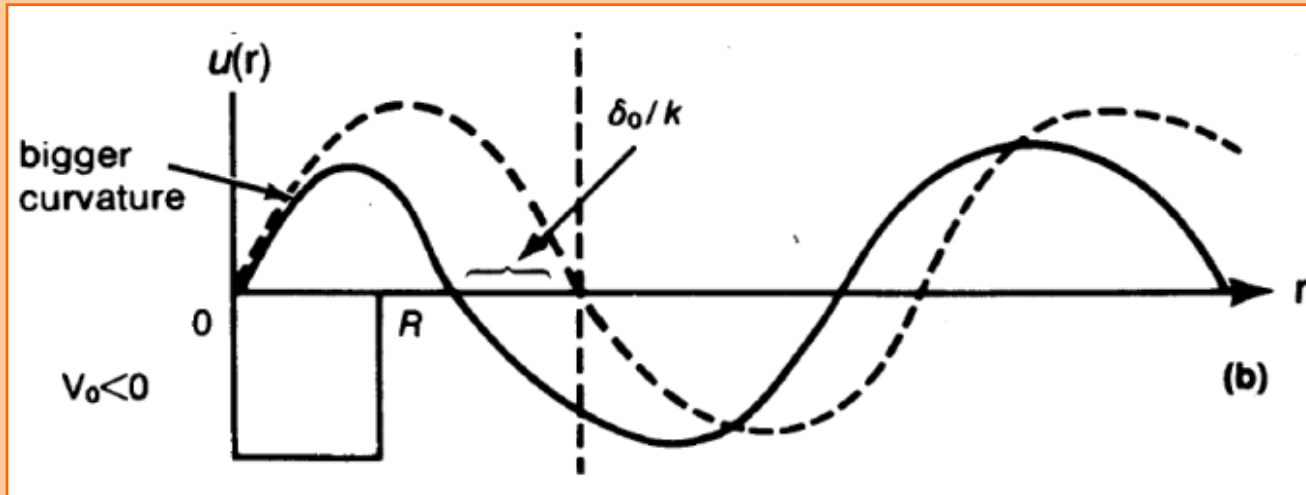
$$V_{\text{ct}}^{(0)}(^1S_0) = \tilde{C}_{^1S_0} = 4\pi (C_S - 3C_T)$$

$$V_{\text{ct}}^{(0)}(^3S_1) = \tilde{C}_{^3S_1} = 4\pi (C_S + C_T).$$

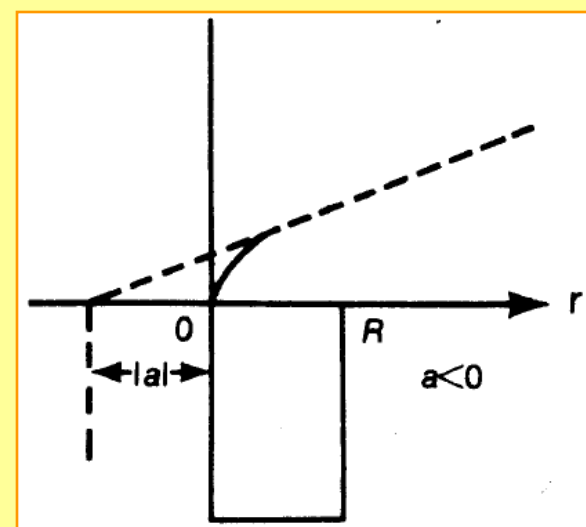
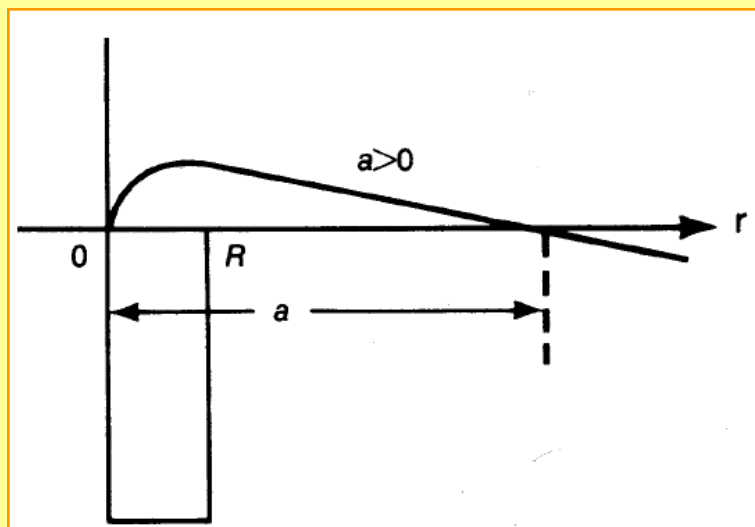
We can determine these parameters by a fit to low-energy nucleon-nucleon phase shifts and scattering lengths.

# The nucleon-nucleon scattering problem

Phase shift is a function of relative momentum  $k$ ; Figure shows s-wave.



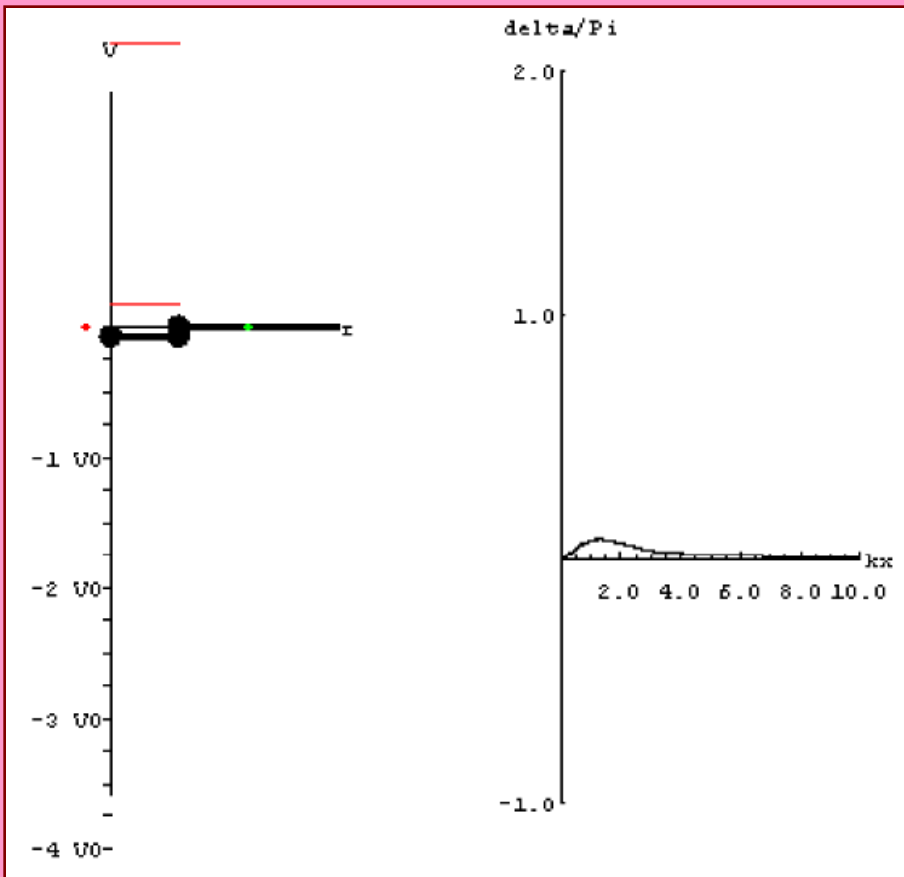
Scattering length:  $k \cot \delta(k) \approx -\frac{1}{a}$ ;  $\sigma_{\text{tot}} \approx 4\pi a^2$  for  $k \rightarrow 0$



# Scattering from a spherical well

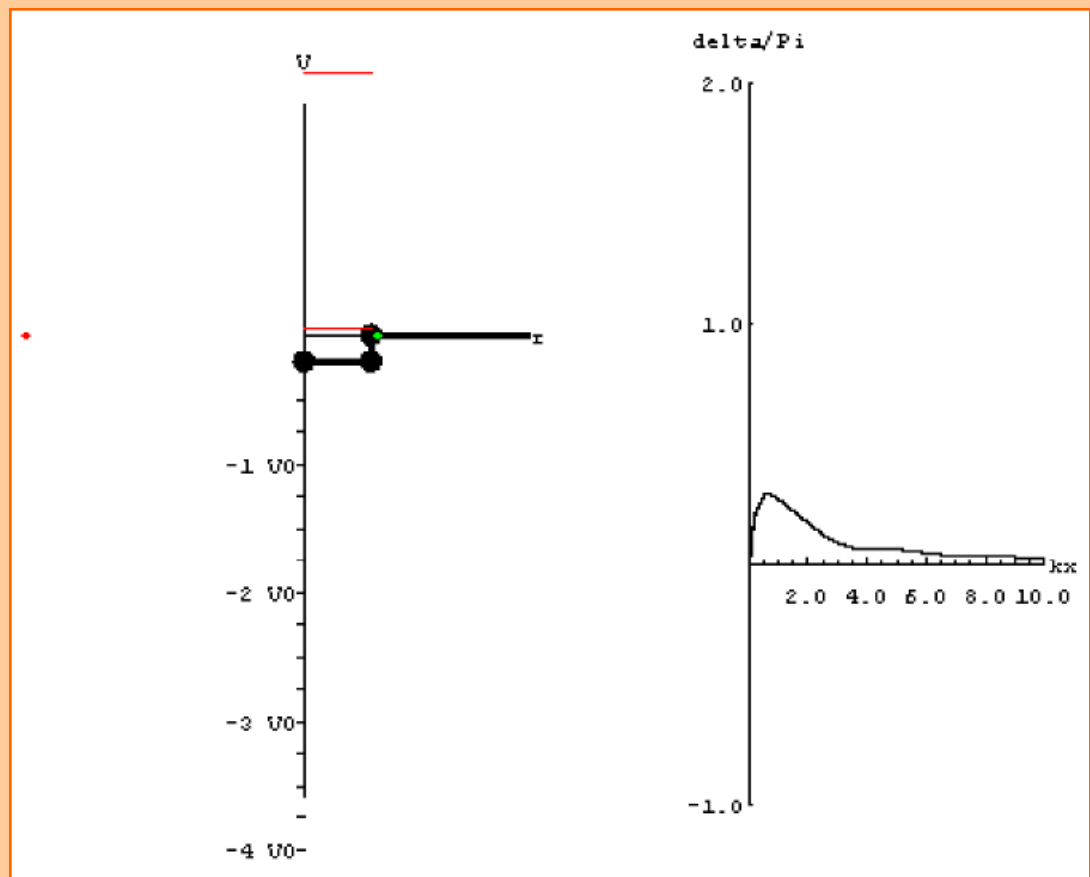
<http://people.ccmr.cornell.edu/~emueller/tutorials.html>

System has no bound state



Increase depth of well:

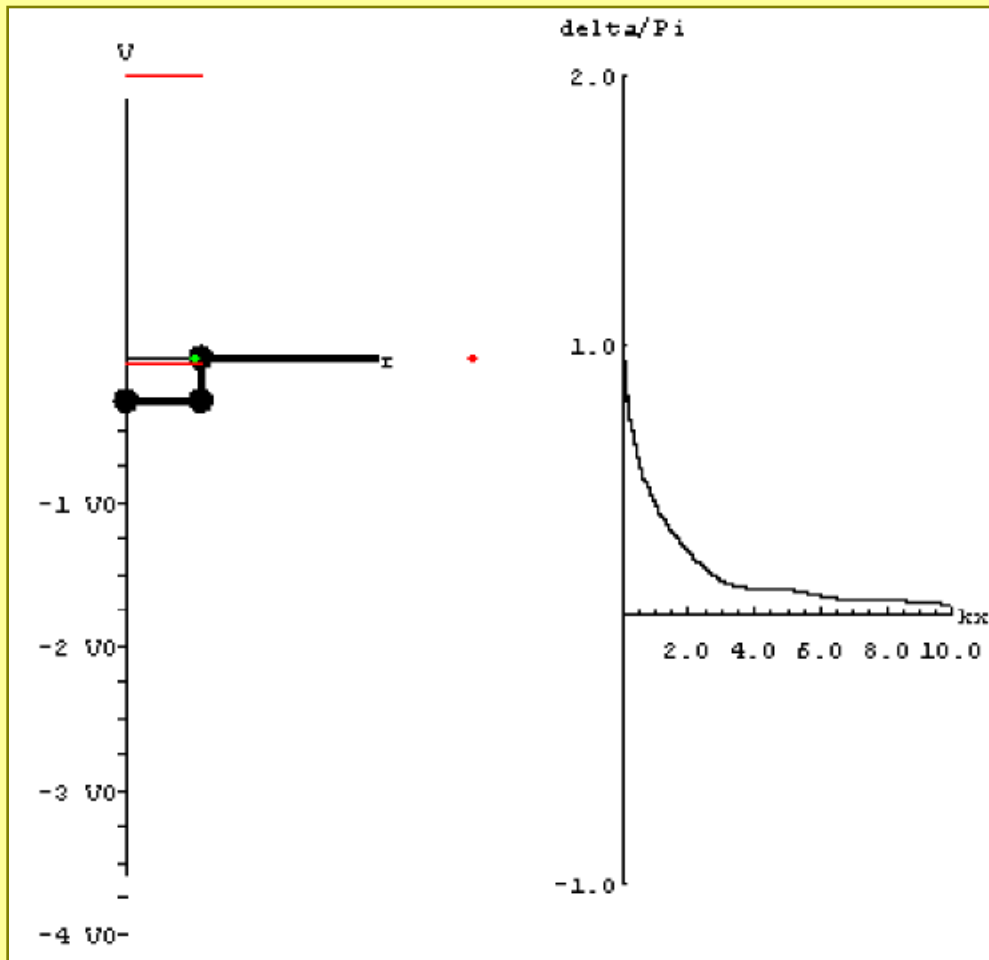
First bound state is about to enter



# Scattering from a spherical well

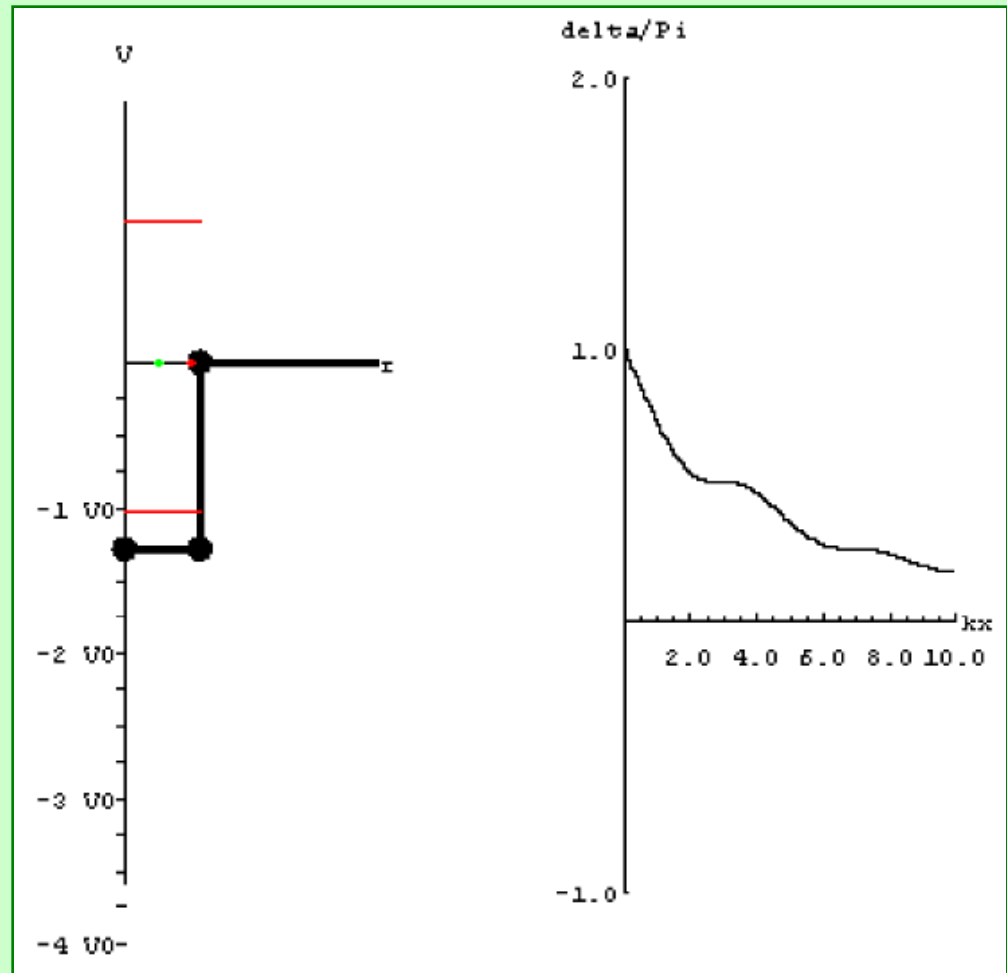
Further increase of depth:

System has one shallow bound state



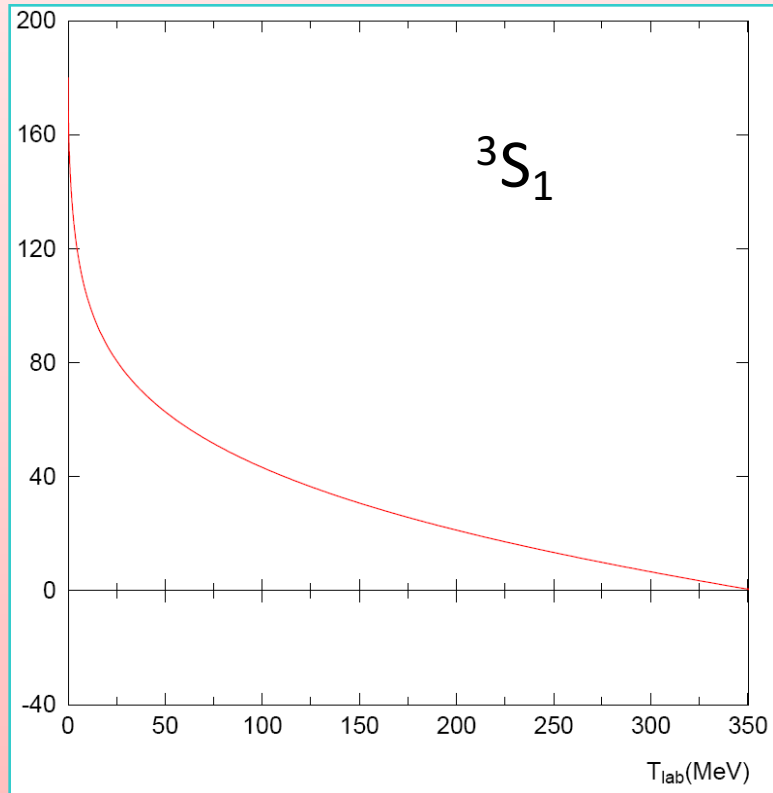
Further increase of depth:

System has one deep bound state



# Nuclear s-wave phase shifts

<http://nn-online.org/>

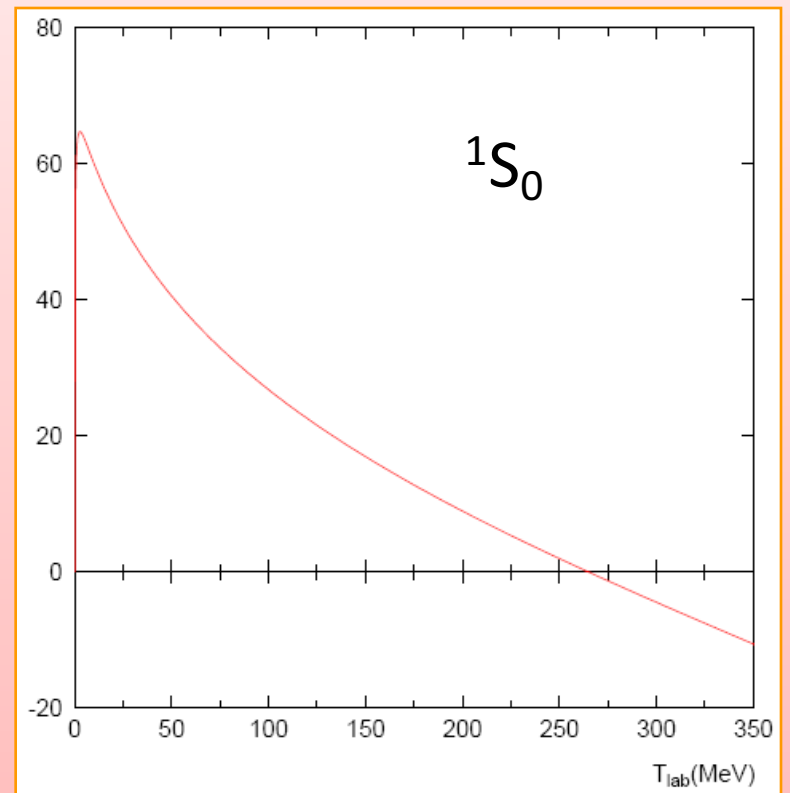


Deuteron is a very weakly bound system!

System has one bound state.

Steep decrease from 180 degrees due to large scattering length  $a = 5.5$  fm.

Acts repulsive due to large (positive) scattering length.

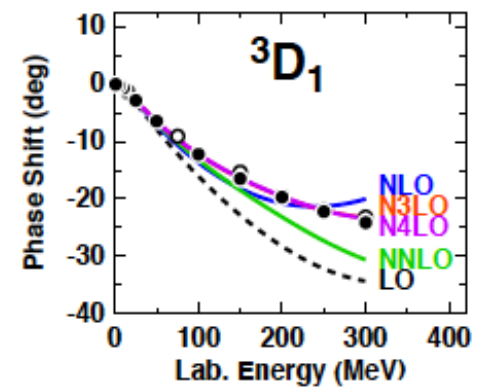
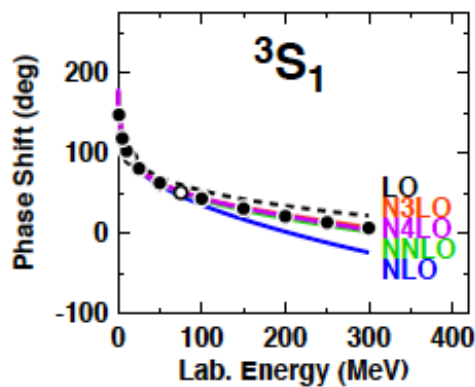
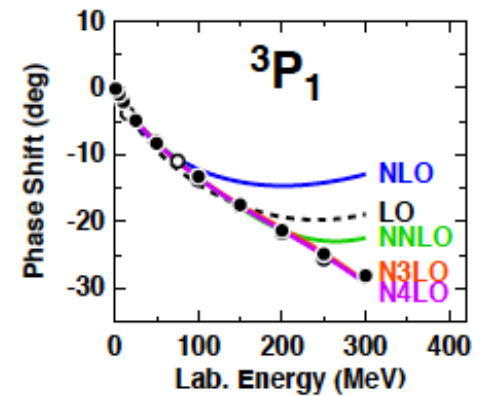
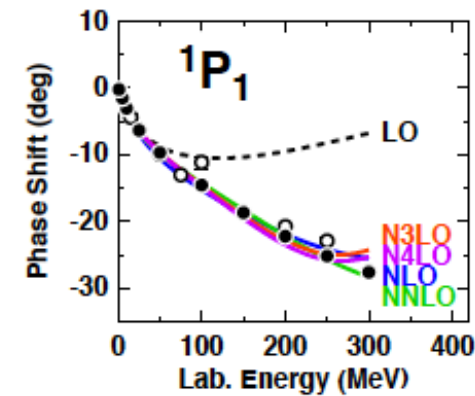
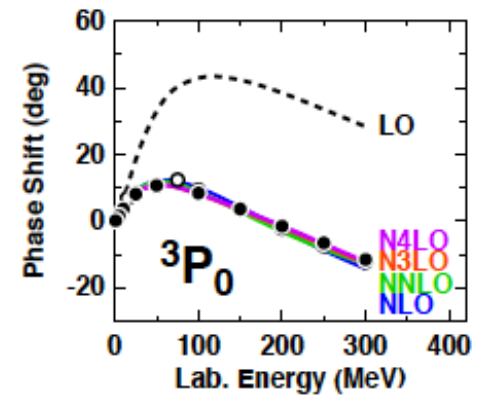
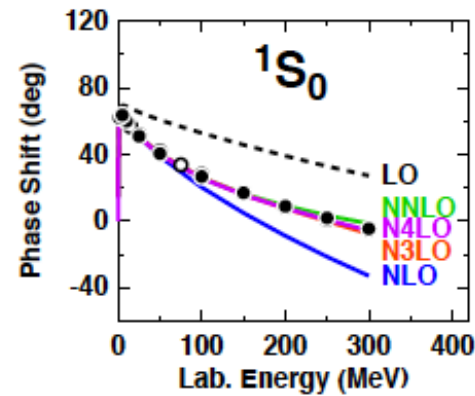
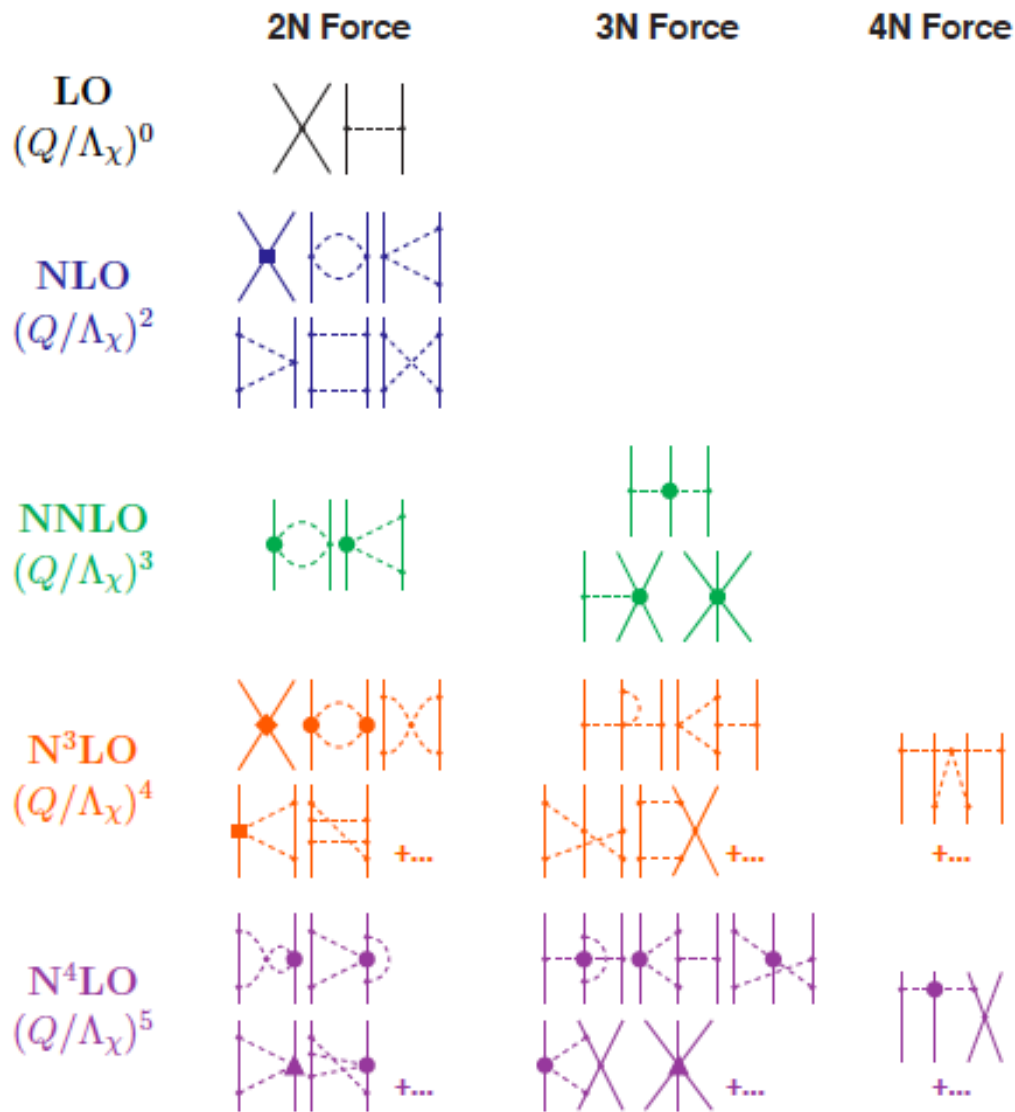


System (barely) fails to exhibit bound state.

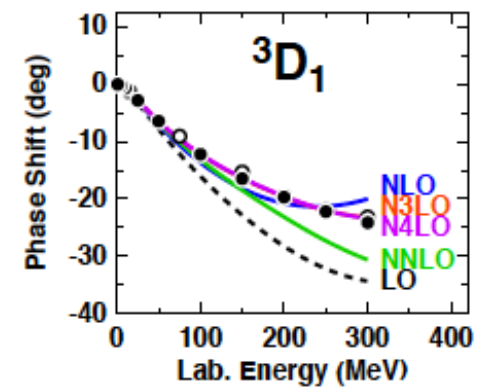
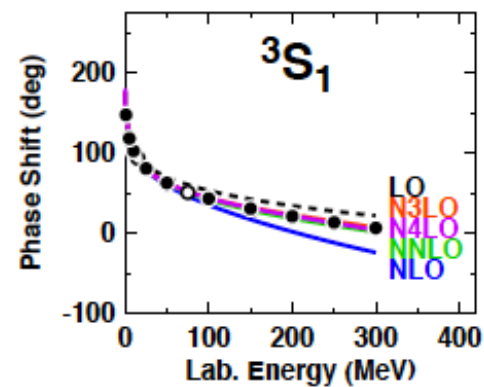
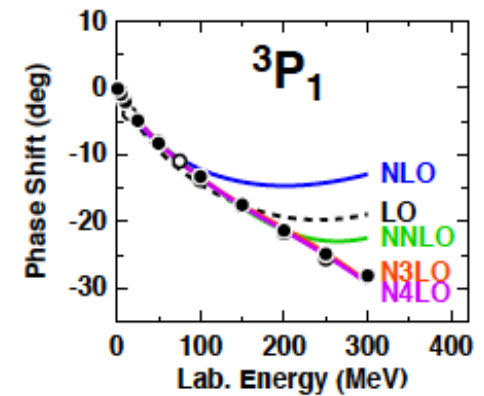
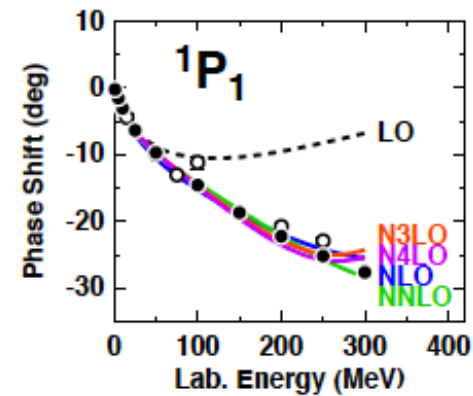
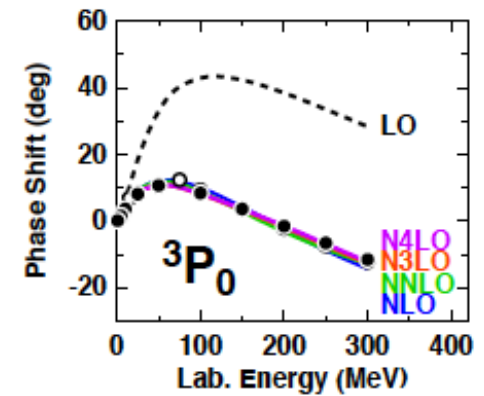
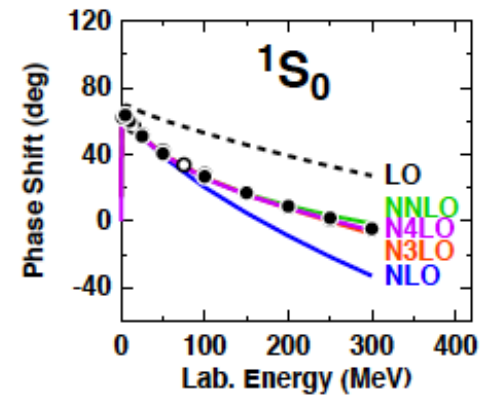
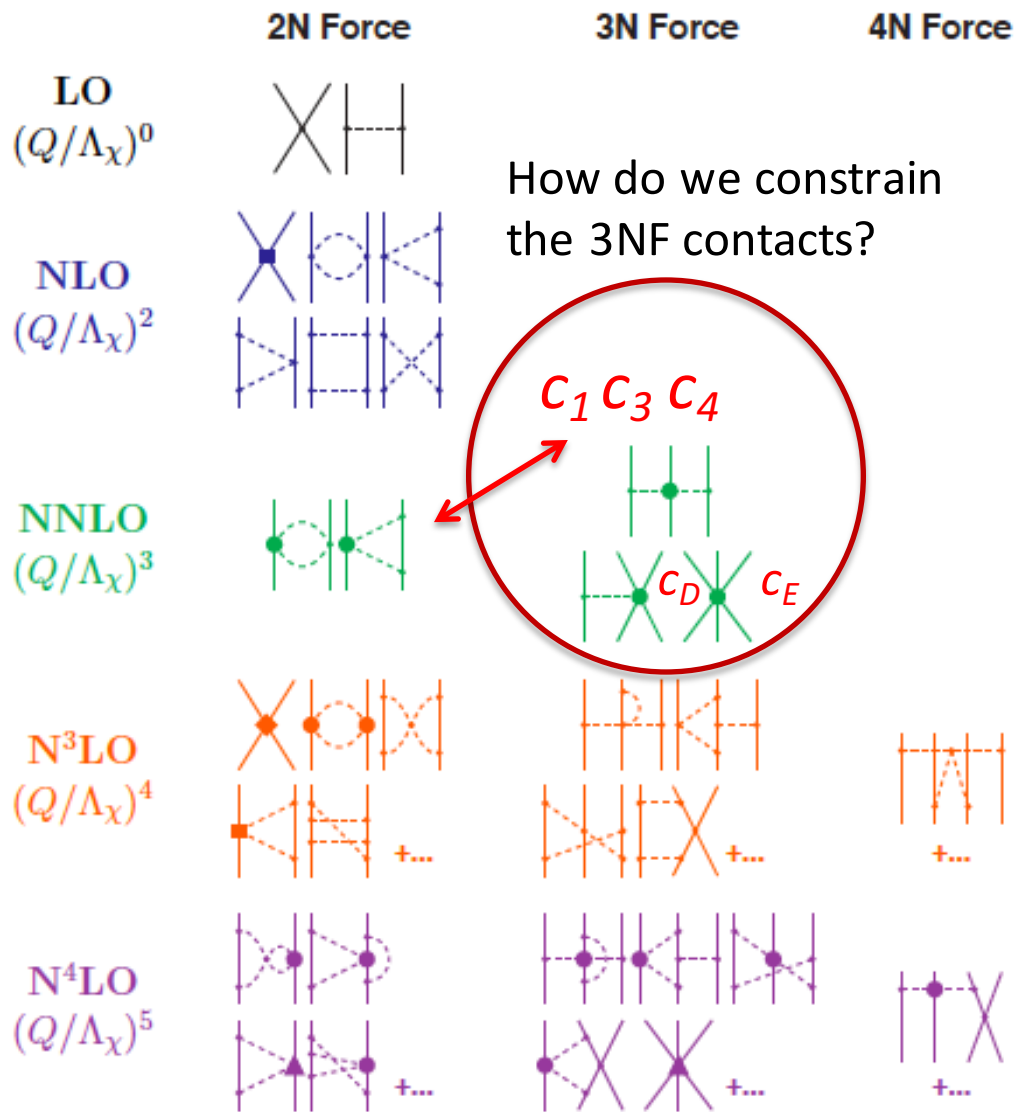
Steep rise at 0 due to large scattering length  $a = -18$  fm.

Monotonous decrease due to hard core.

# Nucleon-nucleon phase shifts to N<sup>4</sup>LO



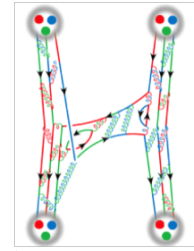
# Nucleon-nucleon phase shifts to N<sup>4</sup>LO



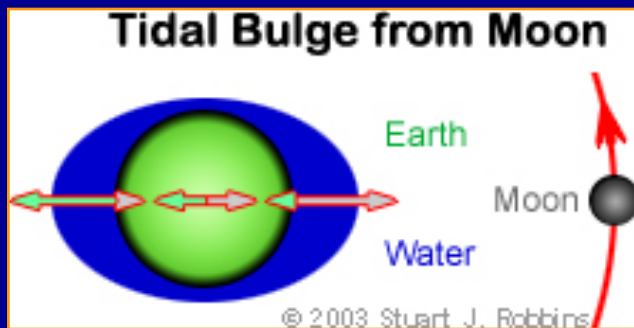


# Three-nucleon forces – Why?

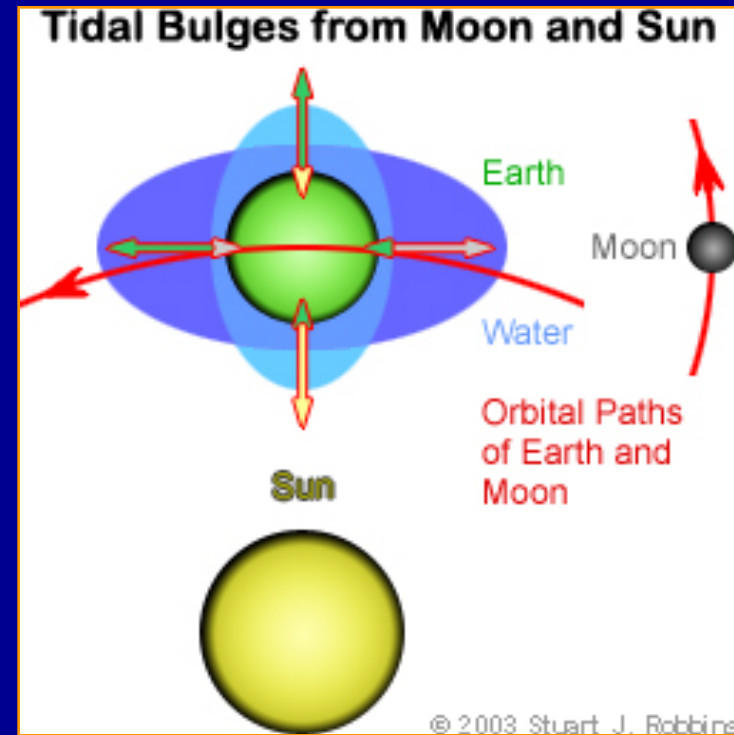
- Nucleons are not point particles (i.e. not elementary).
- We neglected some internal degrees of freedom (e.g.  $\Delta$ -resonance, “polarization effects”, ...), and unconstrained high-momentum modes.



**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

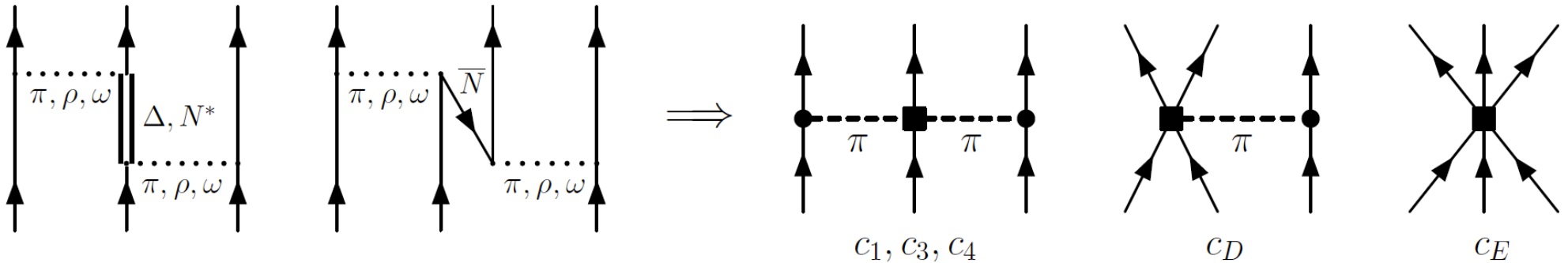


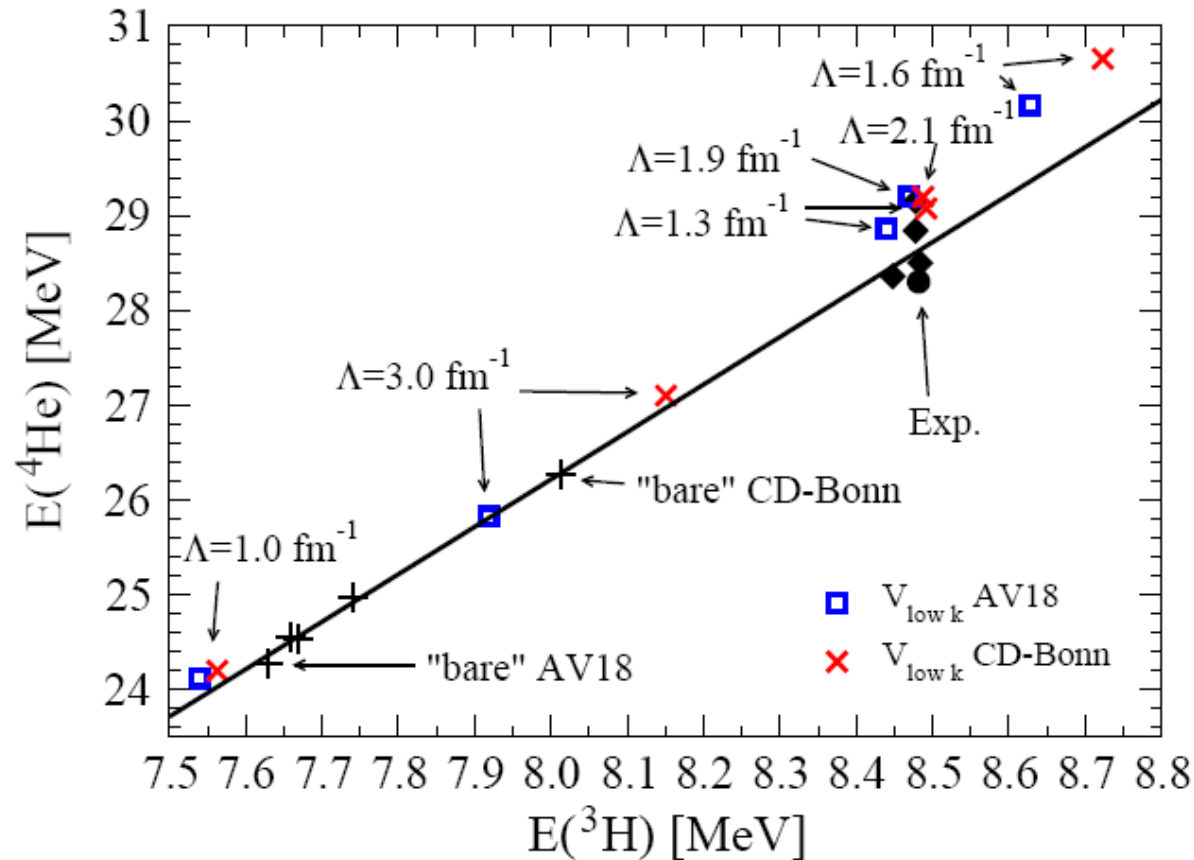
Figure 23: Eliminating degrees of freedom leads to three-body forces.  
 (taken from Bogner, Furnstahl, Schwenk, arXiv:0912.3688)

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?**

# Non-uniqueness of three-nucleon forces



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

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  $^4\text{He}$  would require four-nucleon forces!

# **3NFs play an important but complicated role in nuclear physics**

LECs of 3NFs are tuned together with, and depend on, the underlying nucleon-nucleon interaction

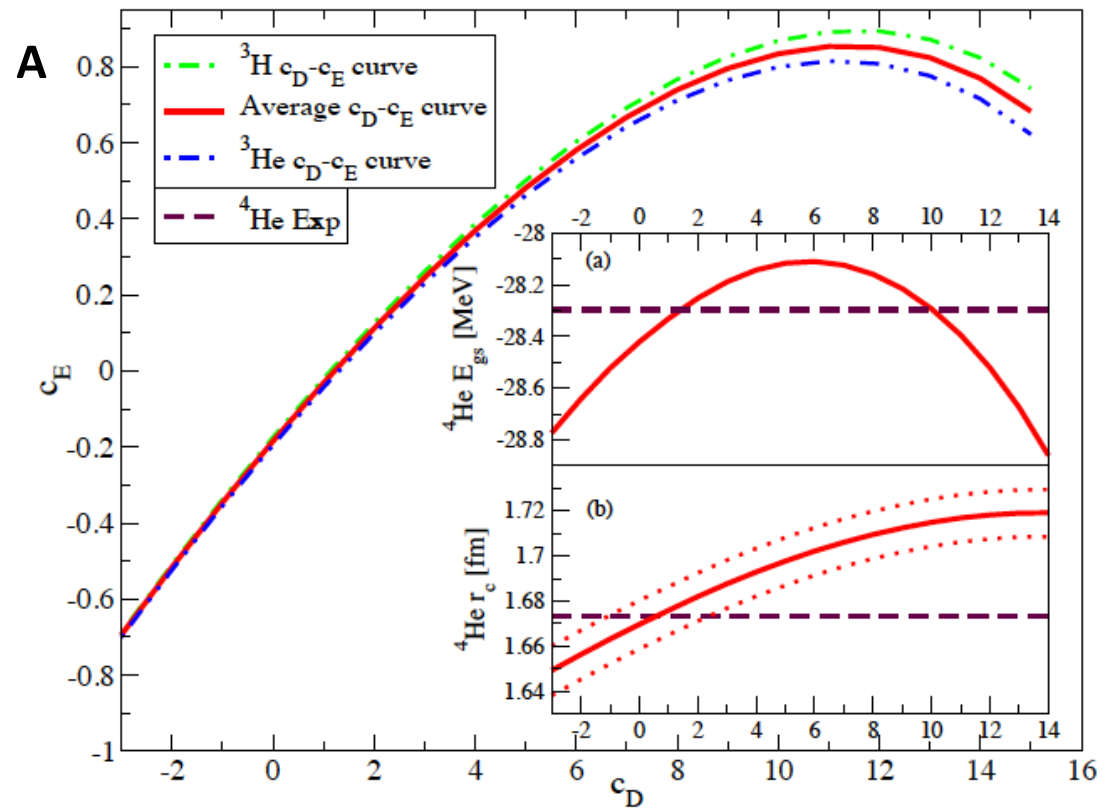
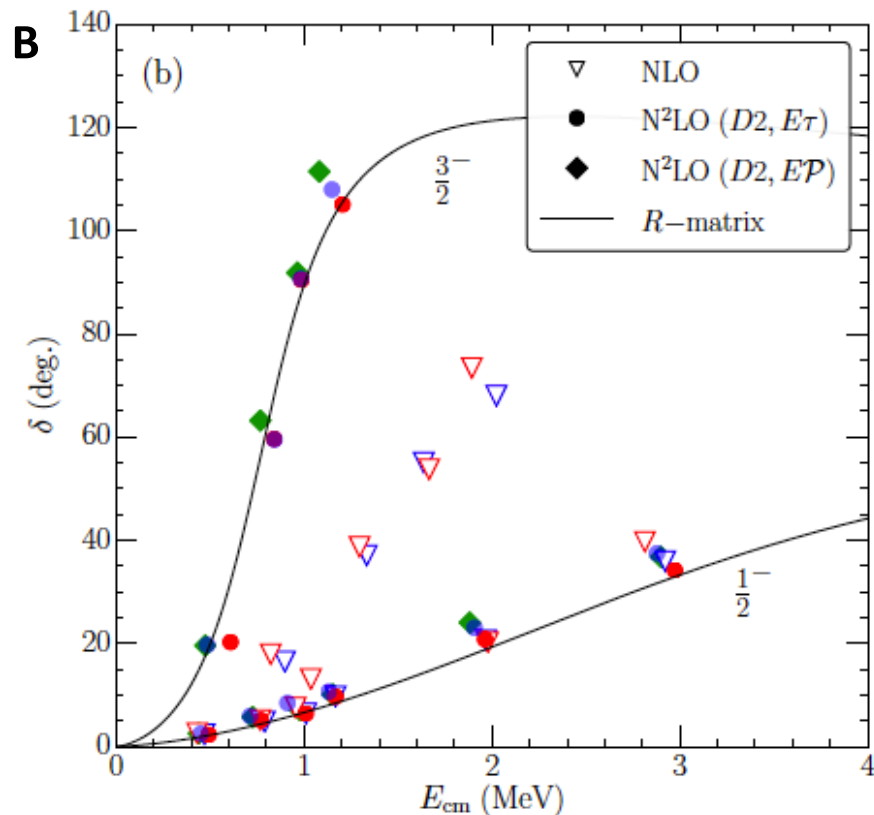
Examples:

- Light nuclei
- Nuclear matter
- Neutron drip line

# Determine the LECs of the 3NF

A. From fit to the  ${}^3\text{H}$ ,  ${}^3\text{He}$ , and  ${}^4\text{He}$  BE and radii. (P. Navratil arXiv:0904.0463)

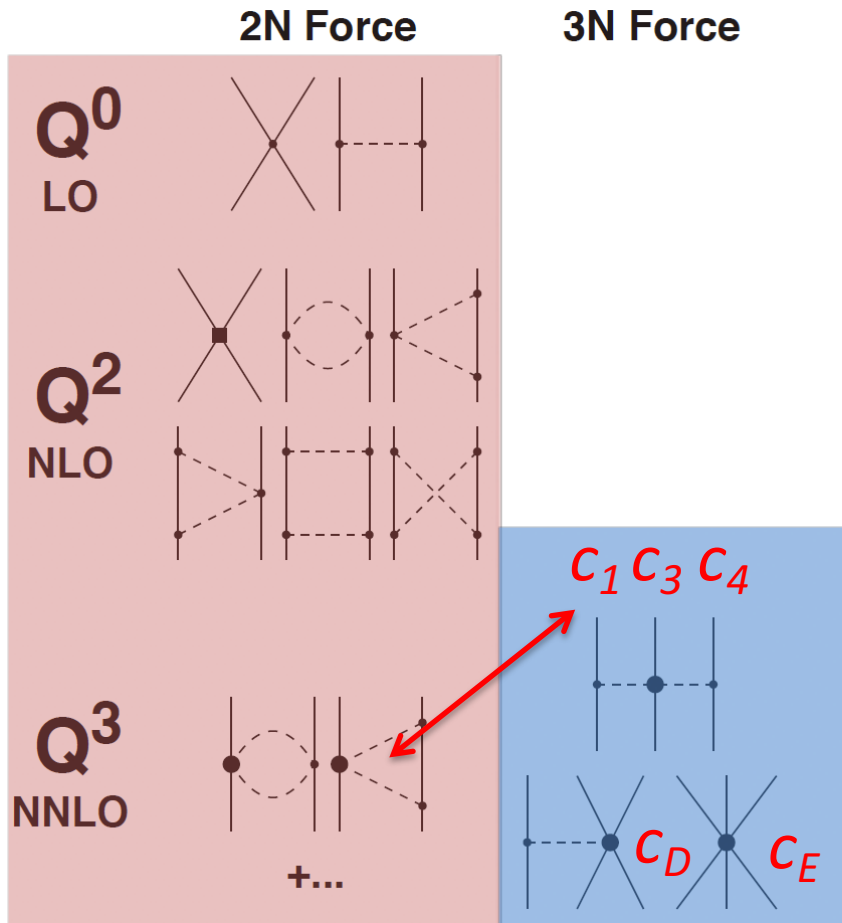
B. Fit to n-alpha scattering (J. E. Lynn, PRL 116, 062501 (2016))



BE of  $A = 3, 4$  nuclei are not independent observables.

Can we use electromagnetic probes to constrain the LECs of the 3NF?

# Meson exchange currents from chiral EFT

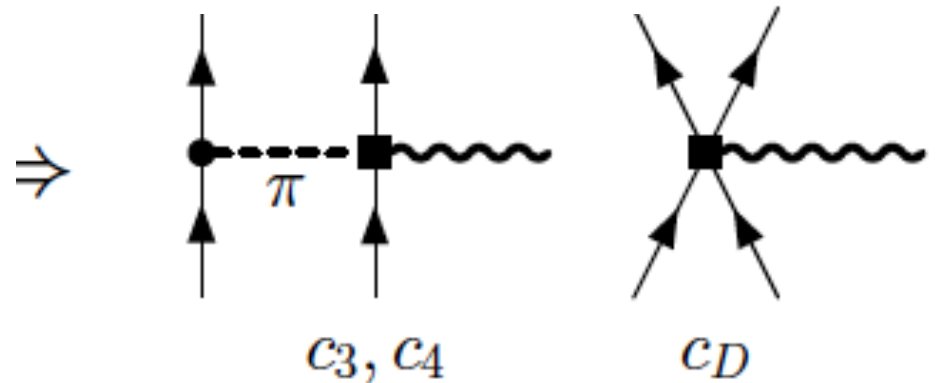


Nuclear currents describe the interactions with external electromagnetic probes:

$$j(\mathbf{q}) = \sum_i j_i(\mathbf{q}) + \sum_{i<j} j_{ij}(\mathbf{q}) + \sum_{i<j<k} j_{ijk}(\mathbf{q})$$

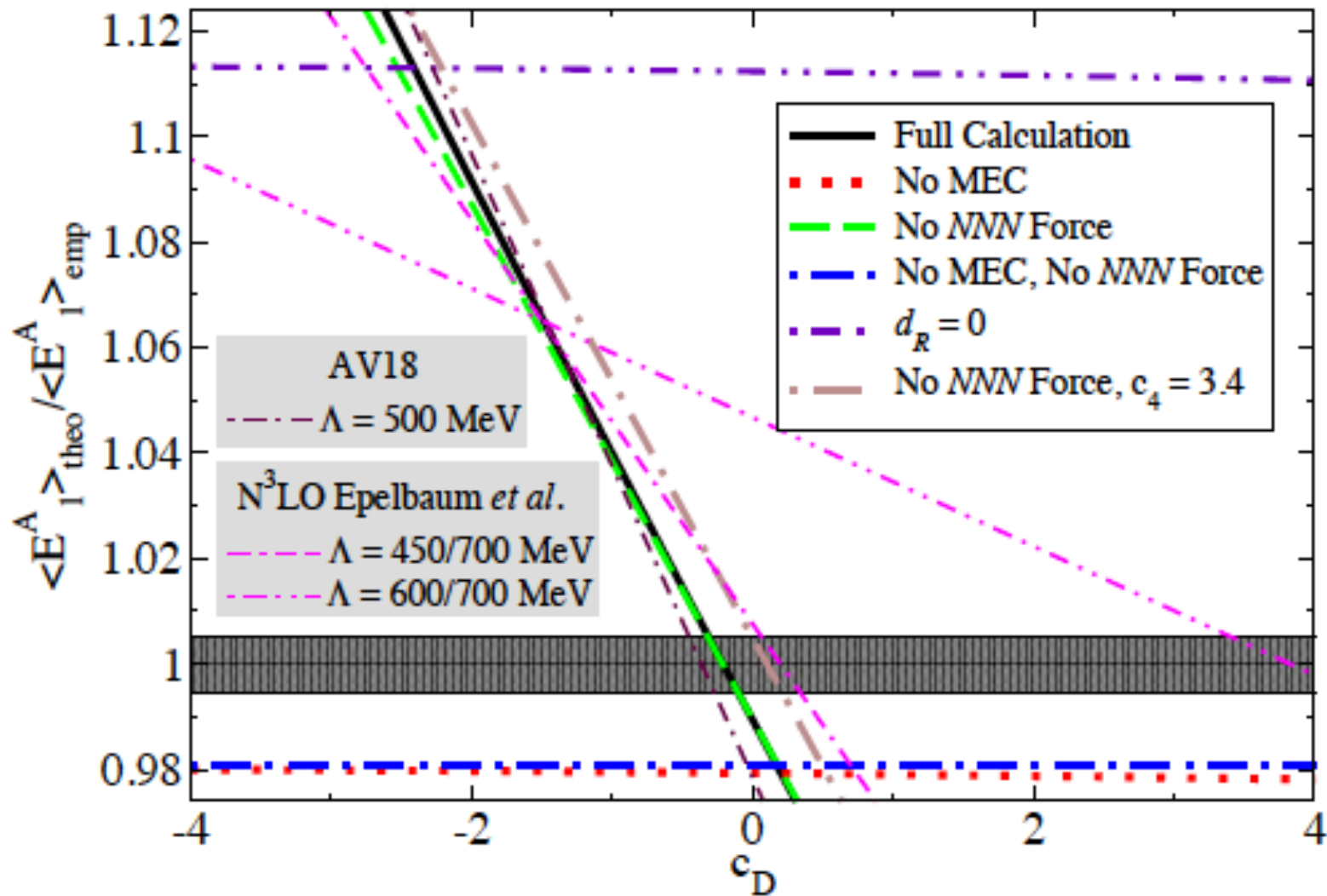
They satisfy the current conservation relation:

$$\mathbf{q} \cdot \mathbf{j}(\mathbf{q}) = [H, \rho(\mathbf{q})]$$



# Determine the LECs of the 3NF

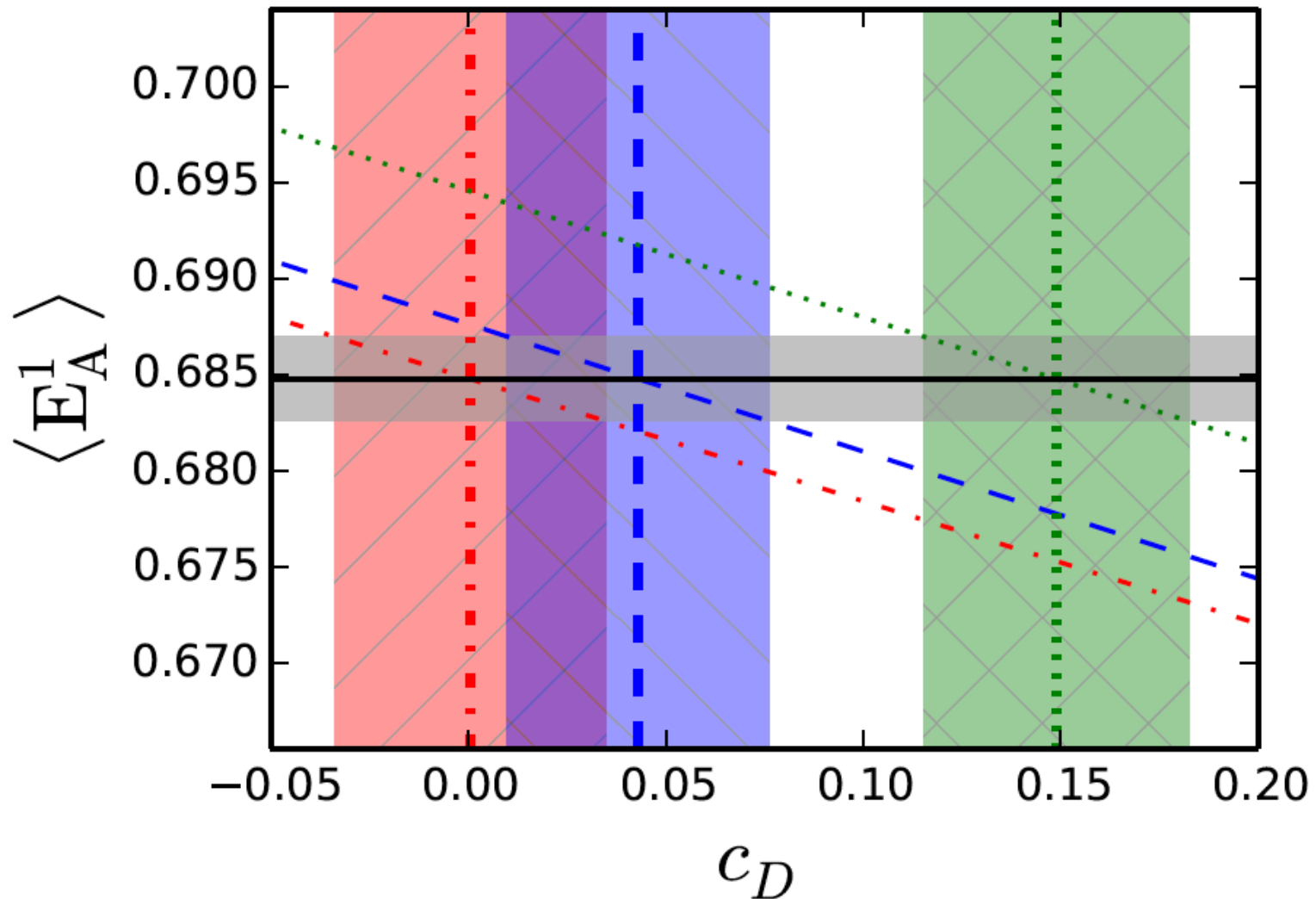
From fit to the triton half life and binding energy (D. Gazit, PRL 2009)



# Optimization of chiral interactions currents at NNLO

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

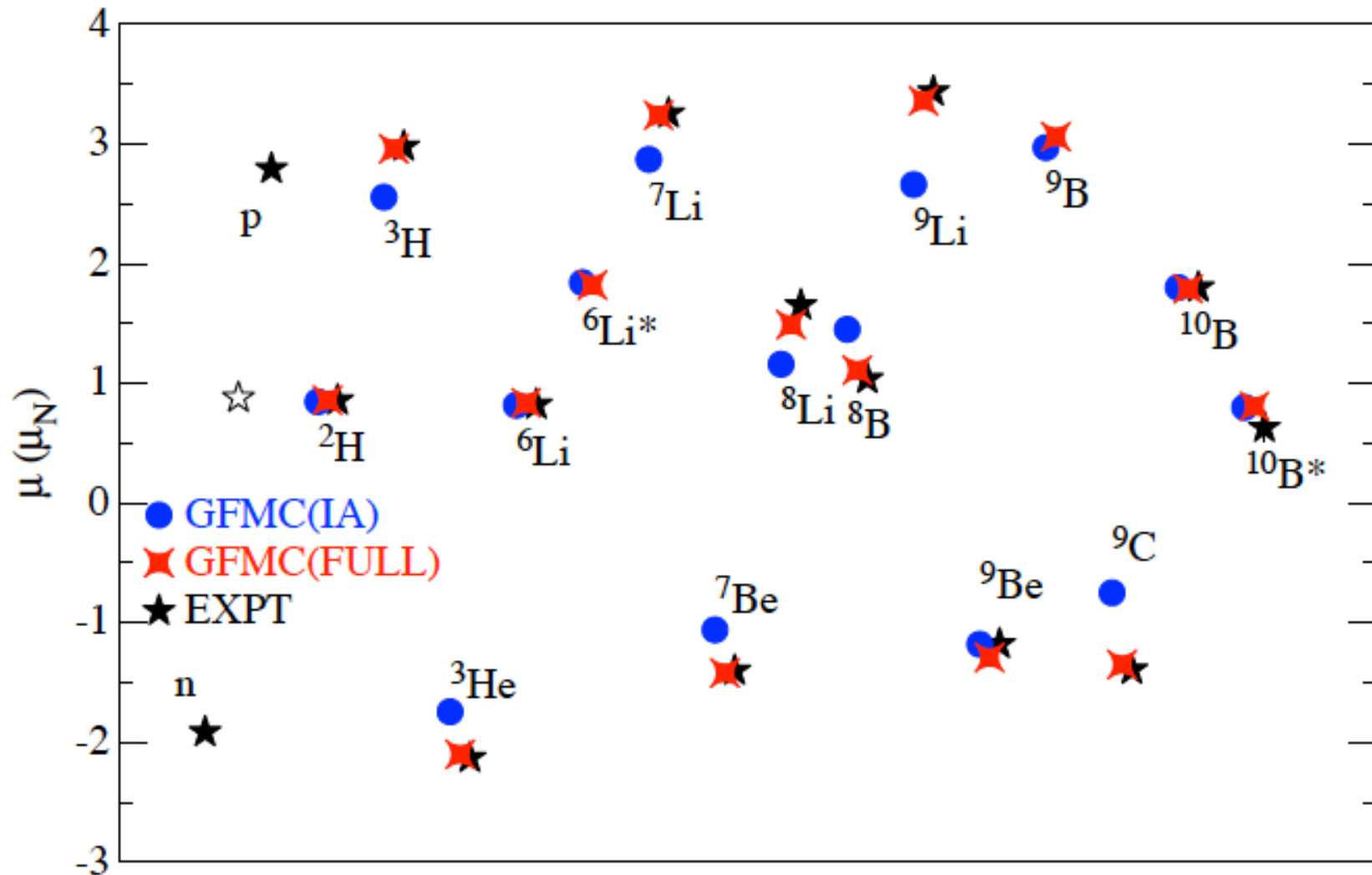
$c_D - c_E$  fit of  $A=3$  binding energies and the  ${}^3\text{H}$  half life at NNLO for chiral cutoffs  $\Lambda = 450, 500, 550$  MeV  $[c_D, c_E] = [0.043, -0.501]$





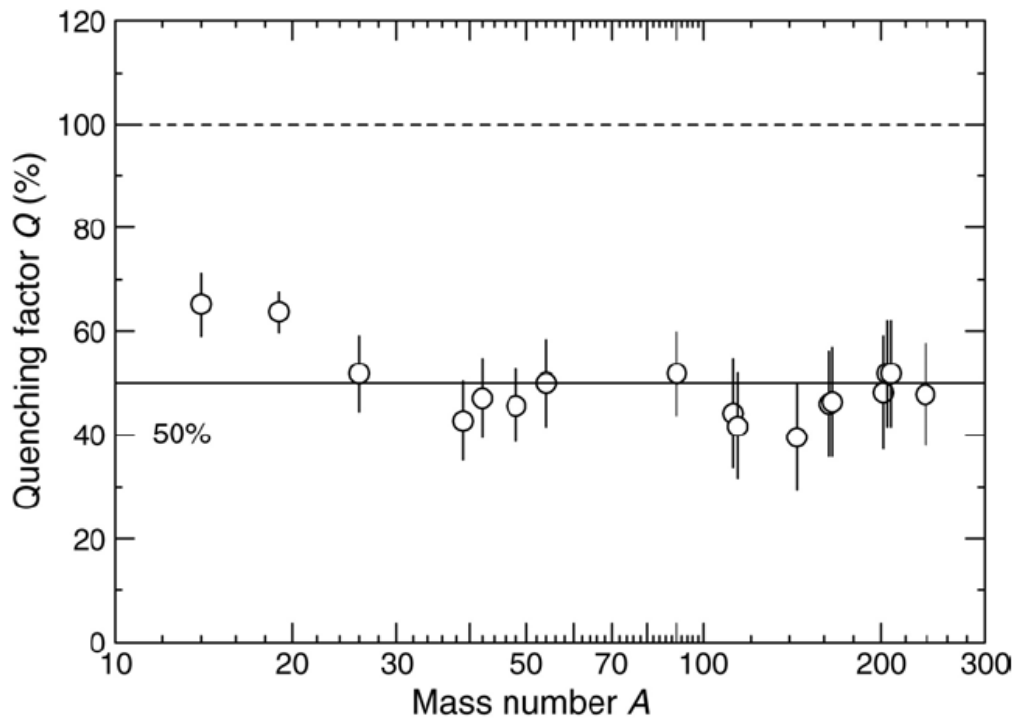
# Role of two-body currents on magnetic moments in light nuclei from GFMC

From S. Pastori arXiv:1508.07363



# Quenching of Gamow-Teller strength in nuclei

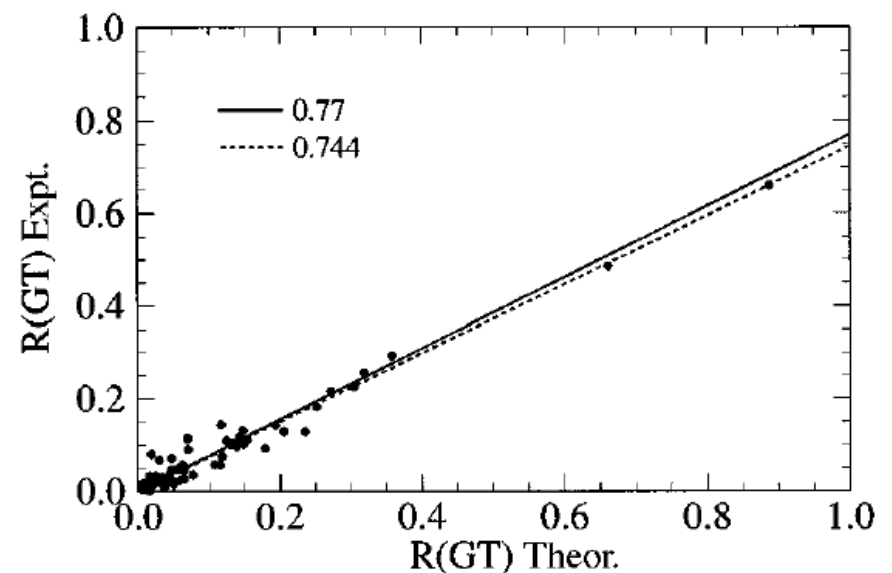
**Long-standing problem:** Experimental beta-decay strengths quenched compared to theoretical results.



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

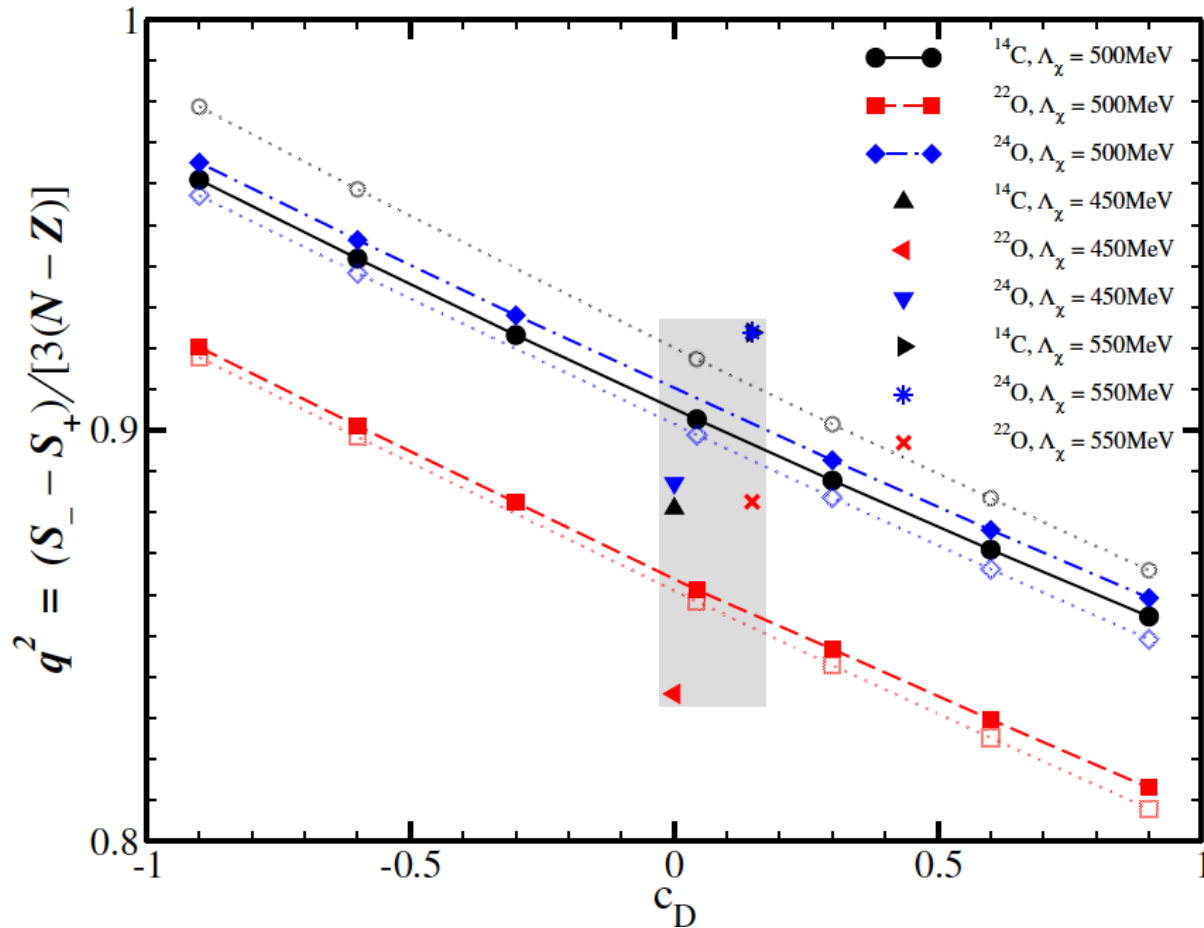
- Renormalizations of the Gamow-Teller operator?
- Missing correlations in nuclear wave functions?
- Model-space truncations?
- Meson exchange currents (2BCs)?

G. Martinez-Pinedo et al, PRC **53**, R2602 (1996)



# Quenching of Ikeda sum rule in $^{14}\text{C}$

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



Quenching factor:

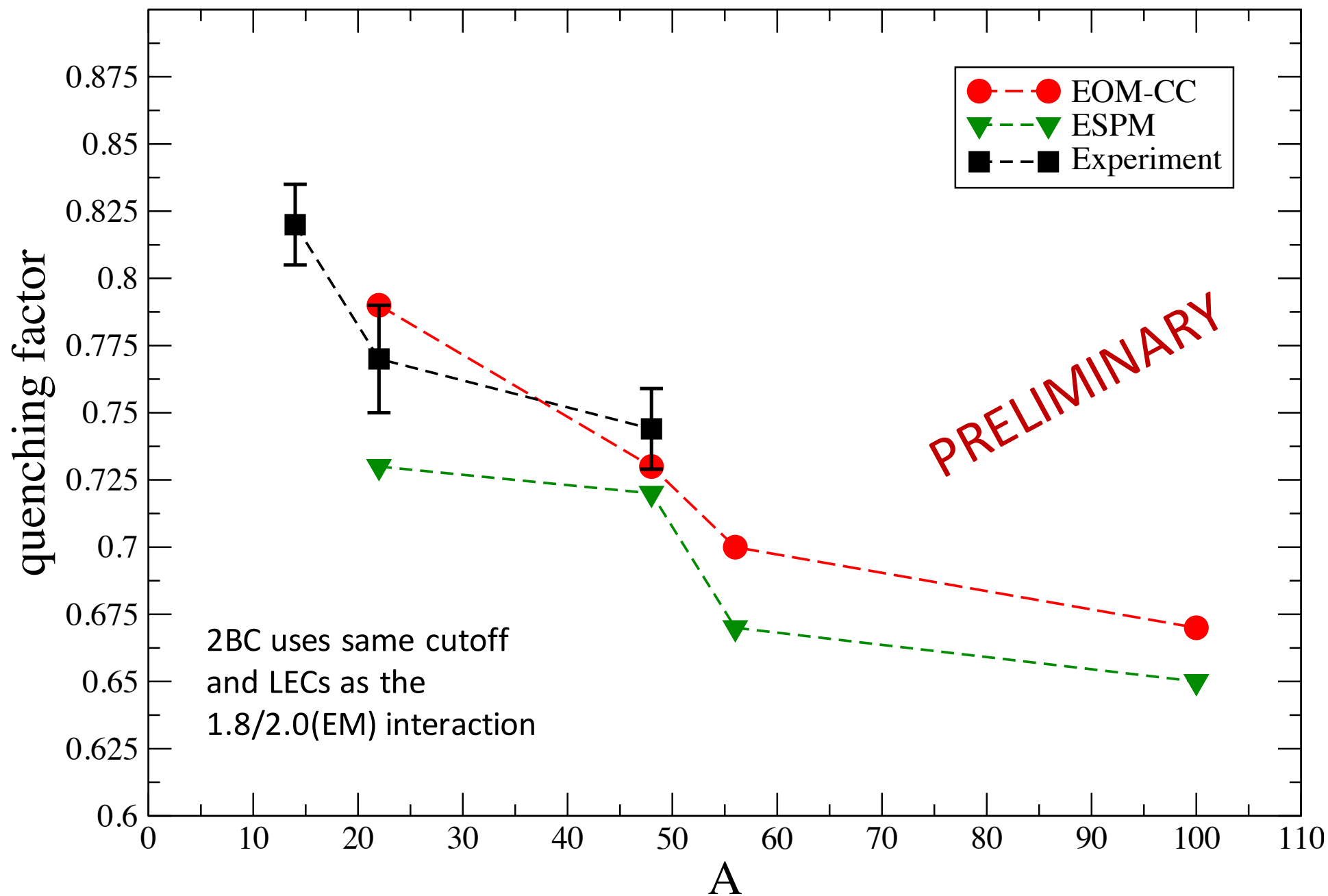
$$Q = \frac{S_{\text{GT}}^-(\omega_{\text{top}}^-) - S_{\text{GT}}^+(\omega_{\text{top}}^+)}{3(N - Z)}$$

Sum rule calculated in CC:

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

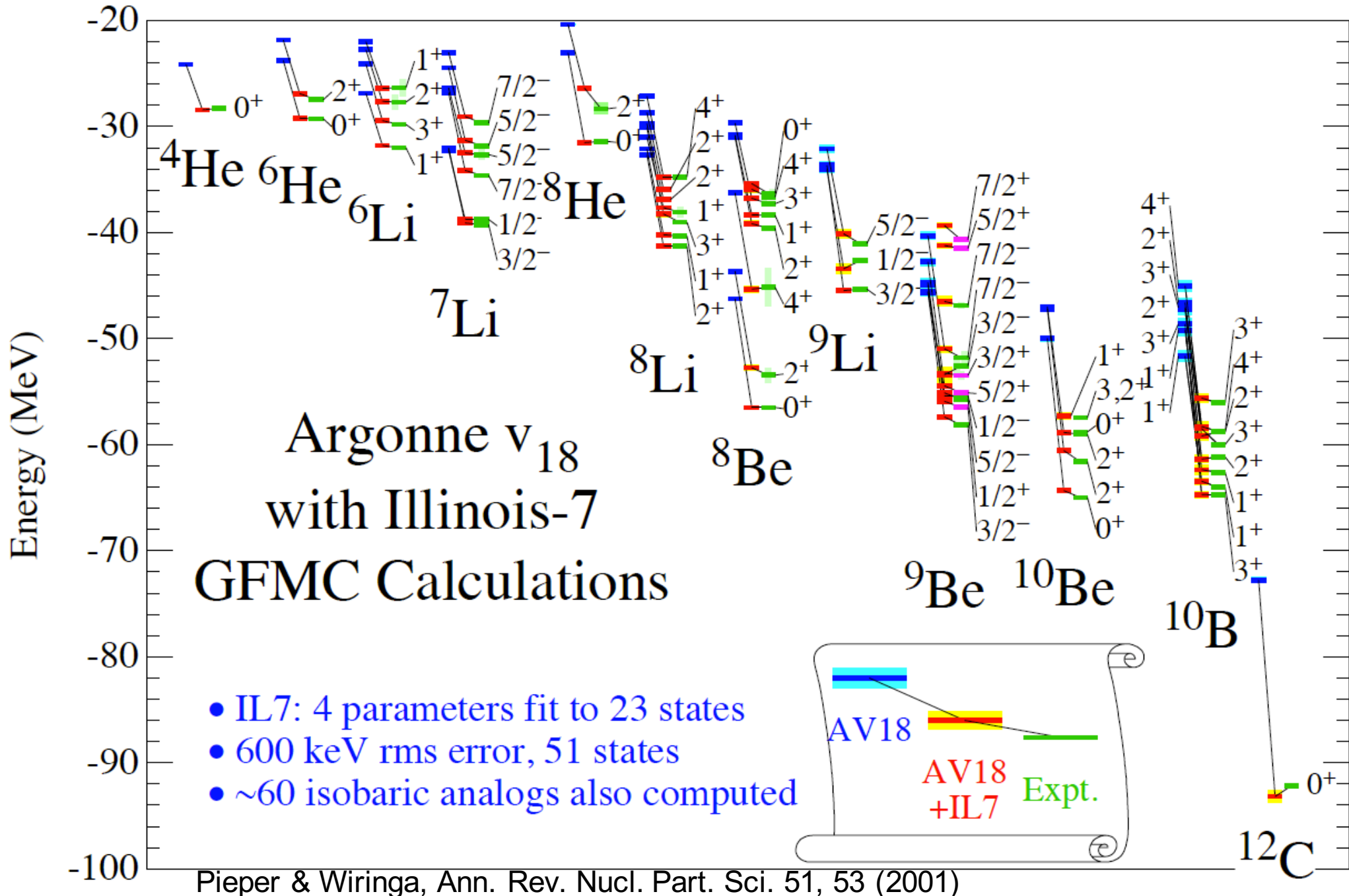
$$S_+ = \langle \Lambda | \overline{\hat{O}_{\text{GT}}} \cdot \overline{\hat{O}_{\text{GT}}^\dagger} | \text{HF} \rangle$$

# Quenching of $g_A$ from two-body currents

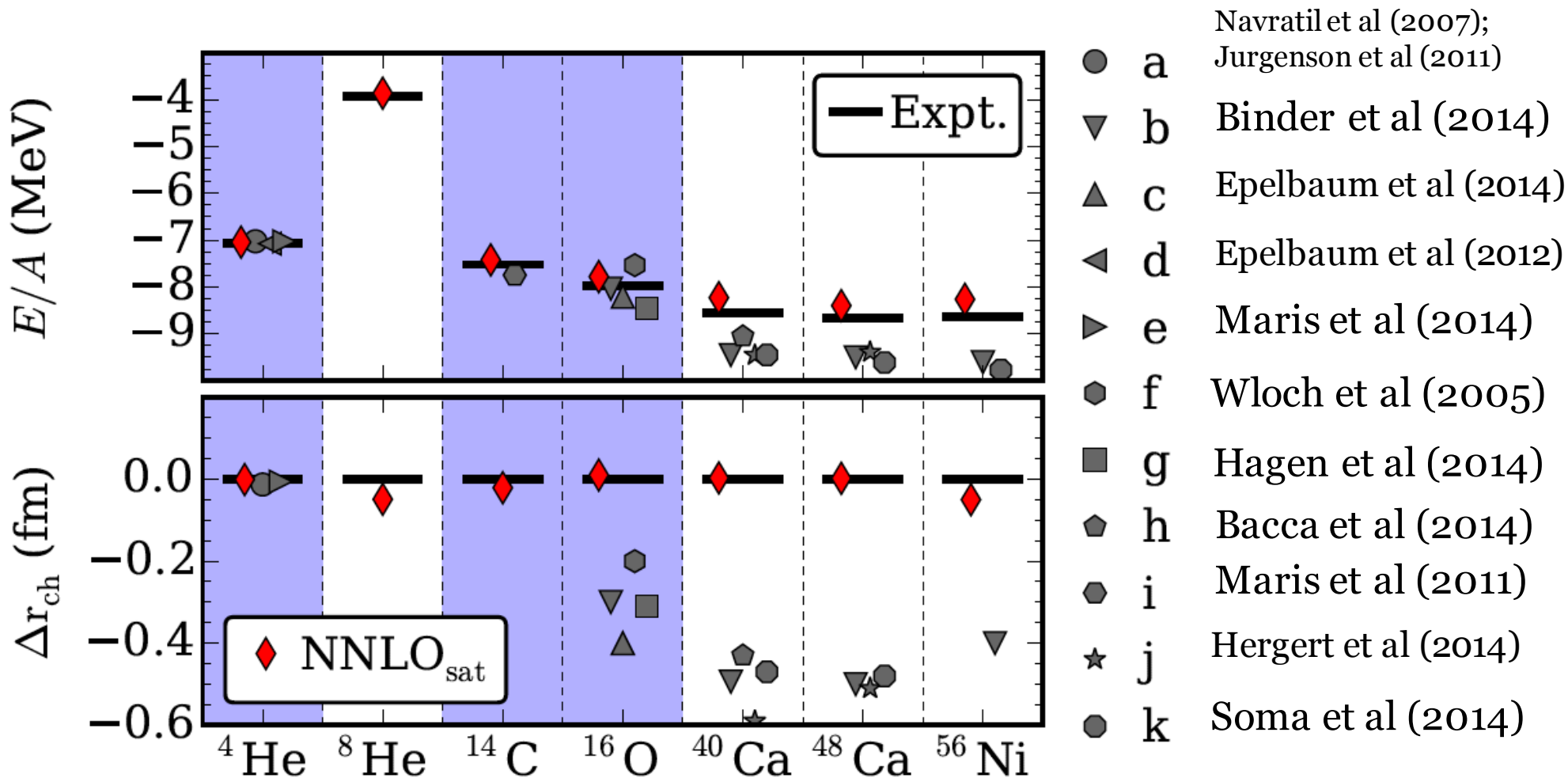


# Green's function Monte Carlo computations

Demonstration that light nuclei can be built from scratch



# Accurate binding energies and radii from a chiral interaction



**Solution:** Simultaneous optimization of NN and 3NFs

Include charge radii and binding energies of  ${}^3\text{H}$ ,  ${}^{3,4}\text{He}$ ,  ${}^{14}\text{C}$ ,  ${}^{16}\text{O}$  in the optimization ( $\text{NNLO}_{\text{sat}}$ )

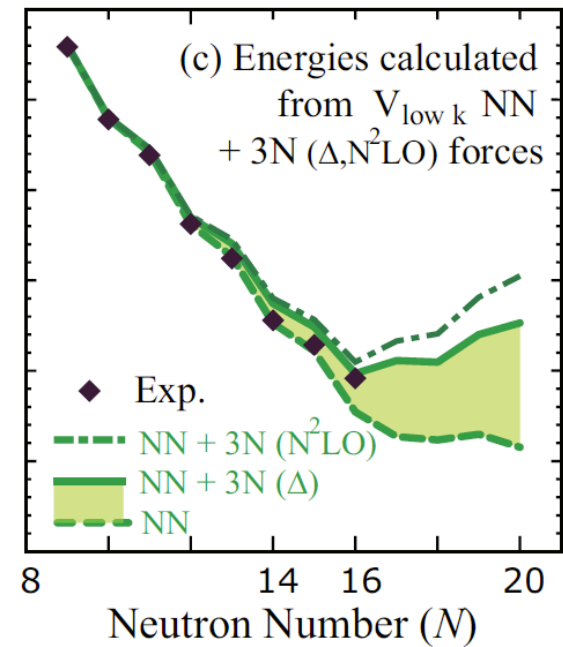
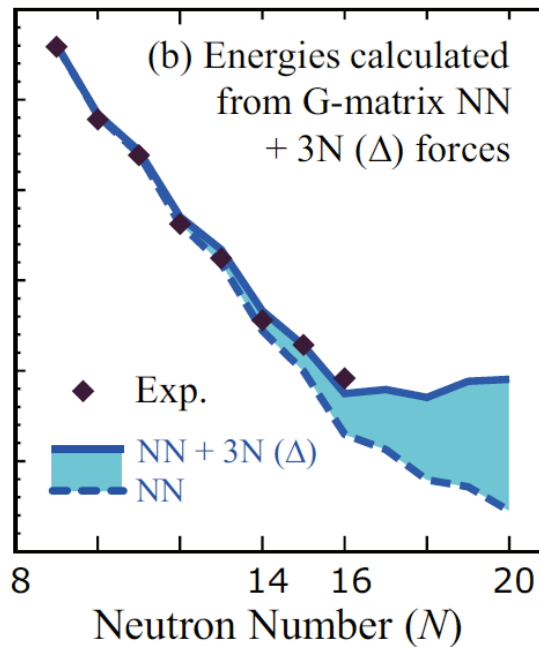
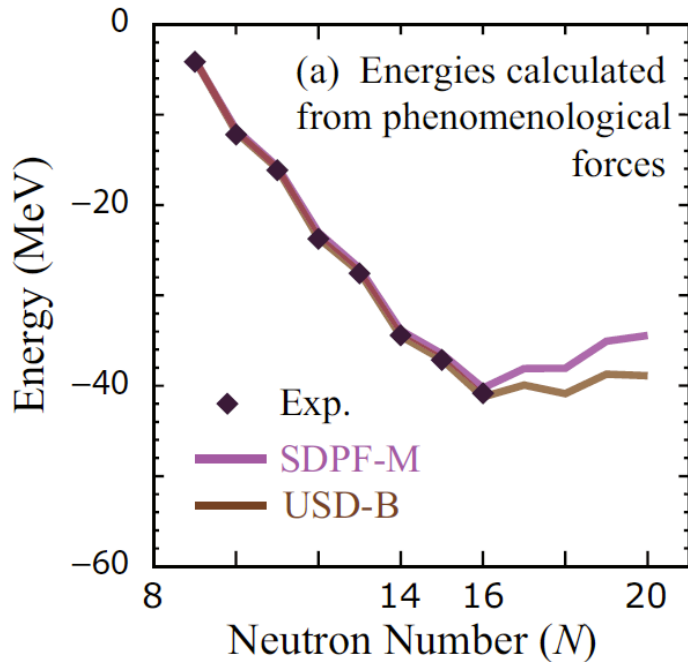
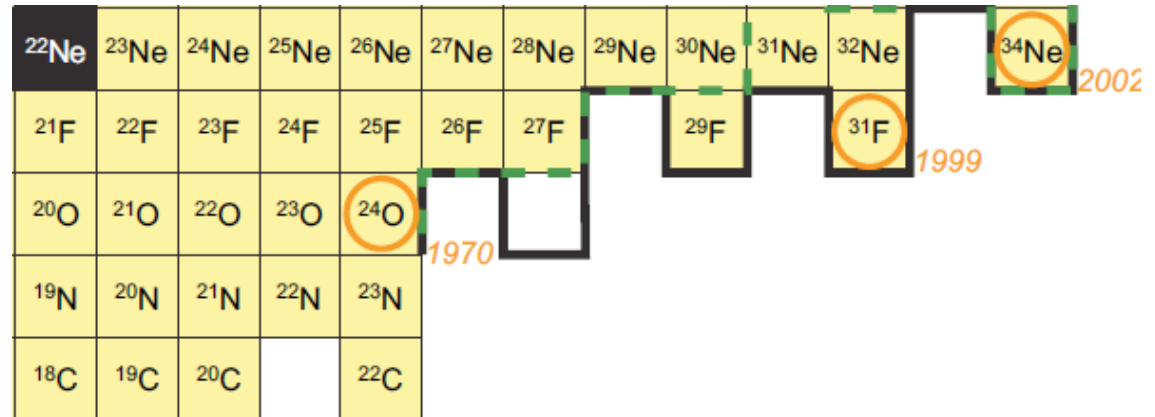
A. Ekström *et al*, Phys. Rev. C **91**, 051301(R) (2015).

G. Hagen *et al*, Phys. Scr. **91**, 063006 (2016).

# The role of 3NFs on nuclear dripline

## Experimental situation

- “Last” stable oxygen isotope  $^{24}\text{O}$
- $^{25}\text{O}$  unstable (Hoffman et al 2008)
- $^{26}\text{O}$  unstable (Lunderberg et al 2012)
- $^{31}\text{F}$  exists (adding on proton shifts drip line by 6 neutrons)



Shell model (sd shell) with monopole corrections based on three-nucleon force predicts  $^{24}\text{O}$  as last stable isotope of oxygen. [Otsuka, Suzuki, Holt, Schwenk, Akaishi, PRL (2010), arXiv:0908.2607; see also NN forces only by Volya & Zelevinsky, PRL 94, 052501 (2005)]

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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3. Which interaction are you looking at? ✓
4. Answers 2 & 3 are correct.

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.**

# Intermession

- Systematic construction of nuclear forces within (chiral) effective field theory
- There is a recipe to follow
- Highlights: power counting, hierarchy of NN  $\gg$  NNN  $\gg$  NNNN forces
- Approach is model independent
- Resulting potential depends on regularization scheme and cutoff
- There are (infinitely) many good ways to implement this

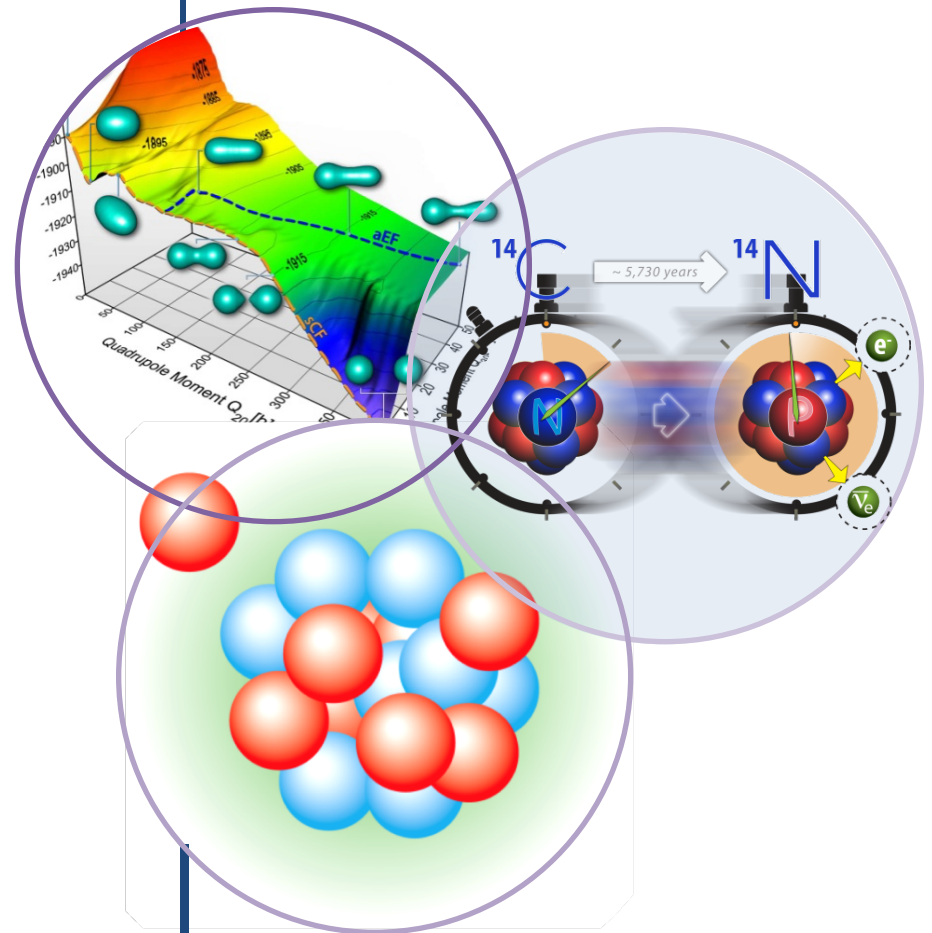
# Nuclear Structure Theory II

**Aim of this lecture:**

**Present recent results ab initio computations with emphasis on the coupled-cluster method**

**Gaute Hagen (ORNL)**

ANL, EBSS, July 25<sup>th</sup>, 2017



# No free lunch

Not well known



Well known

DFT



Shell model



Ab-initio



Interactions



EFT



QCD

Easy to solve



Difficult to solve

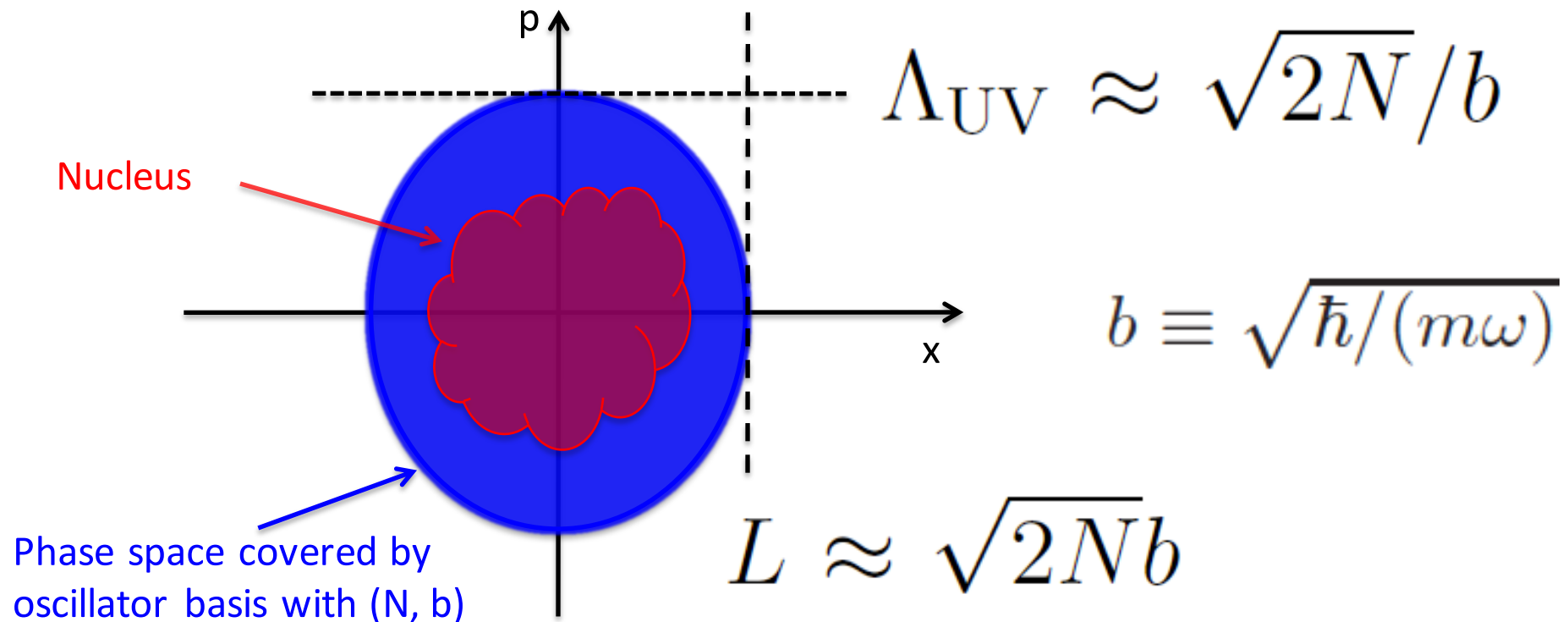
These lectures presents several aspects of this duality.

# Wave function based ab-initio approaches

$$\Psi = \sum_{N=0}^{\infty} C_N R_N(r)$$

Expand the wave-function in harmonic oscillator functions with  $N = 2n+l$

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); König *et al.*, PRC (2014)]

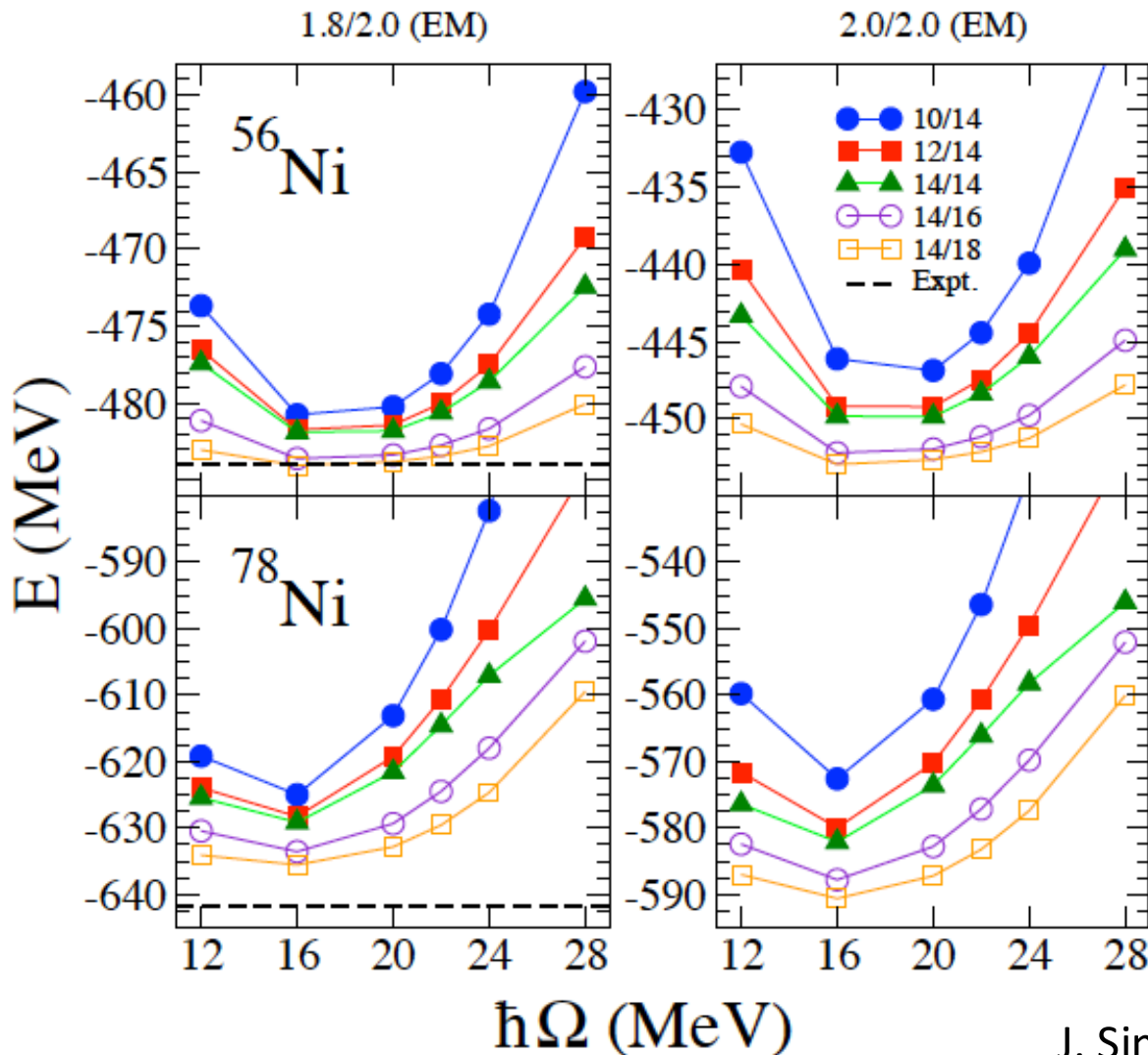


- Nucleus needs to “fit” into basis:
- Nuclear radius  $R < L$
  - cutoff of interaction  $\Lambda < \Lambda_{UV}$

# Wave function based ab-initio approaches

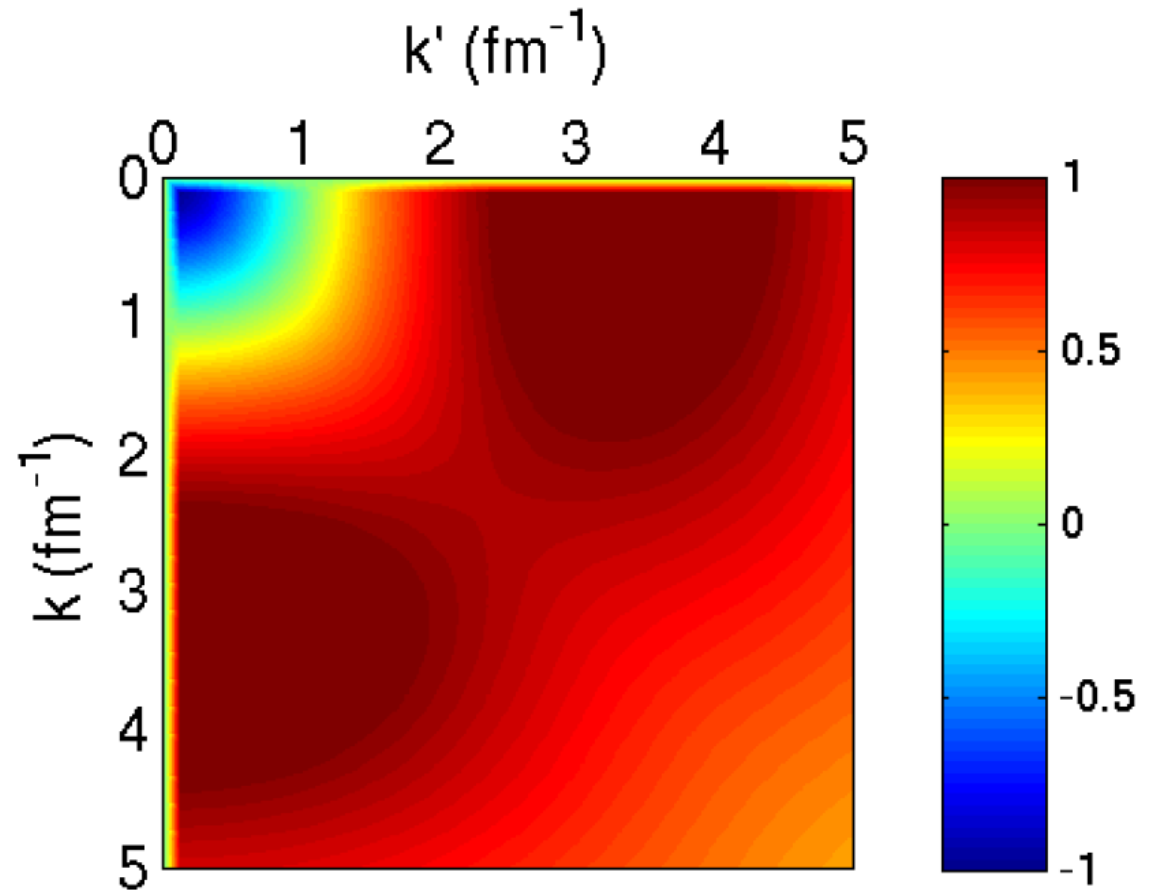
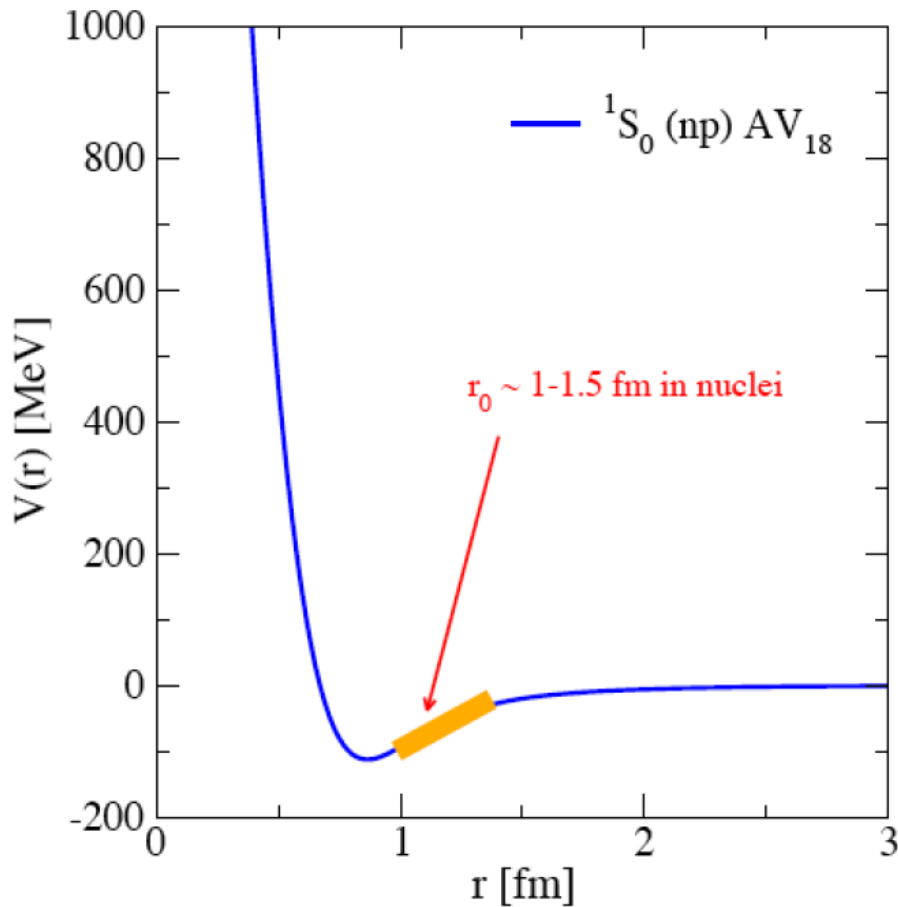
$$\Psi = \sum_{N=0}^{\infty} C_N R_N(r)$$

Expand the wave-function in harmonic oscillator functions with  $N = 2n+l$

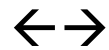


To claim converged results for energies and other observables they should be independent of the size of the basis and frequency of the basis

# Momentum dependence of phenomenological potentials

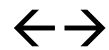


Configuration space



momentum space

Hard core



high-momentum modes

# Similarity renormalization group (SRG) transformation

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

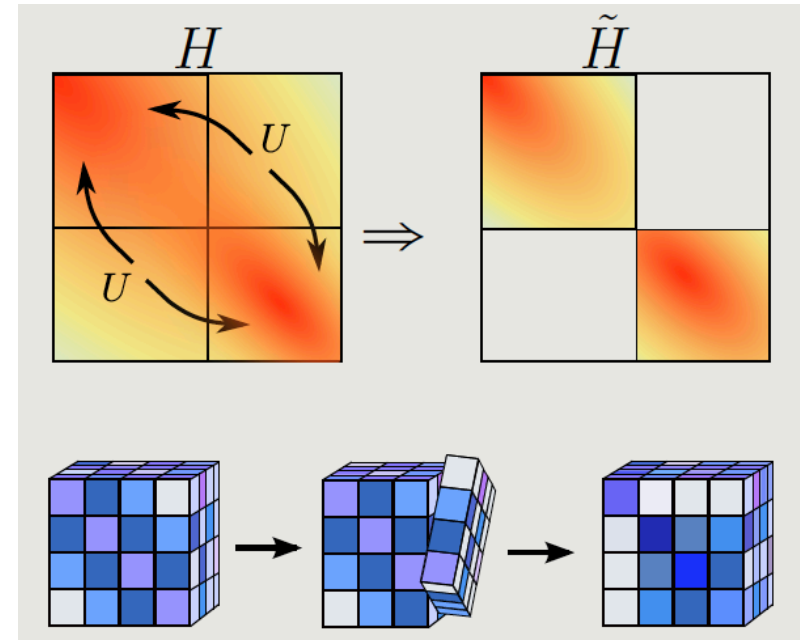
Decouple low from high momenta via a series of (unitary) similarity transformations

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

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

**Pricetag:** induces many-body forces.

From R. S. Stroberg



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

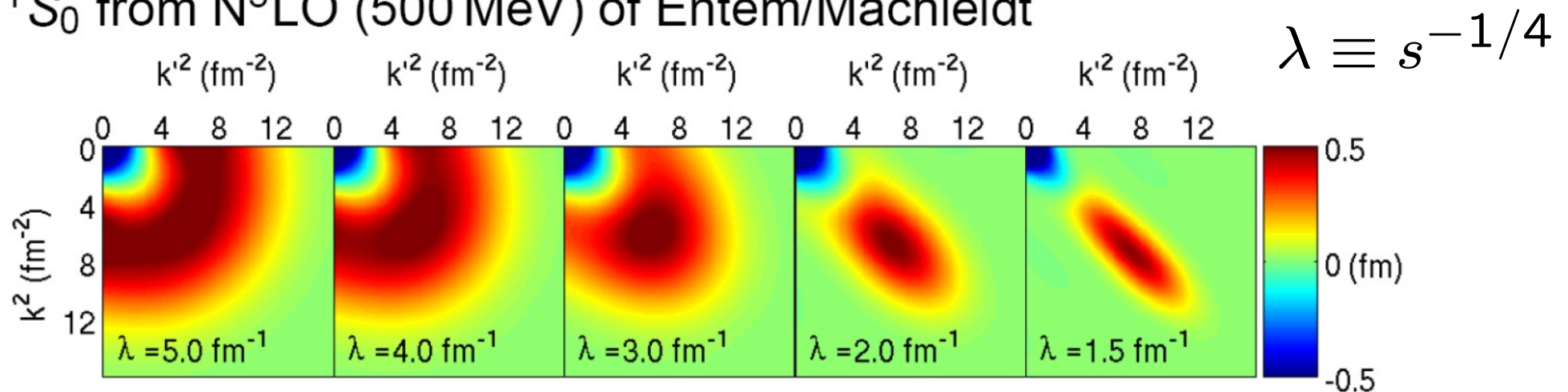


Fig.: Bogner & Furnstahl. See <http://www.physics.ohio-state.edu/~ntg/srg>



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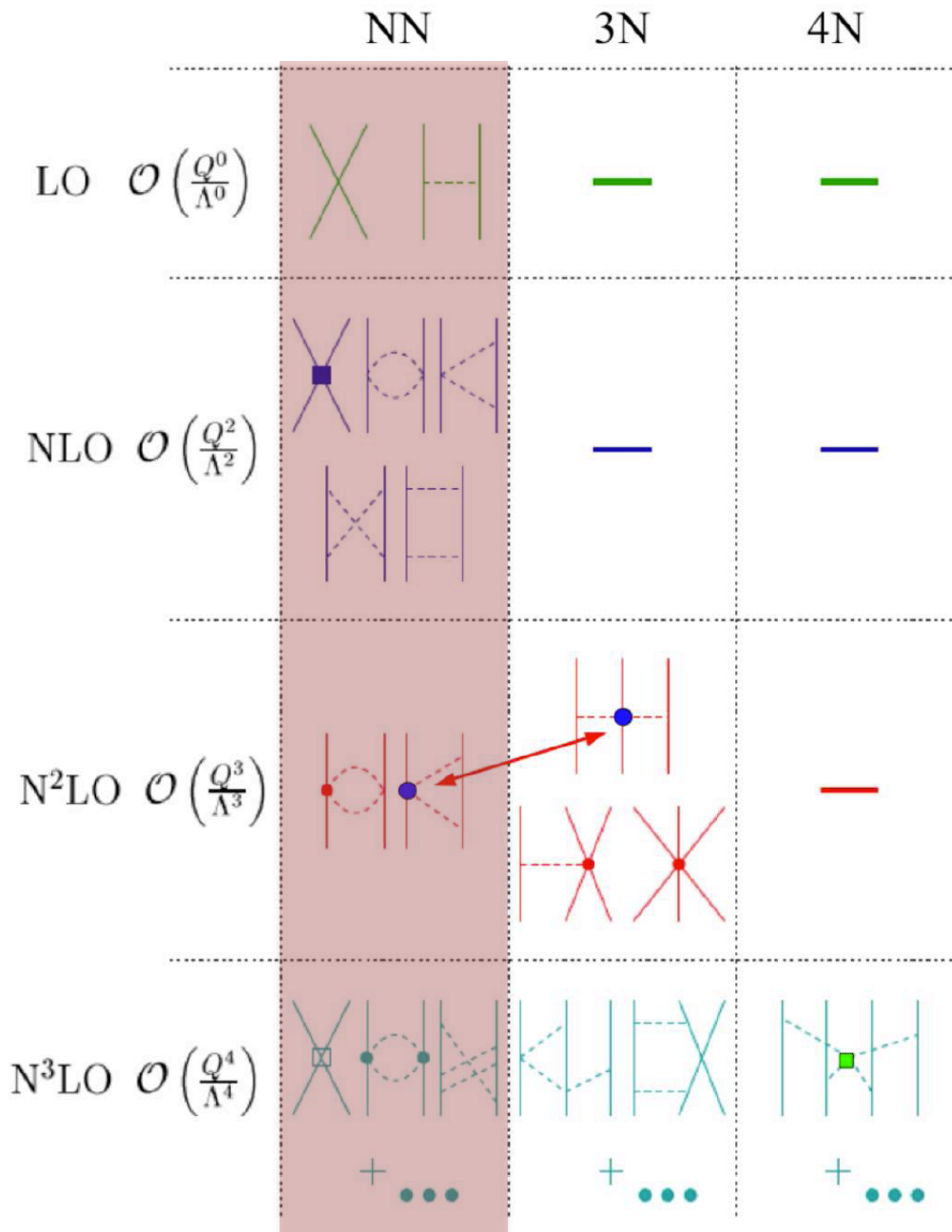
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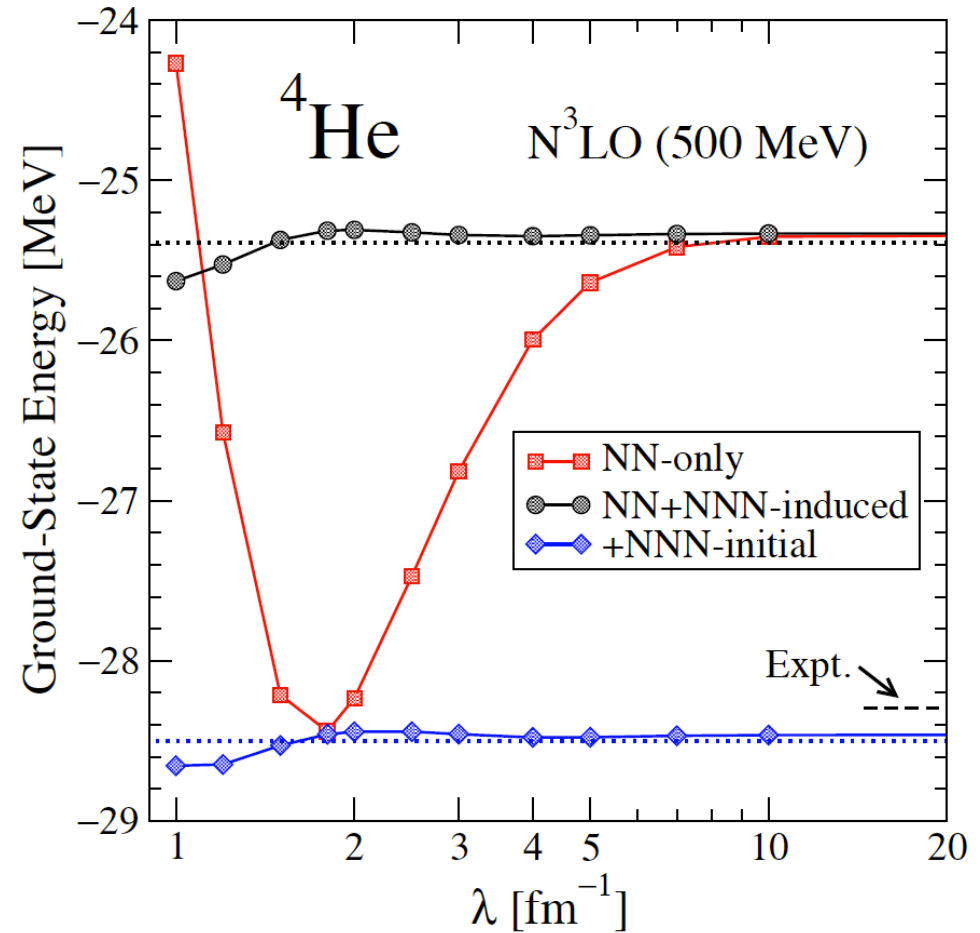
1. Perform a computation with and without SRG and compare.
2. Check how results in the A-body system depend on the cutoff/evolution parameter ✓

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

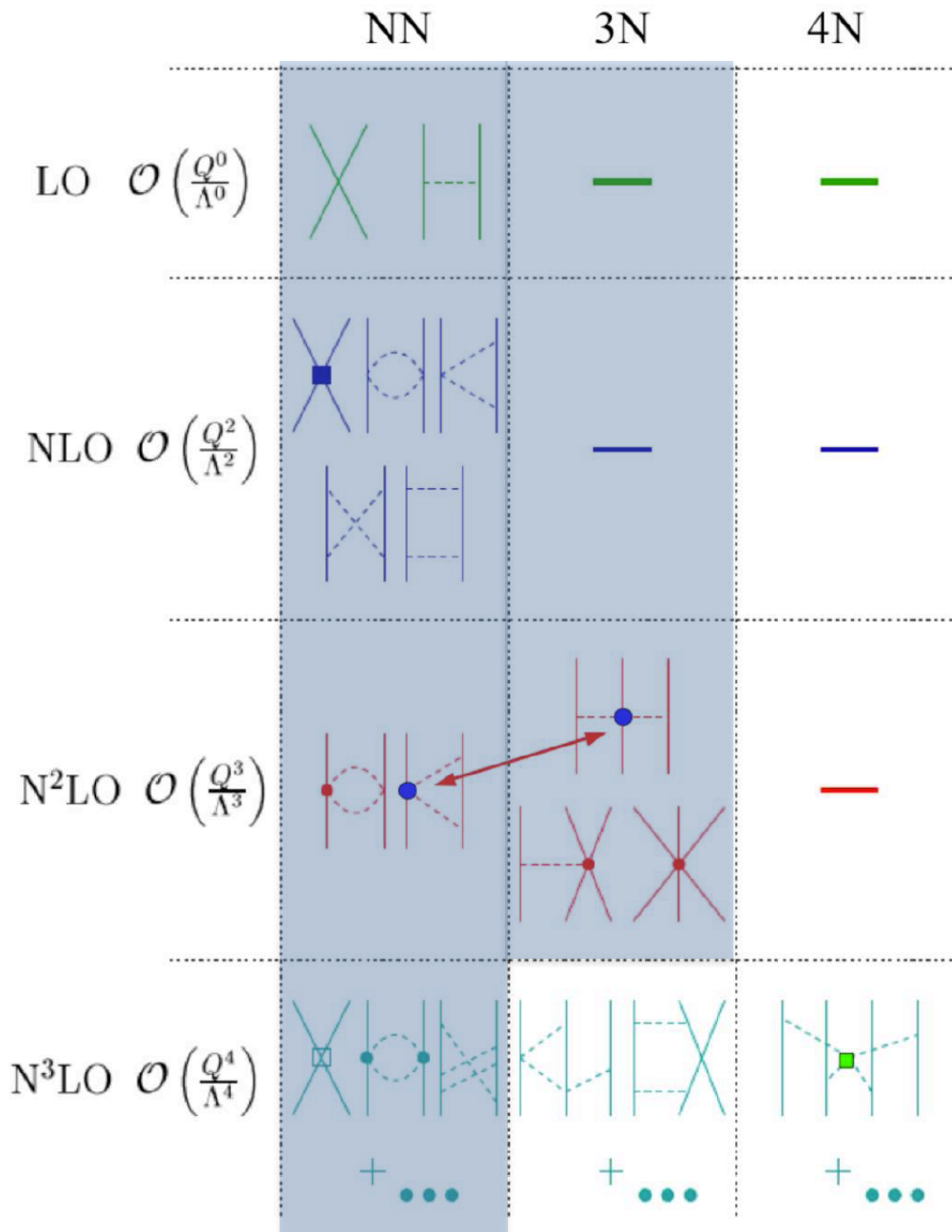
# Nuclear forces from chiral effective field theory



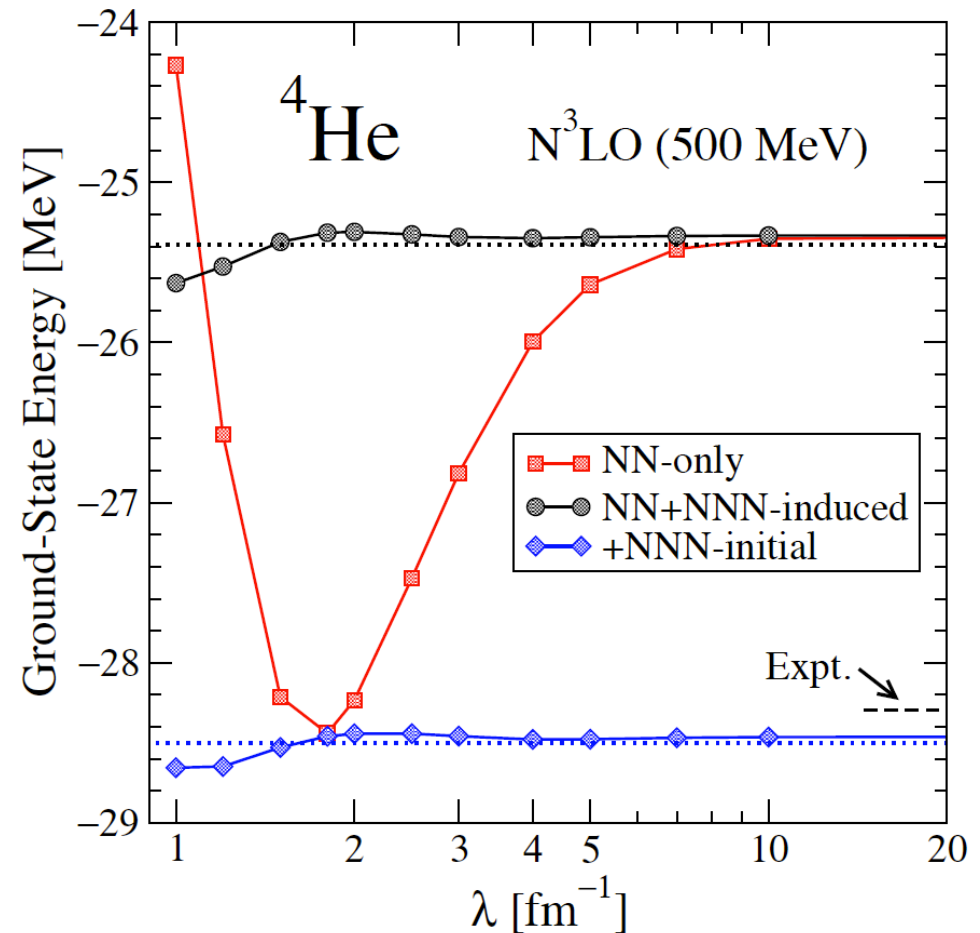
Jurgenson, Navratil & Furnstahl, Phys. Rev. Lett. 103, 082501 (2009), arXiv:0905.1873



# Nuclear forces from chiral effective field theory



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



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

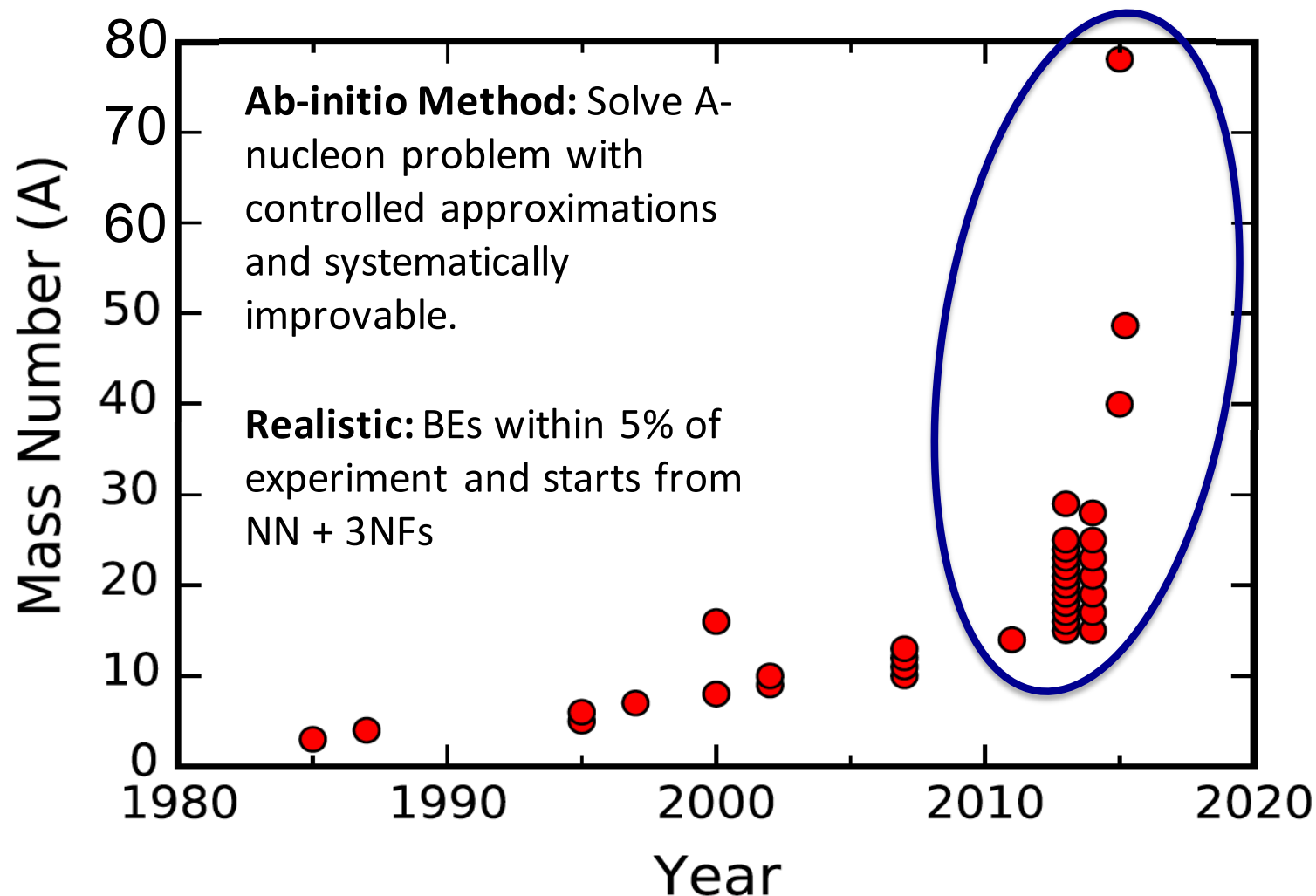
# Intermission

- Introduction to main ideas behind nuclear forces from chiral EFT
- Model-independent approach
- Potentials are not observables, and one can shuffle things around (e.g. via different regularization and renormalization schemes, or via unitary transformations)
- A high cutoff carries a high computational price tag
- Similarity renormalization group transformations very useful tools for study and practical computations

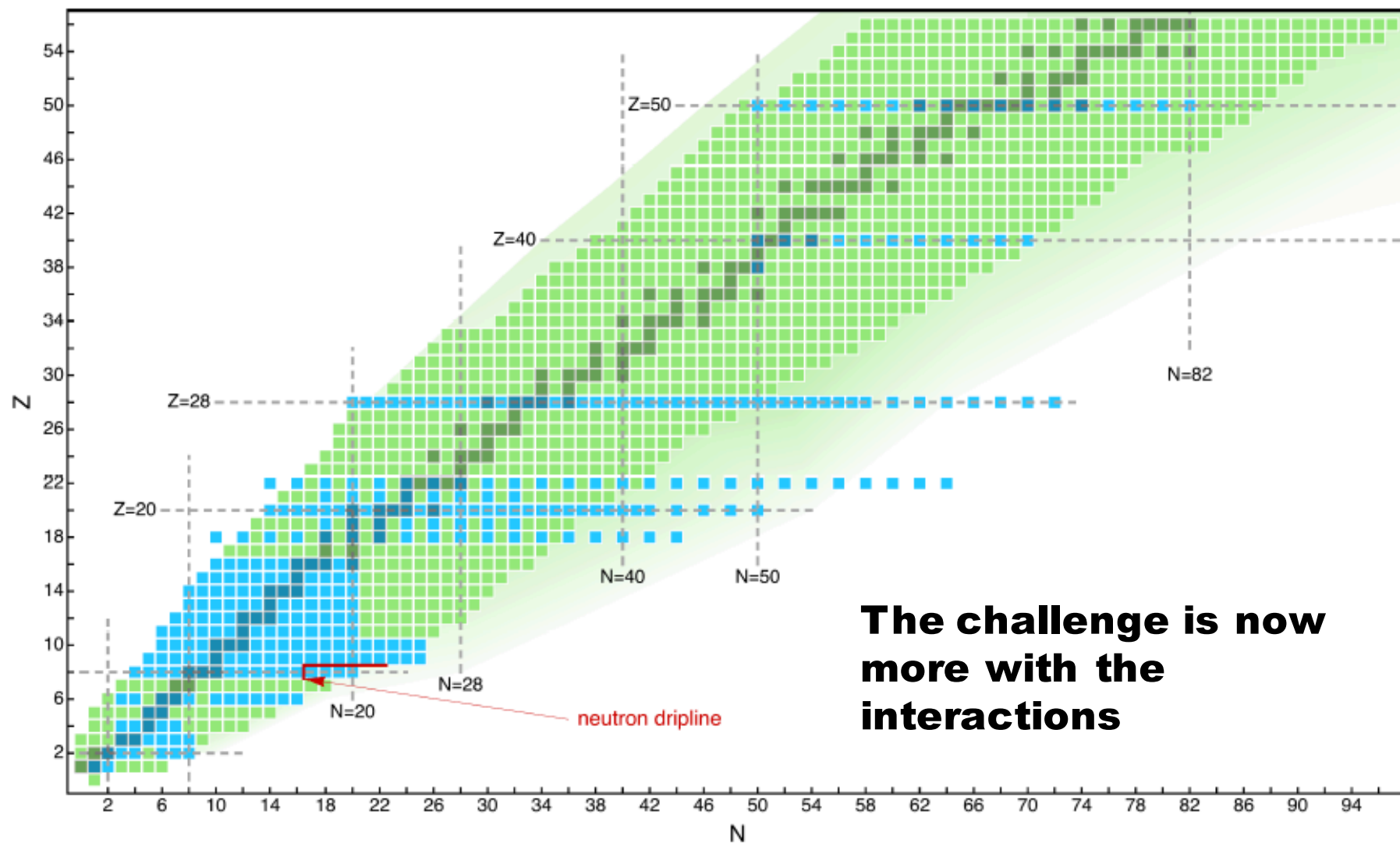
# Trend in realistic ab-initio calculations

**Explosion of many-body methods** (Coupled clusters, Green's function Monte Carlo, In-Medium SRG, Lattice EFT, MCSM, No-Core Shell Model, Self-Consistent Green's Function, UMOA, ...)

**Application of ideas from EFT and renormalization group** ( $V_{\text{low-k}}$ , Similarity Renormalization Group, ...)



# Reach of ab-initio computations of nuclei



H. Hergert *et al*, Physics Reports 621, 165-222 (2016)



# Solving the nuclear many-body problem

- Coupled-cluster method
- No-core shell model
- Greens function Monte Carlo
- Lattice Monte Carlo
- In-Medium SRG
- Self consistent Green's function

Reading suggestions:

## Coupled cluster method:

T. Crawford and H. Schaefer, *Rev. Comp. Chem.* 14, 33 (2000); I. Shavitt and R. Bartlett, *Many-Body Methods in Chemistry and Physics: MBPT and Coupled-Cluster Theory* (Cambridge, 2009); Hagen, TP, Hjorth-Jensen & Dean, arXiv:1312.7872.

## No-core shell model:

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

## GFMC:

Pieper & Wiringa: *Ann. Rev. Nucl. Part.Sci.* 51, 53 (2001); nucl-th/0103005

## Lattice Monte Carlo:

Dean Lee, *Prog. Part. Nucl. Phys.* 63 117-154 (2009); arXiv:0804.3501

## In-medium SRG:

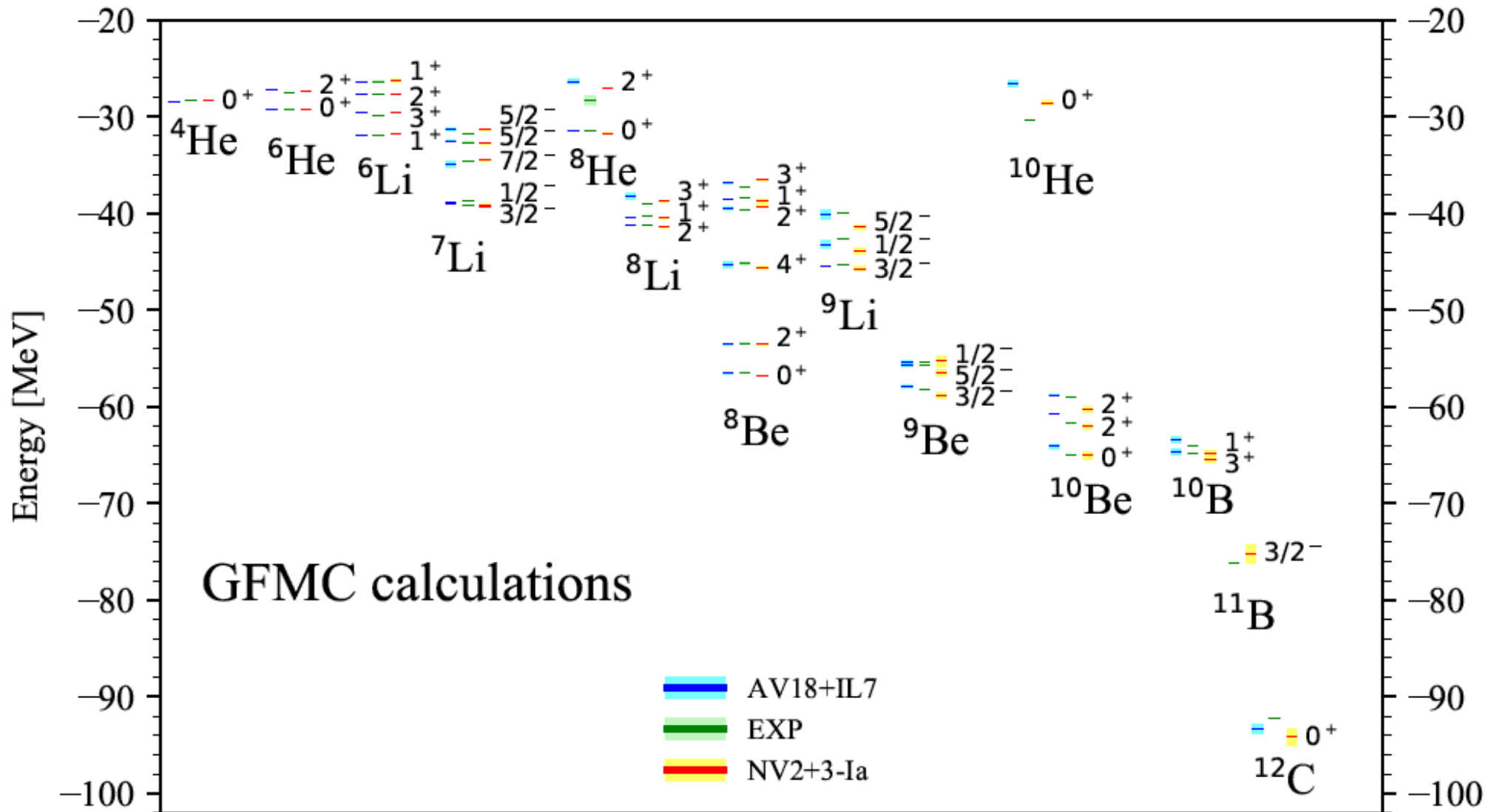
Hergert et al., *Phys. Rep.* 621, 165 (2016); arXiv:1512.06956

## Self-consistent Green's functions:

A. Carbone and C. Barbieri, *Lecture Notes in Physics*, arXiv:1611.03923 (2017)

# Green's function Monte Carlo computations

Demonstration that light nuclei can be built from scratch



Piarulli et al, arXiv:1707.02883 (2017)

# Brief introduction to coupled-cluster theory (CCSD)

Ansatz:

$$|\Psi\rangle = e^T |\Phi\rangle$$

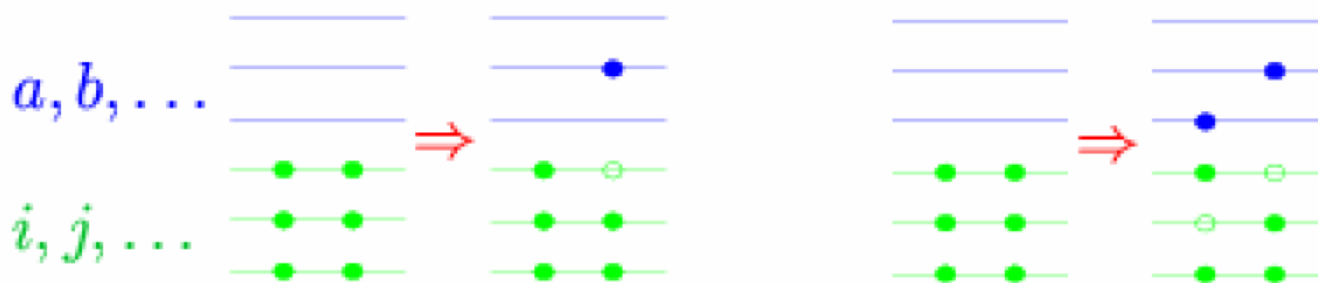
$$T = T_1 + T_2 + \dots$$

$$T_1 = \sum_{ia} t_i^a a_a^\dagger a_i$$

$$T_2 = \sum_{ijab} t_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i$$

- ☺ Scales gently (polynomial) with increasing problem size  $o^2u^4$ .
- ☺ Truncation is the only approximation.
- ☺ Size extensive (error scales with A)

Correlations are *exponentiated* 1p-1h and 2p-2h excitations. Part of np-nh excitations included!



How do we deal with this ansatz / how do we choose the parameters of the cluster operator?

# Coupled-cluster method (CCSD approximation)

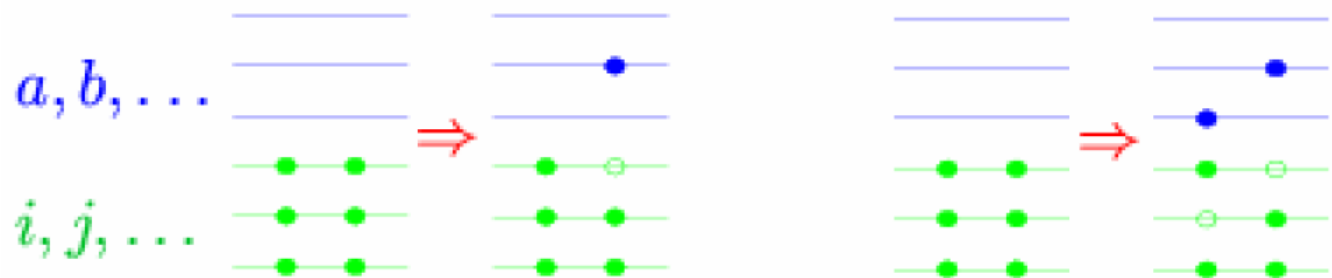
$$\begin{aligned}
 B_1 &= T_1 \\
 B_2 &= T_2 + \frac{1}{2} T_1^2 \\
 B_3 &= T_3 + T_2 T_1 + \frac{1}{6} T_1^3 \\
 B_4 &= T_4 + T_3 T_1 + \frac{1}{2} T_2^2 + \frac{1}{2} T_2 T_1^2 + \frac{1}{24} T_1^4 \\
 &\dots
 \end{aligned}$$

CCSD  
CCSDT

Disconnected quadruples  
Connected quadruples

- CCSD captures most of the 3p3h and 4p4h excitations (scales as  $n_o^2 n_u^4$ )
- In order to describe  $\alpha$ -cluster states need to include full quadruples (CCSDTQ) (scales  $n_o^4 n_u^6$ )

Correlations are *exponentiated* 1p-1h and 2p-2h excitations. Part of np-nh excitations included!



# Coupled-cluster method

Schrödinger equation

$$\hat{H}|\Psi\rangle = E|\Psi\rangle$$

Exponential ansatz for correlation operator

$$\hat{H}e^{\hat{T}}|\Phi_0\rangle = Ee^{\hat{T}}|\Phi_0\rangle$$

yields Schrödinger equation for similarity transformed Hamiltonian

$$e^{-\hat{T}}\hat{H}e^{\hat{T}}|\Phi_0\rangle = E|\Phi_0\rangle$$

Similarity-transformed Hamiltonian is not Hermitian.

$$\overline{H} \equiv e^{-\hat{T}}\hat{H}e^{\hat{T}}$$

# Coupled-cluster equations (in CCSD approximation)

Multiply with 0p0h, 1p1h, and 2p2h bras and obtain coupled-cluster equations.

$$\begin{aligned}\langle \Phi_0 | \overline{H} | \Phi_0 \rangle &= E \\ \langle \Phi_i^a | \overline{H} | \Phi_0 \rangle &= 0 \\ \langle \Phi_{ij}^{ab} | \overline{H} | \Phi_0 \rangle &= 0\end{aligned}$$

The 1p1h and 2p2h excitations are defined as

$$\begin{aligned}|\Phi_i^a\rangle &= \hat{a}_a^\dagger \hat{a}_i |\Phi_0\rangle \\ |\Phi_{ij}^{ab}\rangle &= \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i |\Phi_0\rangle\end{aligned}$$

**CCSD approximation: The similarity-transformed Hamiltonian has no 1p1h and no 2p2h excitations from the reference state.**

First, one needs to solve the CCSD equations. This yields the cluster amplitudes  $t_i^a$  and  $t_{ij}^{ab}$  that define the similarity-transformed Hamiltonian.

Second, the ground-state energy can be computed.

# It's all about the similarity-transformed Hamiltonian

Structure of similarity-transformed Hamiltonian after the CCSD equations are solved

$$\bar{H}_{\text{CCSD}} = \begin{array}{ccc} & \begin{array}{ccc} 0p0h & 1p1h & 2p2h \end{array} & \\ \begin{array}{c} 0p0h \\ 1p1h \\ 2p2h \end{array} & \left( \begin{array}{ccc} E_{\text{CCSD}} & \bar{H}_{0S} & \bar{H}_{0D} \\ 0 & \bar{H}_{SS} & \bar{H}_{SD} \\ 0 & \bar{H}_{DS} & \bar{H}_{DD} \end{array} \right) & \end{array}$$

For excited states and expectation values: Solve the right and left eigenvalue problems

$$\begin{aligned} \bar{H}|R_n\rangle &= E_n|R_n\rangle \\ \langle L_n|\bar{H} &= E_n\langle L_n| \end{aligned}$$

Benefits:

- small model space (2p-2h) excitations are not too numerous)
- similarity transformed Hamiltonian has up to three-body operators in this space

# Computation of the similarity-transformed Hamiltonian

Baker Campbell Hausdorff relation

$$e^{-\hat{T}} \hat{H} e^{\hat{T}} = \hat{H} + [\hat{H}, \hat{T}] + \frac{1}{2!} [[\hat{H}, \hat{T}], \hat{T}] + \frac{1}{3!} [[[\hat{H}, \hat{T}], \hat{T}], \hat{T}] + \frac{1}{4!} [[[[\hat{H}, \hat{T}], \hat{T}], \hat{T}], \hat{T}] + \dots$$

Key observation:

1. When expressed in a diagrammatic way, no unlinked diagrams will be produced by the exponential similarity transform  $\rightarrow$  size extensive approach
2. All terms of the cluster operator  $T$  commute with each other as annihilation and creation operators refer to different sets of single-particle orbitals (occupied and unoccupied single-particle states)

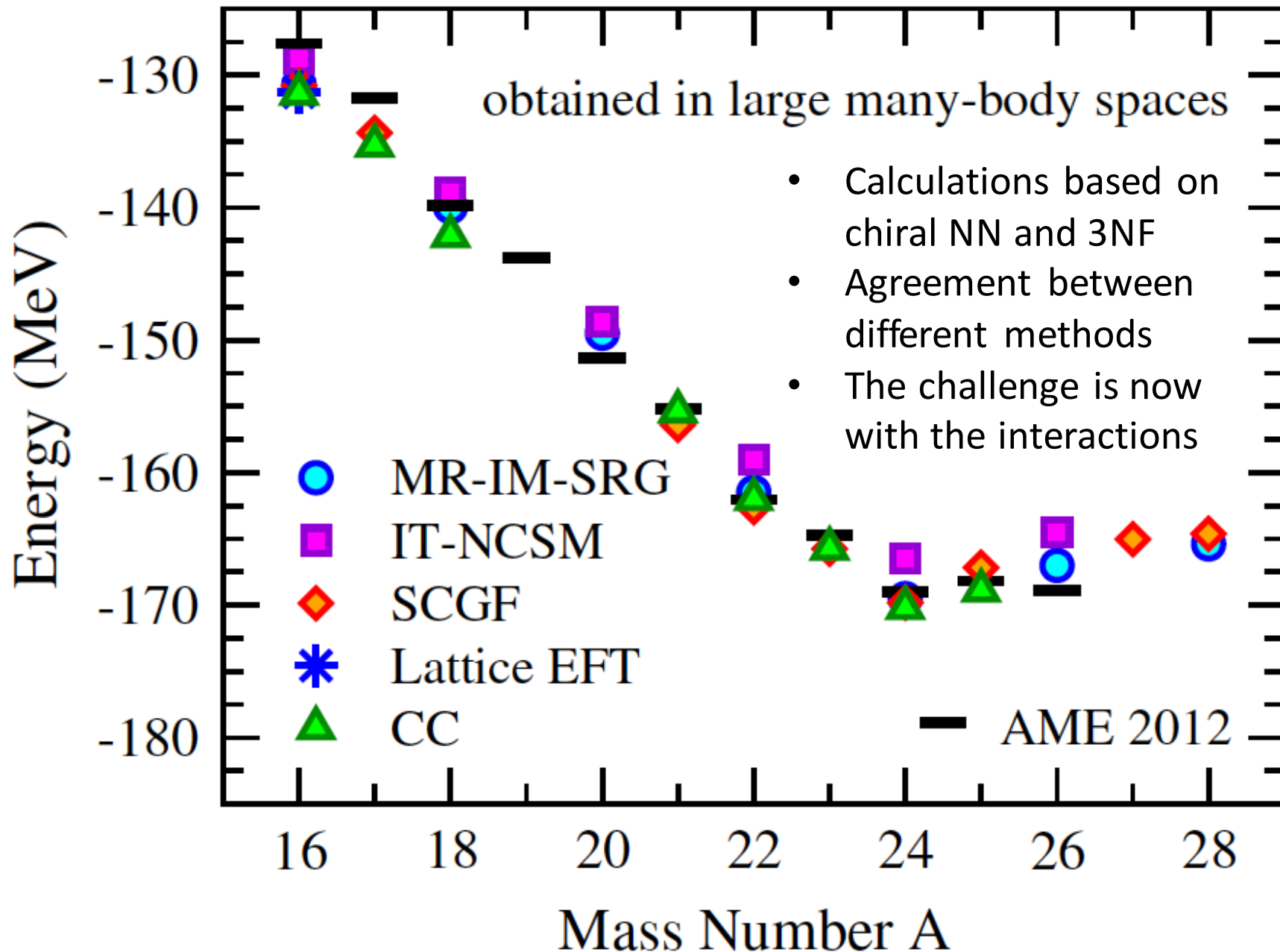
Consequences (of second point)

## The BCH expansion is finite

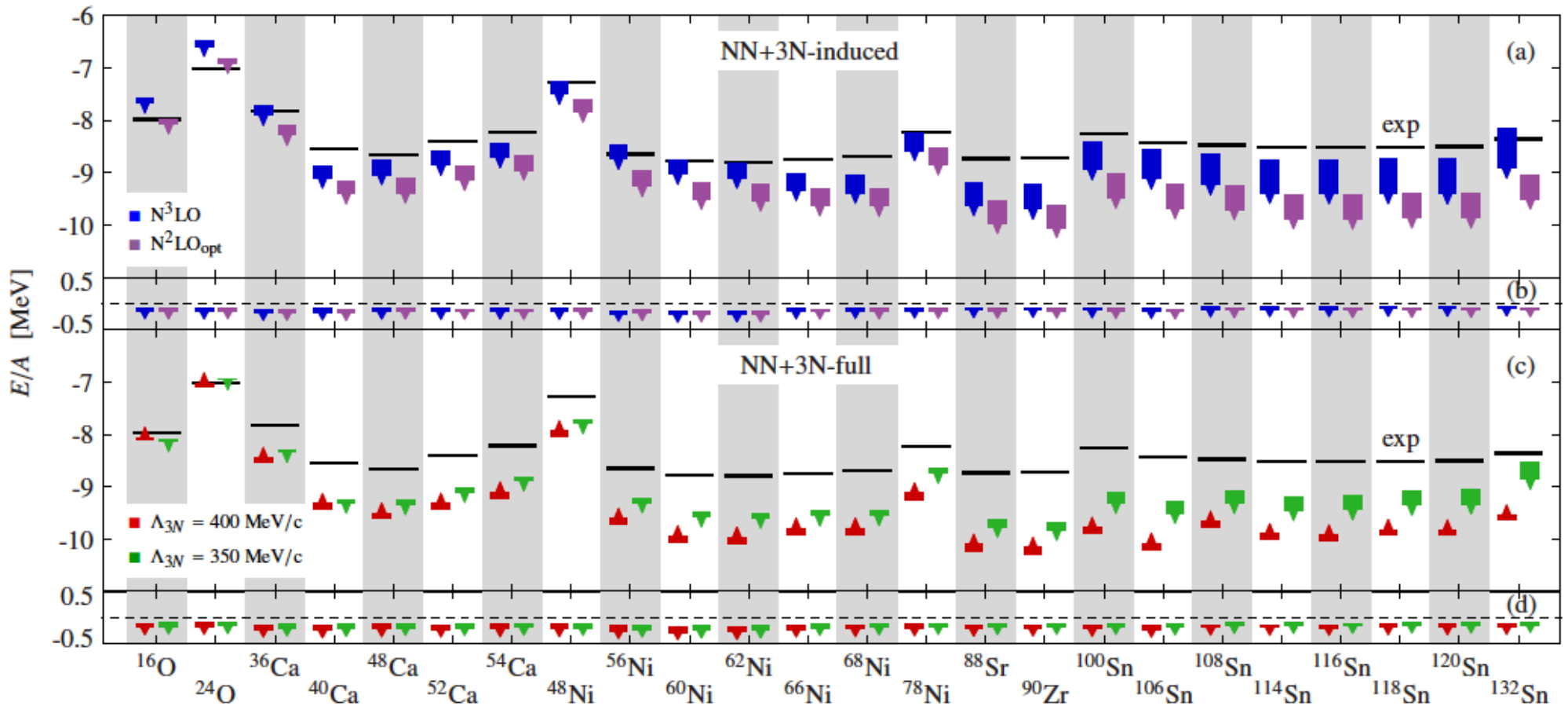
It terminates at 4-fold nested commutators (as shown above) because we deal with a two-body Hamiltonian and generates up to six-body induced terms. This makes the method very efficient.



# Oxygen chain with interactions from chiral EFT



# Ab-initio computations towards heavy nuclei

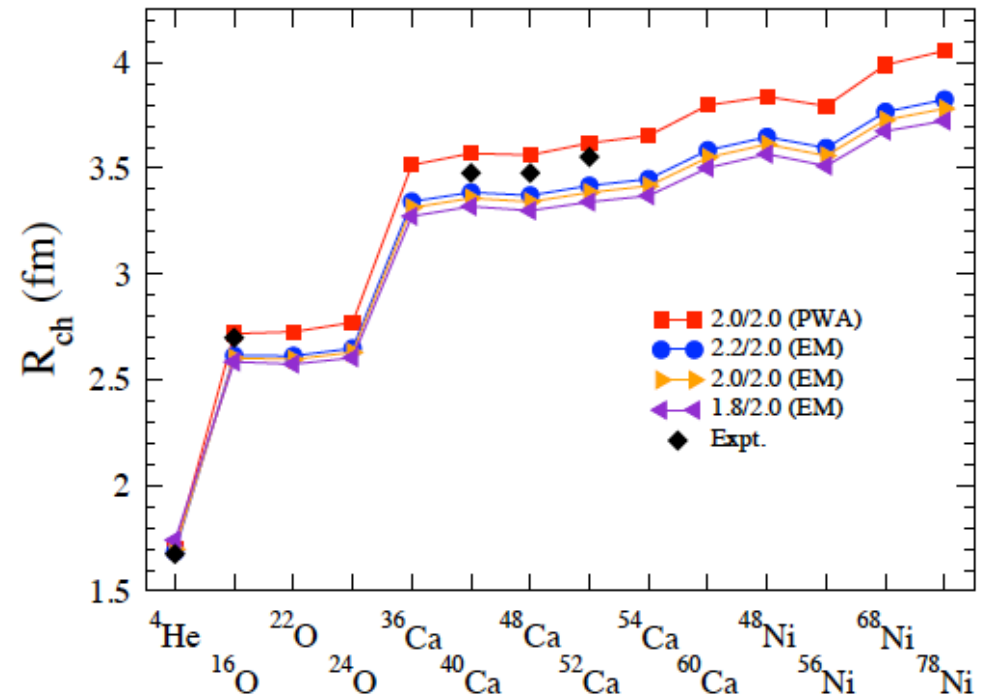
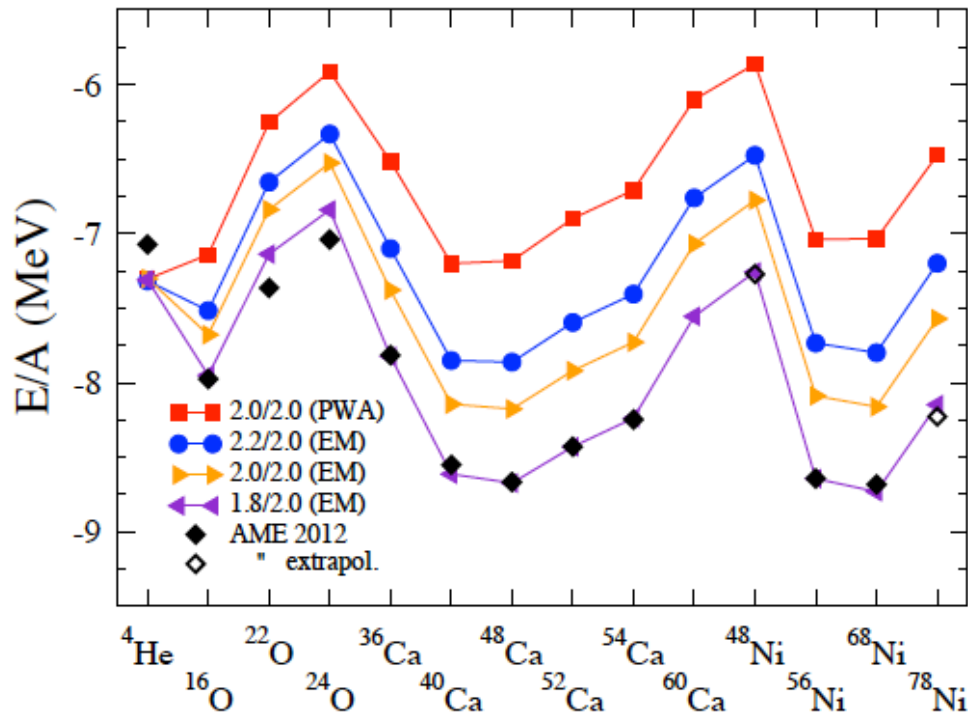


S. Binder et al, Physics Letters B 736 119, (2014)

- Overbinding of 1-2 MeV/A for increasing mass  $A$
- **The challenge is now with the interactions**

# The role of 3NFs on saturation and finite nuclei

J. Simonis et al, PRC 96, 014303 (2017)

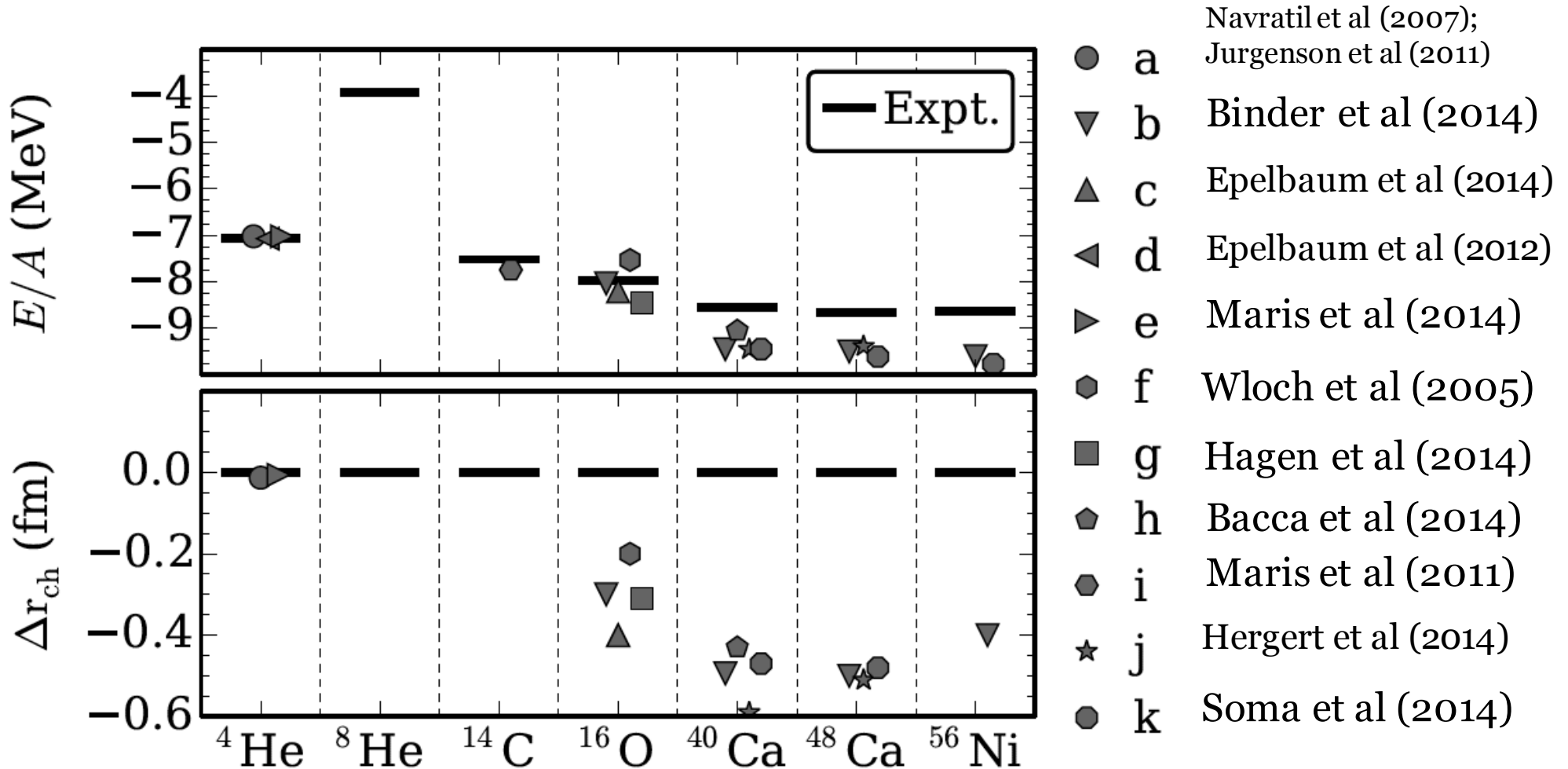


Binding energy per nucleon and charge radii for a set of chiral interactions fit to the triton and  $^4\text{He}$  binding energy and charge radius

Large spread in predictions. One interaction in particular performs extraordinary well for binding energies but underestimate the charge radius. **This is not well understood!**

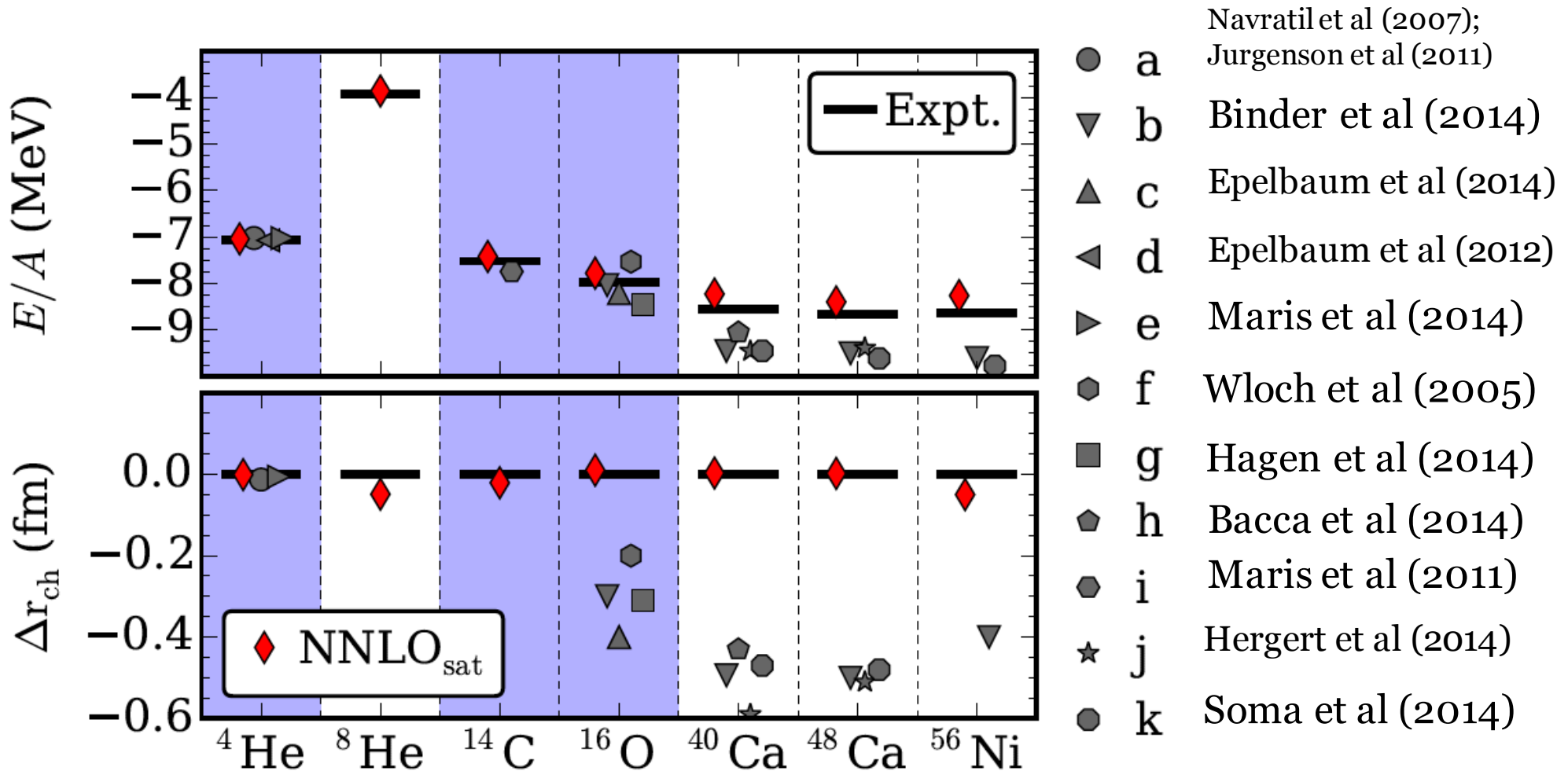
**Can we have both?**

# Accurate nuclear binding energies and radii from a chiral interaction



- Chiral interactions have failed at describing both binding energies and radii of nuclei
- Predictive power does not go together with large extrapolations
- Nuclear saturation may be viewed as an emergent property

# Accurate nuclear binding energies and radii from a chiral interaction



**Solution:** Simultaneous optimization of NN and 3NFs

Include charge radii and binding energies of  ${}^3\text{H}$ ,  ${}^{3,4}\text{He}$ ,  ${}^{14}\text{C}$ ,  ${}^{16}\text{O}$  in the optimization (NNLO<sub>sat</sub>)

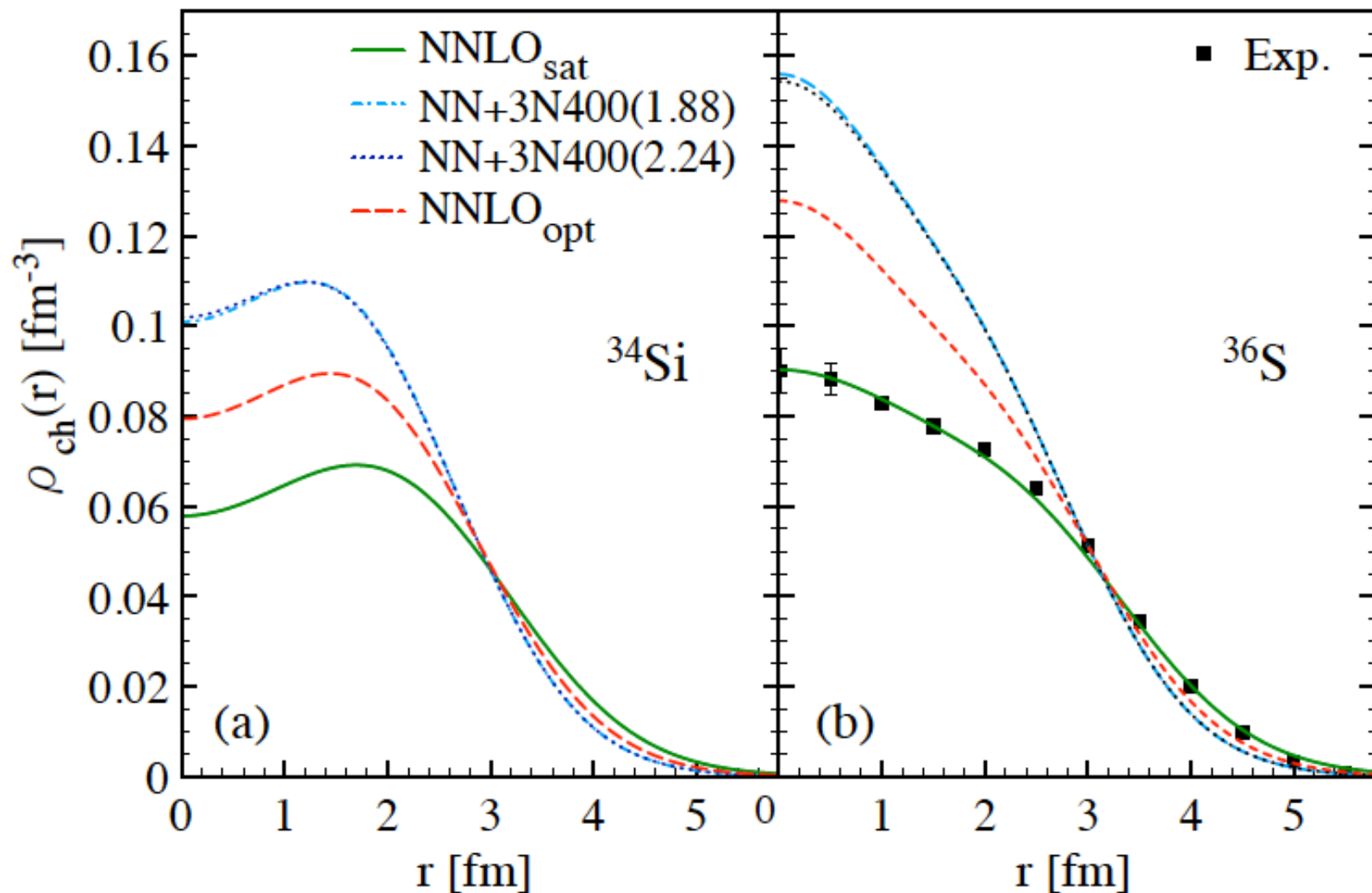
A. Ekström *et al*, Phys. Rev. C **91**, 051301(R) (2015).

G. Hagen *et al*, Phys. Scr. **91**, 063006 (2016).

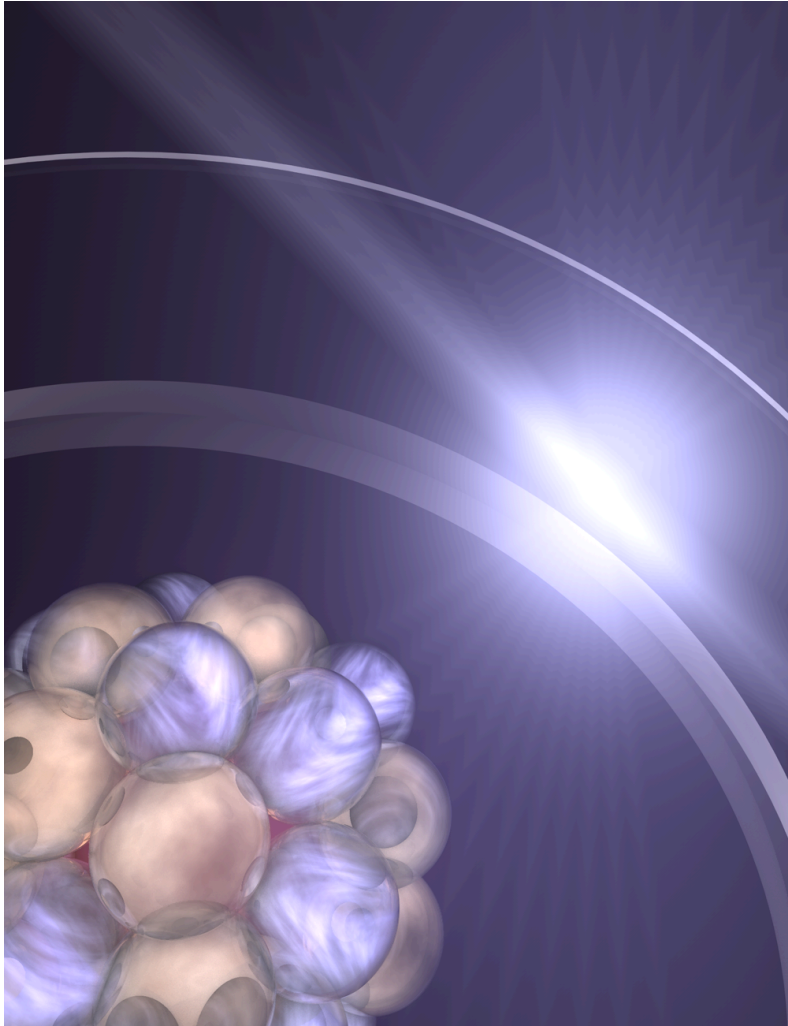
# Ab-initio predictions of bubble nucleus $^{34}\text{Si}$

- Self consistent Green's function calculations of the charge density of  $^{34}\text{Si}$  and  $^{36}\text{S}$  from state-of-the-art chiral interactions
- Pronounced bubble structure in  $^{34}\text{Si}$  is predicted with  $\text{NNLO}_{\text{sat}}$

T. Duguet et al, Phys. Rev. C 95, 034319 (2017)



# What is the neutron skin of $^{48}\text{Ca}$ ?



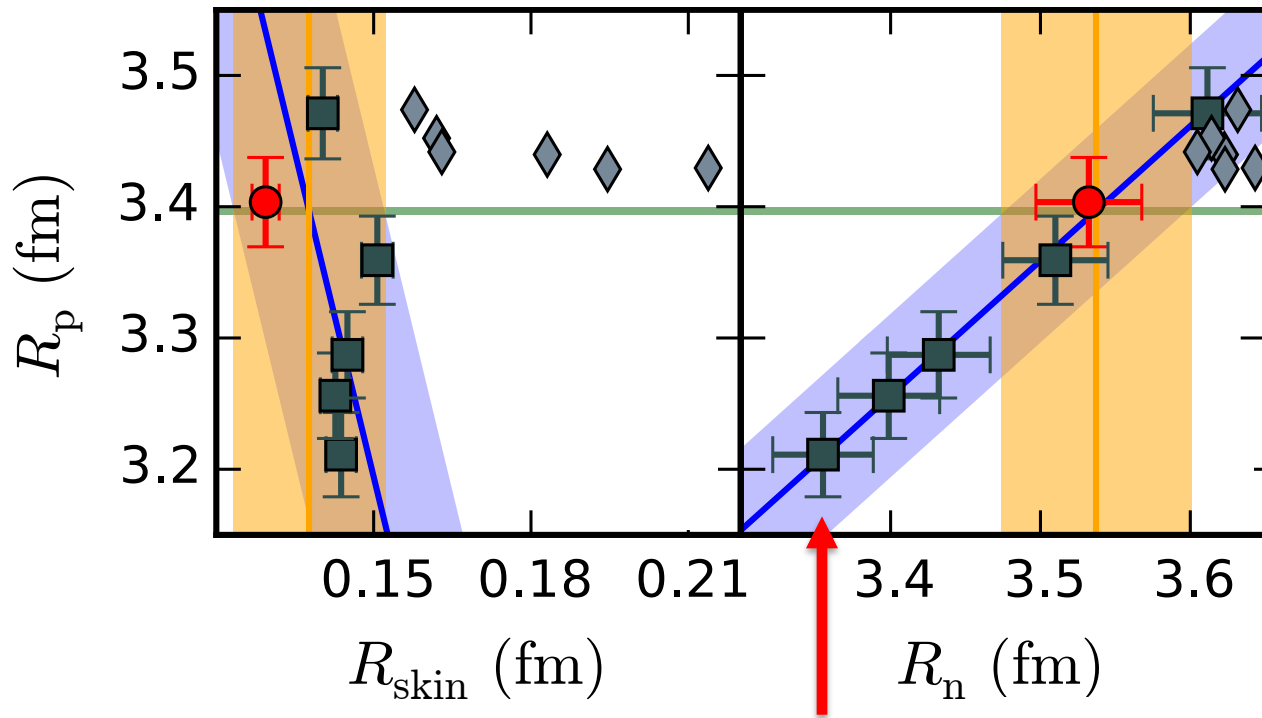
**Neutron skin** = Difference between radii of neutron and proton distributions

Relates atomic nuclei to neutron stars via neutron EOS

Correlated quantity: dipole polarizability

Model-independent measurement of weak charge form factor is possible via parity-violating electron scattering (P-REX/C-REX at JLab)

# Neutron radius and skin of $^{48}\text{Ca}$



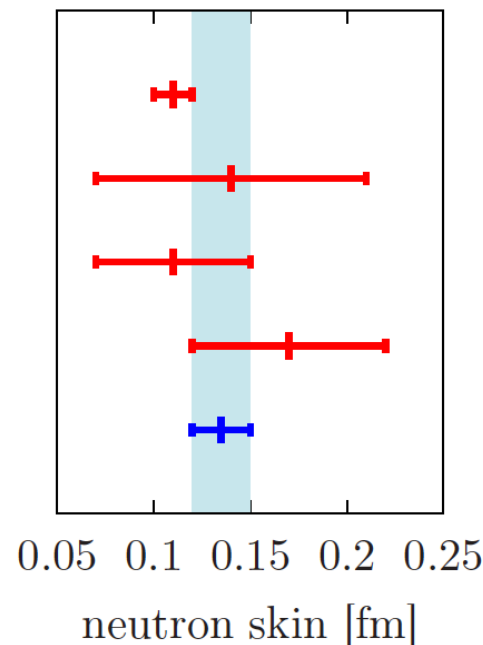
G. Hagen *et al*, Nature Physics  
**12**, 186–190 (2016)

Uncertainty estimates from  
family of chiral interactions:  
K. Hebeler *et al* PRC (2011)

**DFT:**  
SkM\*, SkP, Sly4, SV-min,  
UNEDF0, and UNEDF1

- Neutron skin significantly smaller than in DFT
- Neutron skin almost independent of the employed Hamiltonian
- Our predictions for  $^{48}\text{Ca}$  are consistent with existing data

1.8/2.0 (EM)



$\bar{p}$  atoms - Trzcinska

$\pi$  - Friedman

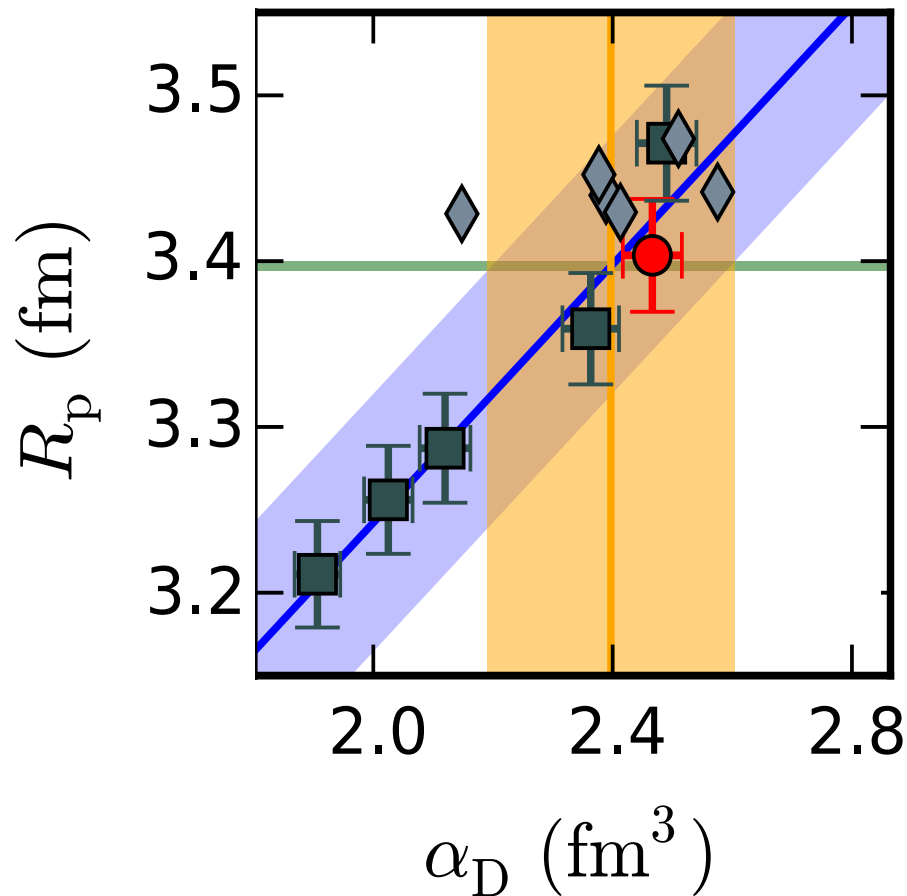
$\pi$  - Gibbs & Dedonder

$\alpha$ -scattering - Gils

Theory - Hagen



# Dipole polarizability of $^{48}\text{Ca}$

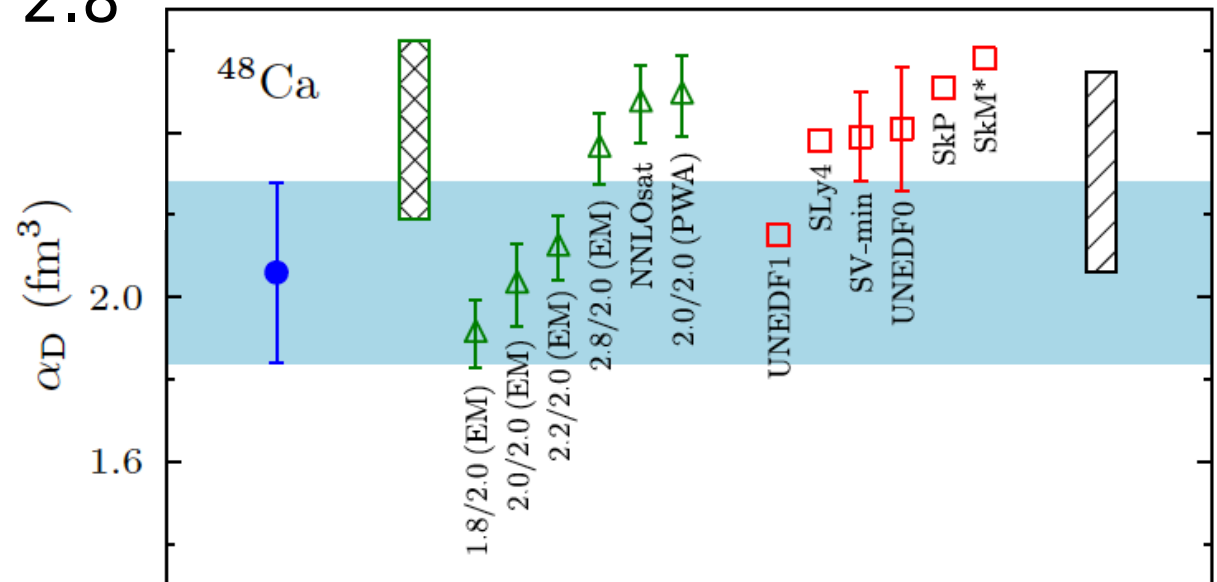


G. Hagen *et al*, Nature Physics  
**12**, 186–190 (2016)

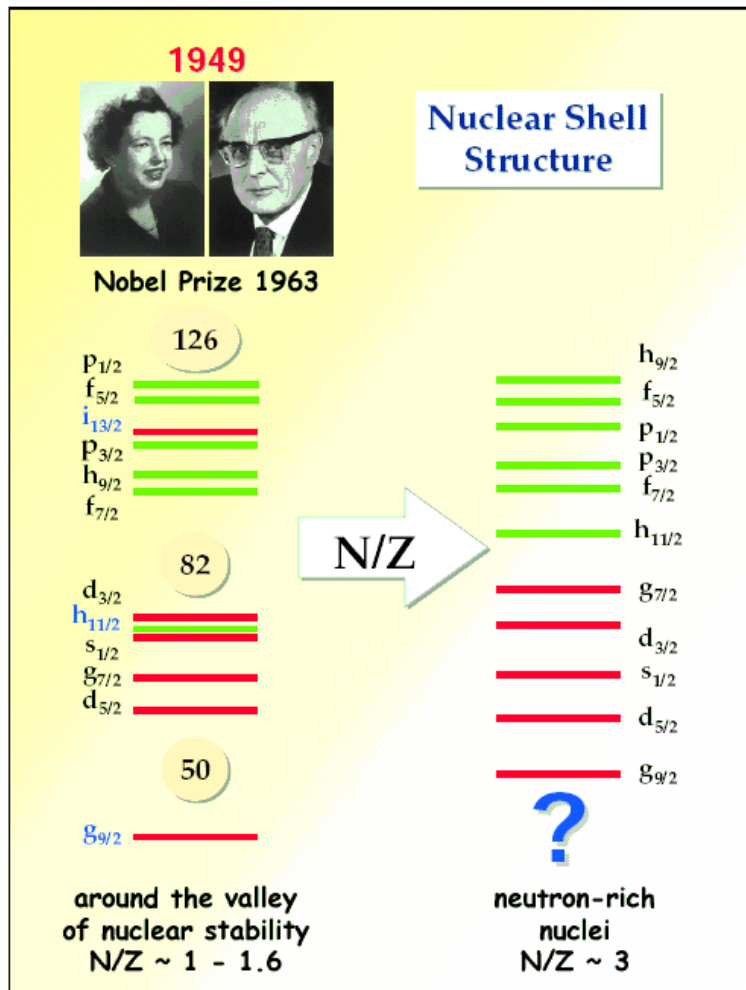
*Ab-initio* prediction from correlation with  $R_p$ :  
 $2.19 \lesssim \alpha_D \lesssim 2.60 \text{ fm}^3$

- DFT results are consistent and within band of ab-initio results
- Data has been analyzed by Osaka-Darmstadt collaboration
- Ab-initio prediction overlaps with experimental uncertainty

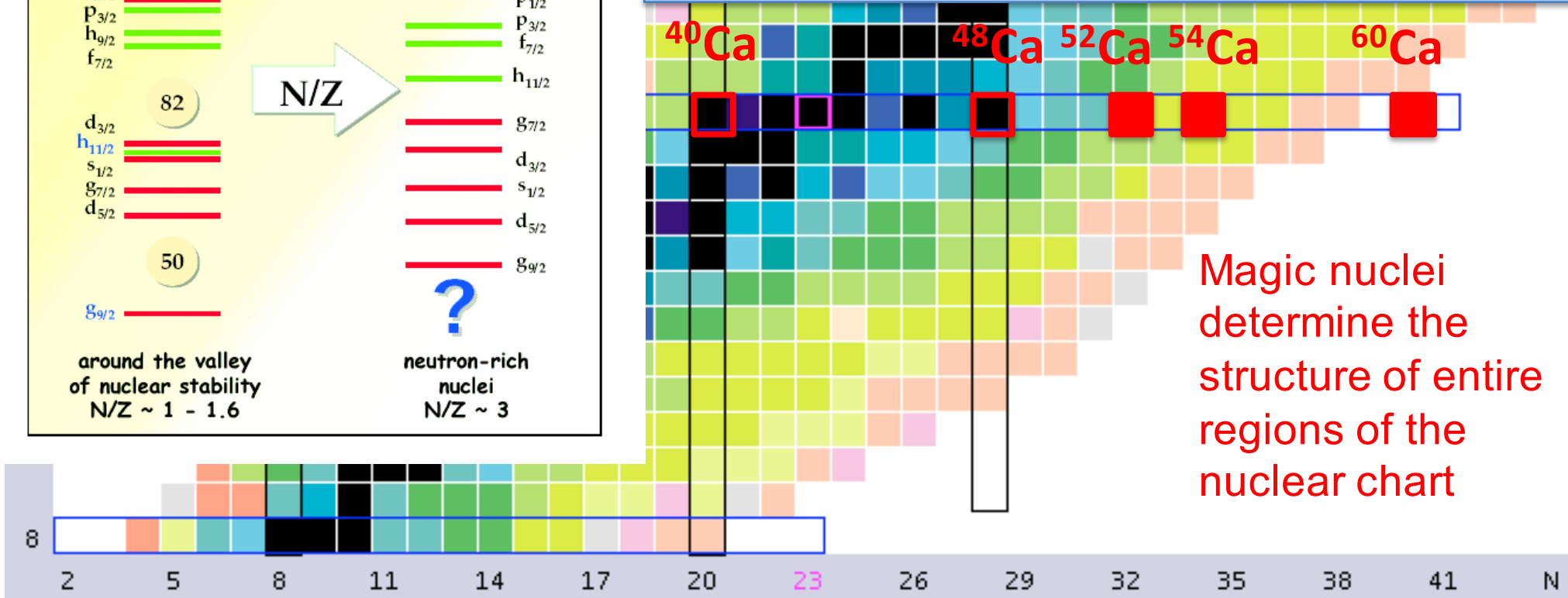
J. Birkhan et al, Phys. Rev. Lett. 118, 252501 (2017)



# Evolution of shell structure in neutron rich calcium



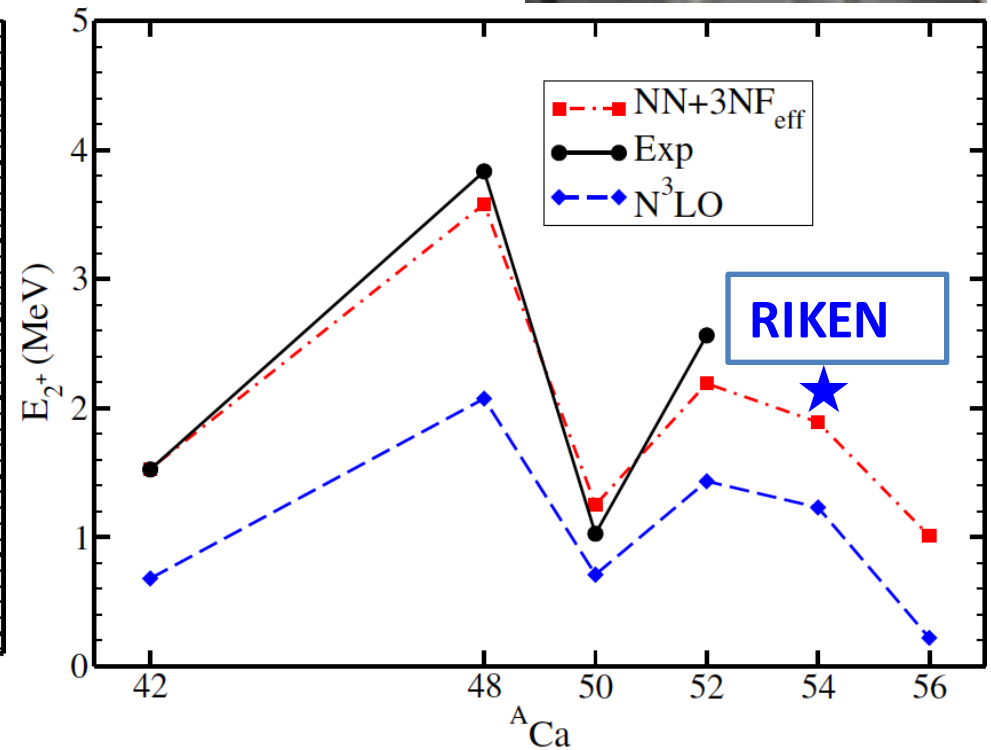
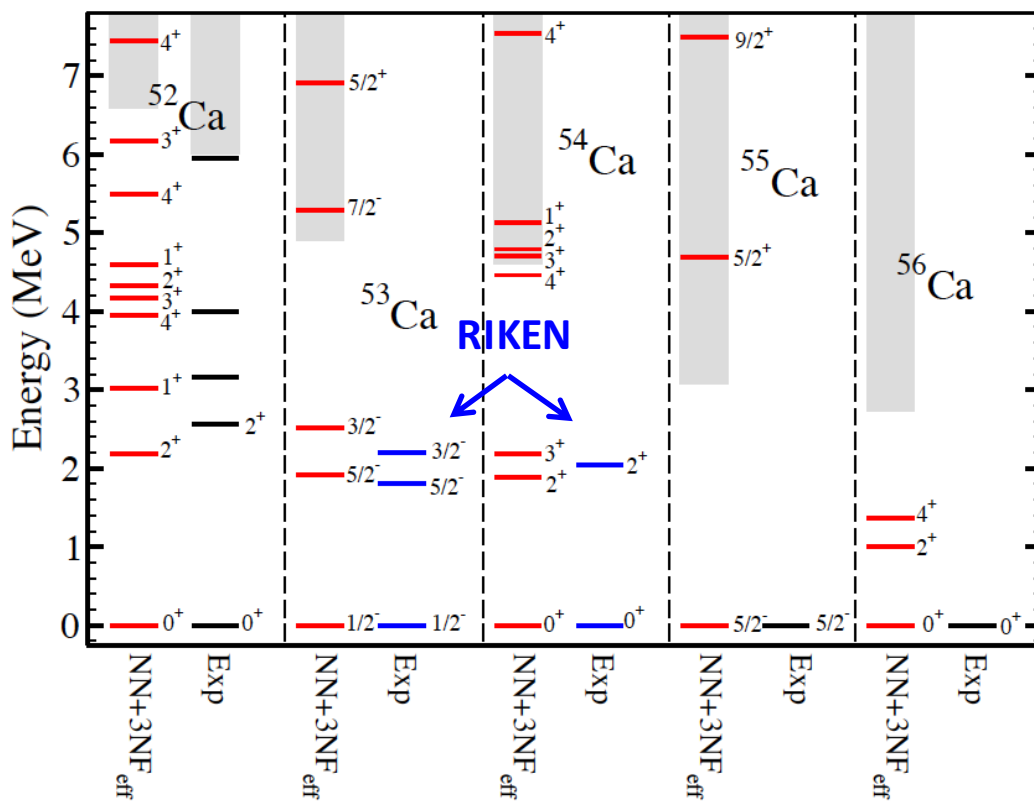
- How do shell closures and magic numbers evolve towards the dripline?
- Is the naïve shell model picture valid at the neutron dripline?
- What are the mechanisms for new shell structure?



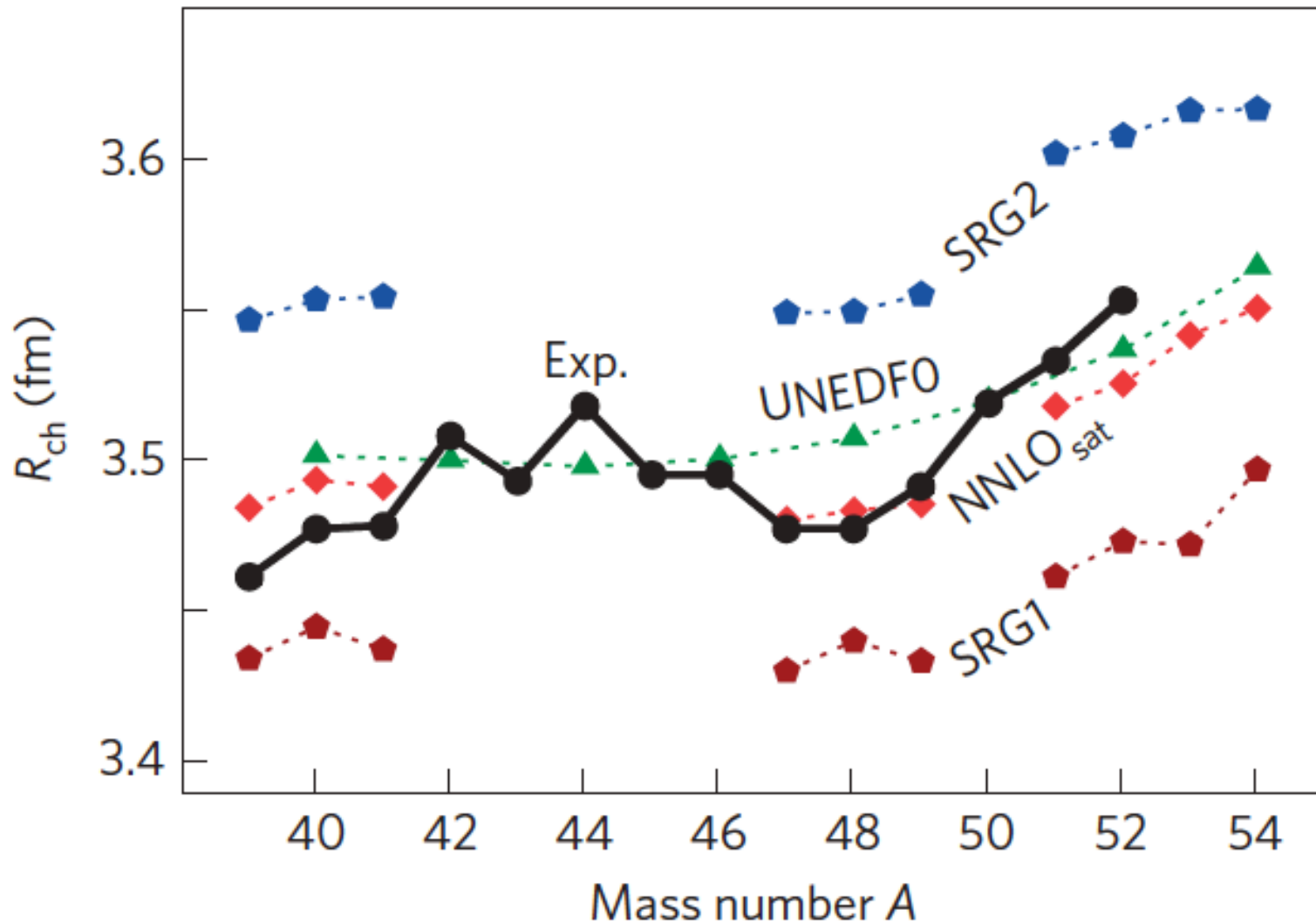
# Evolution of shell structure in neutron rich calcium

- Effects of three-nucleon forces and continuum is essential to describe shell structure
- We predict an inversion of the *gds* shell-model orbitals
- Our prediction for excited states in  $^{53}\text{Ca}$  and weak sub-shell closure in  $^{54}\text{Ca}$  was verified by experiment at RIKEN (Nature 2013, D. Steppenbeck et al)

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

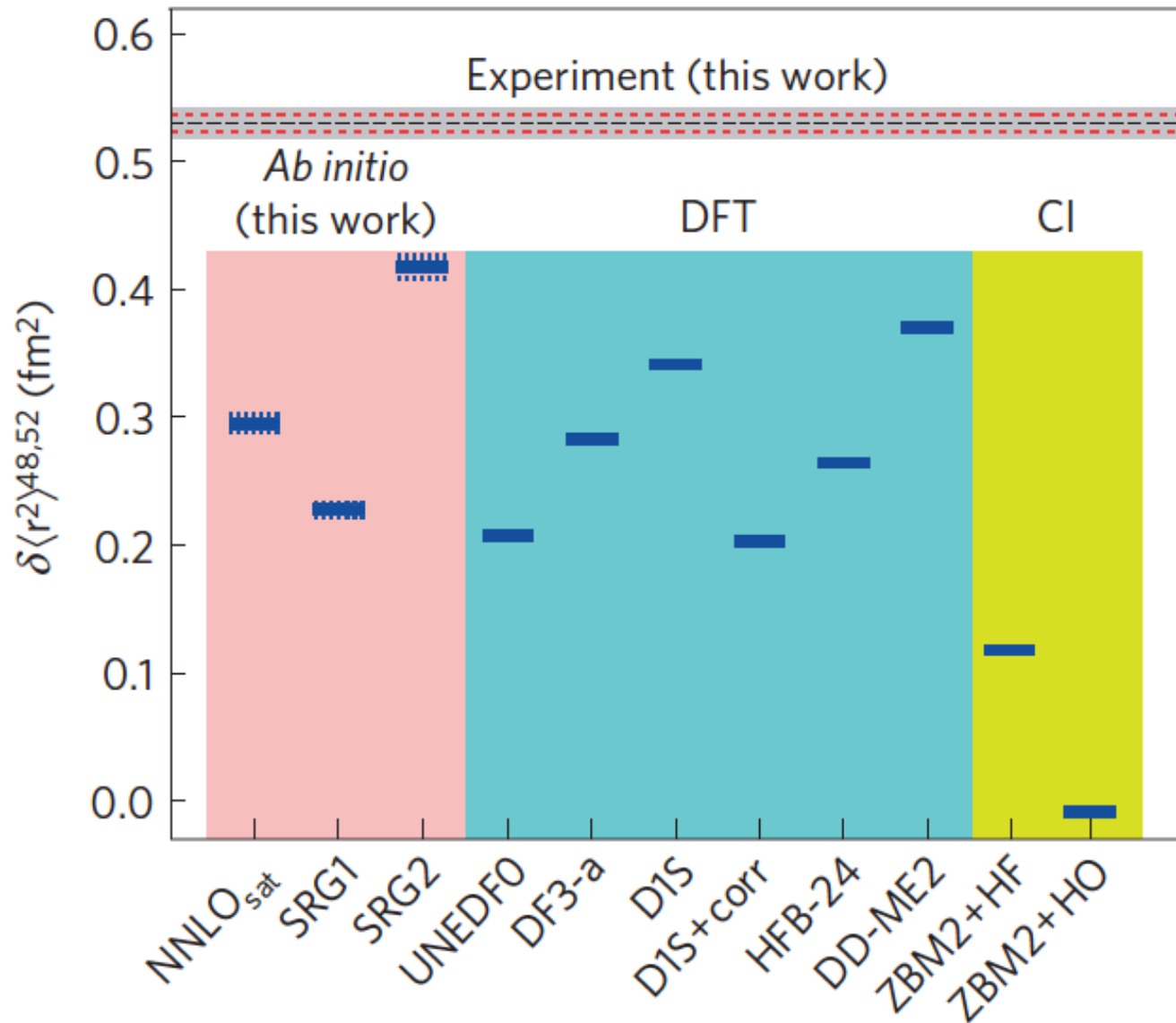


# Charge radii of neutron-rich calcium isotopes



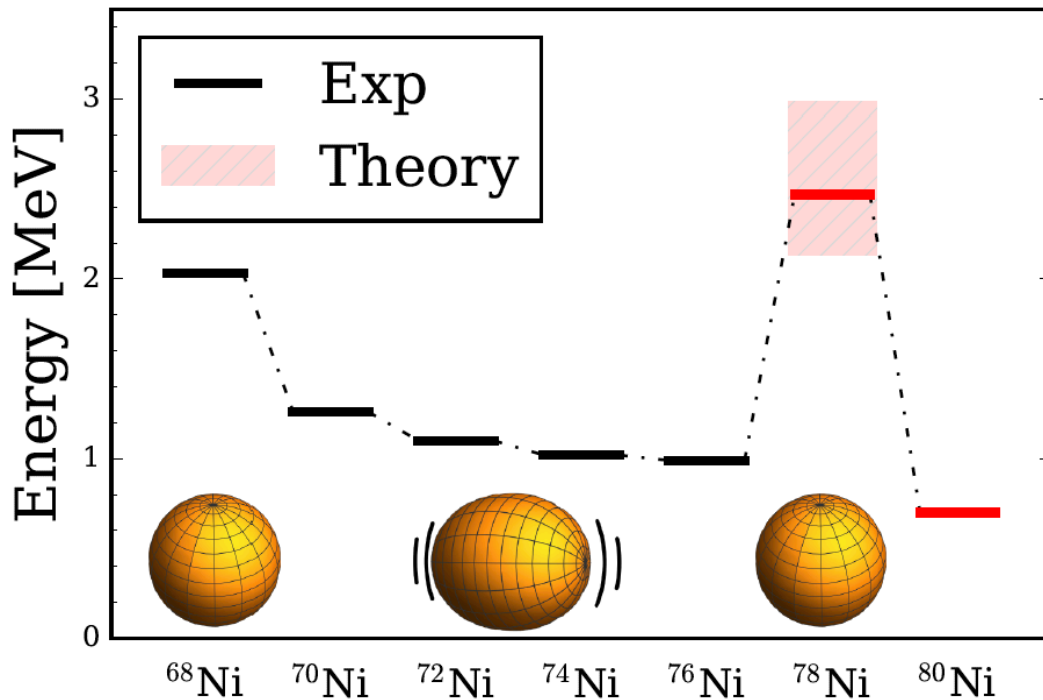
... question the magicity at N=32.

# Theory challenge: Charge radius of $^{52}\text{Ca}$



R. F. Garcia Ruiz *et al*, Nature Physics (2016) **12**, 594–598 (2016)

# Structure of $^{78}\text{Ni}$ from first principles



A high  $2^+$  energy in  $^{78}\text{Ni}$  indicates that this nucleus is doubly magic

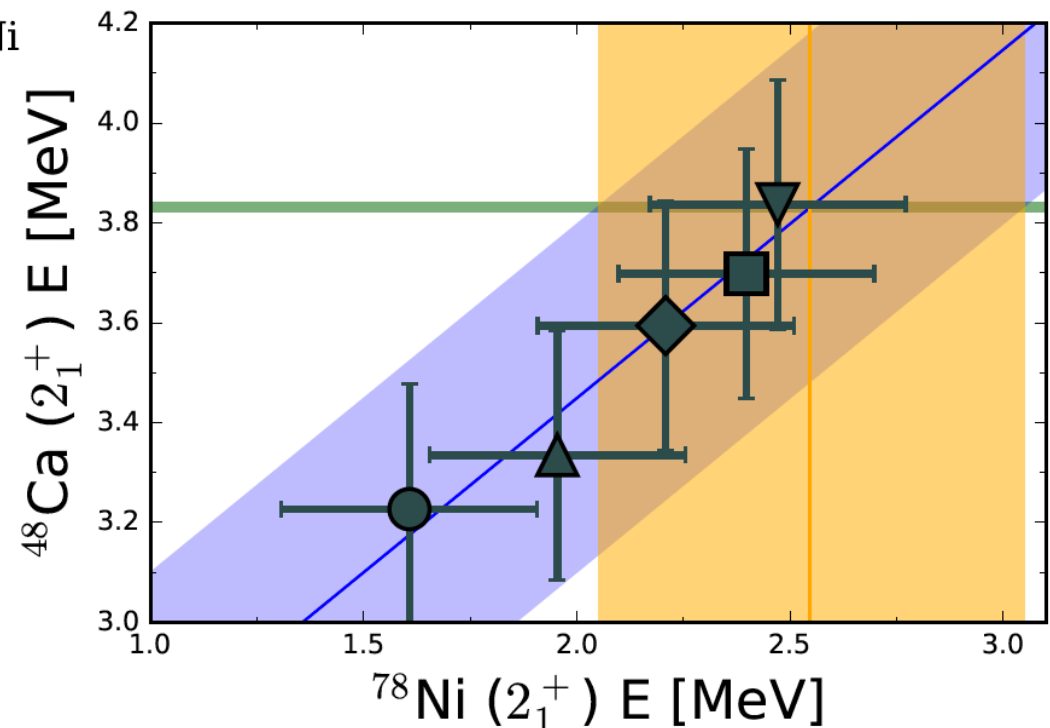
A measurement of this state has been made at RIBF, RIKEN

R. Taniuchi *et al.*, in preparation

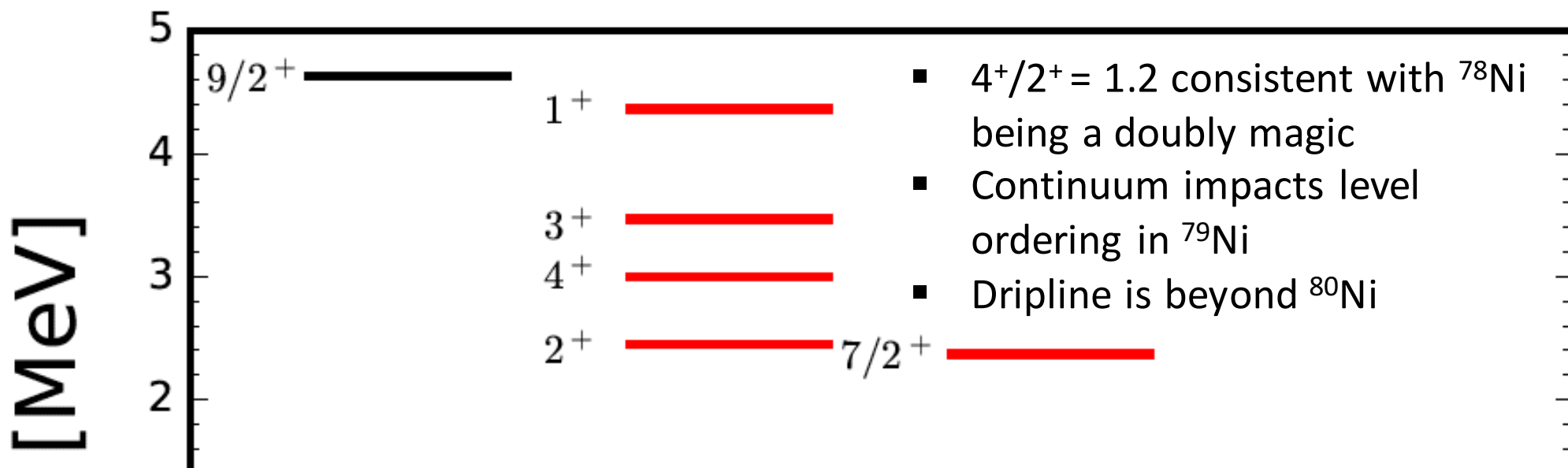
Consistent with recent shell-model studies

F. Nowacki *et al.*, PRL 117, 272501 (2016)

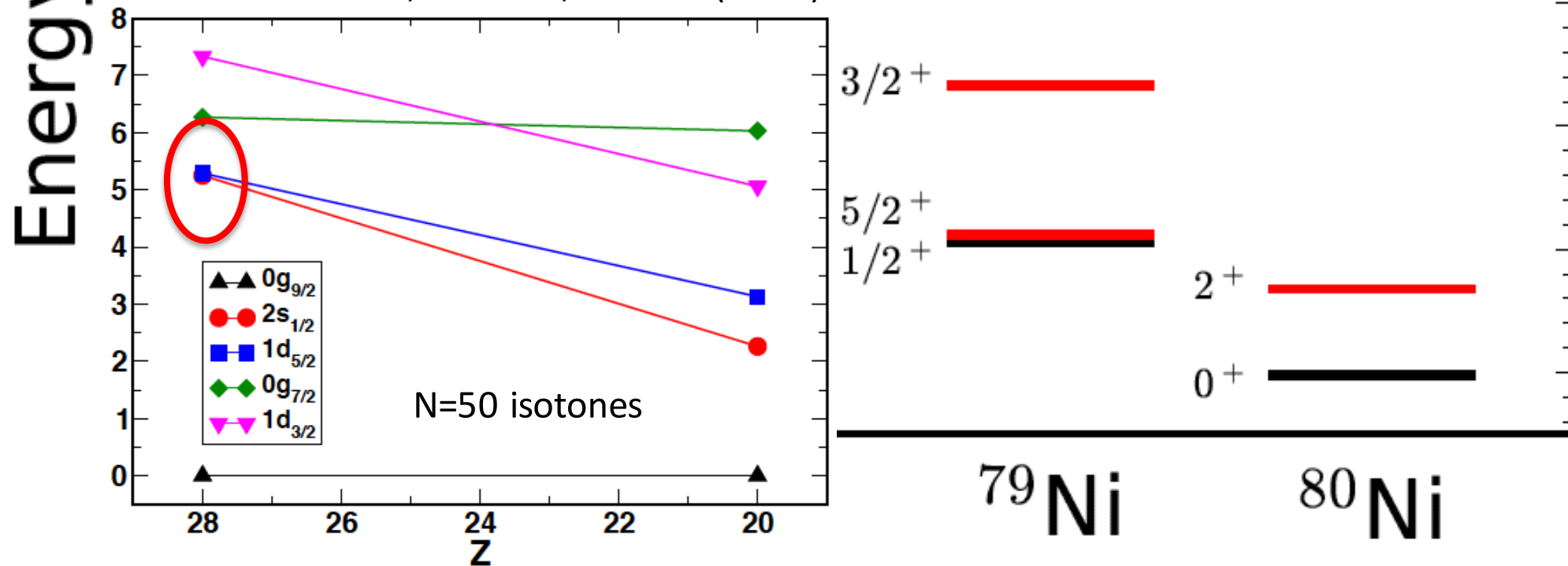
- From an observed correlation we predict the  $2^+$  excited state in  $^{78}\text{Ni}$  using the experimental data for the  $2^+$  state in  $^{48}\text{Ca}$
- Similar correlations have been observed in other nuclei, e.g. Tjon line in light nuclei



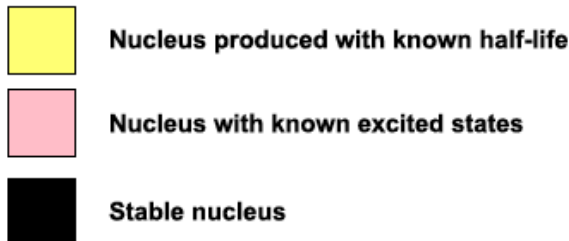
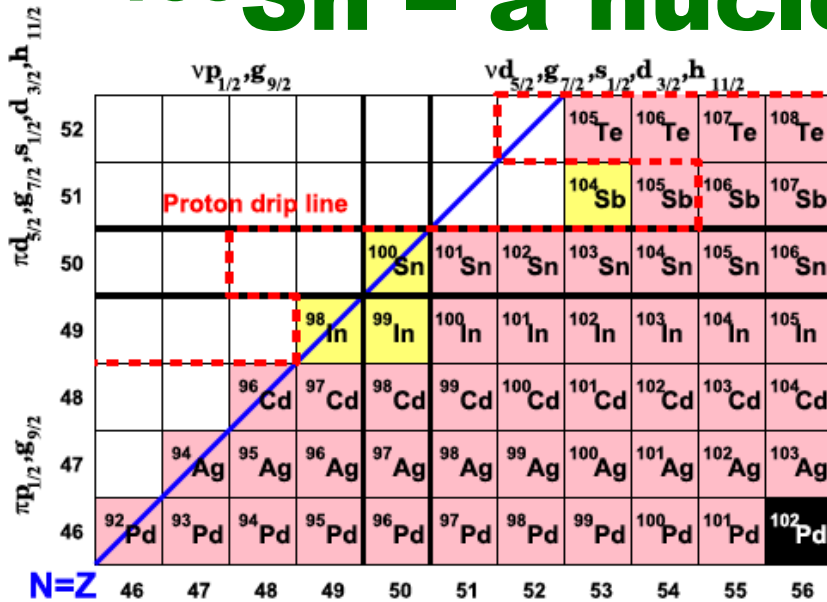
# Excited states in $^{78}\text{Ni}$ and its neighbors



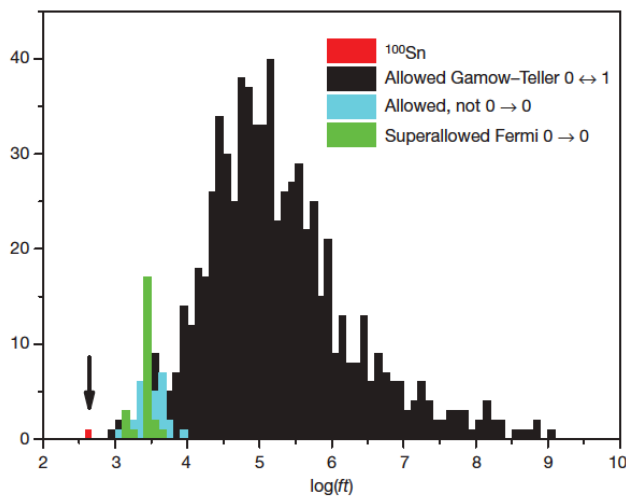
F. Nowacki *et al.*, PRL 117, 272501 (2016)



# $^{100}\text{Sn}$ – a nucleus of superlatives



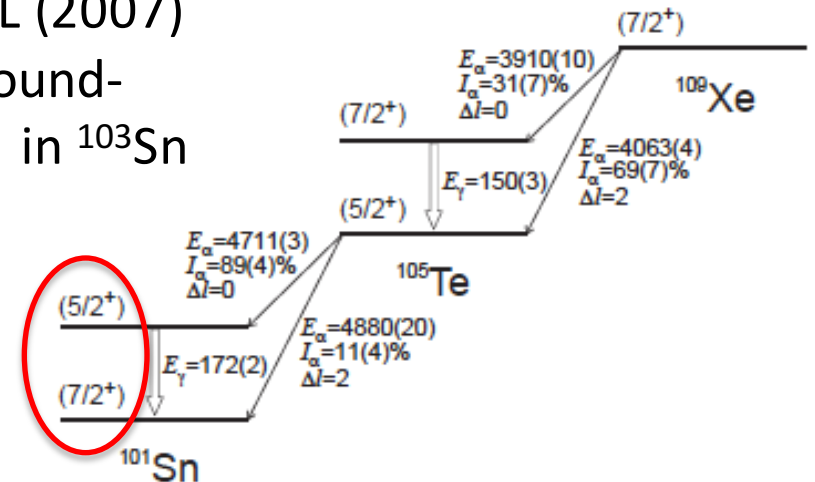
- Heaviest self-conjugate doubly magic nucleus
- Largest known strength in allowed nuclear  $\beta$ -decay
- In the closest proximity to the proton dripline
- At the endpoint of the rapid proton capture process (Sn-Sb-Te cycle)
- Unresolved controversy regarding s.p. structure of  $^{101}\text{Sn}$



Hinke et al, Nature (2012)

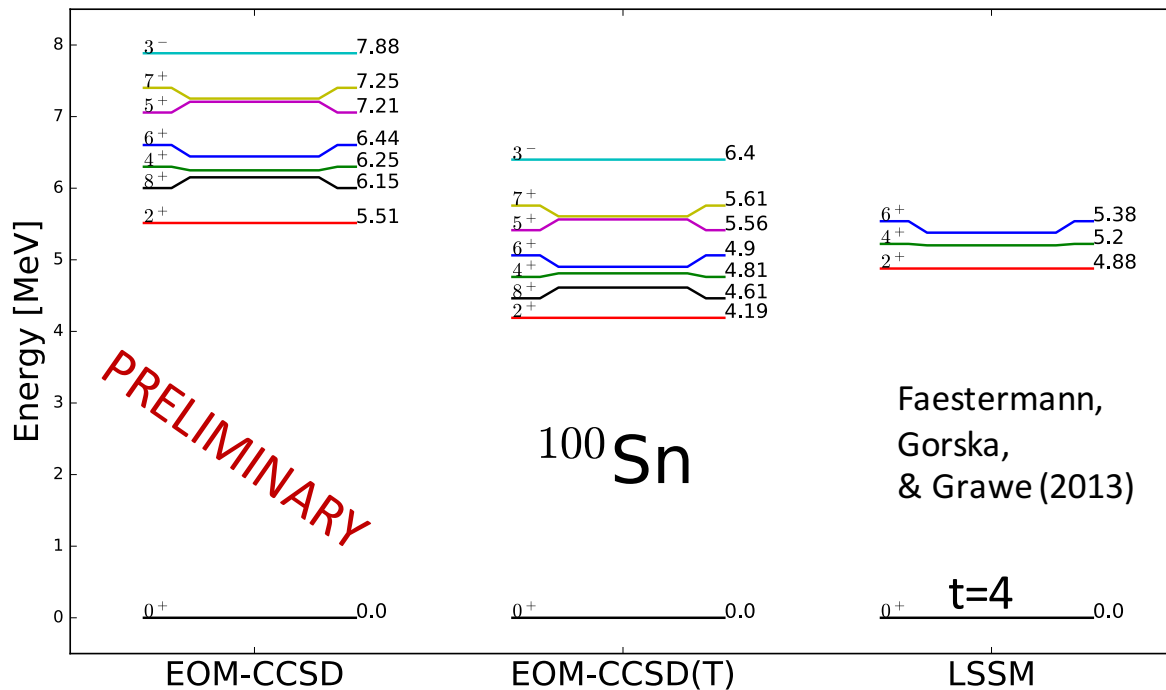
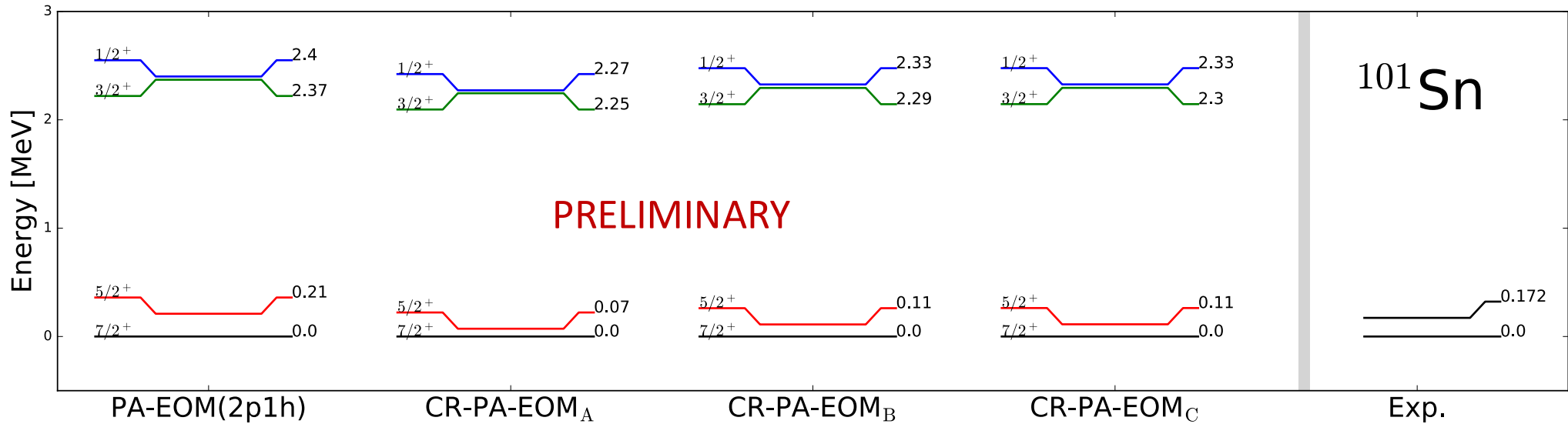
Sewernyiak et al PRL (2007) predicted a  $5/2^+$  ground-state as presumably in  $^{103}\text{Sn}$

Darby et al, PRL (2010)



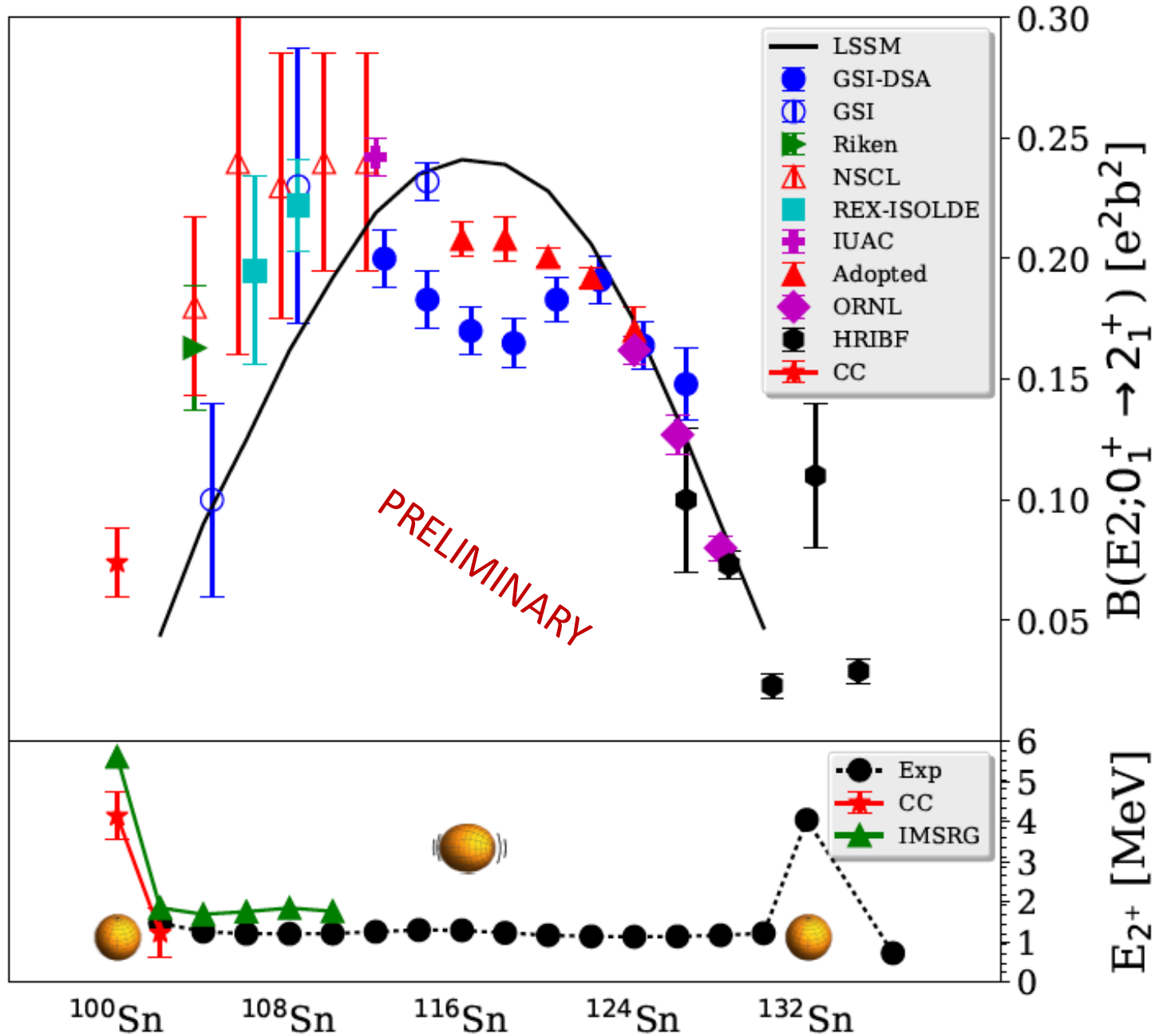


# Structure of the lightest tin isotopes

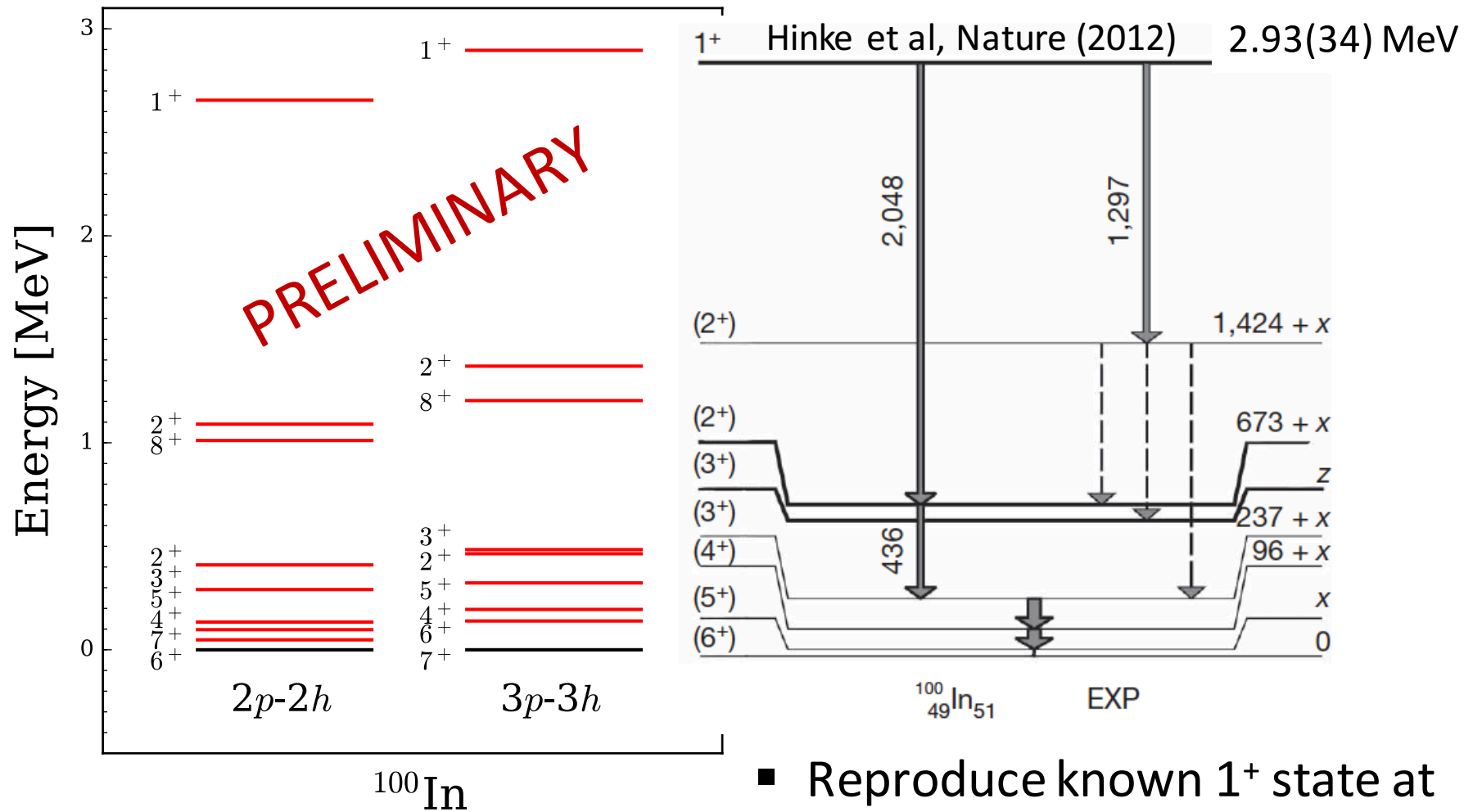


- High  $2^+$  energy in  $^{100}\text{Sn}$
- Predict  $7/2^+$  ground-state in  $^{101}\text{Sn}$
- Experimental splitting between  $7/2^+$  and  $5/2^+$  reproduced
- Ground-state spins of  $^{101-121}\text{Sn}$  will be measured at CERN (CRIS collaboration)

# Structure of the lightest tin isotopes



# $^{100}\text{In}$ from charge exchange coupled-cluster equation-of-motion method

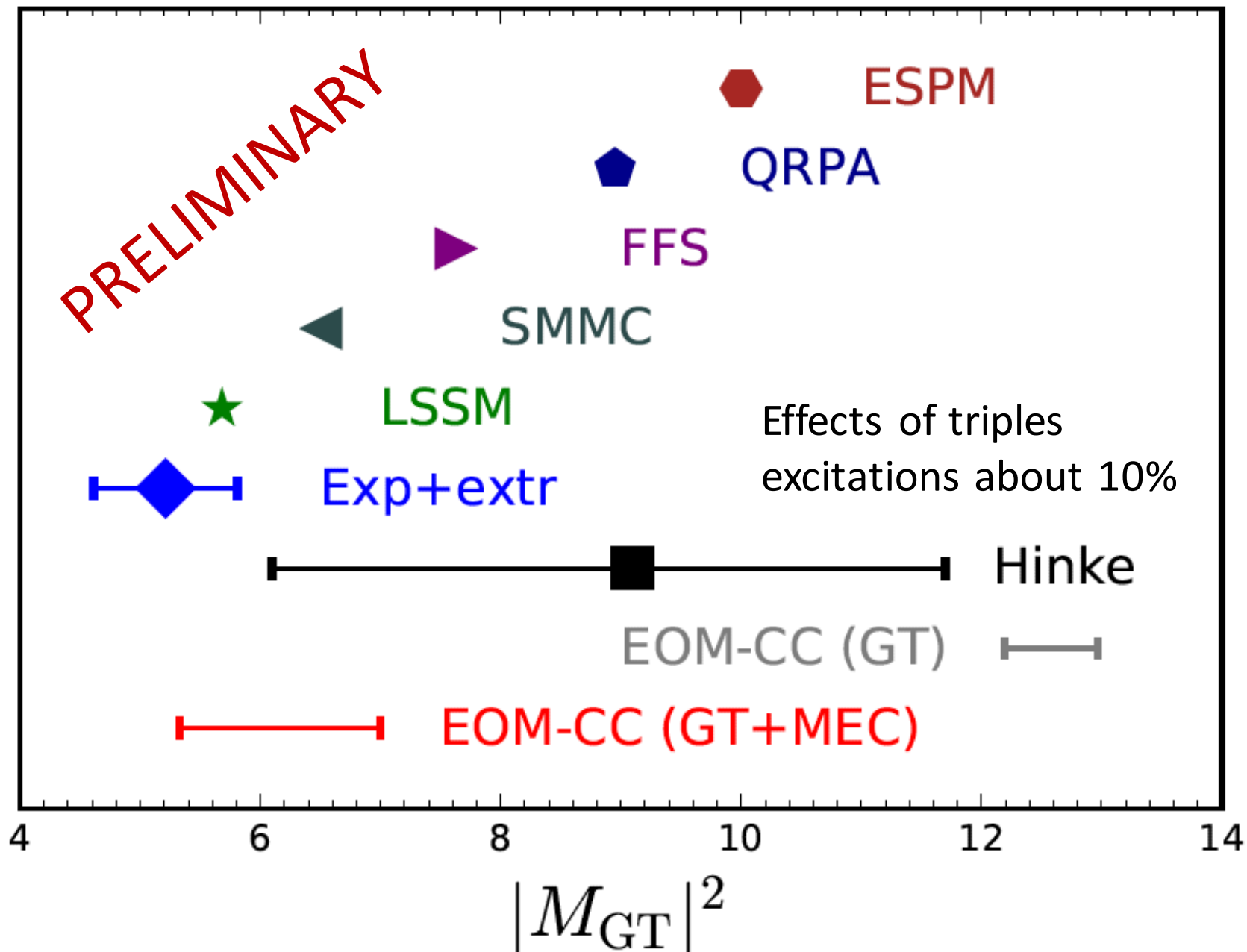


3p-3h charge-exchange EOM:

$$\overline{H}_N R_\mu |\Phi_0\rangle = E_\mu R_\mu |\Phi_0\rangle$$

- Reproduce known  $1^+$  state at 2.93(34) MeV
- Predict a  $7^+$  ground-state for  $^{100}\text{In}$
- Ground-state spin of  $^{100}\text{In}$  can be measured by CRIS collab. at CERN

# Super allowed Gamow-Teller decay of $^{100}\text{Sn}$



# Accomplishments of ab-initio nuclear structure calculations

- Demonstration that nuclei can be built from scratch
- Demonstration that three-nucleon forces must be included in the description
- Determination of low-energy constants of potentials from chiral EFT
- Probing of effective interactions in medium-mass nuclei
- Providing a solid basis that other methods can build on and link to (→ UNEDF [www.unedf.org](http://www.unedf.org), NUCLEI [www.computingnuclei.org](http://www.computingnuclei.org) projects)

Several methods with complementary properties available