Recent advances in nuclear theory

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and

OAK RIDGE NATIONAL LABORATORY

SciDAC Scientific Discovery through Advanced Computing

TRIUMF Colloquium
February 25, 2016

NUCLEI Nuclear Computational Low-Energy Initiative

Research partly funded by the US Department of Energy

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@ CERN: COLLAPS Collaboration **(R. Garcia Ruiz** et al.)

Energy scales and relevant degrees of freedom

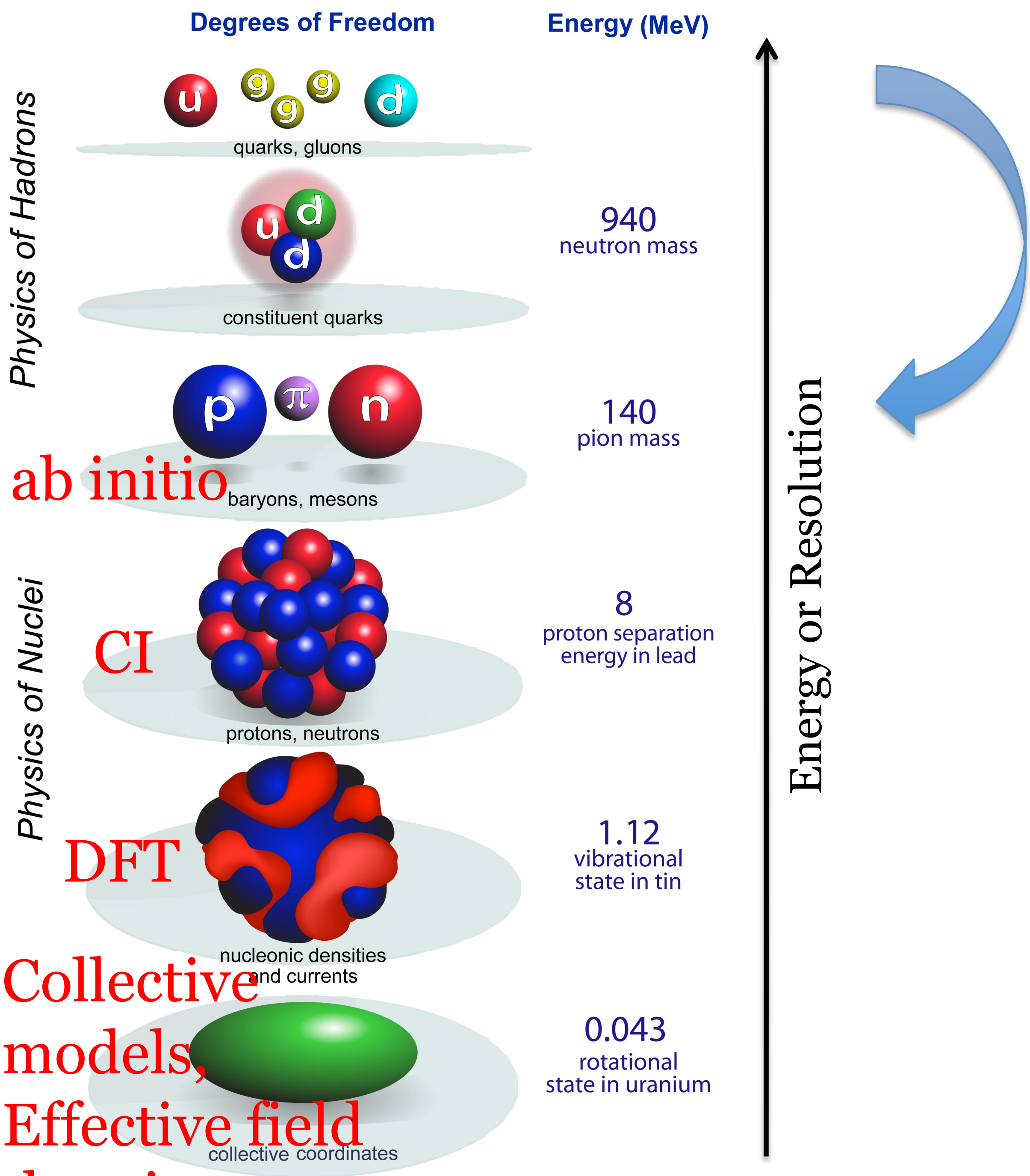


Fig.: Bertsch, Dean, Nazarewicz, SciDAC review (2007)

Chiral symmetry is broken

Pion is Nambu-Goldstone boson

Tool: Chiral effective field theory

Other EFTs:

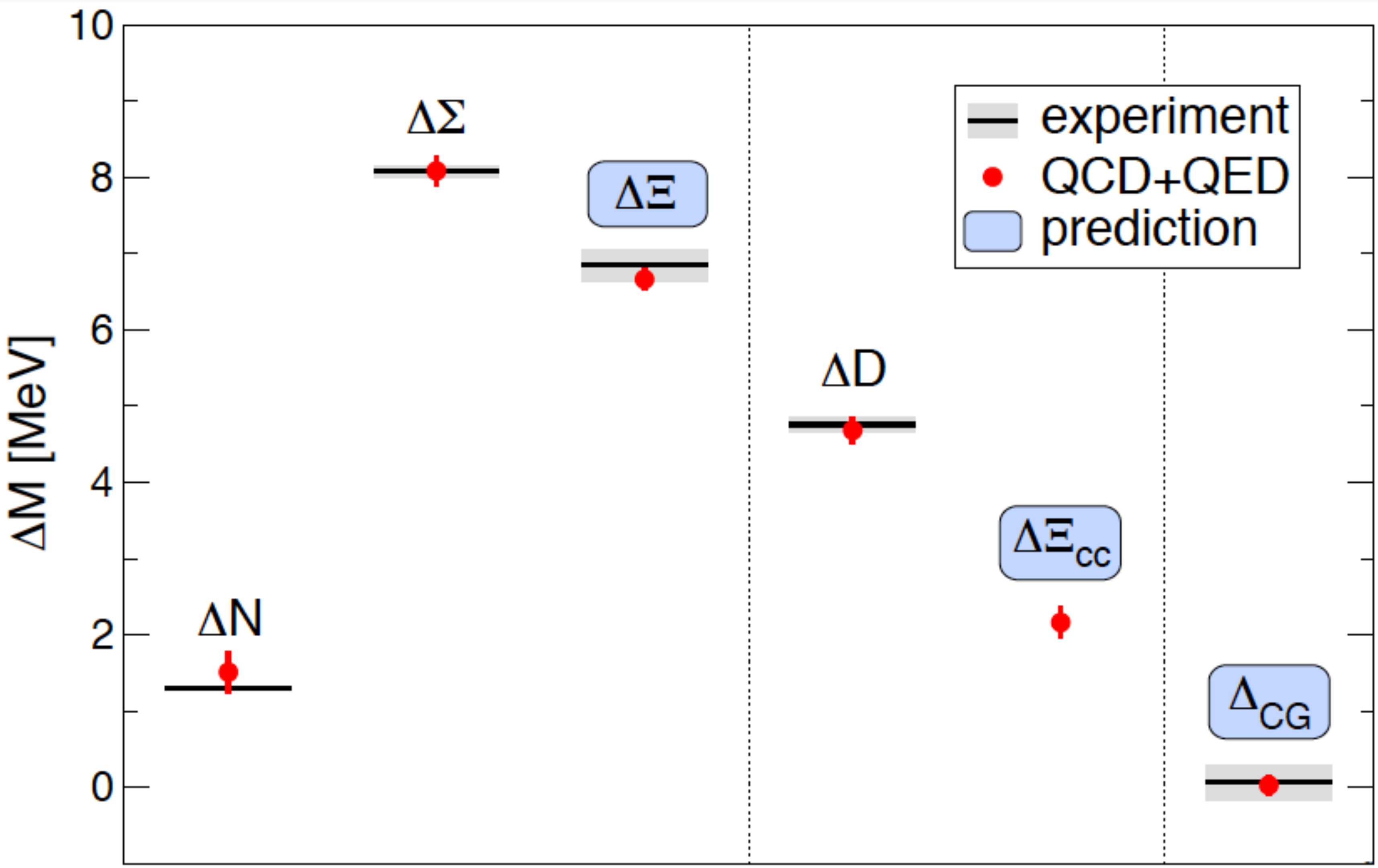
Pion-less EFT

EFT for halo nuclei

EFT for nuclear vibrations

EFT for deformed nuclei

Lattice QCD describes the nucleon



Mass splittings from lattice QCD & QED
Borsanyi et al., Science (2015)

Toward bridging QCD and nuclei

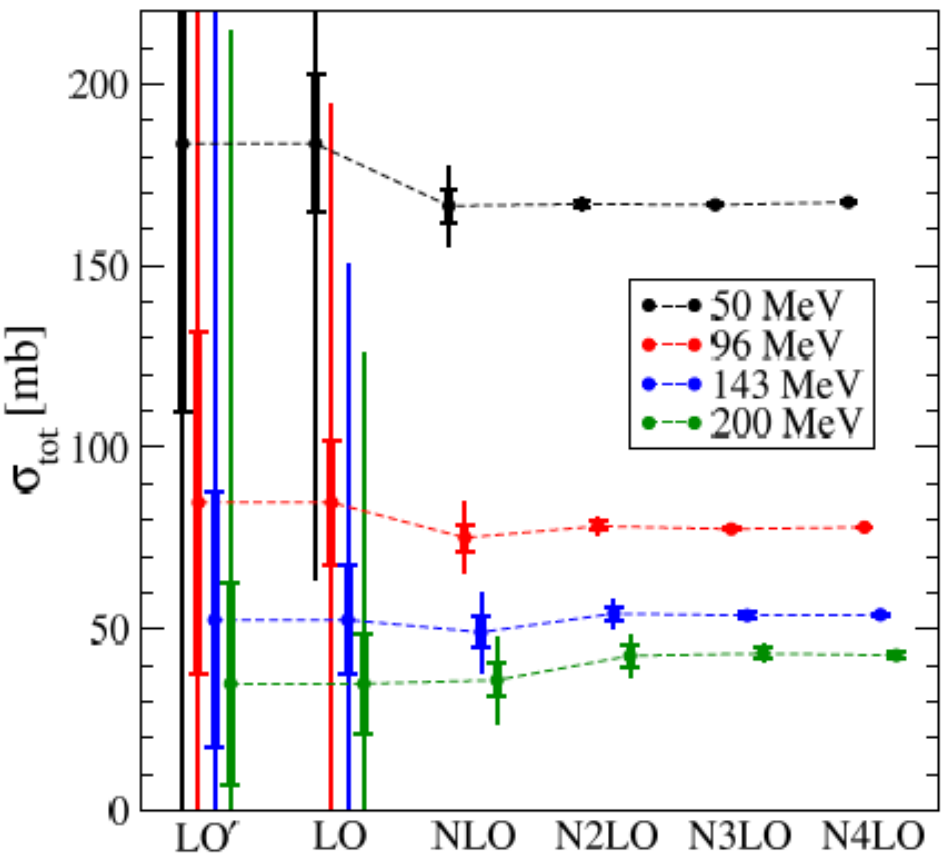
m_π	140	510	805	805
Nucleus	[Nature]	[5]	[6]	[This work]
n	939.6	1320.0	1634.0	1634.0
p	938.3	1320.0	1634.0	1634.0
nn	-	7.4 ± 1.4	15.9 ± 3.8	15.9 ± 3.8 *
D	2.224	11.5 ± 1.3	19.5 ± 4.8	19.5 ± 4.8 *
^{3}n	-			-
^{3}H	8.482	20.3 ± 4.5	53.9 ± 10.7	53.9 ± 10.7 *
^{3}He	7.718	20.3 ± 4.5	53.9 ± 10.7	53.9 ± 10.7
^{4}He	28.30	43.0 ± 14.4	107.0 ± 24.2	89 ± 36
^{5}He	27.50			98 ± 39
^{5}Li	26.61			98 ± 39
^{6}Li	32.00			122 ± 50

Match pion-less EFT to lattice QCD at large pion masses.
Not yet in the phase of spontaneously broken chiral symmetry.
Barnea et al., PRL (2015)

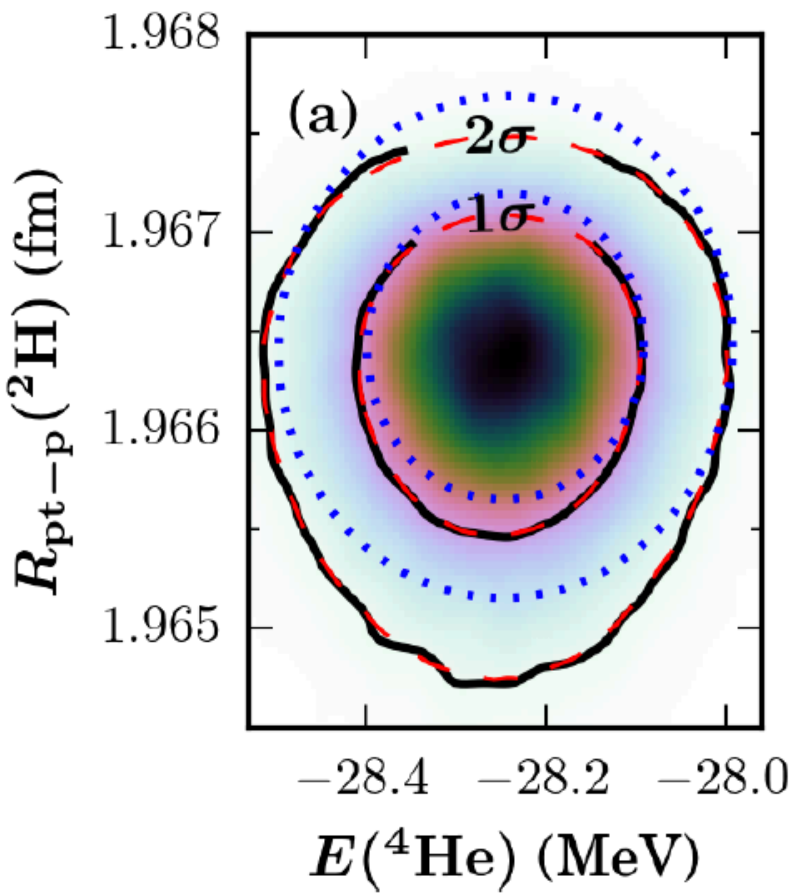
Quantified theoretical uncertainties

EFTs provide us with advantages over models:

- Uncertainty estimates readily available (based on power counting)
- Quantified uncertainties (based on Bayesian statistics *and* testable assumptions)



Furnstahl et al., PRC (2015)



Carlsson et al., PRX (2016)

Computation of emergent phenomena

Emergent phenomena

- Nuclear saturation
- Nuclear deformation and vibrations
- Clustering (α particles, halos, ...)

Really hard to compute from first principles

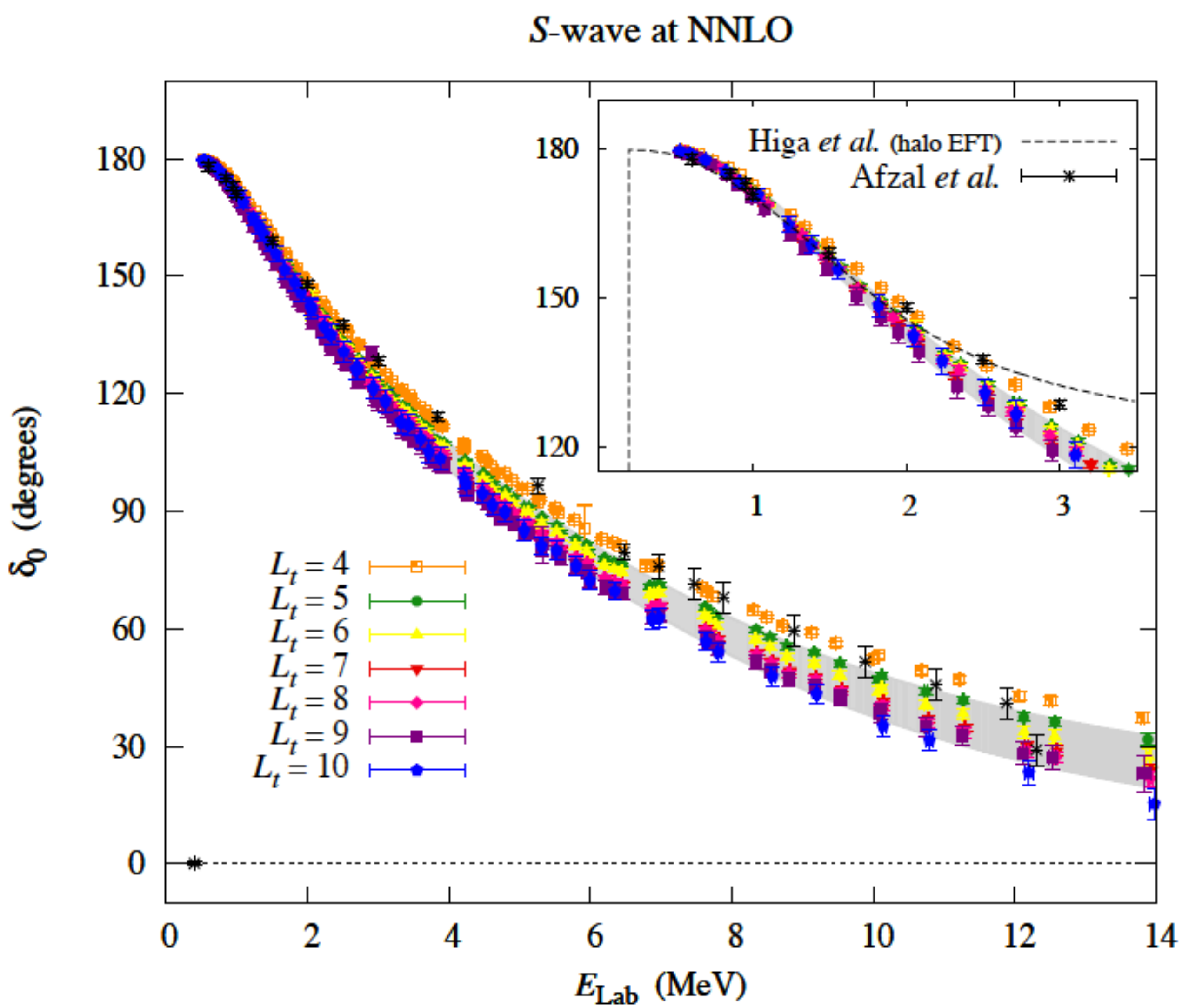
- Finely tuned
- Emergent low-energy scales / multi-scale problem
- Complex and collective in nature

Usually fixed in models

- ħω sets nuclear saturation & radii in shell model
- Deformed shell model, collective & algebraic models
- α-particle cluster models of the nucleus

Opportunities for EFTs & challenges for ab initio approaches

α-α scattering from lattice EFT

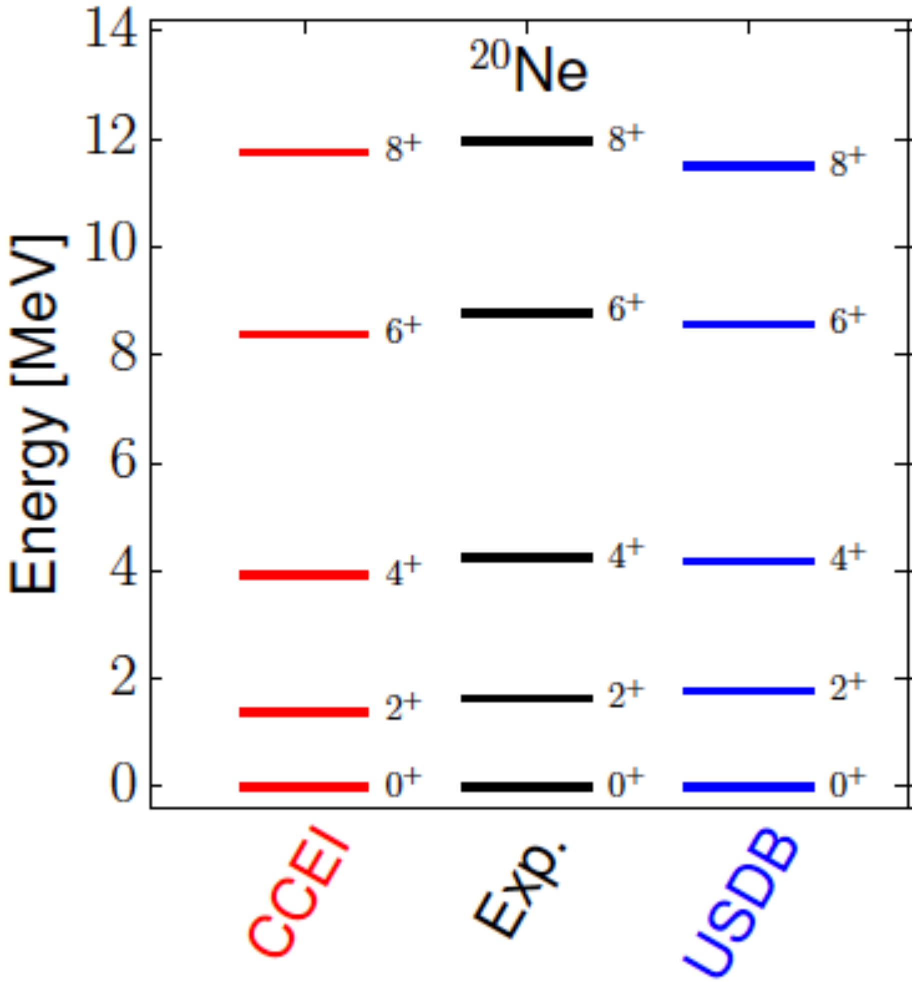


S. Elhatisari et al., Nature 528, 111 (2015)

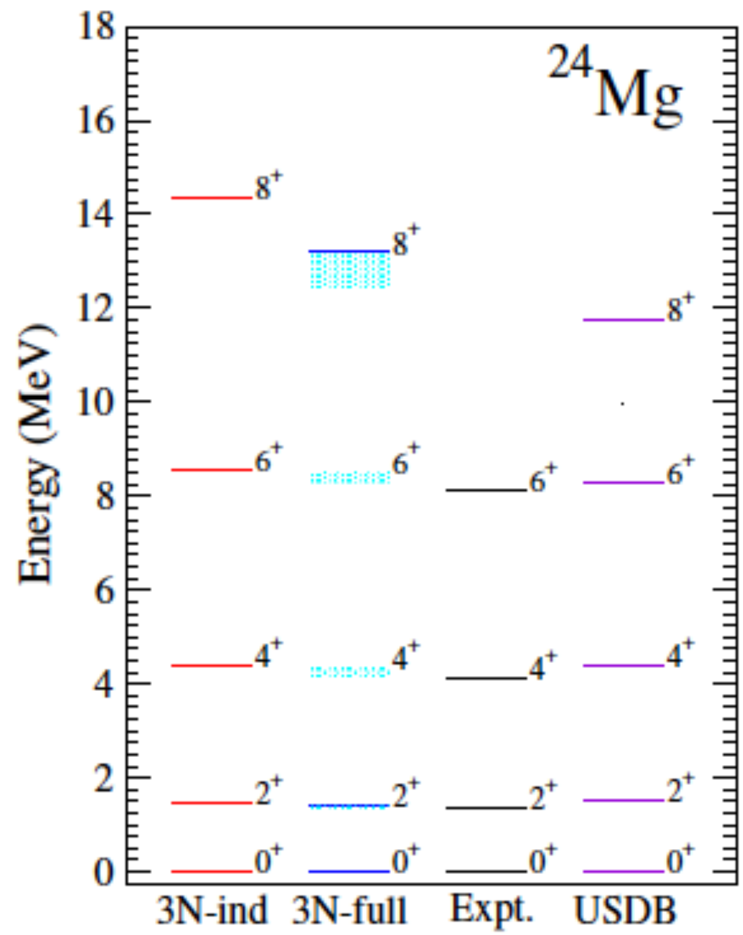
Recent reviews on ab initio reactions:
Bacca & Pastore (2014);
Navrátil, Quaglioni, Hupin, Romero-Redondo, Calci (2016).

Electroweak processes:
Pastore et al. (2013);
Lovato et al. (2013);
Carlson et al. (2015).

Nuclear deformation from first principles



Jansen et al., 1511.00757



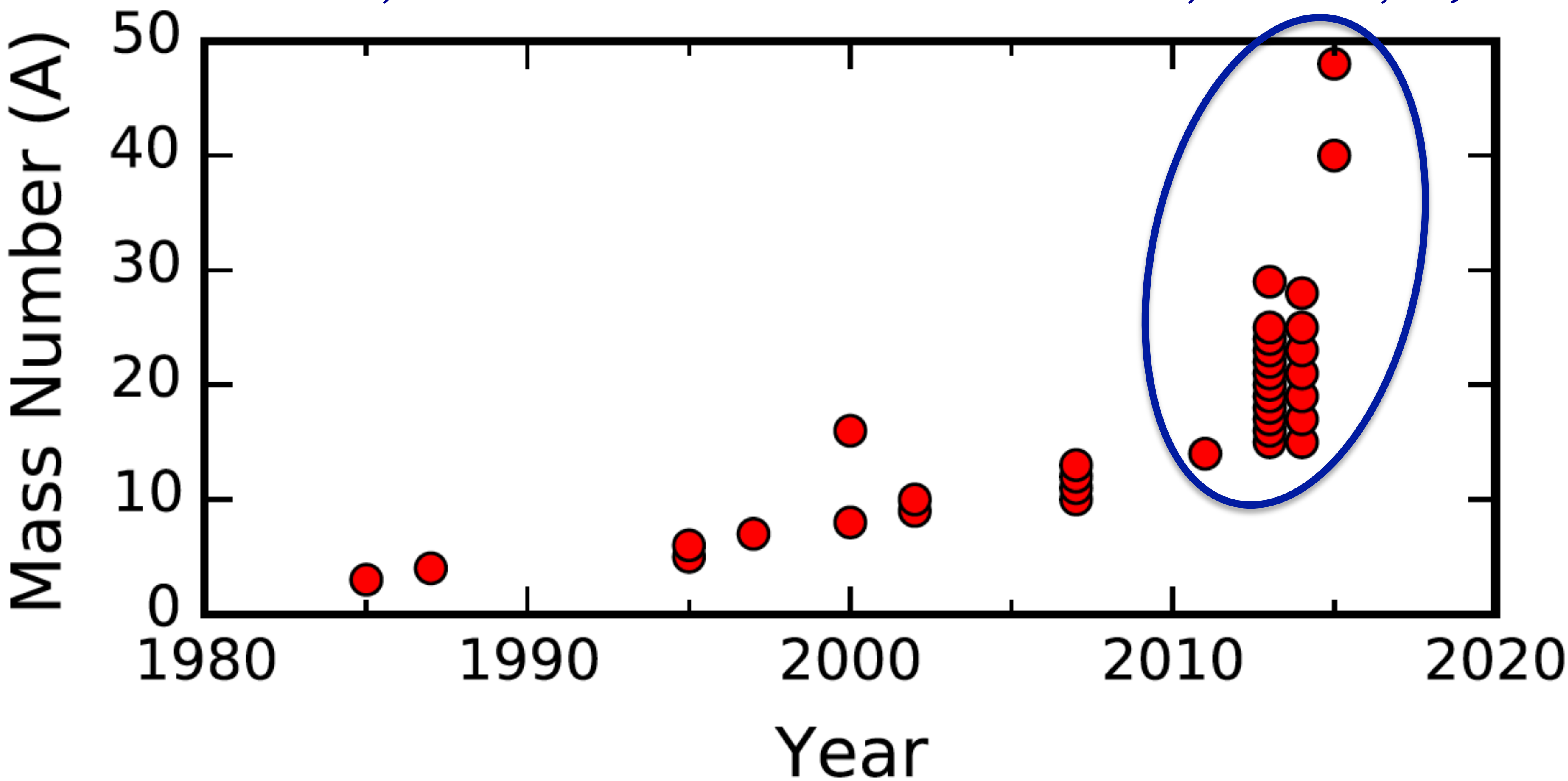
Stroberg et al., 1511.02802

Deformation in *p*-shell nuclei:

Caprio, Maris & Vary, PLB (2013); Caprio et al., IJMPE (2015); Dytrych et al., PRL (2013)

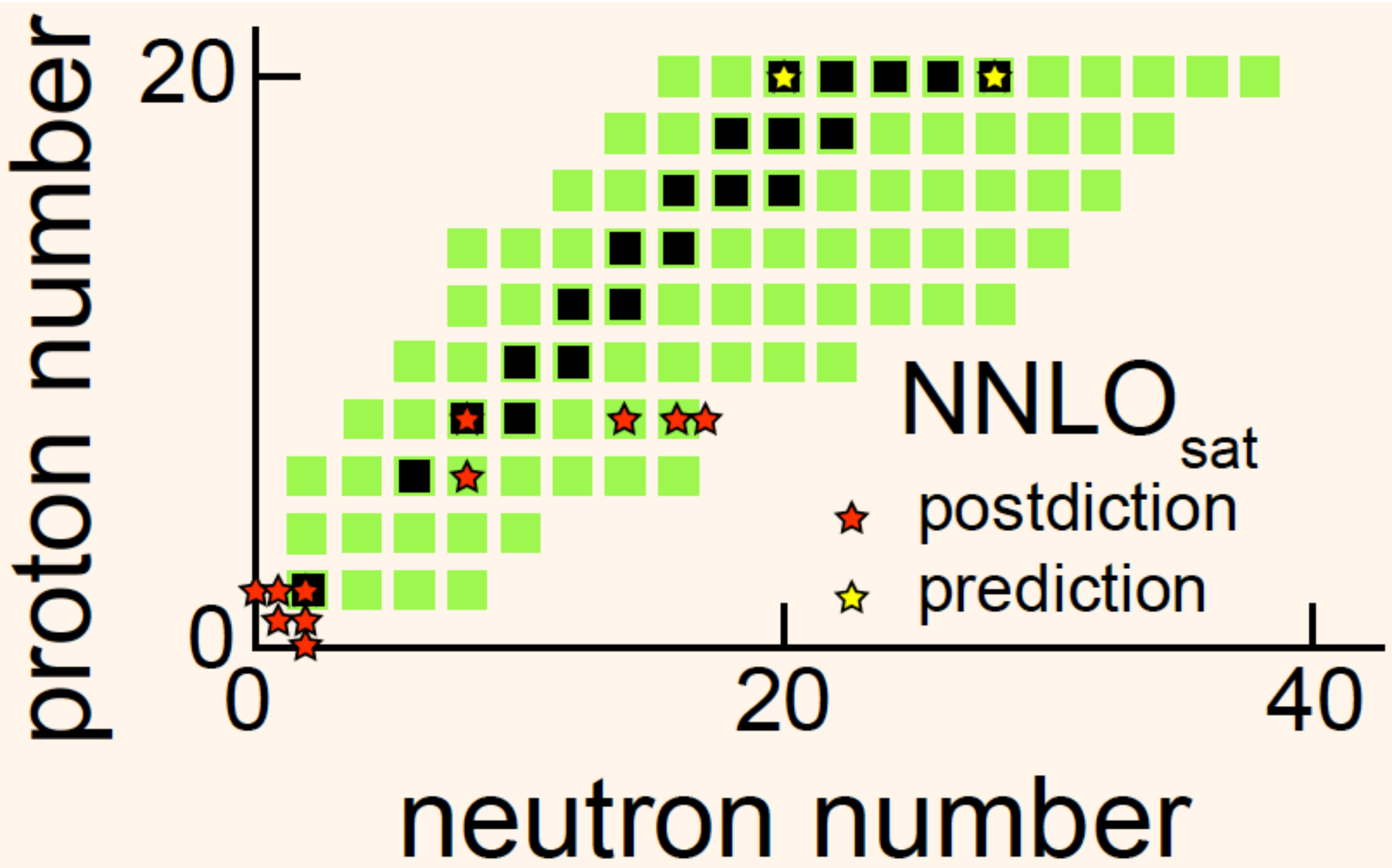
Trend in realistic *ab initio* calculations

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, …)

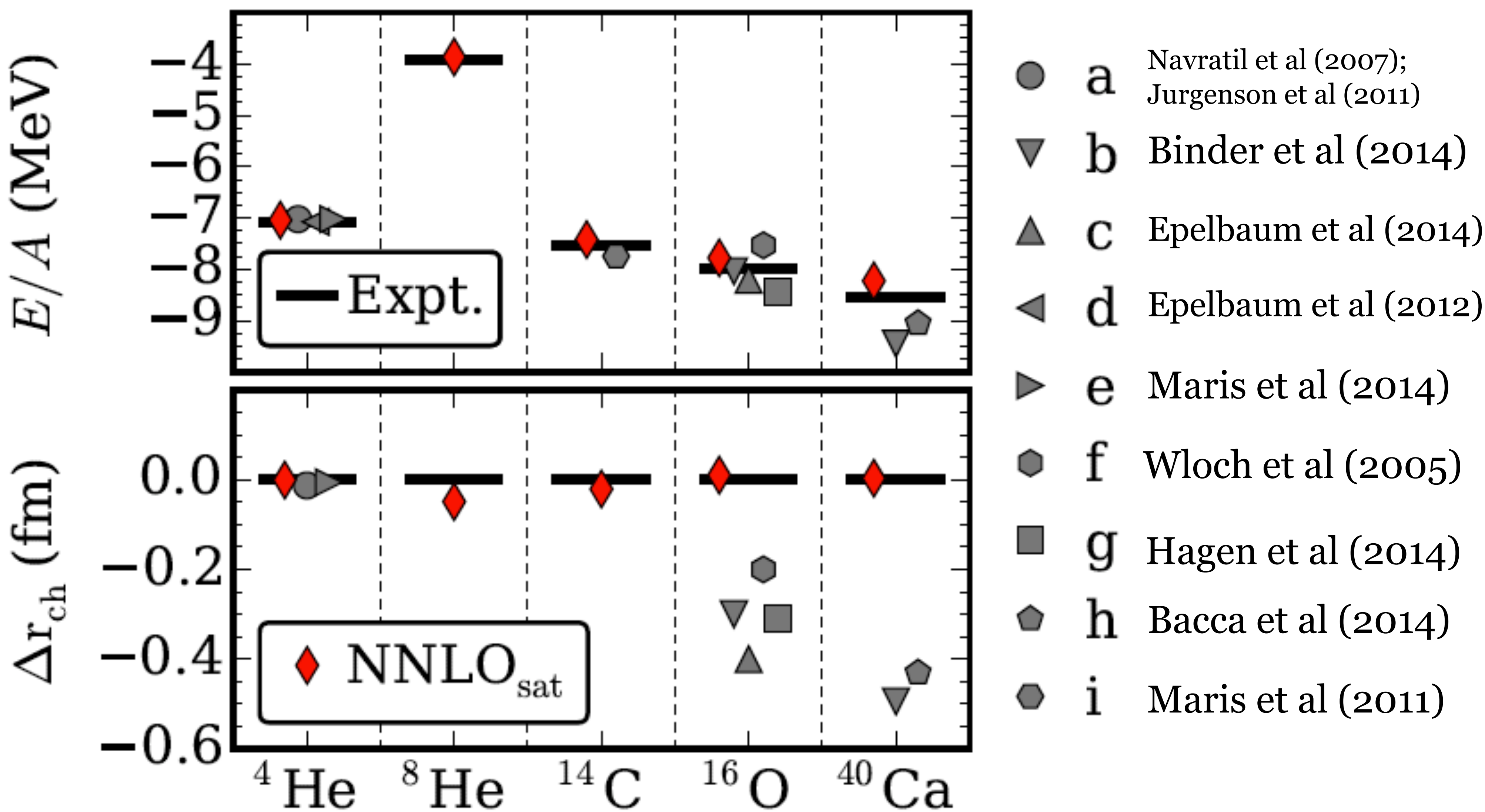


Computational capabilities exceed accuracy of available interactions
[Binder *et al*, Phys. Lett. B 736 (2014) 119]

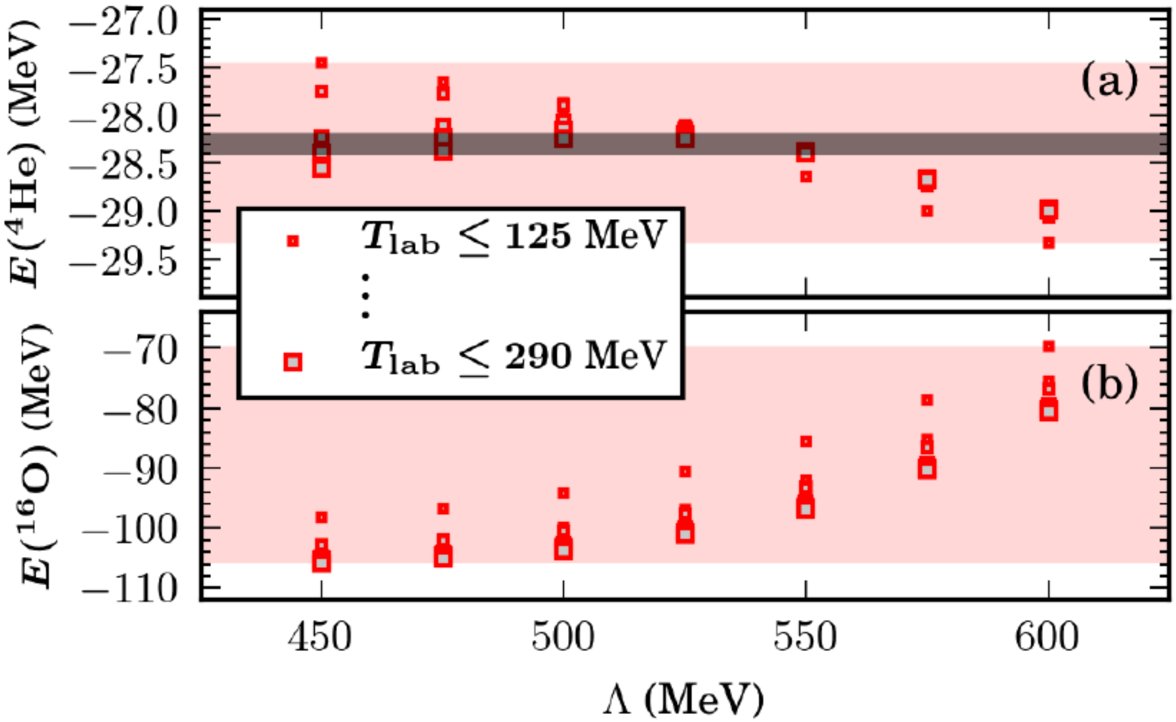
Chiral interaction $NNLO_{sat}$



$NNLO_{sat}$ – improved binding and radii by construction

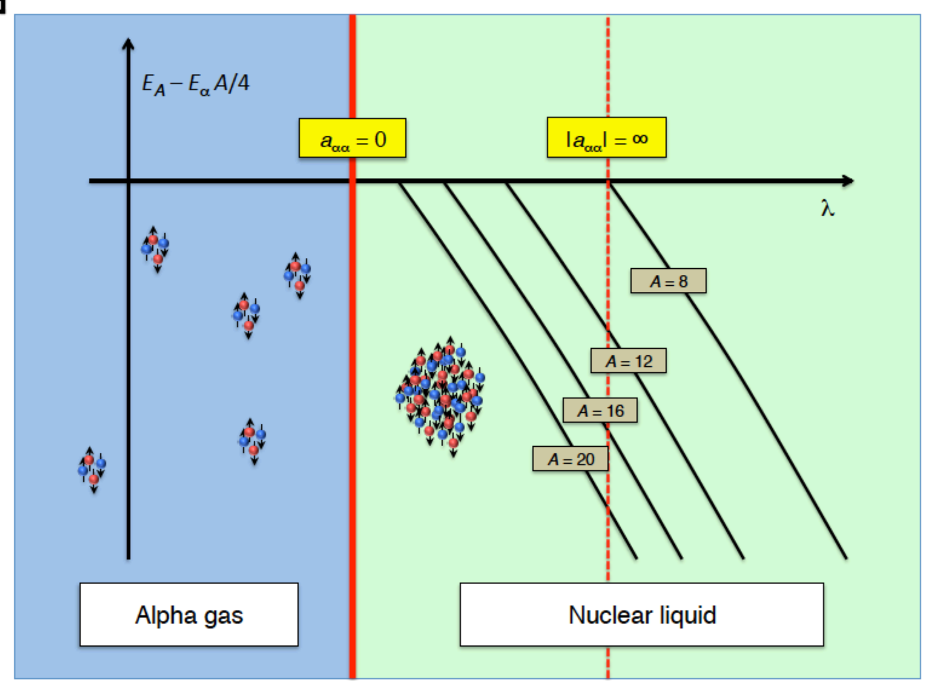


Nuclear saturation is finely tuned



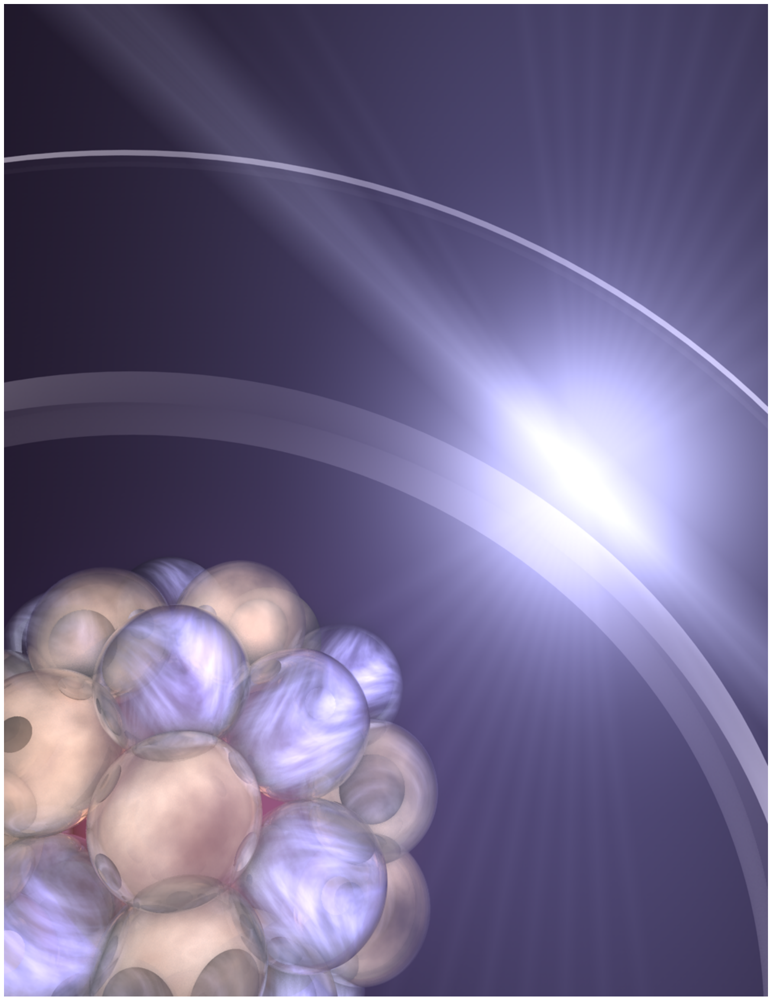
Lattice EFT suggests that nuclei are close to a quantum phase transition [Elhatisari et al., (2016)]

A 4% change in the binding energy of ^{4}He yields a 15% change in ^{16}O [B. Carlsson, A. Ekström, C. Forssén et al., PRX **6**, 011019 (2016)].



Light nuclei:
Illinois 3NF fitted to 7 states in A≤8 nuclei [Pieper et al. (2001)].

What is the neutron skin in ^{48}Ca?



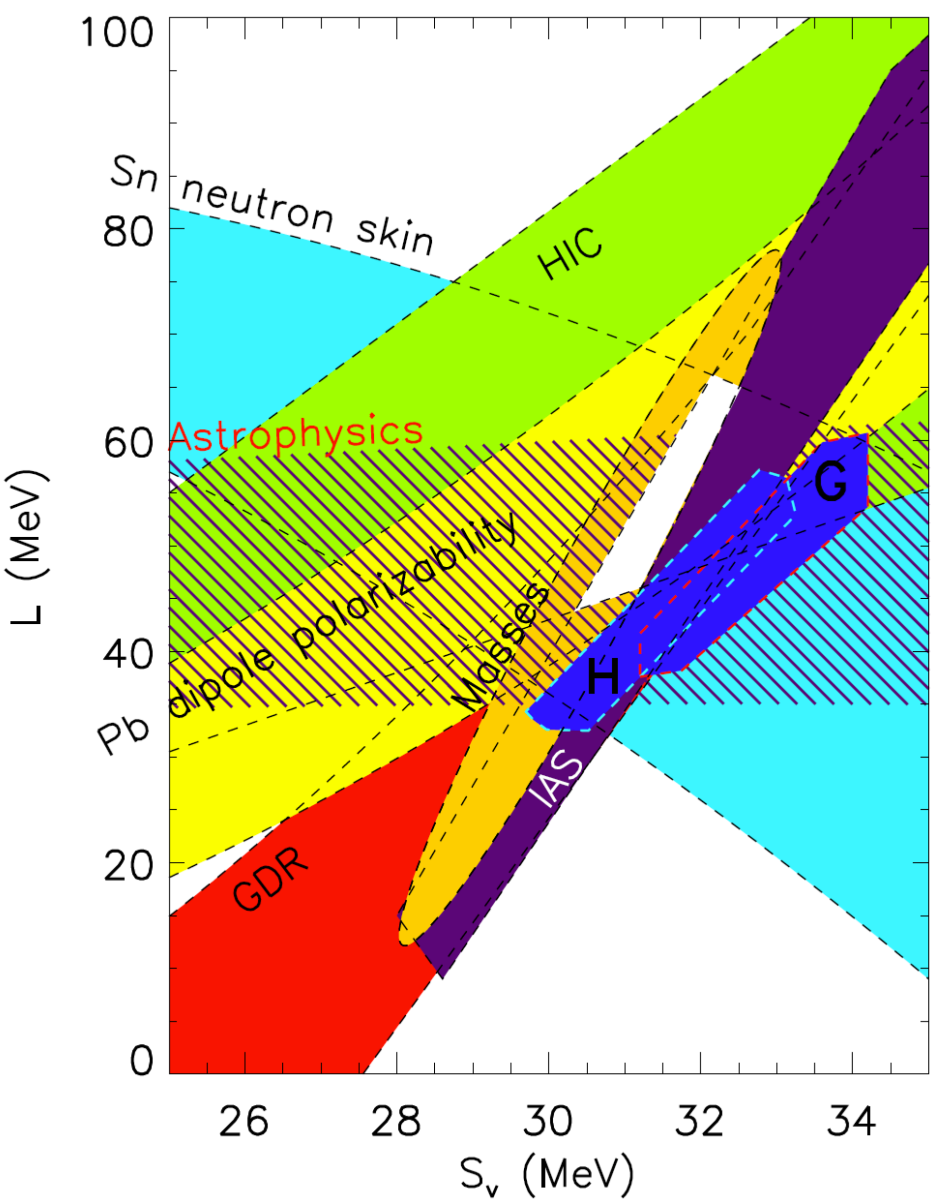
Neutron skin = Difference between radii of neutron and proton distributions

Relates atomic nuclei to neutron stars via neutron EOS

Correlated quantity: dipole polarizability

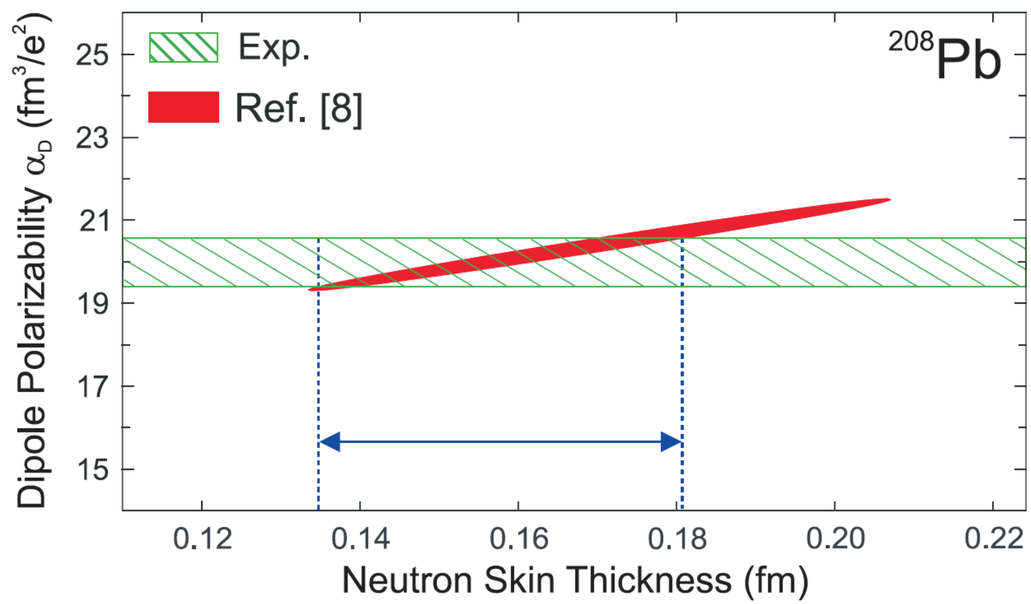
Model-independent measurement possible via parity-violating electron scattering

Neutron radii and dipole polarizabilities



Lattimer & Steiner, EPJA 50 (2014) 40

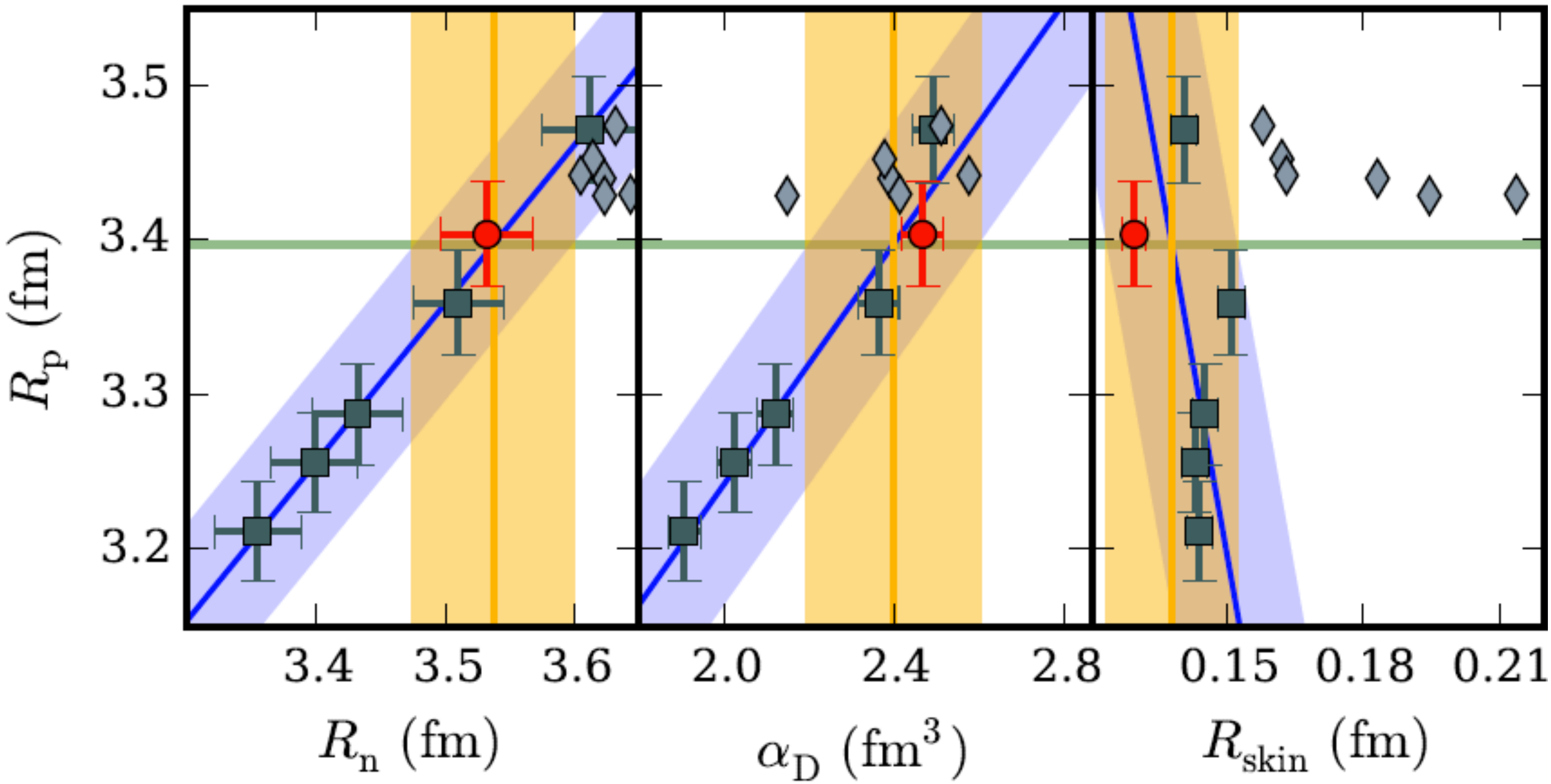
Brown, PRL 2000, Piekarewicz & Horowitz, PRL 2001; Furnstahl, NPA 2002; Reinhard & Nazarewicz, PRC 2010; Piekarewicz et al., PRC 2012; Horowitz et al, PRC 2012; …



α_D: ^{208}Pb by Tamii et al, PRL 2011; ^{68}Ni by Rossi et al, PRL 2013; ^{120}Sn by Hashimoto et al. (2015); ^{48}Ca coming soon …

R_n: ^{208}Pb by Abrahamyan et al, PRL 2012; ^{48}Ca → CREX

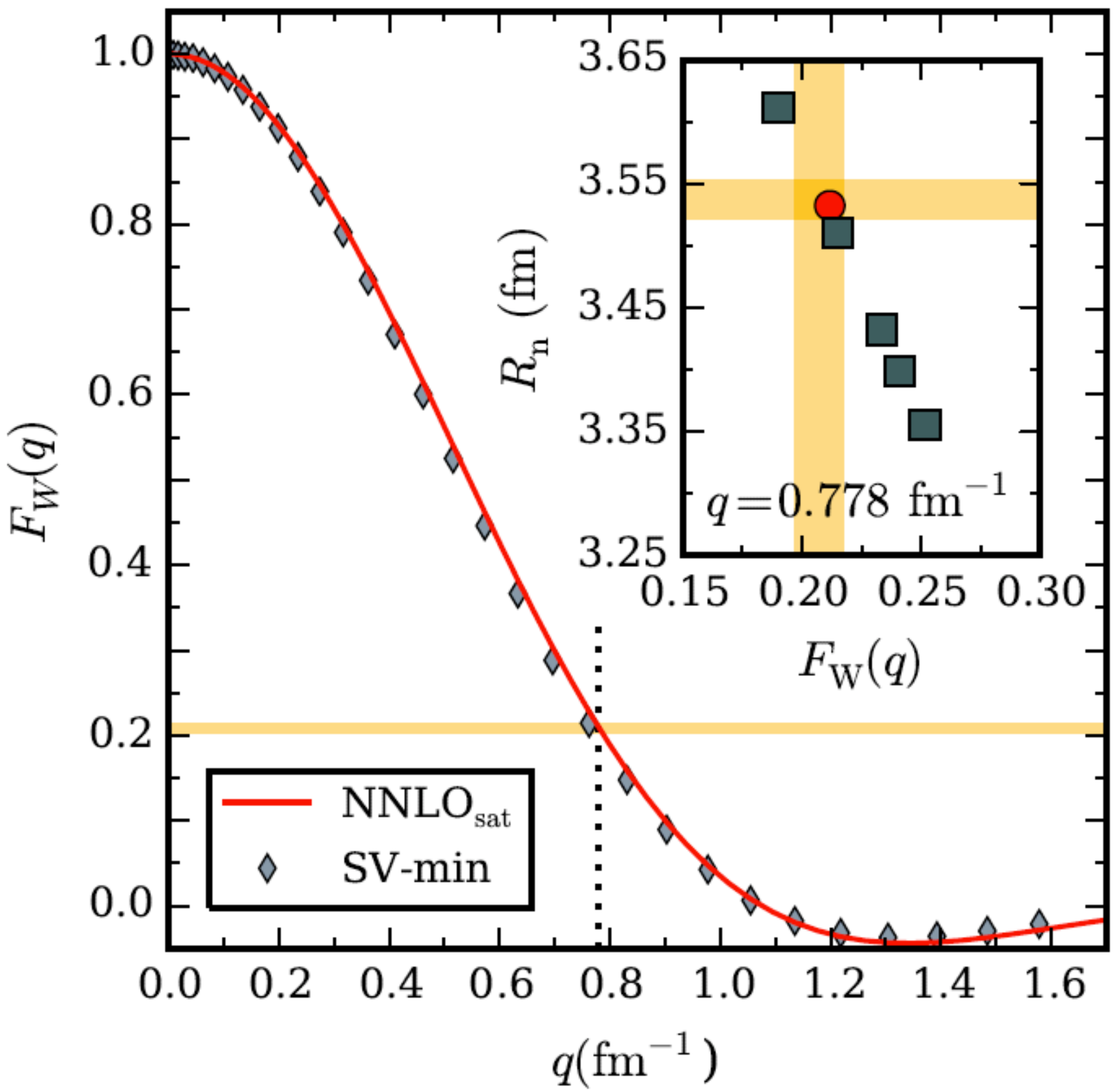
Correlations of critical observables



Uncertainty estimates from family of chiral interactions [NNLO$_{sat}$, other potentials from Hebeler (2011), and DFT].

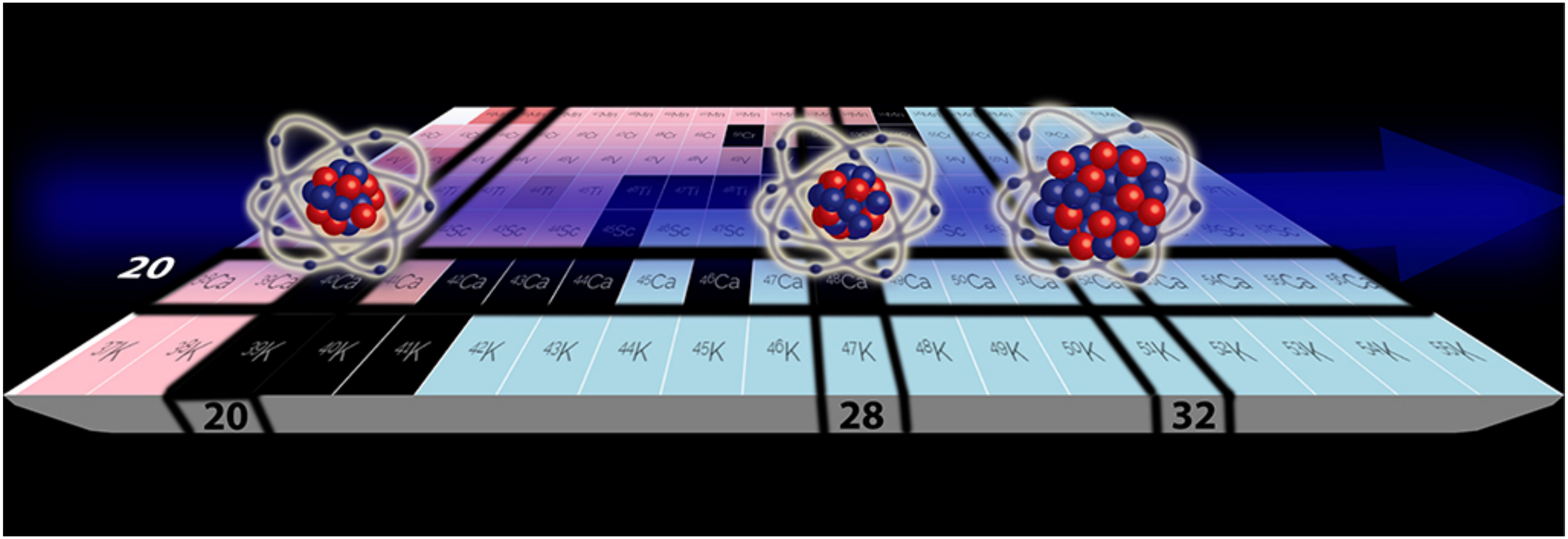
G. Hagen et al., Nature Physics 12, 186 (2016)

Weak form factor



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

Magicity in calcium isotopes

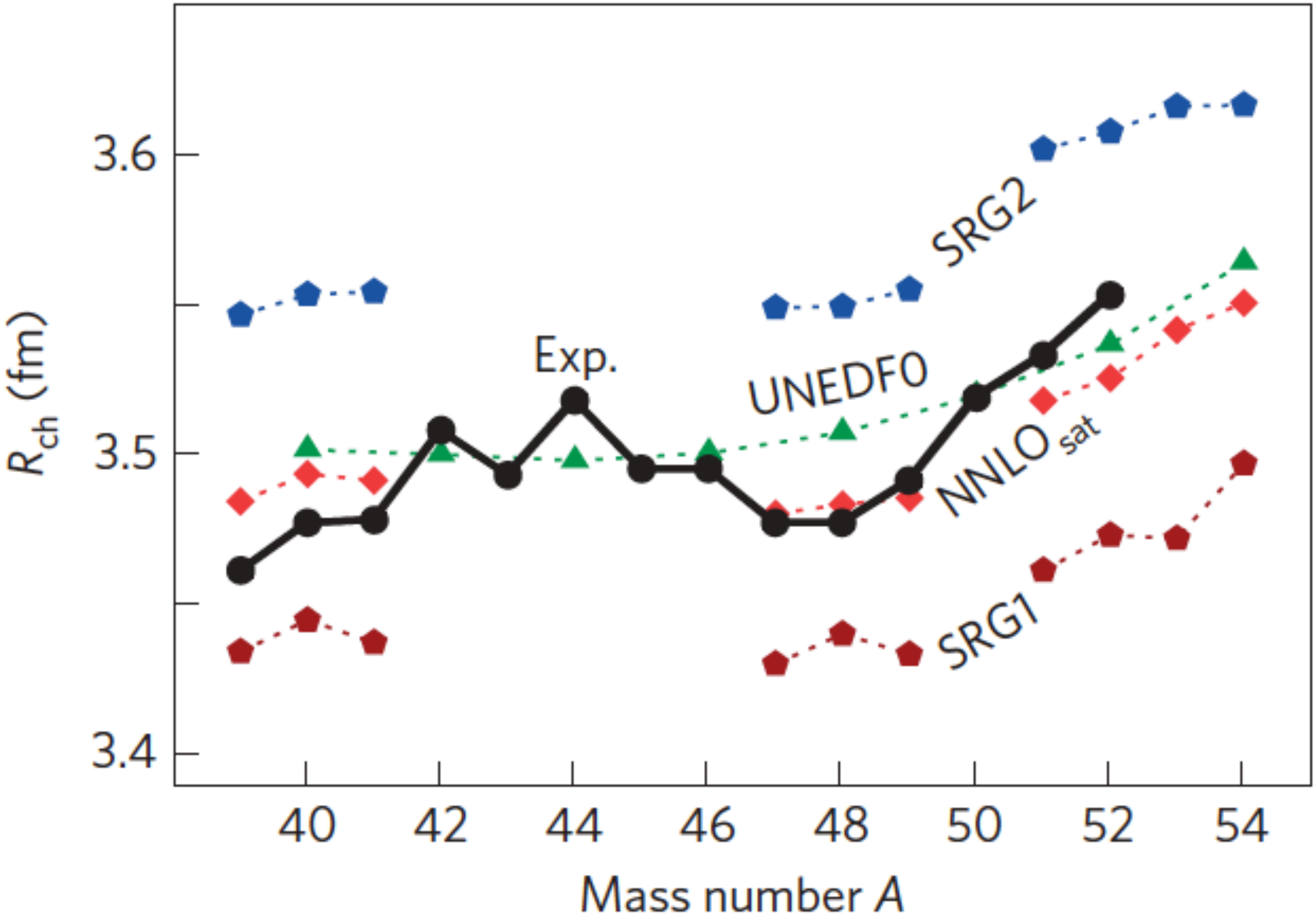


Magicity manifests itself through many observables:

- Separation energies
- Energy of 2^+ excited state
- Charge radii
- …

Figure: R. Garcia Ruiz and COLLAPS collaboration

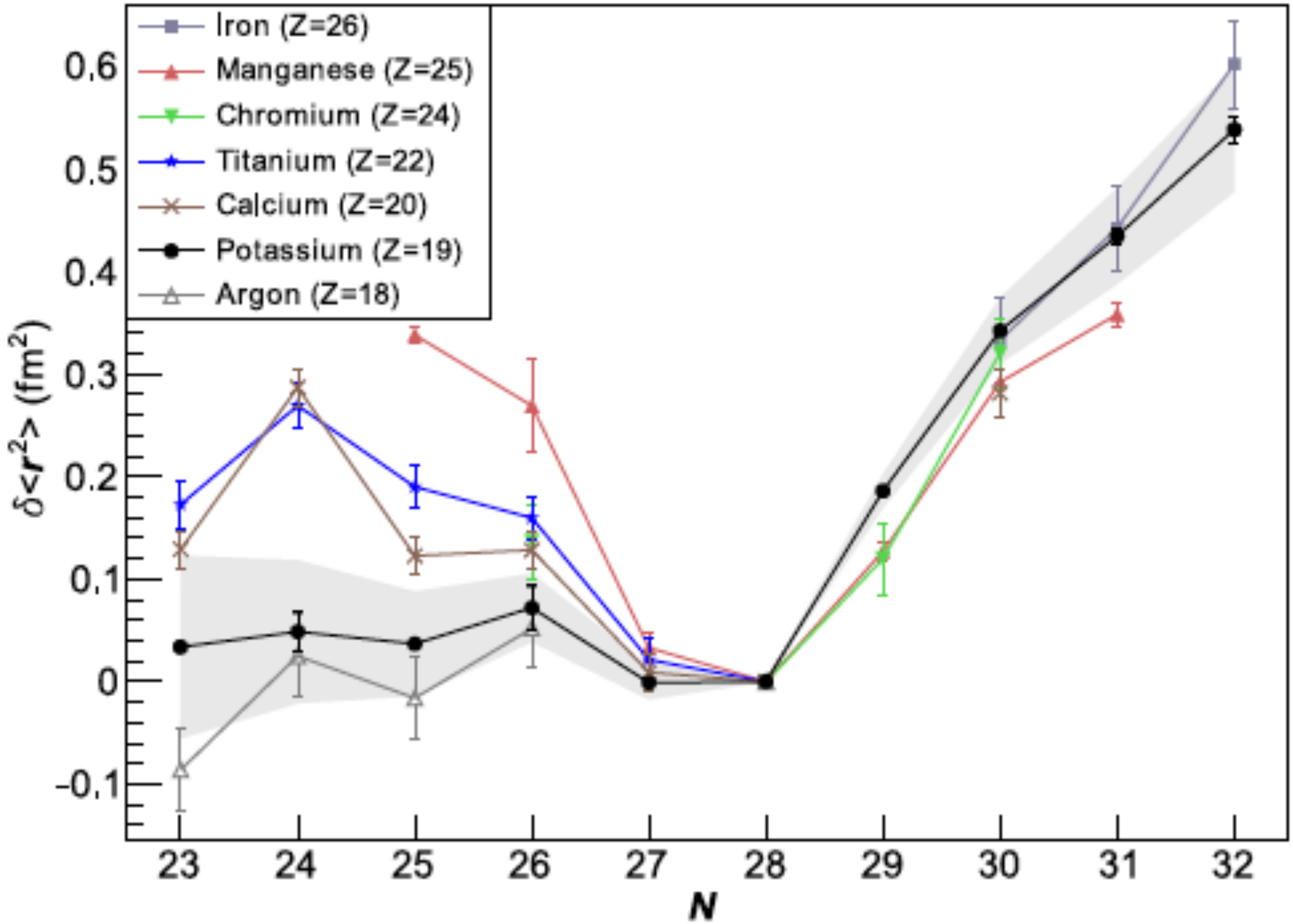
Charge radii in calcium isotopes



... question the magicity at N=32.

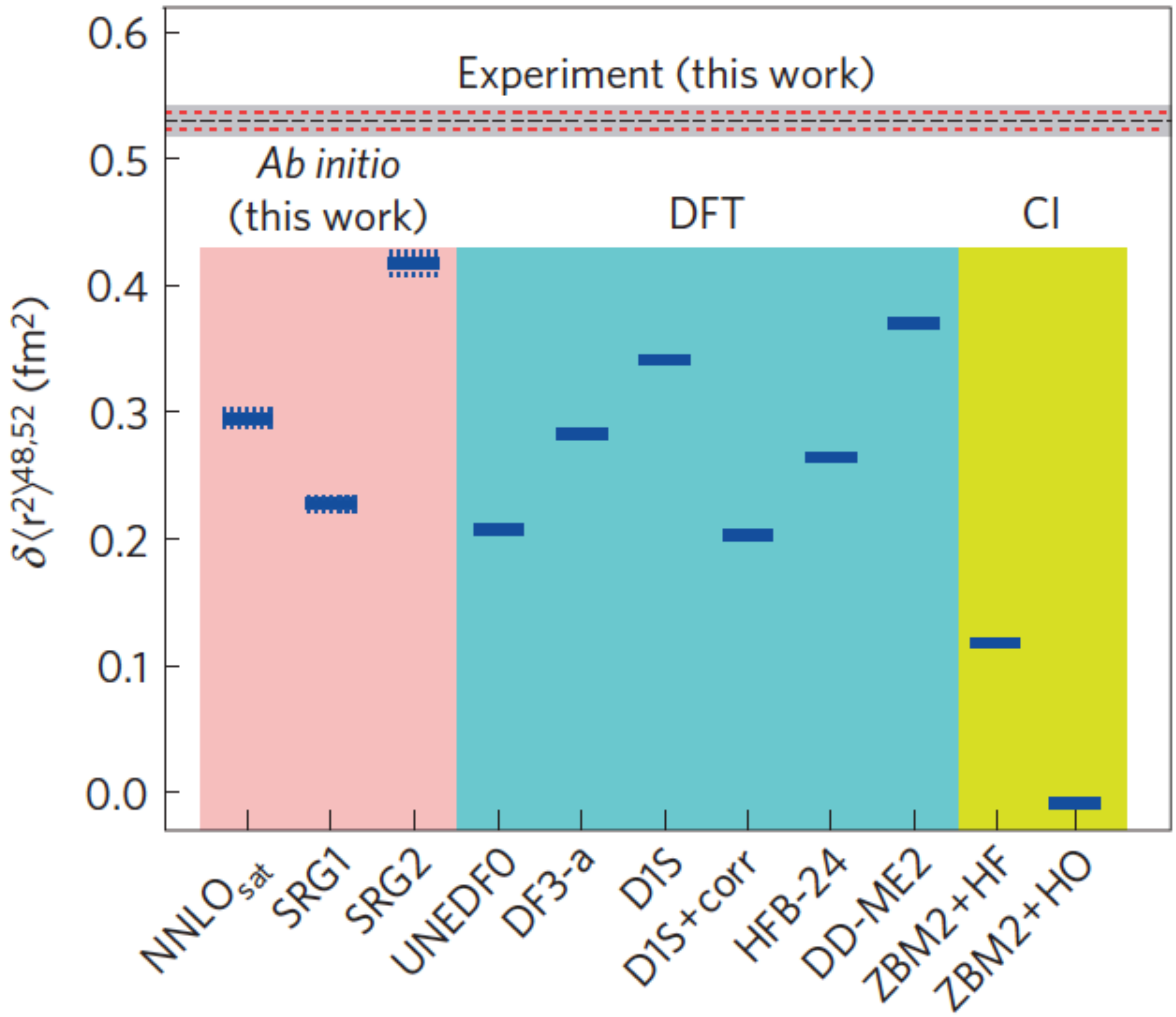
R. Garcia Ruiz et al., Nature Physics (advance online, 2016)

Isotope shifts around N=28

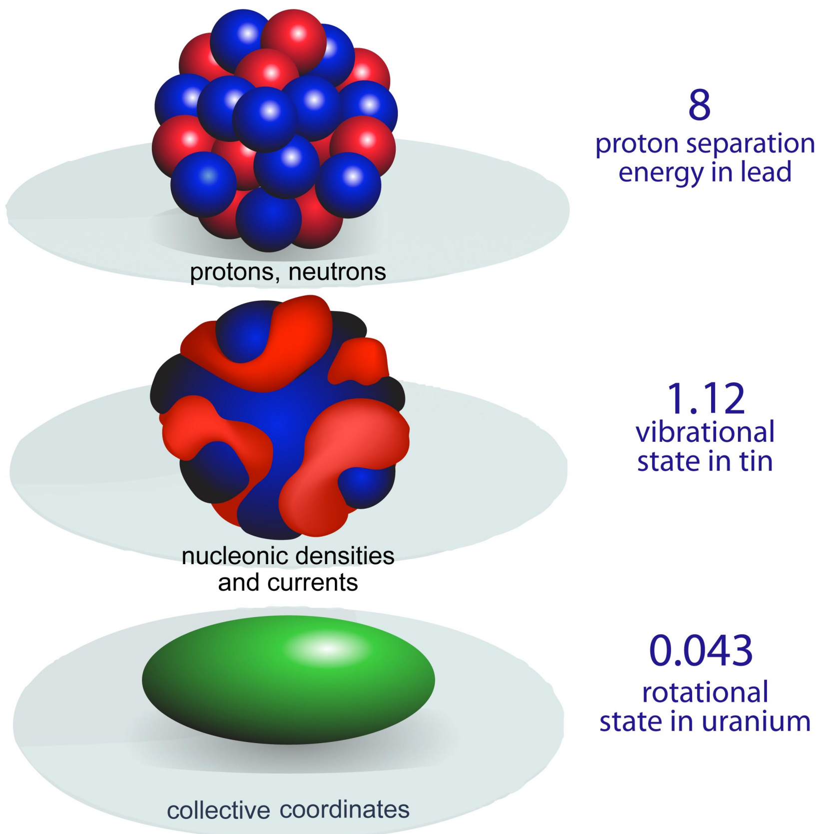


Kreim et al., PLB (2014)

Theory challenge: Charge radius in ^{52}Ca

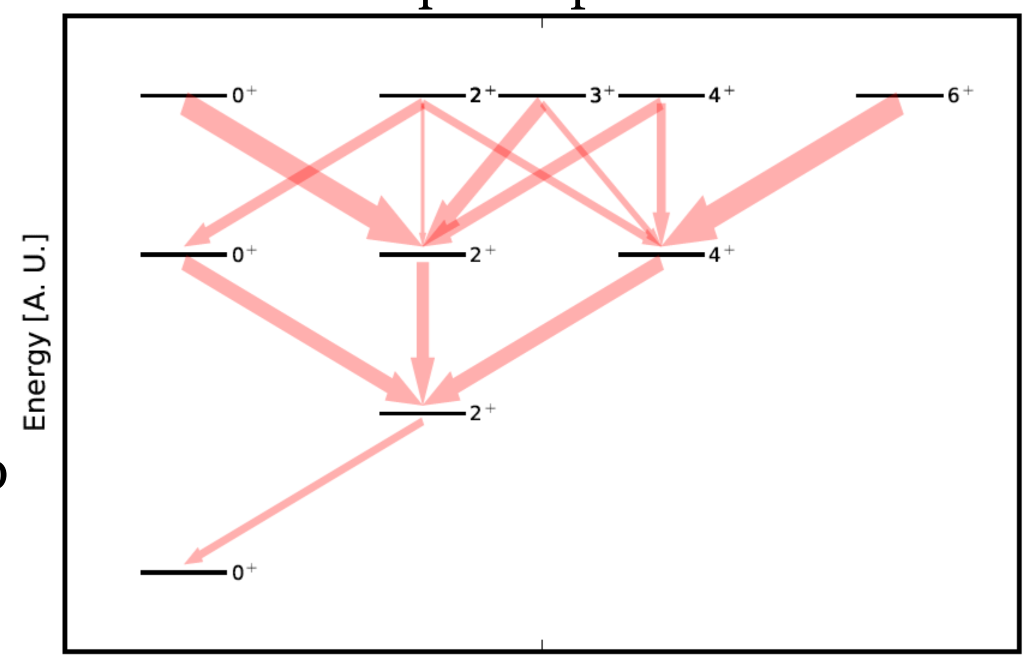


EFT for nuclear vibrations
[with E. A. Coello Pérez, PRC 92, 064309 (2015)]



EFT for nuclear vibrations

Harmonic quadrupole oscillator

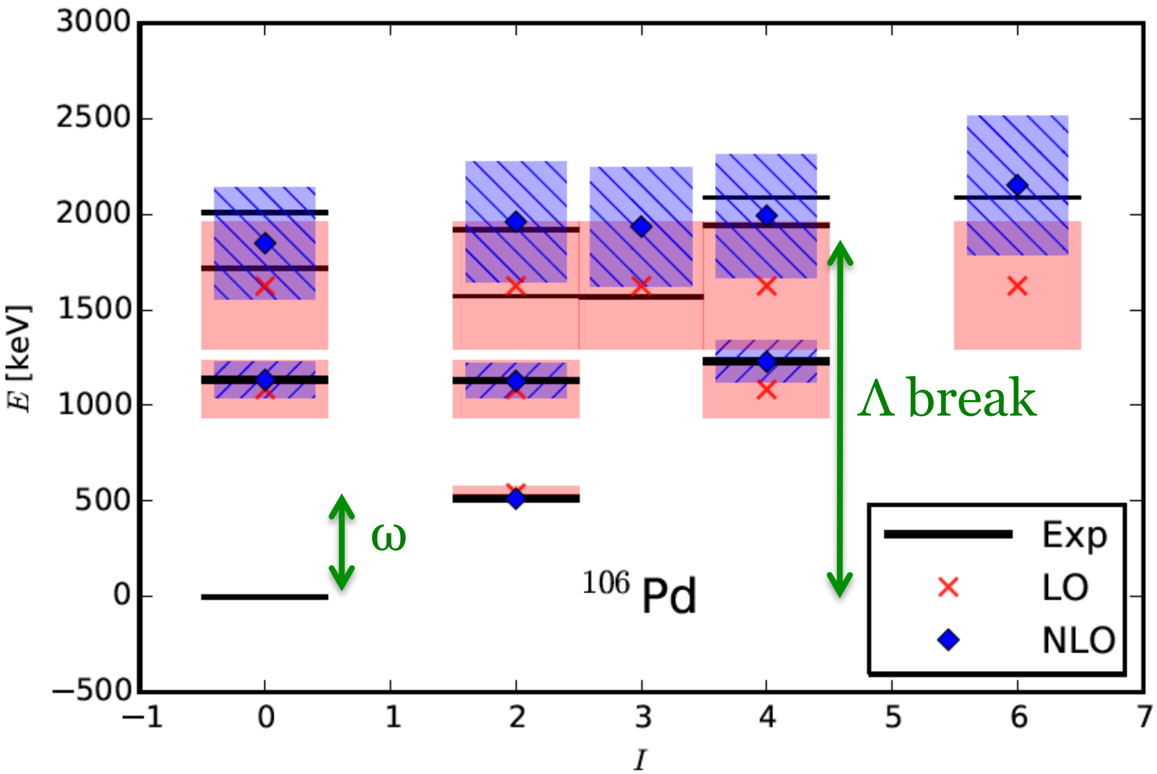


Spectrum and B(E2) transitions

While spectra of certain nuclei appear to be harmonic, B(E2) transitions do not.

Garrett & Wood (2010): “Where are the qudrupole vibrations in atomic nuclei?”

EFT for nuclear vibrations



EFT ingredients:

- quadrupole degrees of freedom
- breakdown scale around three-phonon levels
- "small" expansion parameter: ratio of vibrational energy to breakdown scale: $\omega/\Lambda \approx 1/3$

- Uncertainties show 68% DOB intervals from Bayesian analysis of EFT truncation effects, following [Cacciari & Houdeau (2011); Bagnaschi et al (2015); Furnstahl, Klco, Phillips & Wesolowski (2015)]
  - Expand observables according to power counting
  - Employ "naturalness" assumptions as log-normal priors in Bayes' theorem
  - Compute distribution function of uncertainties due to EFT truncation
  - Compute degree-of-believe (DOB) intervals.

Hamiltonian

LO Hamiltonian $\hat{H}_{\rm LO} = \omega \hat{N}$

NLO correction $\hat{h}_{\rm NLO} = g_N \hat{N}^2 + g_v \hat{\Lambda}^2 + g_I \hat{I}^2$

with
$$\hat{N}^2 = (d^\dagger \cdot \tilde{d})^2,$$
$$\hat{\Lambda}^2 = -(d^\dagger \cdot d^\dagger)(\tilde{d} \cdot \tilde{d}) + \hat{N}^2 - 3\hat{N},$$
$$\hat{I}^2 = 10(d^\dagger \otimes \tilde{d})^{(1)} \cdot (d^\dagger \otimes \tilde{d})^{(1)}.$$

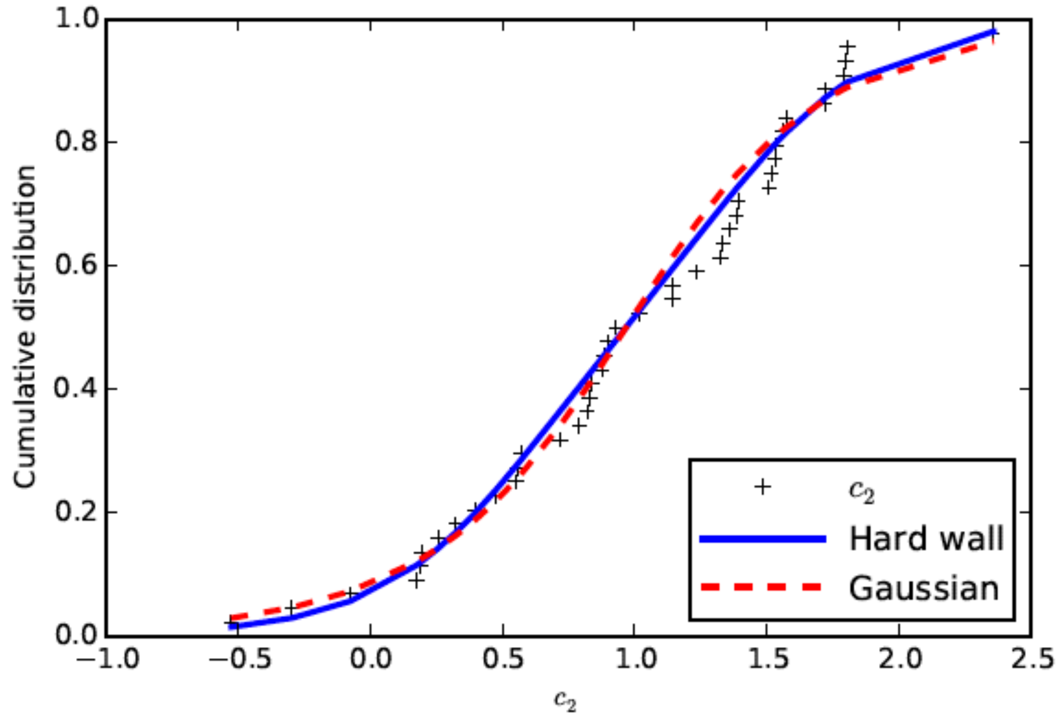
Small expansion parameter $\varepsilon \equiv (N\omega/\Lambda)$

Uncertainty quantification

$$E_{\text{NLO}} = \omega N + g_\omega N + g_N N^2 + g_v v(v+3) + g_I I(I+1)$$

$$c_2 \equiv c_2(N, v, I) = \frac{g_\omega N + g_N N^2 + g_v v(v+3) + g_I I(I+1)}{\varepsilon^2 \omega}$$

$$X = X_0 \sum_{n=0}^{\infty} c_n \varepsilon^n$$



Linear combinations of LECs enter observables. LECs are random, but with EFT expectations, i.e. log-normal distributed. Making assumptions about these distributions then allows one to quantify uncertainties. The assumptions can be tested.

$$\Delta_k^{(M)} = \sum_{n=k+1}^{k+M} c_n \varepsilon^n$$

$$p_M(\Delta | c_0, \ldots, c_k) = \frac{\int_0^\infty \mathrm{d}c \; \mathrm{pr}(c) p_M(\Delta | c) \prod_{m=0}^{k} \mathrm{pr}(c_m | c)}{\int_0^\infty \mathrm{d}c \; \mathrm{pr}(c) \prod_{m=0}^{k} \mathrm{pr}(c_m | c)}$$

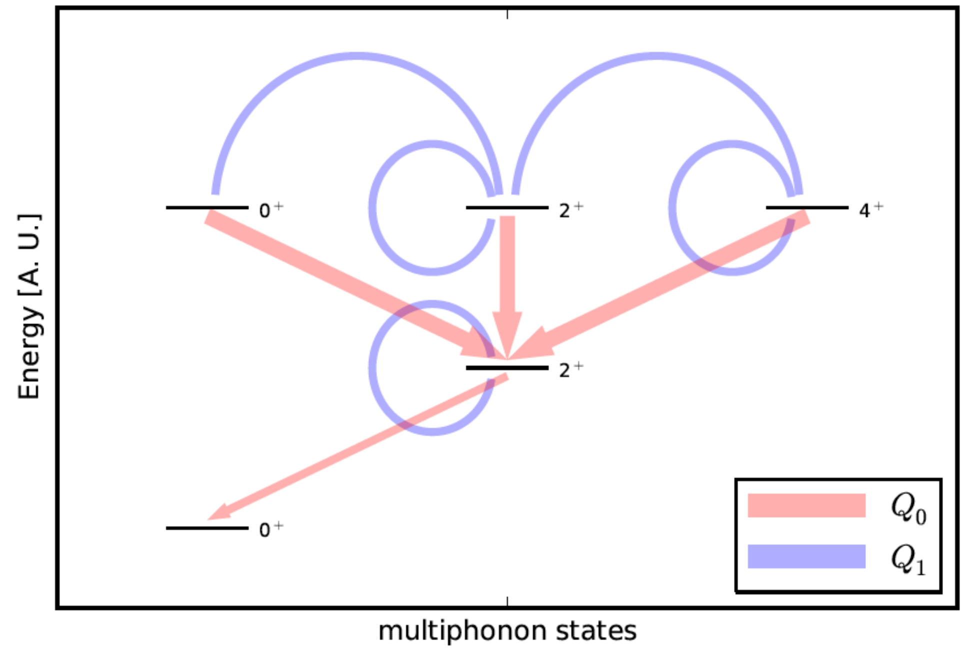
EFT result: sizeable quadrupole matrix elements are natural

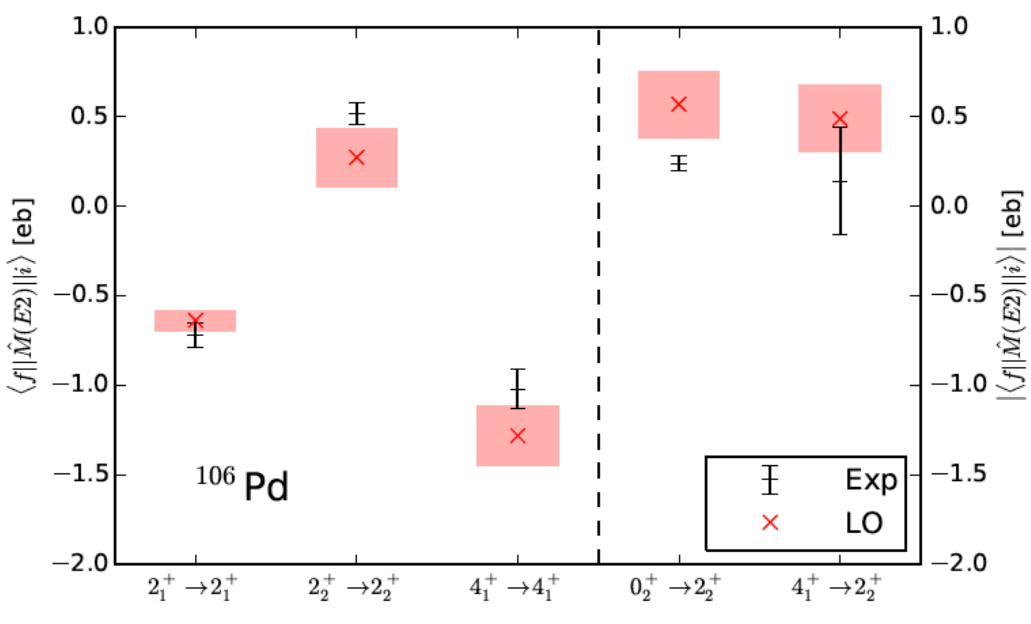
In the EFT, the quadrupole operator is also expanded:

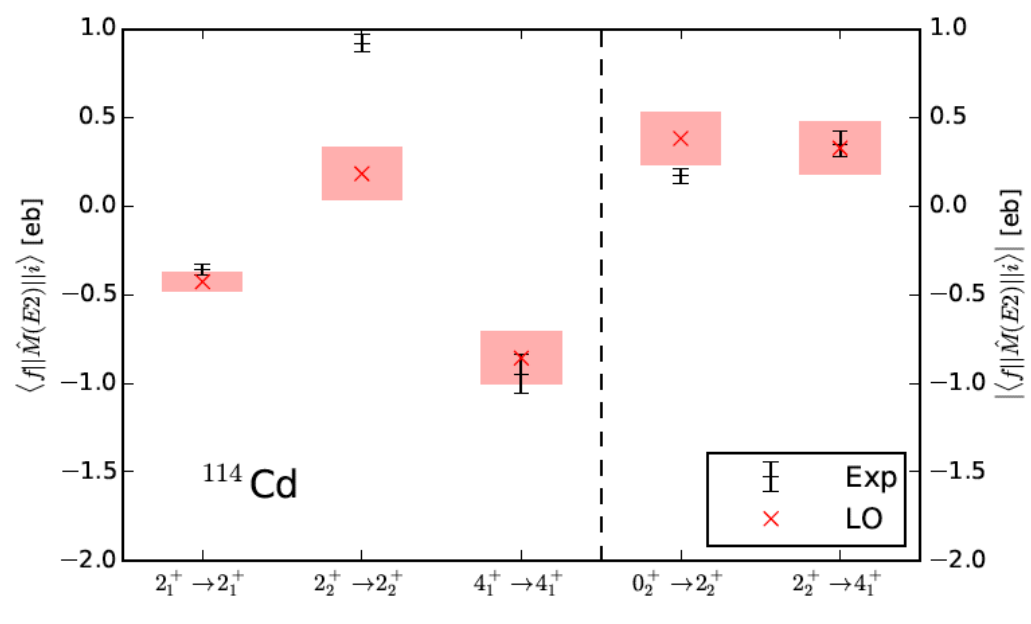
$$\hat{Q}_\mu = Q_0 \left(d^\dagger_\mu + \tilde{d}_\mu \right) + Q_1 \left(d^\dagger \times d^\dagger + \tilde{d} \times \tilde{d} + 2 d^\dagger \times \tilde{d} \right)^{(2)}_\mu$$

Subleading corrections are sizable:

$$Q_1 \sim \left(\frac{\omega}{\Lambda} \right)^{1/2} Q_0$$



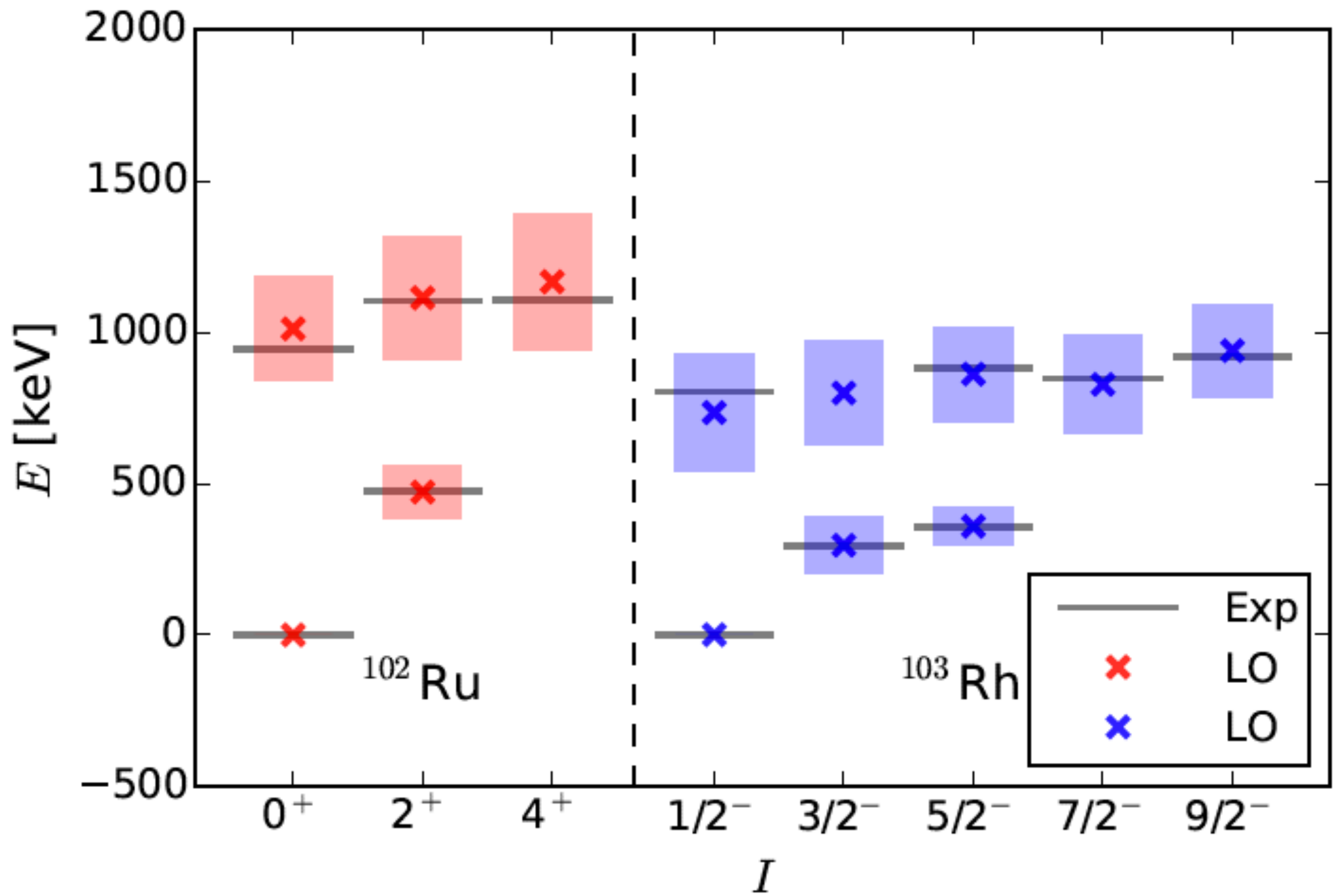




Work in progress: Fermion coupled to vibrating nucleus

Idea: In the spirit of Halo EFT [Bertulani, Hammer, van Kolck (2002); Higa, Hammer, van Kolck (2008); Hammer & Philipps (2011); Ryberg et al. (2014)], add a fermion to describe odd-mass neighbors

Two new LECs enter at LO



E. A. Coello Pérez & TP, preliminary results

Magnetic moments: Relations between even-even and even-odd nuclei

Nucleus	I_i^π	$\mu_{\rm exp}(I_i^\pi)$	$\mu_{\rm EFT}(I_i^\pi)$
^{102}Ru	2_1^+	$0.85(3)^*$	0.85(16)
	2_2^+		0.85(33)
	4_1^+		2.08(33)
^{103}Rh	$\frac{1}{2}_1$	-0.088^*	$-0.088(16)$
	$\frac{3}{2}_1$	0.77(7)	0.78(16)
	$\frac{5}{2}_1$	1.08(4)	0.79(16)
	$\frac{7}{2}_1$	2.0(6)	2.0(3)
	$\frac{9}{2}_1$	2.8(5)	2.0(3)

Nucleus	I_i^π	$\mu_{\rm exp}(I_i^\pi)$	$\mu_{\rm EFT}(I_i^\pi)$
^{106}Pd	2_1^+	$0.79(2)^*$	0.79(15)
	2_2^+	0.71(10)	0.79(30)
	4_1^+	1.8(4)	1.93(30)
^{107}Ag	$\frac{1}{2}_1$	-0.11^*	$-0.11(15)$
	$\frac{3}{2}_1$	0.98(9)	0.74(15)
	$\frac{5}{2}_1$	1.02(9)	0.71(15)
	$\frac{7}{2}_1$		1.9(3)
	$\frac{9}{2}_1$		1.9(3)

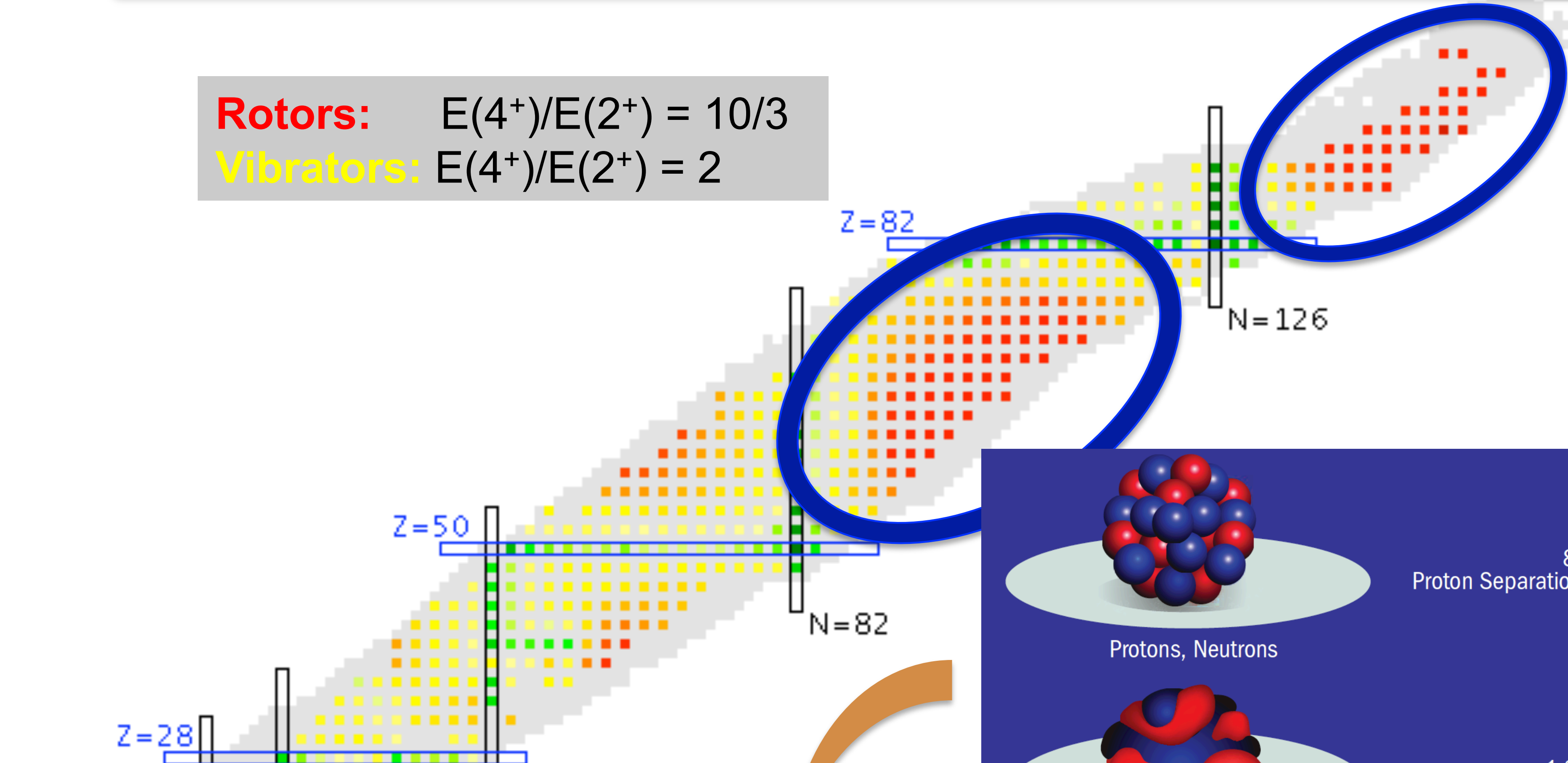
At LO, one new LEC enters to describe odd-mass neighbor

E. A. Coello Pérez & TP, preliminary results

EFT for deformed nuclei

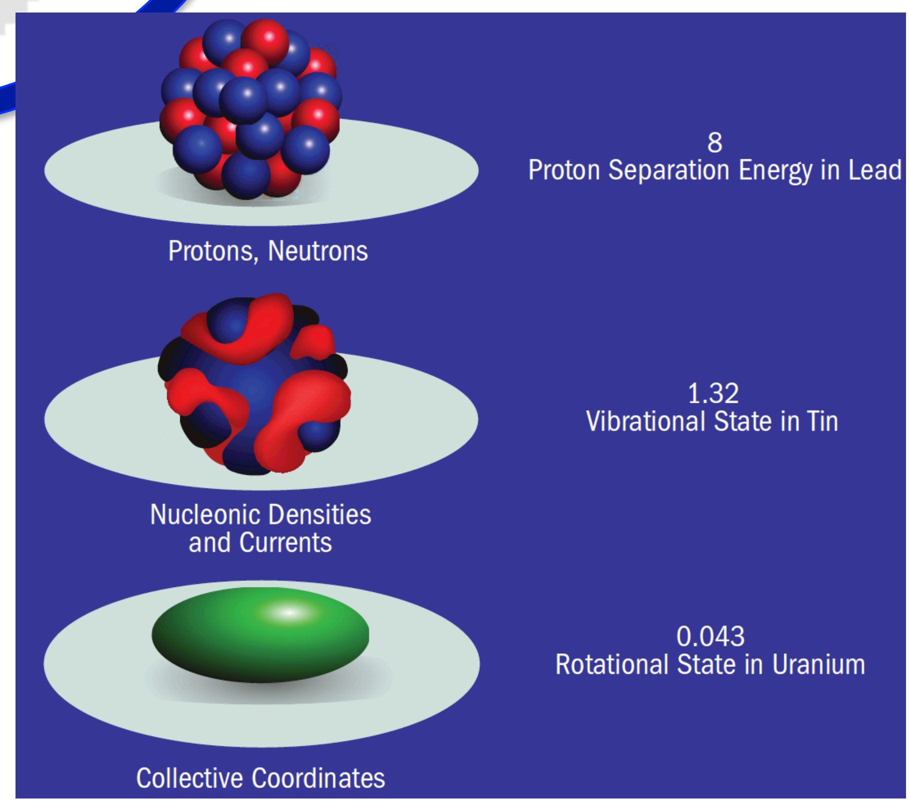
Rotors: $E(4^+)/E(2^+) = 10/3$

Vibrators: $E(4^+)/E(2^+) = 2$



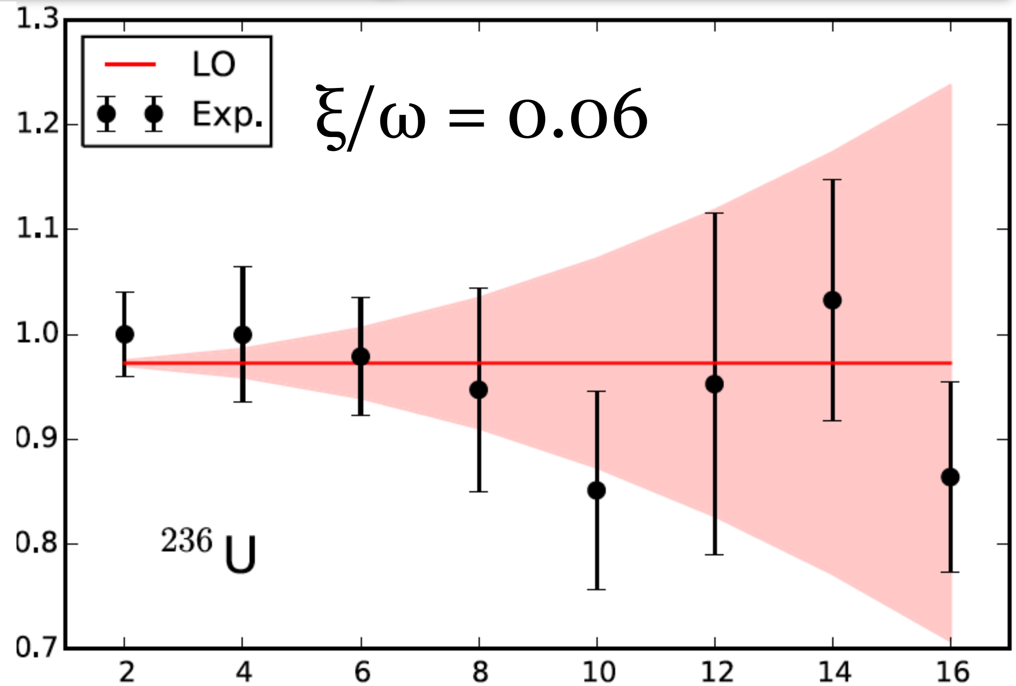
Effective field theory

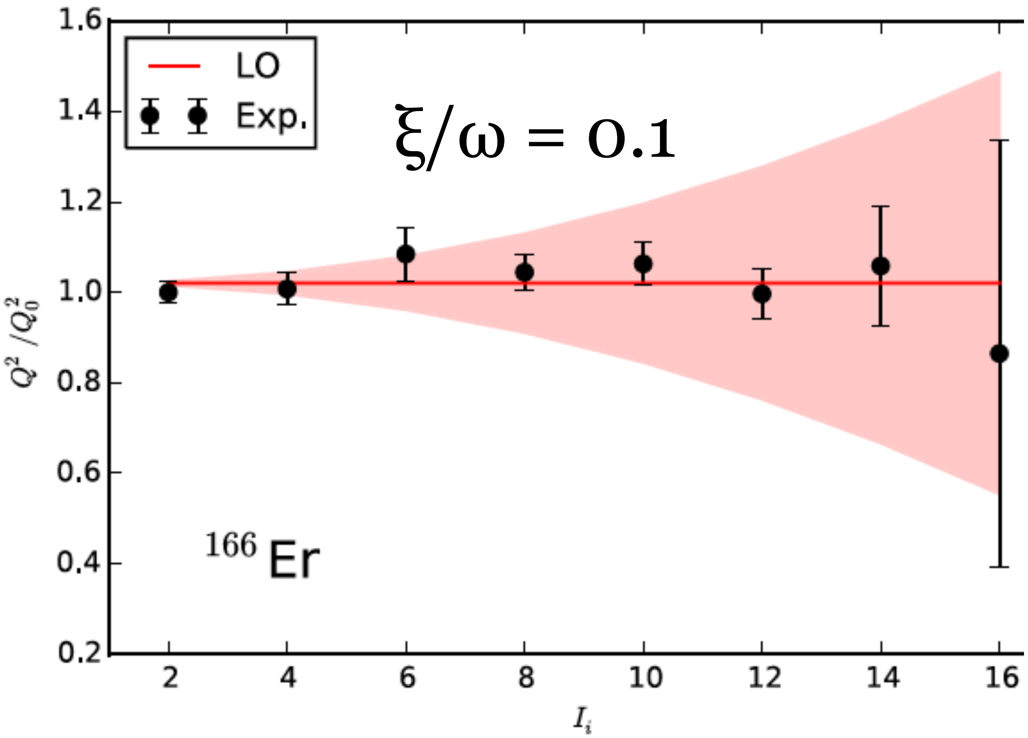
[TP (2011); Weidenmüller & TP (2014); Coello Pérez & TP (2015);

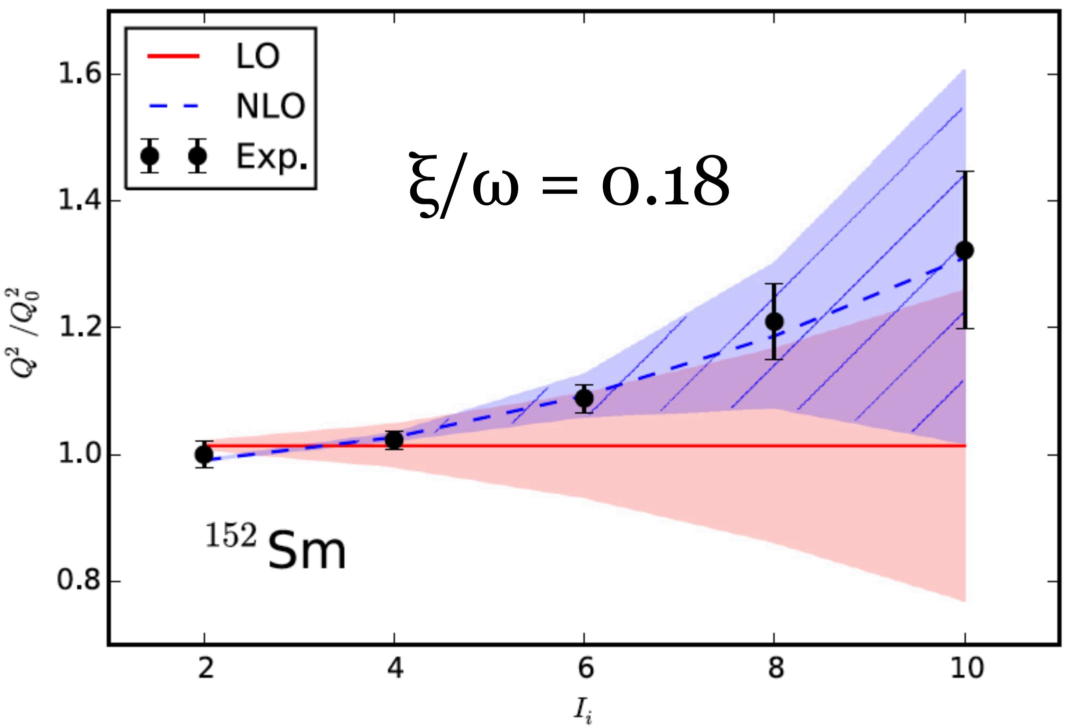


EFT works well for a wide range of rotors

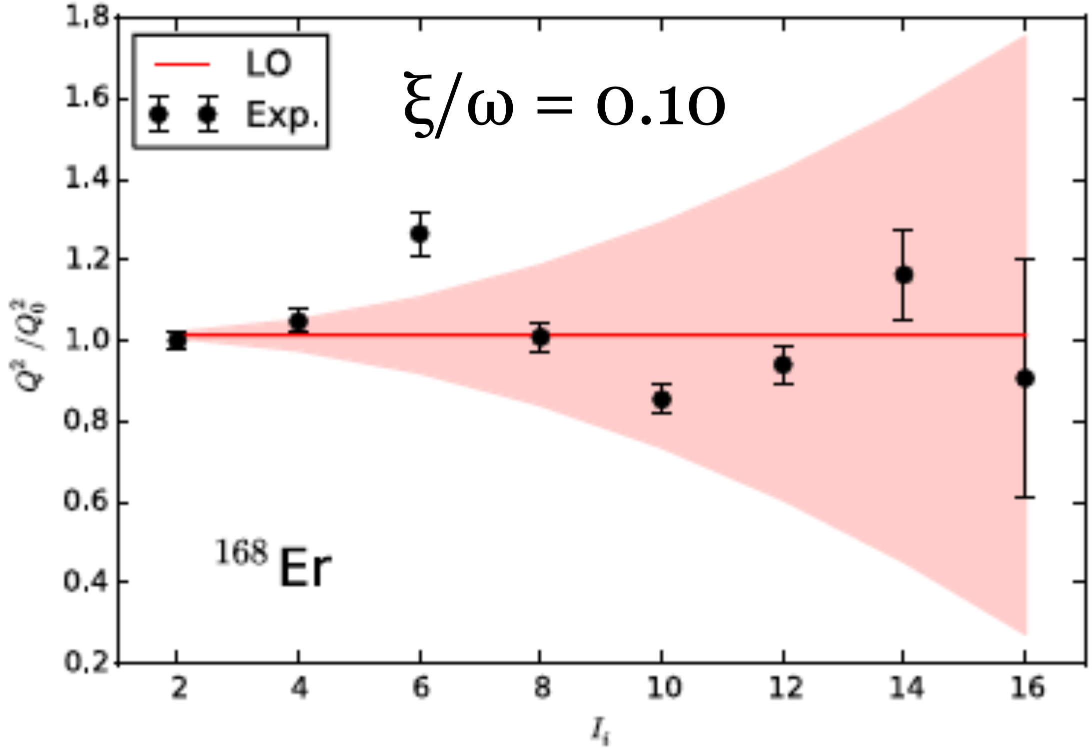
Bohr & Mottelson (1975):
"The accuracy of the present measurements of E2-matrix elements in the ground-state bands of even even nuclei is in most cases barely sufficient to detect deviations from the leading-order intensity relations."







EFT can not explain oscillatory patterns in supposedly "good" rotors ^{168}Er, ^{174}Yb

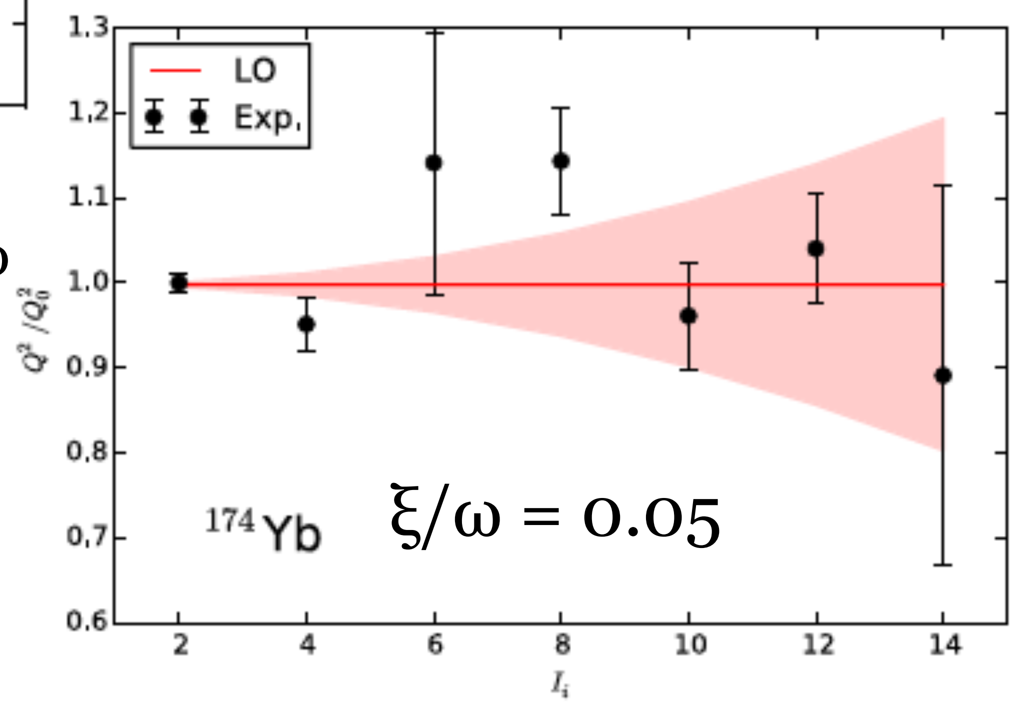


Based on results for molecules, well-deformed nuclei, and transitional nuclei, EFT suggests that a few transitions in text-book rotors could merit re-measurement.

^{168}Er: B(E2) for $6^+ \rightarrow 4^+$ very difficult to understand.

^{174}Yb: B(E2) for $8^+ \rightarrow 6^+$ difficult to reconcile with $4^+ \rightarrow 2^+$.

Theoretical uncertainty estimates relevant.



EFT and weak interband transitions (^{154}Sm)

$i \to f$	$B(E2)_{\text{exp}}$	$B(E2)_{\text{ET}}$	$B(E2)_{\text{CBS}}$	$B(E2)_{\text{BH}}$
$2_g^+ \to 0_g^+$	0.863 (5)	0.863[a]	0.853	0.863
$4_g^+ \to 2_g^+$	1.201 (29)	1.233 (9)	1.231	1.234
$6_g^+ \to 4_g^+$	1.417 (39)	1.358 (23)	1.378	1.355
$8_g^+ \to 6_g^+$	1.564 (83)	1.421 (43)	1.471	1.424
$2_\gamma^+ \to 0_g^+$	0.0093 (10)	0.0110 (28)		0.0492
$2_\gamma^+ \to 2_g^+$	0.0157 (15)	0.0157[a]		0.0703
$2_\gamma^+ \to 4_g^+$	0.0018 (2)	0.0008 (2)		0.0050
$2_\beta^+ \to 0_g^+$	0.0016 (2)	0.0025 (6)	0.0024	0.0319
$2_\beta^+ \to 2_g^+$	0.0035 (4)	0.0035[a]	0.0069	0.0456
$2_\beta^+ \to 4_g^+$	0.0065 (7)	0.0063 (16)	0.0348	0.0821

[a]Values employed to adjust the LECs of the effective theory.

In-band transitions [in e^2b^2] are LO, inter-band transitions are NLO. Effective theory is more complicated than Bohr Hamiltonian both in Hamiltonian and E2 transition operator. EFT correctly predicts strengths of inter-band transitions with natural LECs.

[E. A. Coello Pérez and TP, Phys. Rev. C 92, 014323 (2015)]

Summary

- Exciting times in nuclear theory
  - explosion of many-body solvers
  - many new developments regarding interactions and currents
- Optimization of chiral interaction $\mathrm{NNLO}_{\mathrm{sat}}$: improved radii and binding
- Weak charge, neutron radius, and dipole polarizability in ^{48}Ca
  - predictions for soon-to-be measured quantities
  - charge radii in neutron-rich calcium isotopes not well understood
- EFT for nuclear vibrations
  - Quadrupole moments are of natural size (and sizeable) due to NLO corrections
  - anharmonic vibrations
- EFT for deformed nuclei
  - interband transitions correctly described due to new terms in operator

Outlook

We have fast cars (CCM, GFMC, IMSRG, MCSM, NCSM, UMOA, QMC) ...

but the roads have potholes

New interactions are being worked on ...