Effective field theories for nuclear deformations and vibrations

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Toward Predictive Theories of Nuclear Reactions Across the Isotopic Chart

SciDAC Scientific Discovery through Advanced Computing

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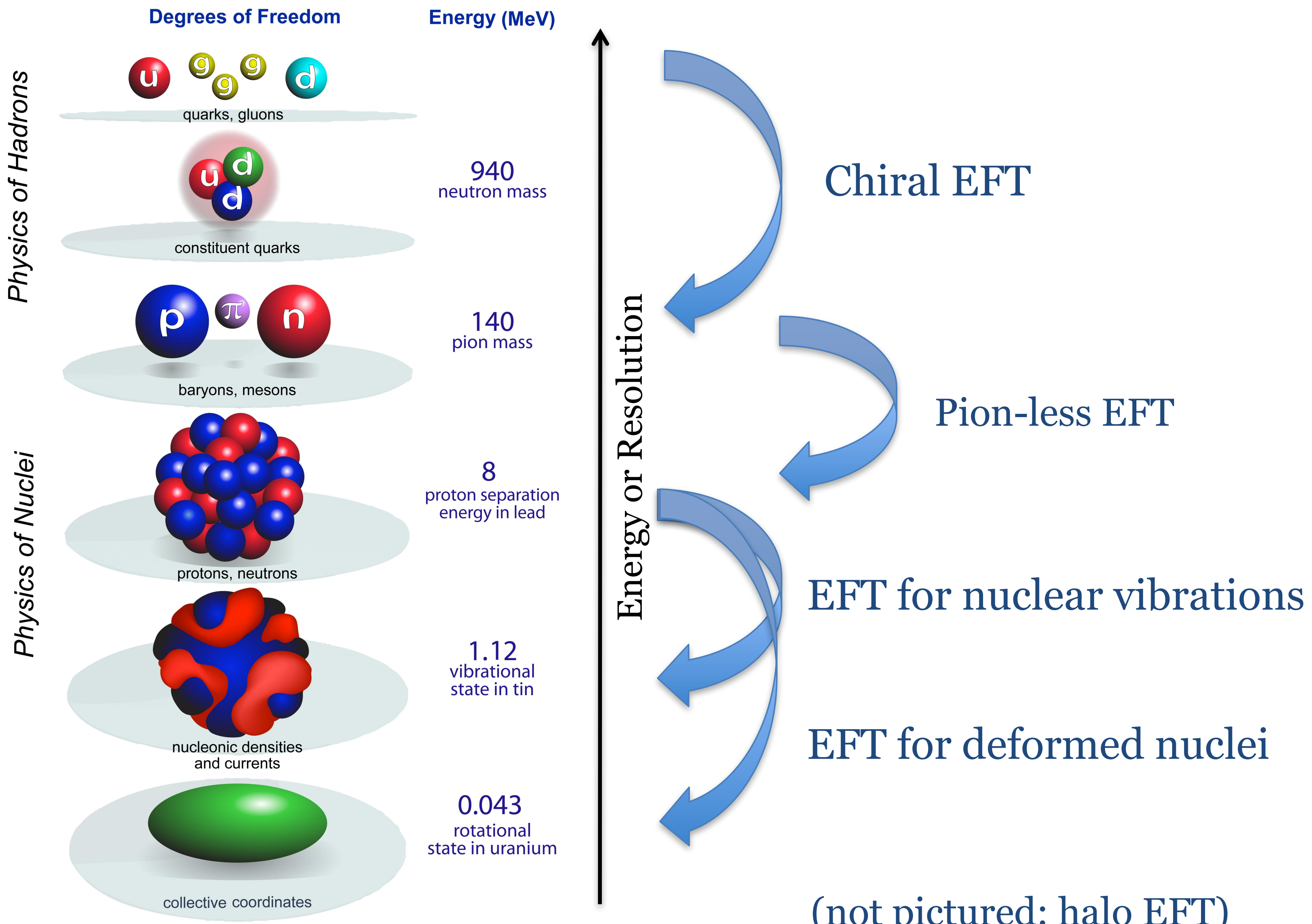
Menu

1. EFT for nuclear vibrations
2. EFT for deformed nuclei
3. Pion-less EFT for ^{16}O and ^{40}Ca
4. IR extrapolations for radiative capture

Energy scales and relevant degrees of freedom



Energy or Resolution

Chiral EFT

Pion-less EFT

EFT for nuclear vibrations

EFT for deformed nuclei

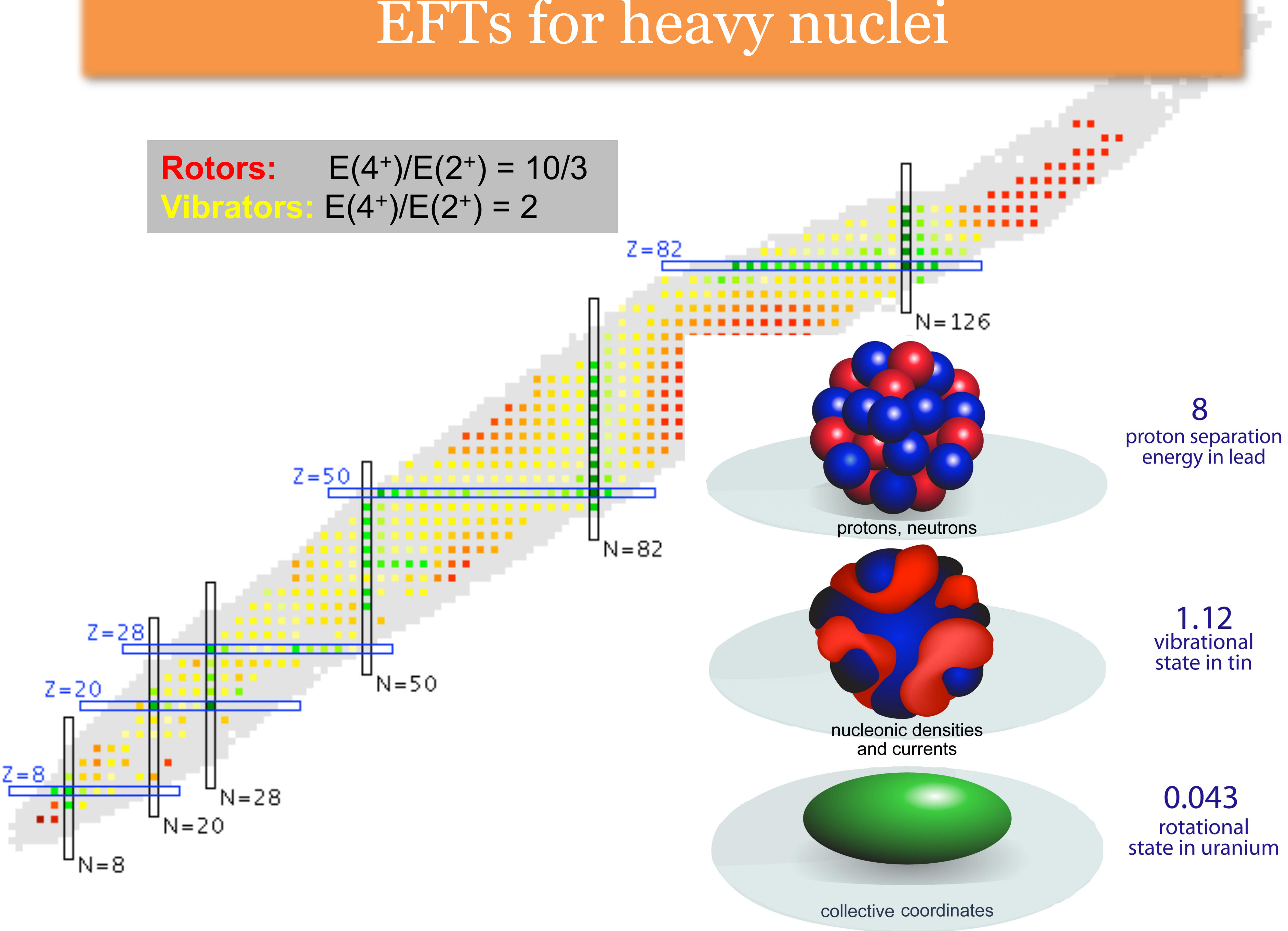
(not pictured: halo EFT)

Fig.: Bertsch, Dean, Nazarewicz (2007)

EFTs for heavy nuclei

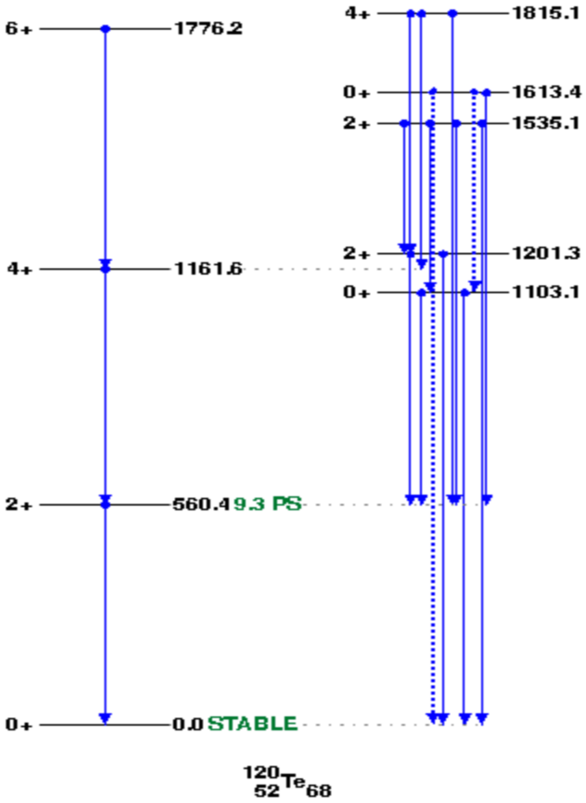
Rotors: $E(4^+)/E(2^+) = 10/3$

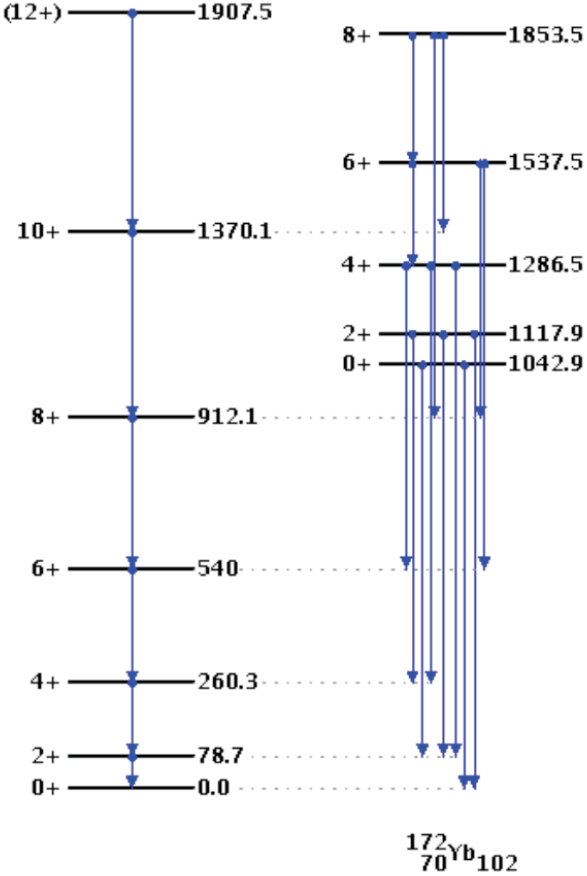
Vibrators: $E(4^+)/E(2^+) = 2$



Two paradigms: vibrations and rotations

Quadrupole degrees of freedom describe spins and parity of low-energy spectra

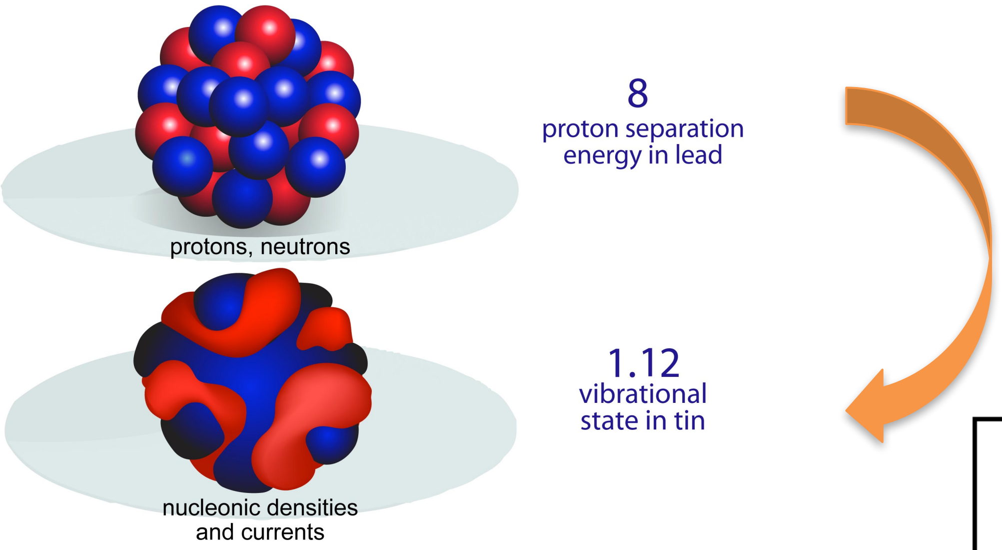




Nuclear vibration: EFT based on linear realization (Wigner / Weyl) of SO(3)

Nuclear rotation: emergent breaking of rotational symmetry of SO(3) → SO(2); EFT based on nonlinear realization (Nambu-Goldstone) of SO(3)

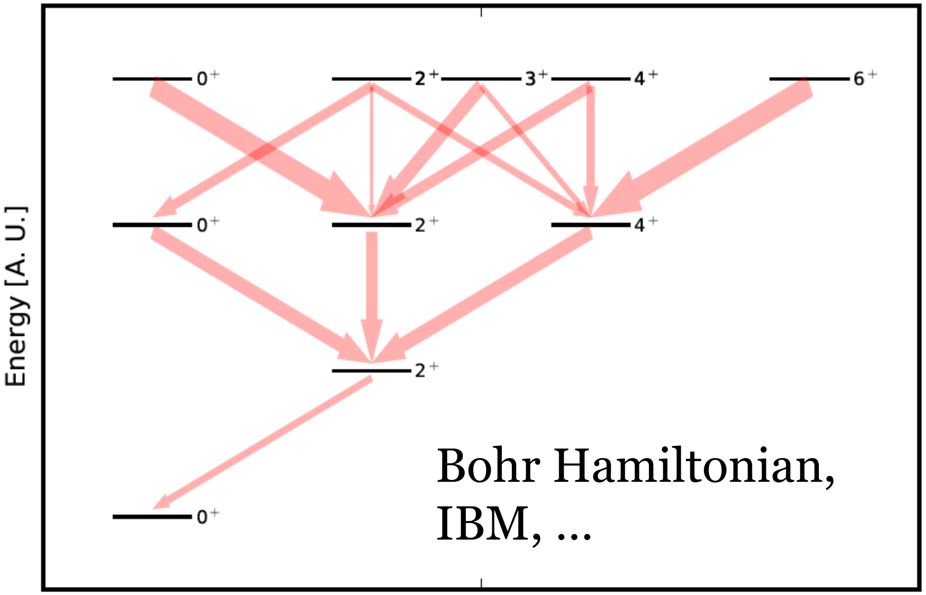
EFT for nuclear vibrations
→ Toño Coello's talk earlier in this program



EFT for nuclear vibrations
[Coello Pérez & TP 2015, 2016]

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

Garrett & Wood (2010): "Where are the quadrupole vibrations in atomic nuclei?"



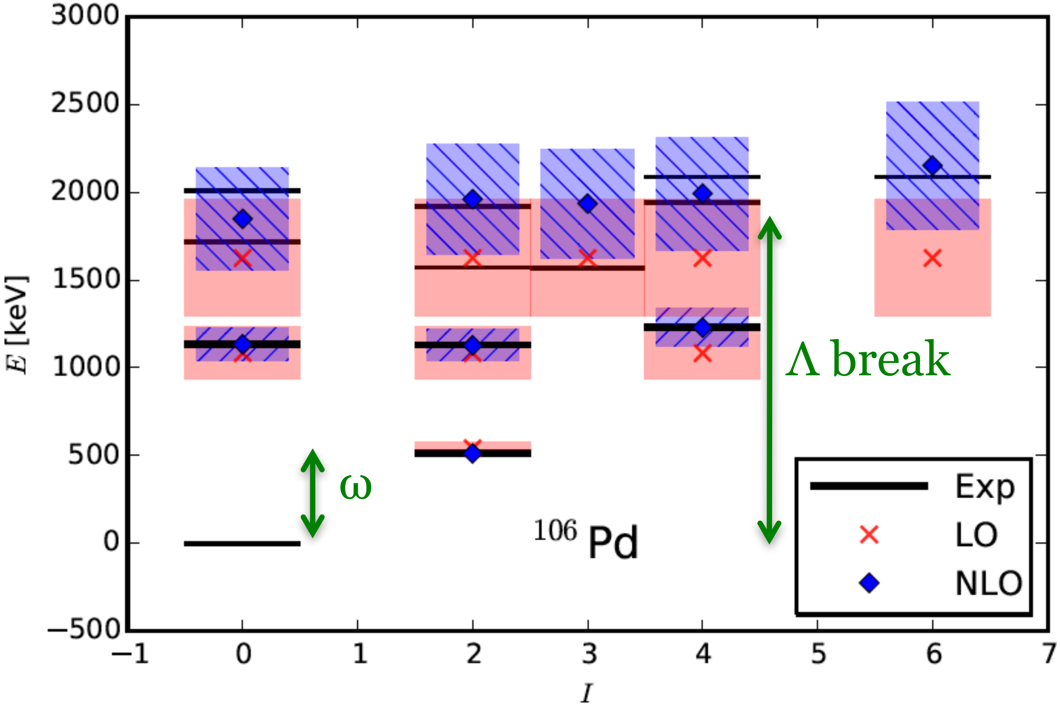
Bohr Hamiltonian,
IBM, …

Spectrum and B(E2) transitions of the *harmonic* quadrupole oscillator

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: $\omega/\Lambda \approx 1/3$



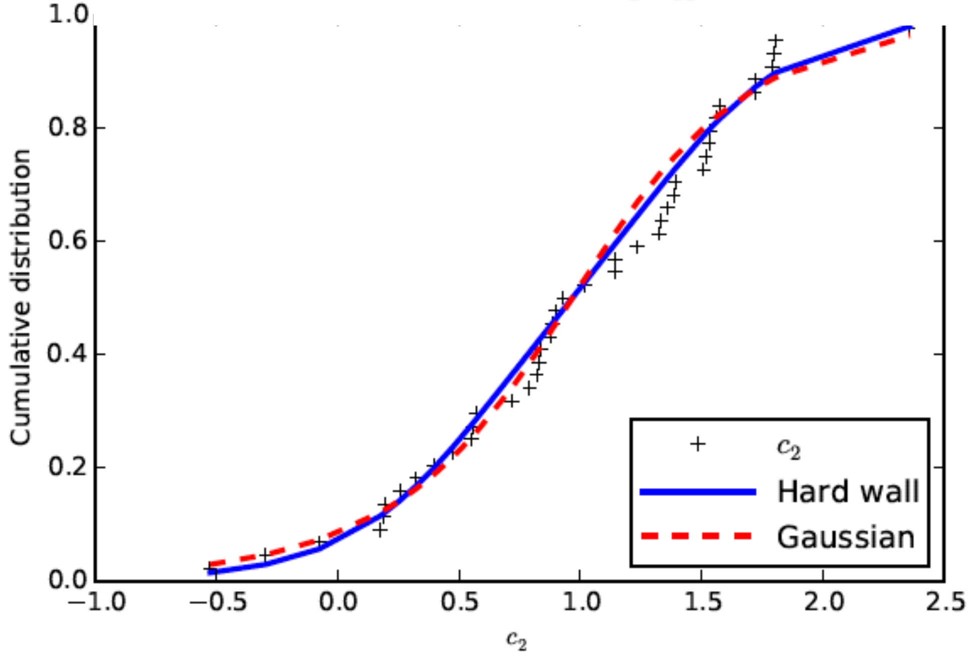
- Uncertainties show 68% DOB intervals from truncating higher EFT orders [Cacciari & Houdeau (2011); Bagnaschi et al (2015); Furnstahl, Klco, Phillips & Wesolowski (2015)]
  - Expand observables according to power counting
  - Employ "naturalness" assumptions as log-normal priors in Bayes' theorem
 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

Uncertainty quantification

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

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

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



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.

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

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

Hamiltonian

LO Hamiltonian $O(\omega)$

$$\hat{H}_{\mathrm{LO}} = \omega \hat{N}$$

NLO correction $O(\frac{\omega^3}{\Lambda^2})$

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

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 $\varepsilon \equiv (N\omega/\Lambda)$

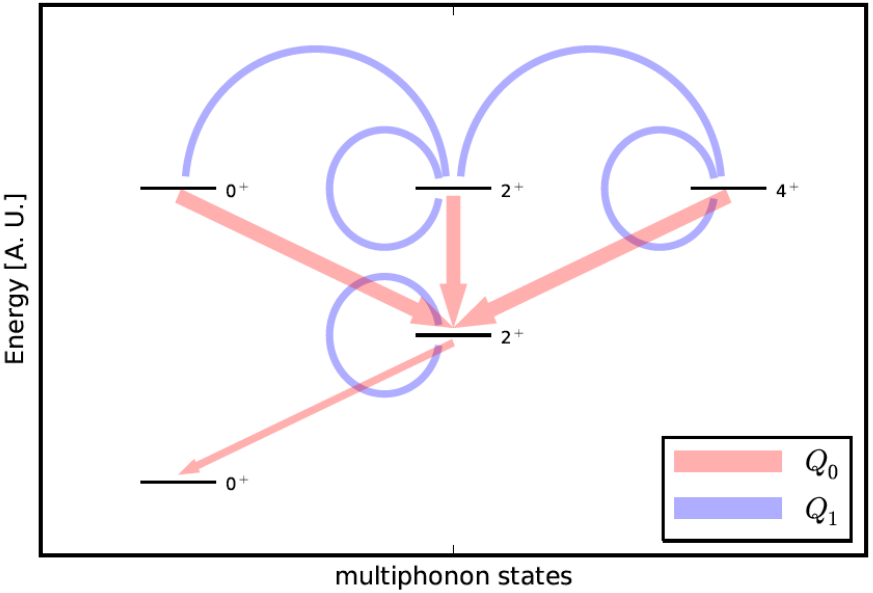
EFT result: sizeable quadrupole matrix elements are natural in size

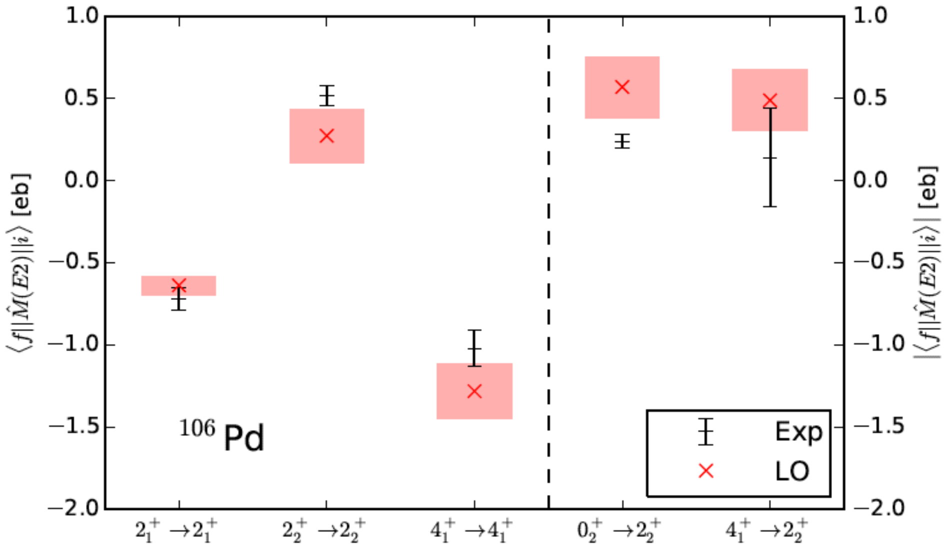
In the EFT, the quadrupole operator is also expanded:

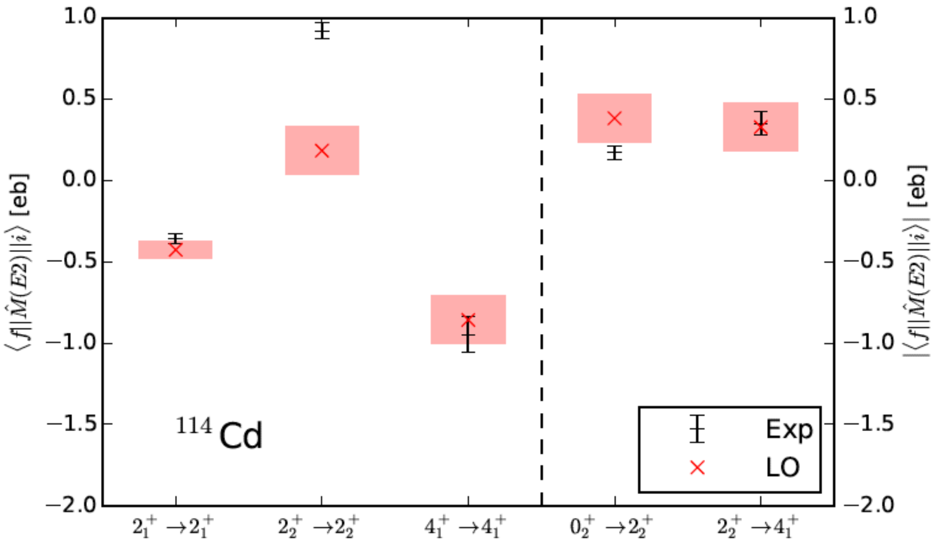
$$\hat{Q}_\mu = Q_0 \left(d^\dagger_\mu + \tilde{d}_\mu \right) + Q_1 \left(d^\dagger \times d^\dagger + \tilde{d} \times \tilde{d} + 2 d^\dagger \times \tilde{d} \right)^{(2)}_\mu$$

Subleading corrections are sizable:

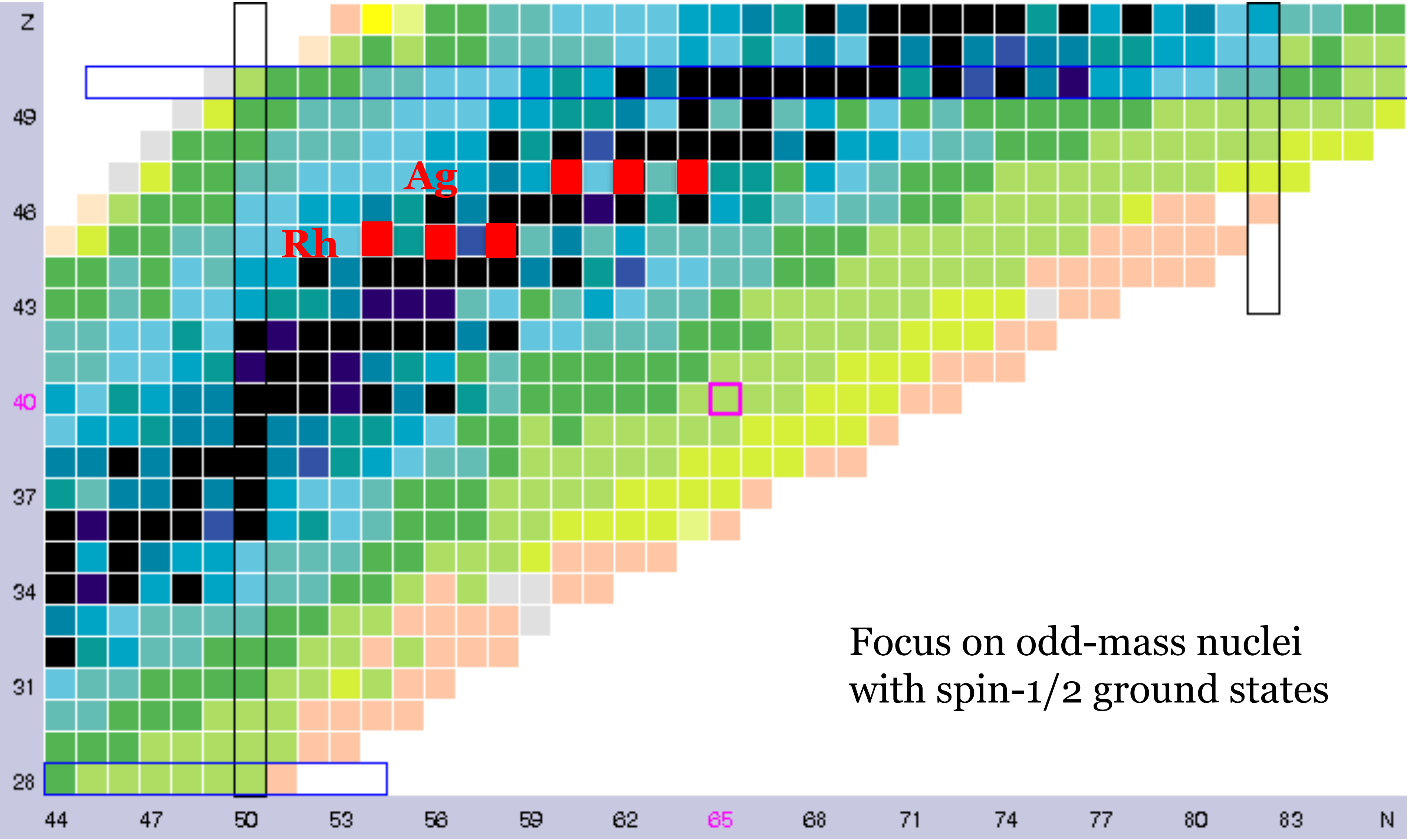
$$Q_1 \sim \left(\frac{\omega}{\Lambda} \right)^{1/2} Q_0$$







Rhodium as a proton coupled to ruthenium
Silver as a proton (hole) coupled to palladium (cadmium)

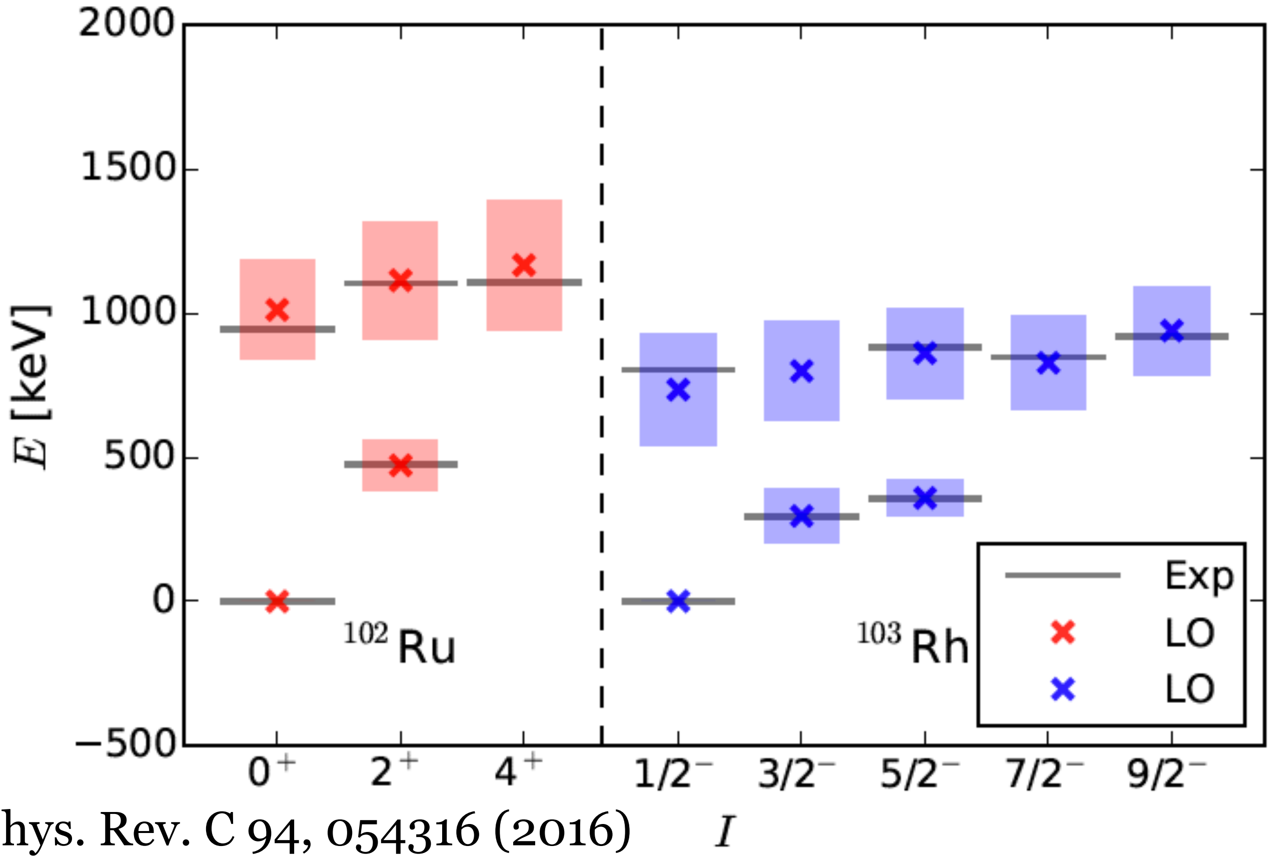


Focus on odd-mass nuclei with spin-1/2 ground states

Fermion coupled to vibrating nucleus

Approach follows halo EFT [Bertulani, Hammer, van Kolck (2002); Higa, Hammer, van Kolck (2008); Hammer & Phillips (2011); Ryberg et al. (2014)], and particle-vibrator models [de Shalit (1961); Iachello & Scholten (1981); Vervier (1982);…]

Two new LECs enter at lowest interesting order



E. A. Coello Pérez & TP, Phys. Rev. C 94, 054316 (2016)

Coupling a spin ½ fermion to vibrations

Number operator $\hat{n} \equiv a^\dagger \cdot \tilde{a}$

Spin $\hat{\mathbf{j}} = \frac{1}{\sqrt{2}}(a^\dagger \otimes \tilde{a})^{(1)}$

Hamiltonian

$$H = H_{\mathrm{b}} + H_{\mathrm{f}} + H_{\mathrm{b\text{-}f}}$$

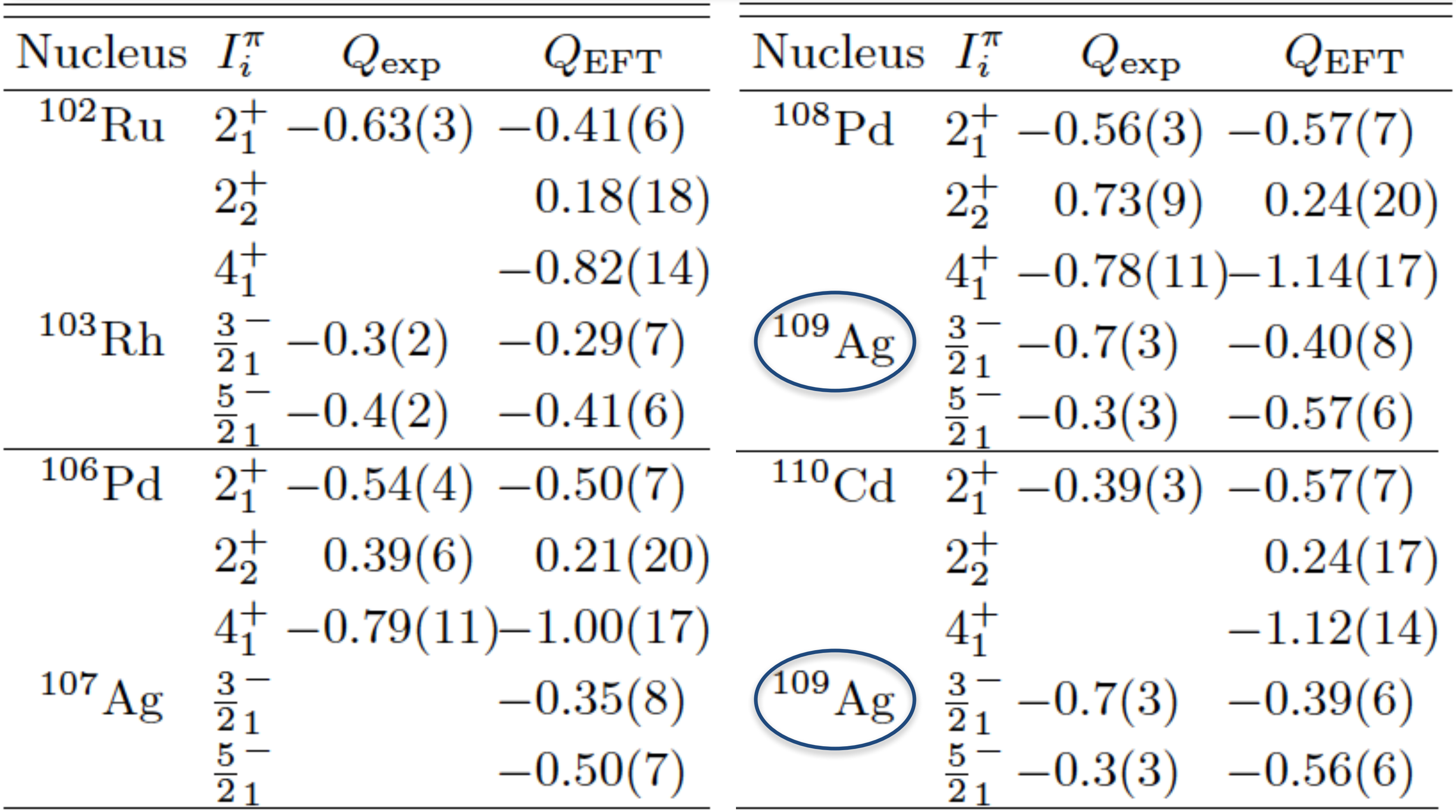
$$\hat{H}_{\mathrm{f}} = -S\hat{n} - \Delta\hat{n}(\hat{n} - 1)$$

$$H_{\mathrm{b\text{-}f}} = g_{Jj}\hat{\mathbf{J}} \cdot \hat{\mathbf{j}} + \omega_2\hat{N}\hat{n} + \omega_3\hat{N}\hat{n}(\hat{n} - 1)$$

Coupling to vibrator (based on empirically small splittings)

$$H_{\mathrm{NLO}} \equiv g_{Jj}\hat{\mathbf{J}} \cdot \hat{\mathbf{j}} + \omega_2\hat{N}\hat{n}$$

Static E2 moments (in eb)



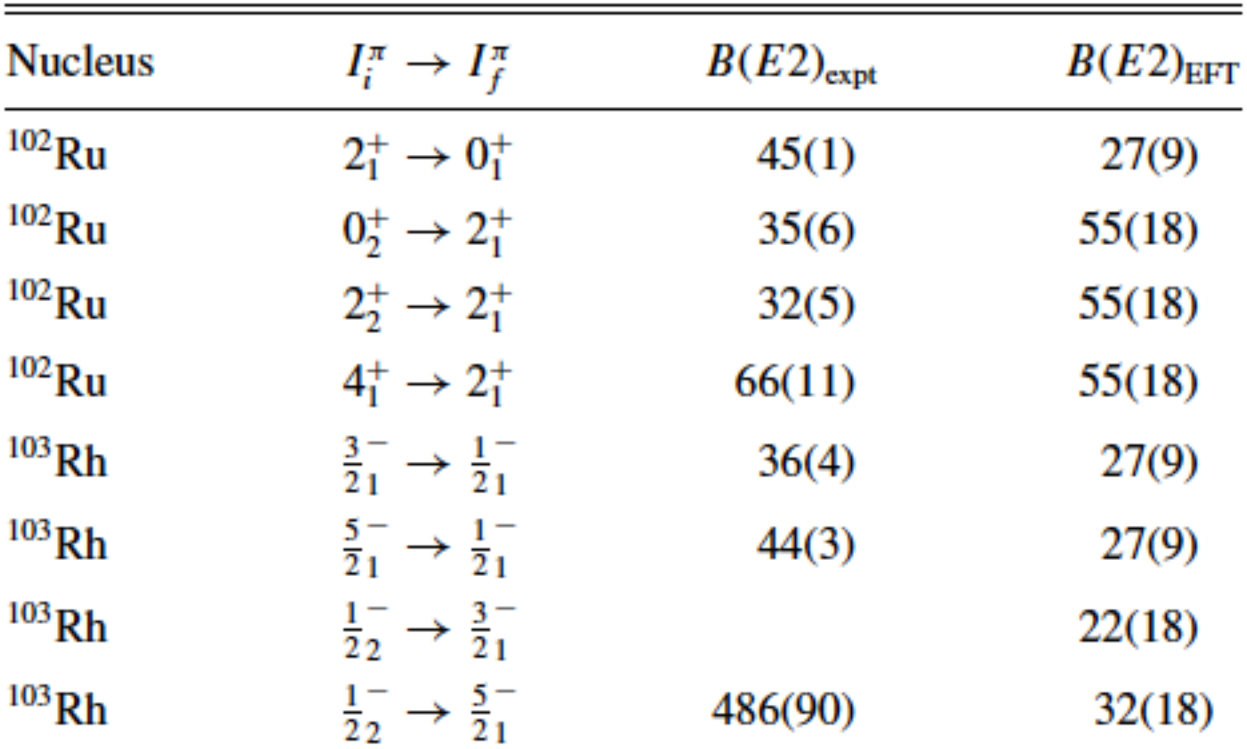
Nucleus	I_i^π	$Q_{\rm exp}$	$Q_{\rm EFT}$	Nucleus	I_i^π	$Q_{\rm exp}$	$Q_{\rm EFT}$
^{102}Ru	2_1^+	$-0.63(3)$	$-0.41(6)$	^{108}Pd	2_1^+	$-0.56(3)$	$-0.57(7)$
	2_2^+		$0.18(18)$		2_2^+	$0.73(9)$	$0.24(20)$
	4_1^+		$-0.82(14)$		4_1^+	$-0.78(11)$	$-1.14(17)$
^{103}Rh	$\frac{3}{2}{}_1^-$	$-0.3(2)$	$-0.29(7)$	^{109}Ag	$\frac{3}{2}{}_1^-$	$-0.7(3)$	$-0.40(8)$
	$\frac{5}{2}{}_1^-$	$-0.4(2)$	$-0.41(6)$		$\frac{5}{2}{}_1^-$	$-0.3(3)$	$-0.57(6)$
^{106}Pd	2_1^+	$-0.54(4)$	$-0.50(7)$	^{110}Cd	2_1^+	$-0.39(3)$	$-0.57(7)$
	2_2^+	$0.39(6)$	$0.21(20)$		2_2^+		$0.24(17)$
	4_1^+	$-0.79(11)$	$-1.00(17)$		4_1^+		$-1.12(14)$
^{107}Ag	$\frac{3}{2}{}_1^-$		$-0.35(8)$	^{109}Ag	$\frac{3}{2}{}_1^-$	$-0.7(3)$	$-0.39(6)$
	$\frac{5}{2}{}_1^-$		$-0.50(7)$		$\frac{5}{2}{}_1^-$	$-0.3(3)$	$-0.56(6)$

Single LEC Q_1 fit to all data with EFT weighting.

$$\hat{Q}_\mu = Q_0(d_\mu^\dagger + \tilde{d}_\mu) + Q_1(d^\dagger \otimes \tilde{d})_\mu^{(2)}$$

E. A. Coello Pérez & TP, Phys. Rev. C 94, 054316 (2016)

E2 transition strengths

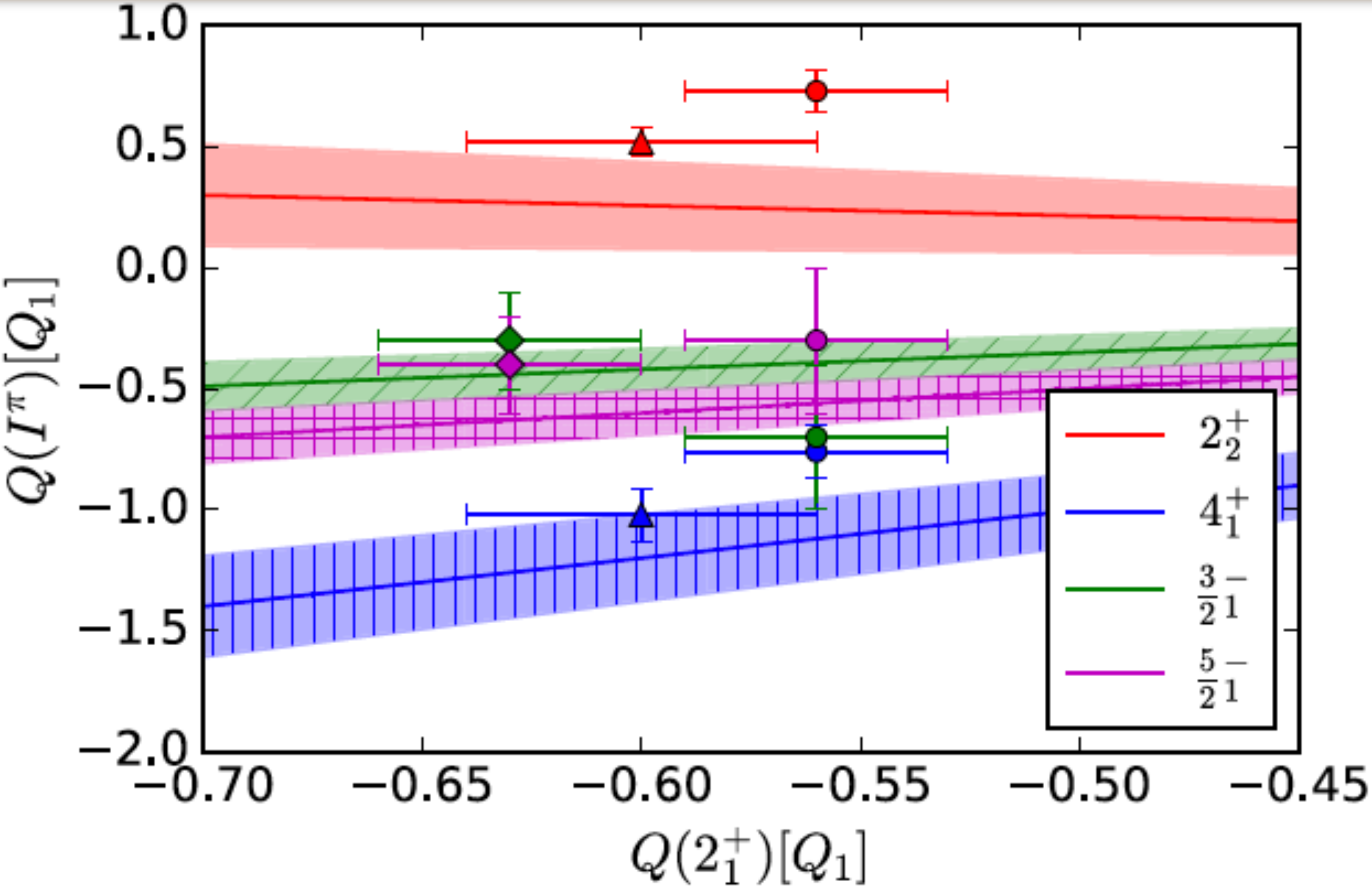


Nucleus	$I_i^\pi \to I_f^\pi$	$B(E2)_{\text{expt}}$	$B(E2)_{\text{EFT}}$
^{102}Ru	$2_1^+ \to 0_1^+$	45(1)	27(9)
^{102}Ru	$0_2^+ \to 2_1^+$	35(6)	55(18)
^{102}Ru	$2_2^+ \to 2_1^+$	32(5)	55(18)
^{102}Ru	$4_1^+ \to 2_1^+$	66(11)	55(18)
^{103}Rh	$\frac{3}{2}{}_1^- \to \frac{1}{2}{}_1^-$	36(4)	27(9)
^{103}Rh	$\frac{5}{2}{}_1^- \to \frac{1}{2}{}_1^-$	44(3)	27(9)
^{103}Rh	$\frac{1}{2}{}_2^- \to \frac{3}{2}{}_1^-$		22(18)
^{103}Rh	$\frac{1}{2}{}_2^- \to \frac{5}{2}{}_1^-$	486(90)	32(18)

Results in Weisskopf units. A single LEC Q_o enters.

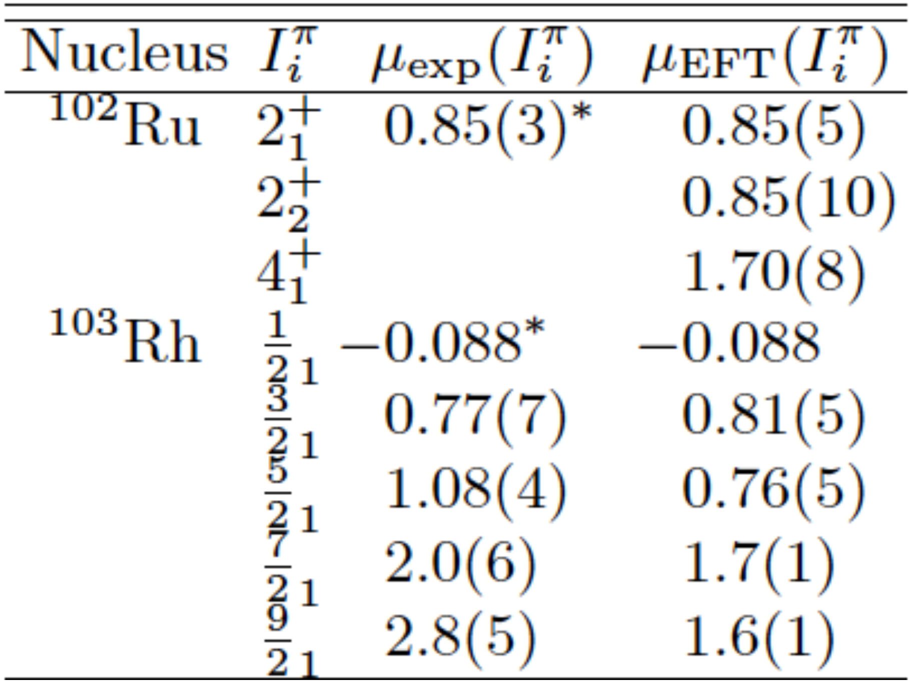
E. A. Coello Pérez & TP, Phys. Rev. C 94, 054316 (2016)

Correlations between static quadrupole moments

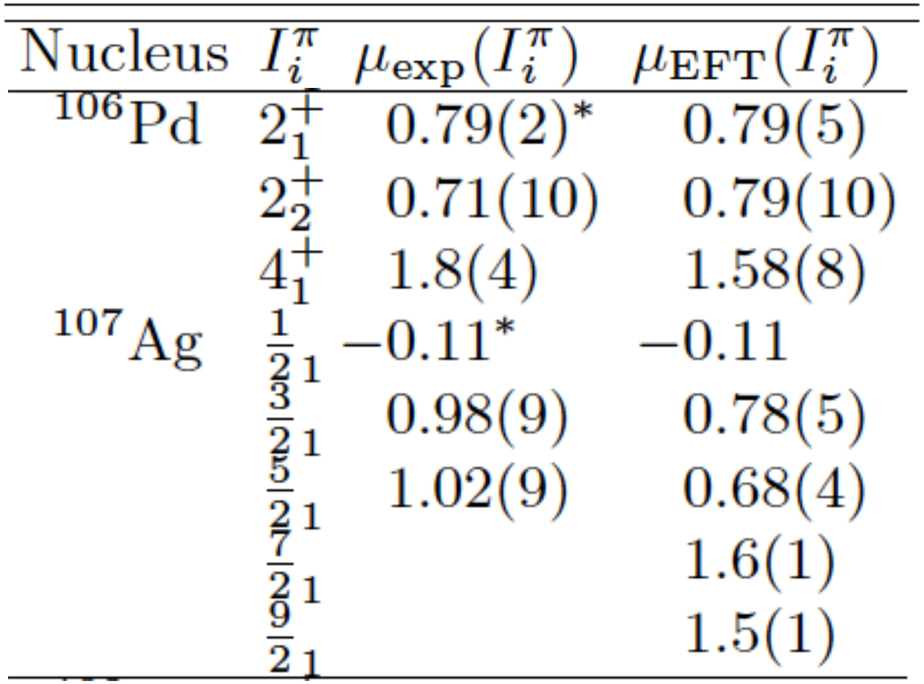


Data for the ^{102}Ru /^{103}Rh, ^{106}Pd /^{107}Ag, and ^{108}Pd /^{109}Ag systems are shown as diamonds, triangles, and circles, respectively.

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(5)
	2_2^+		0.85(10)
	4_1^+		1.70(8)
^{103}Rh	$\frac{1}{2}_1$	−0.088*	−0.088
	$\frac{3}{2}_1$	0.77(7)	0.81(5)
	$\frac{5}{2}_1$	1.08(4)	0.76(5)
	$\frac{7}{2}_1$	2.0(6)	1.7(1)
	$\frac{9}{2}_1$	2.8(5)	1.6(1)



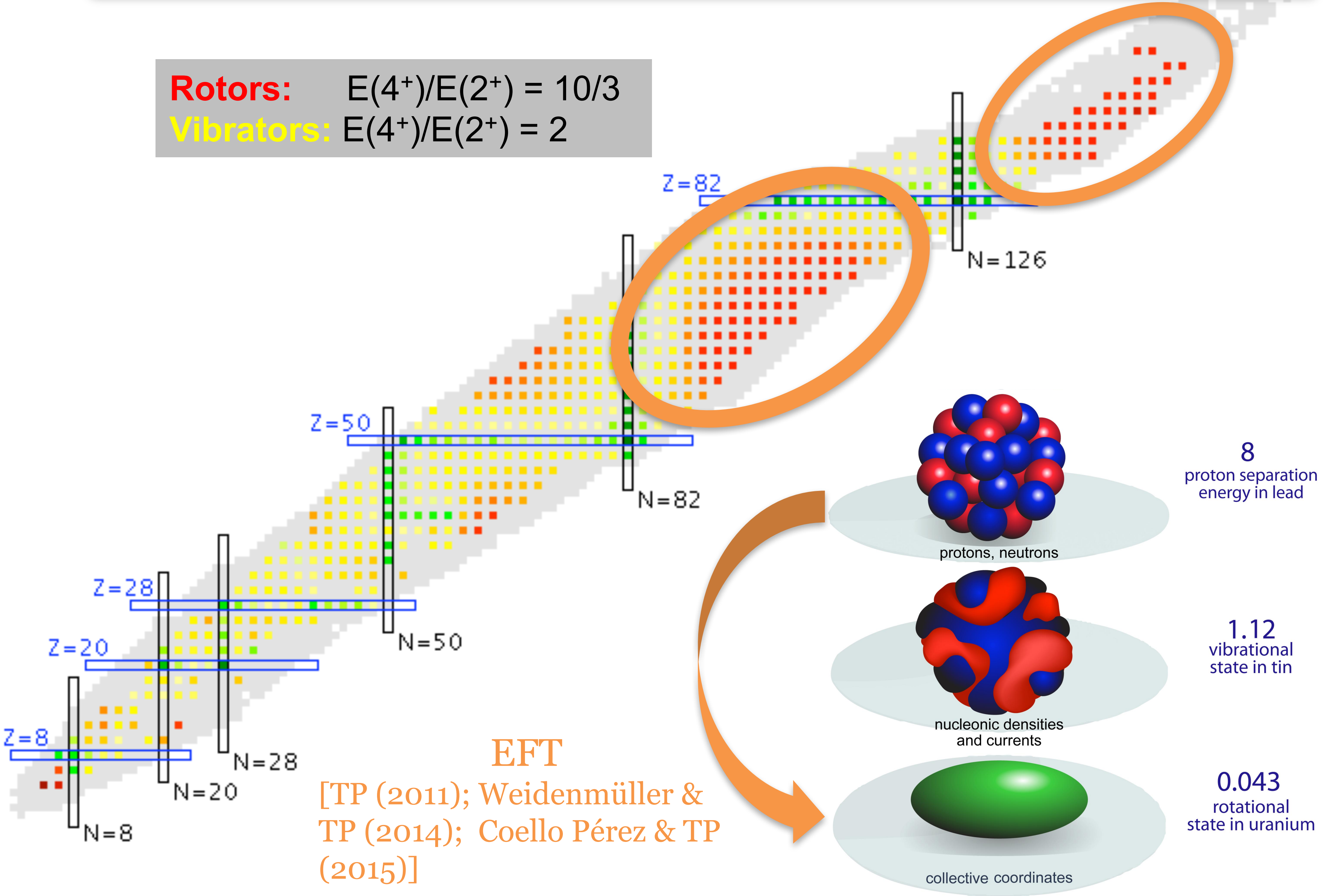
Nucleus	I_i^π	$\mu_{\rm exp}(I_i^\pi)$	$\mu_{\rm EFT}(I_i^\pi)$
^{106}Pd	2_1^+	0.79(2)*	0.79(5)
	2_2^+	0.71(10)	0.79(10)
	4_1^+	1.8(4)	1.58(8)
^{107}Ag	$\frac{1}{2}_1$	−0.11*	−0.11
	$\frac{3}{2}_1$	0.98(9)	0.78(5)
	$\frac{5}{2}_1$	1.02(9)	0.68(4)
	$\frac{7}{2}_1$		1.6(1)
	$\frac{9}{2}_1$		1.5(1)

Results in nuclear magnetons.
At LO, one new LEC enters to describe the magnetic moments in the odd-mass neighbor $\hat{\mu}_\mu = \mu_d \hat{\mathbf{J}}_\mu + \mu_a \hat{\mathbf{j}}_\mu$

E. A. Coello Pérez & TP, Phys. Rev. C 94, 054316 (2016)

EFT for deformed nuclei: rotations

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

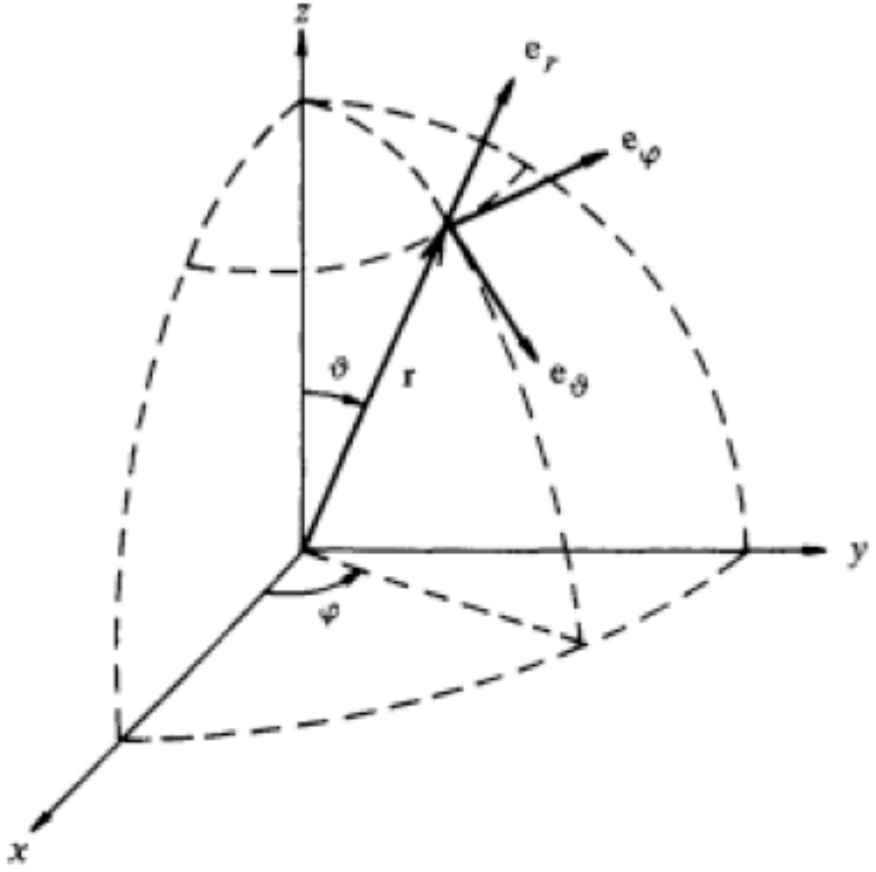


EFT
[TP (2011); Weidenmüller & TP (2014); Coello Pérez & TP (2015)]

Nonlinear realization of rotational symmetry

[follows Weinberg 1967; Coleman, Callan, Wess & Zumino 1969]

Spontaneous breaking of rotational symmetry: Nambu-Goldstone modes parameterize the coset SO(3)/SO(2) ~ S^2, i.e. the two sphere



$$\vec{n}(\theta,\phi) = \begin{pmatrix} \cos\phi\sin\theta \\ \sin\phi\sin\theta \\ \cos\theta \end{pmatrix}$$

Comments:

- Further degrees of freedom in the tangential plane can be added to the tangential plane
- Addition of monopole field yields nuclei with nonzero ground-state spins

[TP & Weidenmüller; Phys. Scr. 91 (2016) 053004]

Emergent symmetry breaking

Finite system cannot exhibit spontaneous symmetry breaking

Instead: Emergent symmetry breaking [Yannouleas & Landman 2007]

Infinite system: Hilbert spaces with different orientations (of the nucleus) are inequivalent. No rotation, i.e. no unitary transformation can connect states in inequivalent Hilbert spaces

Finite system: Hilbert spaces with different orientations are connected by a rotation: Zero mode, i.e. purely time-dependent "Nambu-Goldstone field" has to be added; amplitudes of this mode can be large.

Low-lying modes in finite systems: [Gasser & Leutwyler 1988; Hasenfratz & Niedermayer 1993]

Field theory of (anti)ferromagnet as example of SO(3)→SO(2): [Leutwyler 1987; Roman & Soto 1999; Hofmann 1999; Bär, Imboden & Wiese 2004; Kämpfer, Moser & Wiese 2005]

EFT for deformed nuclei

Spectrum of ground-state band

$$E(I) = \frac{I(I+1)}{2C_0} - \frac{C_2}{4C_0^4}[I(I+1)]^2$$

Strength of quadrupole transitions $I_i \rightarrow I_i - 2$ in ground-state band
(Clebsch-Gordan coefficient divided out)

$$Q_{if}^2 = Q_0^2\left[1 + \frac{b}{a} I_i(I_i - 1)\right]$$

At leading order: EFT reproduces well known results from phenomenological models (e.g. Variable Moment of Inertia, Mikhailov theory…)
EFT provides us with insight in scale of parameters in expansion of observables

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

EFT: expansion parameter & naturalness

Natural sizes as expected!

		Expansion parameter: E_{rot} / E_{vib}	Natural LECs: spectrum	Natural LECs: transitions
	System	$(\xi/\omega)^2$	C_2/C_0^3	b/a
Molecules	N_2	0.000 026	0.000 006	-0.000 011
	H_2	0.0062	0.0015	0.0022
Rotational nuclei	^{236}U	0.0043	0.0011	—
	^{174}Yb	0.0026	0.0010	—
	^{168}Er	0.0094	0.0010	—
	^{166}Er	0.011	0.0020	—
	^{162}Dy	0.0083	0.0017	—
	^{154}Sm	0.0056	0.0033	—
Transitional nuclei	^{188}Os	0.06	0.012	0.008
	^{154}Gd	0.033	0.013	0.006
	^{152}Sm	0.032	0.013	0.003
	^{150}Nd	0.037	0.017	0.011

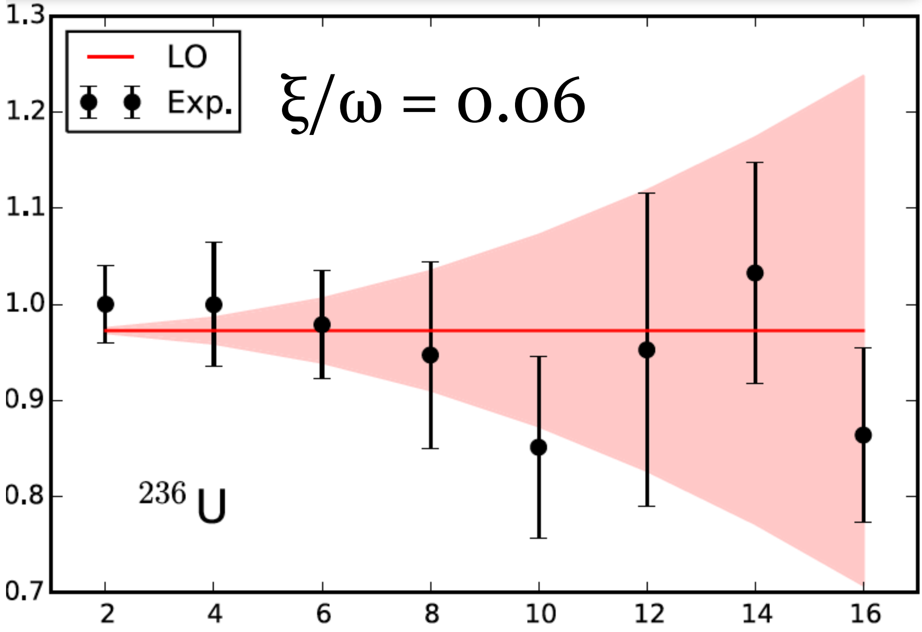
less rigid rotor

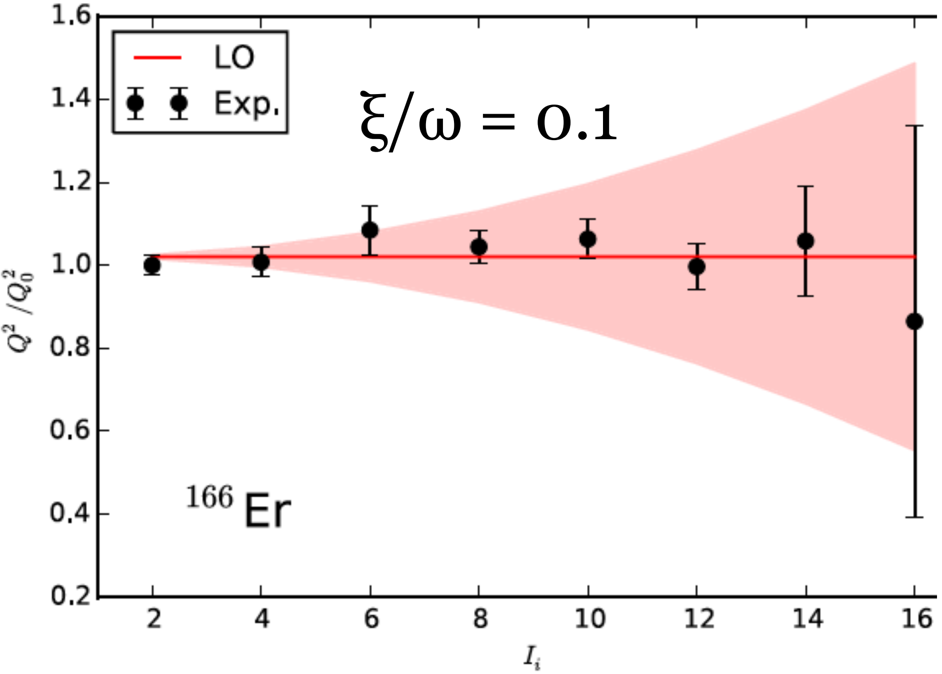
E. A. Coello Pérez and TP, Phys. Rev. C 92, 014323 (2015)

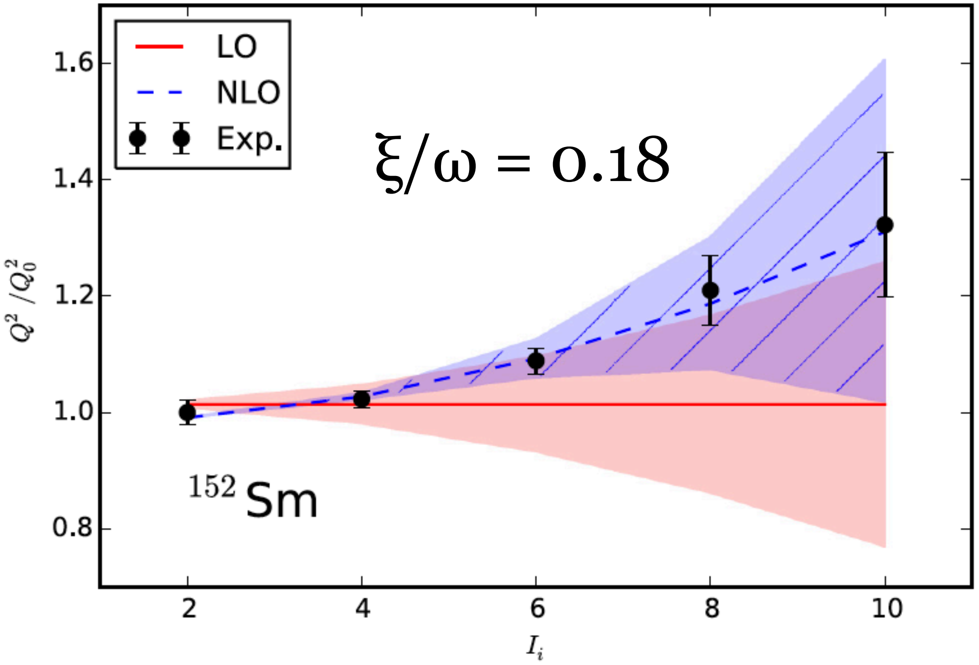
EFT works well for a wide range of rotors

Bohr & Mottelson (1975):

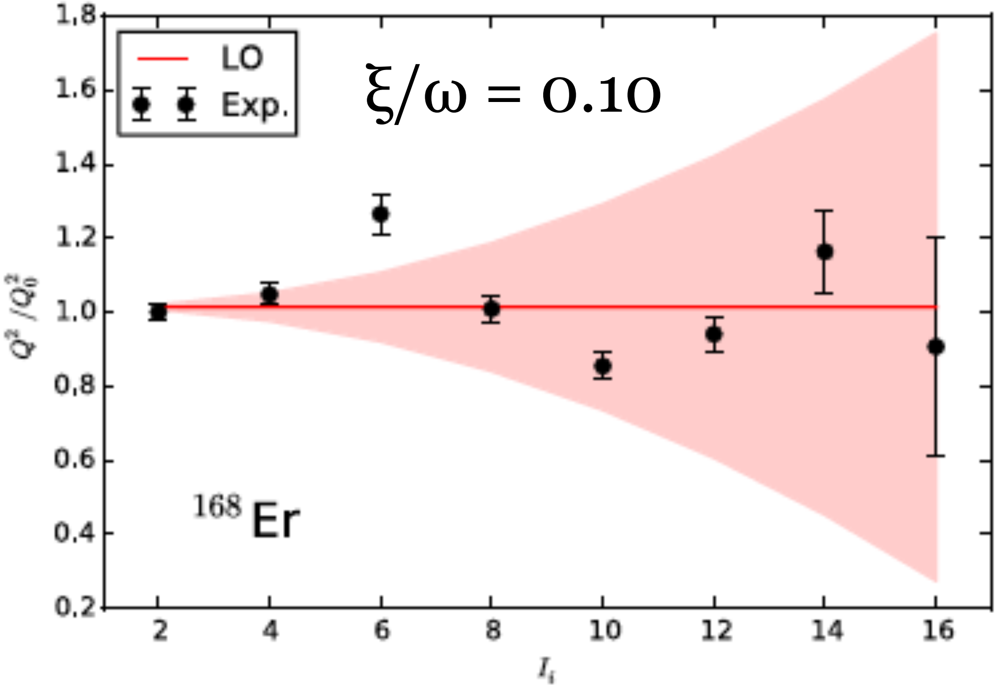
> “The accuracy of the present measurements of E2-matrix elements in the ground-state bands of even even nuclei is in most cases barely sufficient to detect deviations from the leading-order intensity relations.”







Unexpected oscillatory patterns in supposedly “good” rotors ^{168}Er, ^{174}Yb

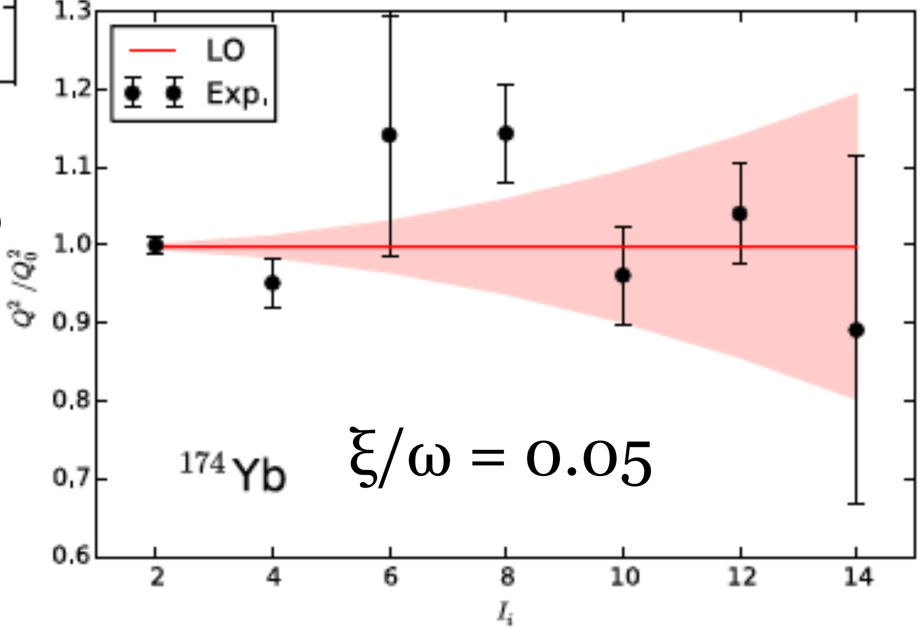


Based on results for molecules, well-deformed nuclei, and transitional nuclei, EFT suggests that a few transitions in text-book rotors could merit re-measurement.

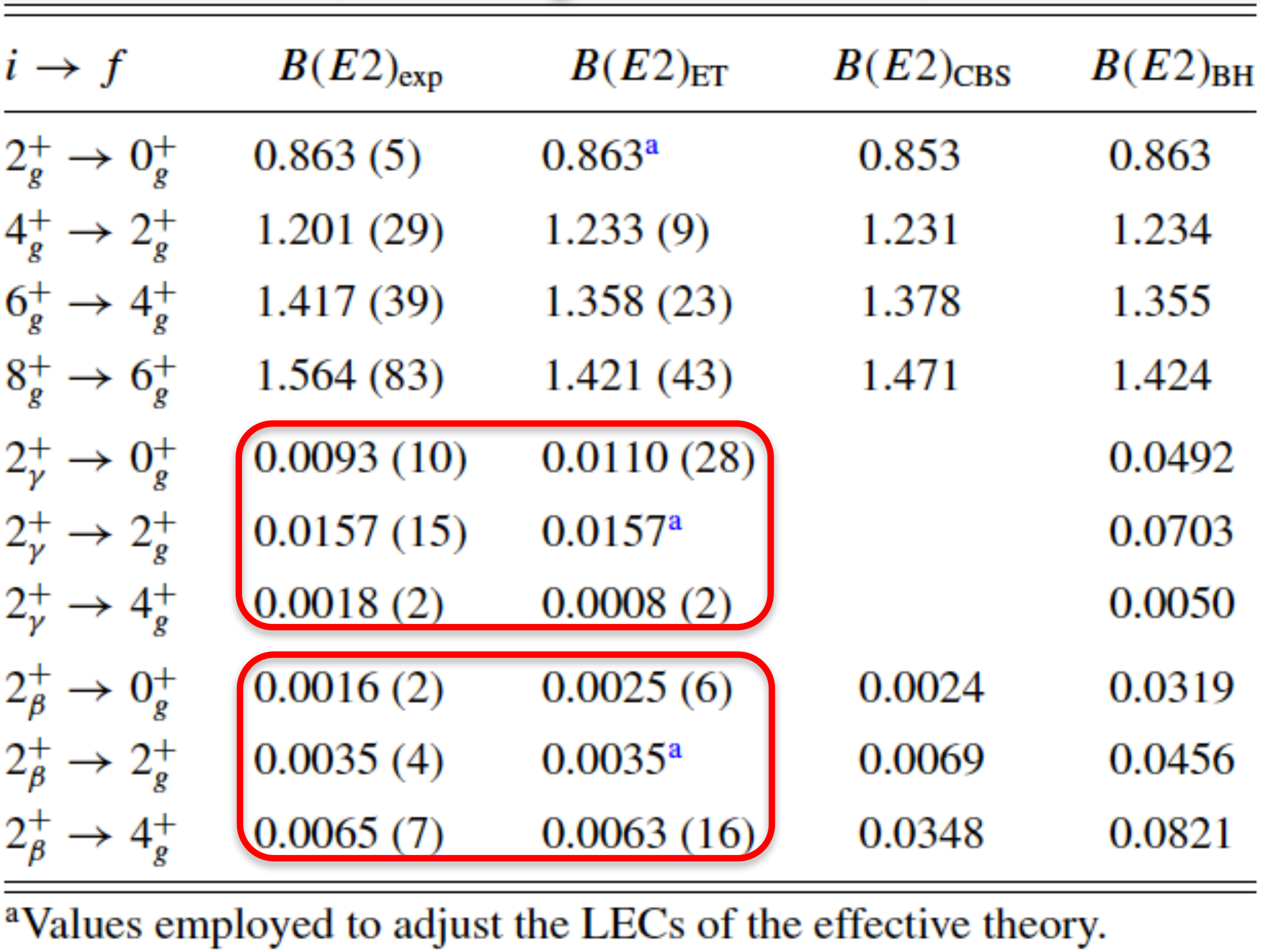
^{168}Er: B(E2) for $6^+ \rightarrow 4^+$ very difficult to understand.

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

Theoretical uncertainty estimates relevant.



Challenge: weak interband transitions (example: ^{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^{2}b^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)]

EFT in harmonic oscillator basis

Motivation: optimize and generate interactions in basis of computation

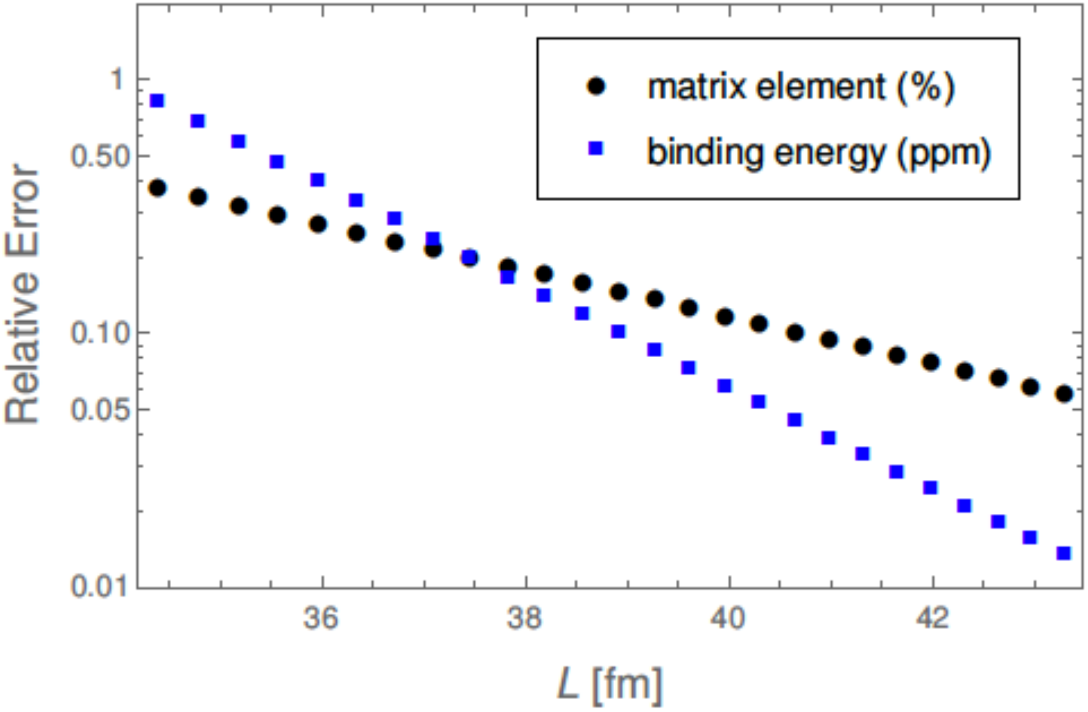
- A finite harmonic oscillator basis exhibits IR and UV cutoffs; indistinguishable from a spherical cavity at low momenta; Lüscher-like extrapolation formulas for many observables [Stetcu, Barrett & van Kolck (2007); Coon *et al.* (2012); Furnstahl, Hagen & TP (2012); …]
- Computation of scattering phase shifts directly in the oscillator basis [Heller & Yamani (1974); Bang et al. (2000); Shirokov et al. (2004)]
- Formulate EFT directly in the oscillator basis [Haxton & Song (2000); Stetcu, Barrett & van Kolck (2007); Tölle, Hammer & Metsch (2011)]
- Discrete momentum eigenstates from diagonalization of p^2 for DVR in oscillator basis [Binder *et al.*, PRC 93, 044332 (2016)]

Extrapolations in finite Hilbert spaces

Radiative capture:

- from continuum to bound state
- Convergence depends on bound-state momentum and is slower than energy convergence

$$\Delta\mathcal{I}_\lambda(k;\eta;L) = \frac{2A_\infty\gamma_\infty}{\gamma_\infty^2+k^2}L^\lambda e^{-\gamma_\infty L}\sin\left(\delta_l+\sigma_l-\frac{\pi l}{2}+kL-\eta\log 2kL\right)$$



Corrections to capture cross sections ~ 1%, even when integrating out to 30 fm.

[Girlanda *et al.* PRL 2010]

Acharya *et al*, arXiv:1608.04699

→ Phys. Rev. C **95**, 031301 (2017)

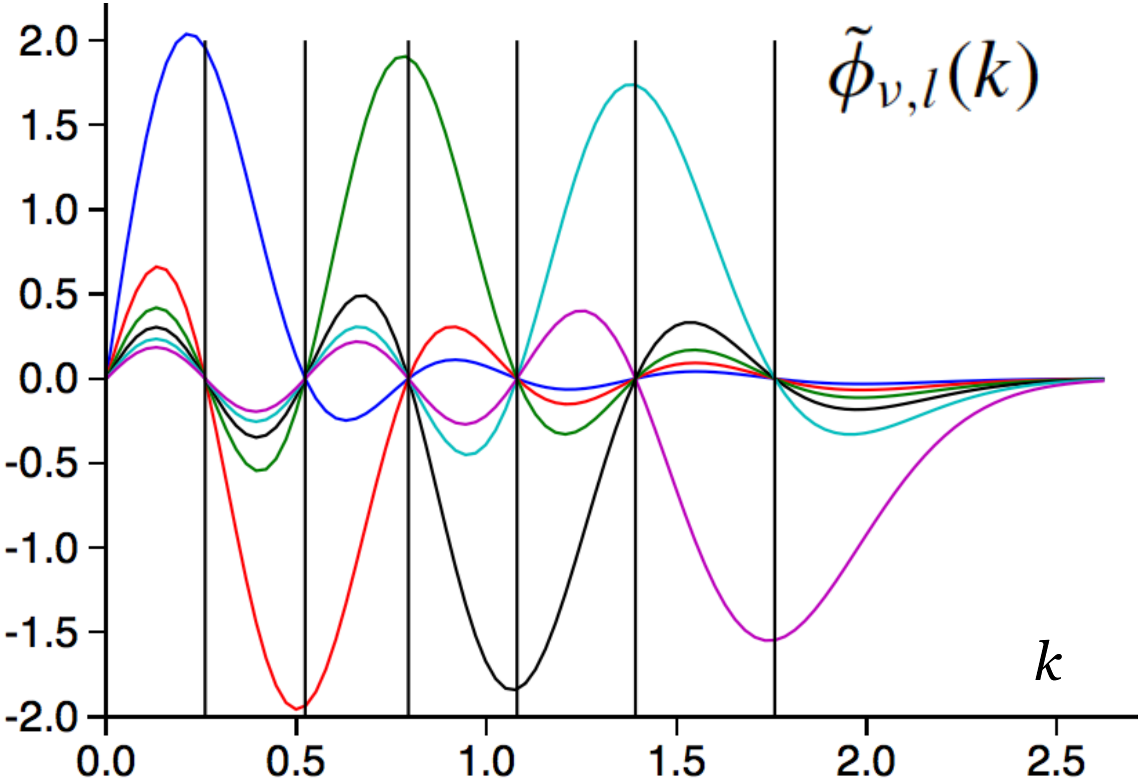
Eigenfunctions and eigenvalues of p^2

For a partial wave l in a Hilbert space with energies up to $(2N+l)\hbar\boldsymbol{\omega}$, the eigenvalues $k_{\mu l}^2$ of p^2 are the roots of the associated Laguerre polynomial $L_{N+1}^{l+1/2}$.

The eigenfunctions of p^2 are a DVR (discrete variable representation).

DVRs see: [Harris, Engerholm, & Gwinn (1965); Light, Hamilton, & Lill (1985); Baye & Heenen (1986); Littlejohn *et al*. (2002); Bulgac & McNeil Forbes (2013).]

Eigenfunctions of p^2 for $l=0$, $N=10$, and $\hbar\boldsymbol{\omega} = 10$ MeV. Vertical lines are eigenvalues $k_{\mu l}$.



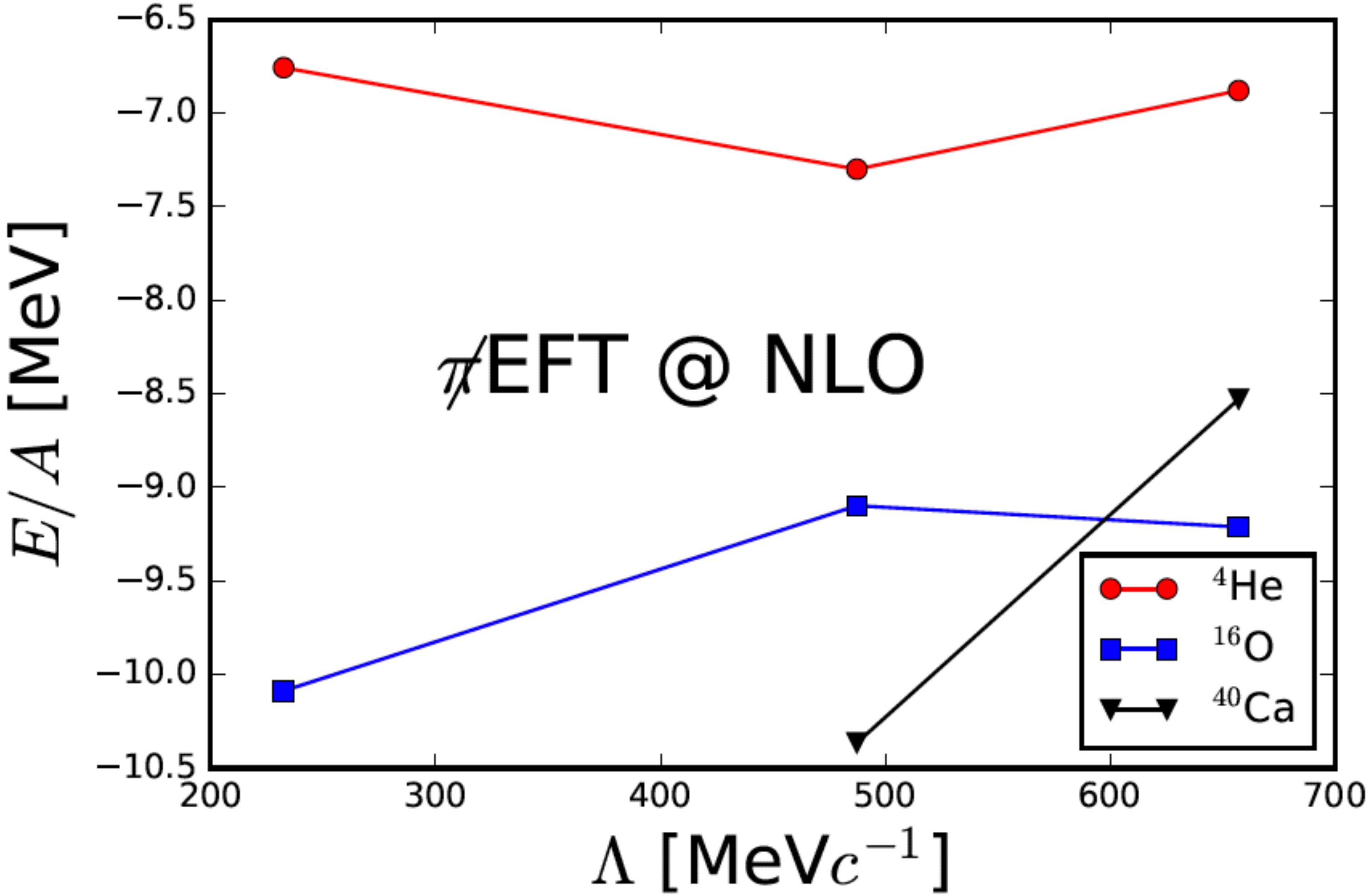
Pionless EFT for A>4

- A>4 nuclei explored only very recently [Kirscher *et al*. 2010; Lensky, Birse & Walet 2016; Contessi *et al*. 2017]
- Used as tool to compute finite nuclei from lattice QCD input (at unphysical pion masses, though)
- At LO, ^{16}O is not bound with respect to decay into four α particles [Contessi *et al*. 2017]

Here:

- Nonperturbative NLO
- Interaction as IR improved DVR in N=8 shells
- Increase kinetic energy until convergence is reached
- Compute ^{4}He, ^{16}O, and ^{40}Ca

Preliminary results



Bansal, Binder, Ekström, Hagen, and TP (in preparation)

Summary

- EFT for nuclear vibrations
    - Anharmonic vibrations consistent with data within uncertainties
    - Sizable quadrupole moments and transitions where models yield null result
    - Predictions for M1 and E2 moments and transitions
- EFT for deformed nuclei
    - LO recovers Bohr Hamiltonian
    - EFT explains weak interband transitions
- IR extrapolations
    - Lüscher-like formulas for energies, radii, quadrupole moments, transitions, radiative capture reactions
- Pion-less EFT
    - Bound ^{16}O, ^{40}Ca in nonperturbative NLO for cutoffs $200 < \Lambda < 700$ MeV