From EFTs to Nuclei

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and

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SciDAC
Scientific Discovery through Advanced Computing

INT Program
Nuclear Physics from Lattice QCD
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NUCLEI
Nuclear Computational Low-Energy Initiative

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Energy scales and relevant degrees of freedom

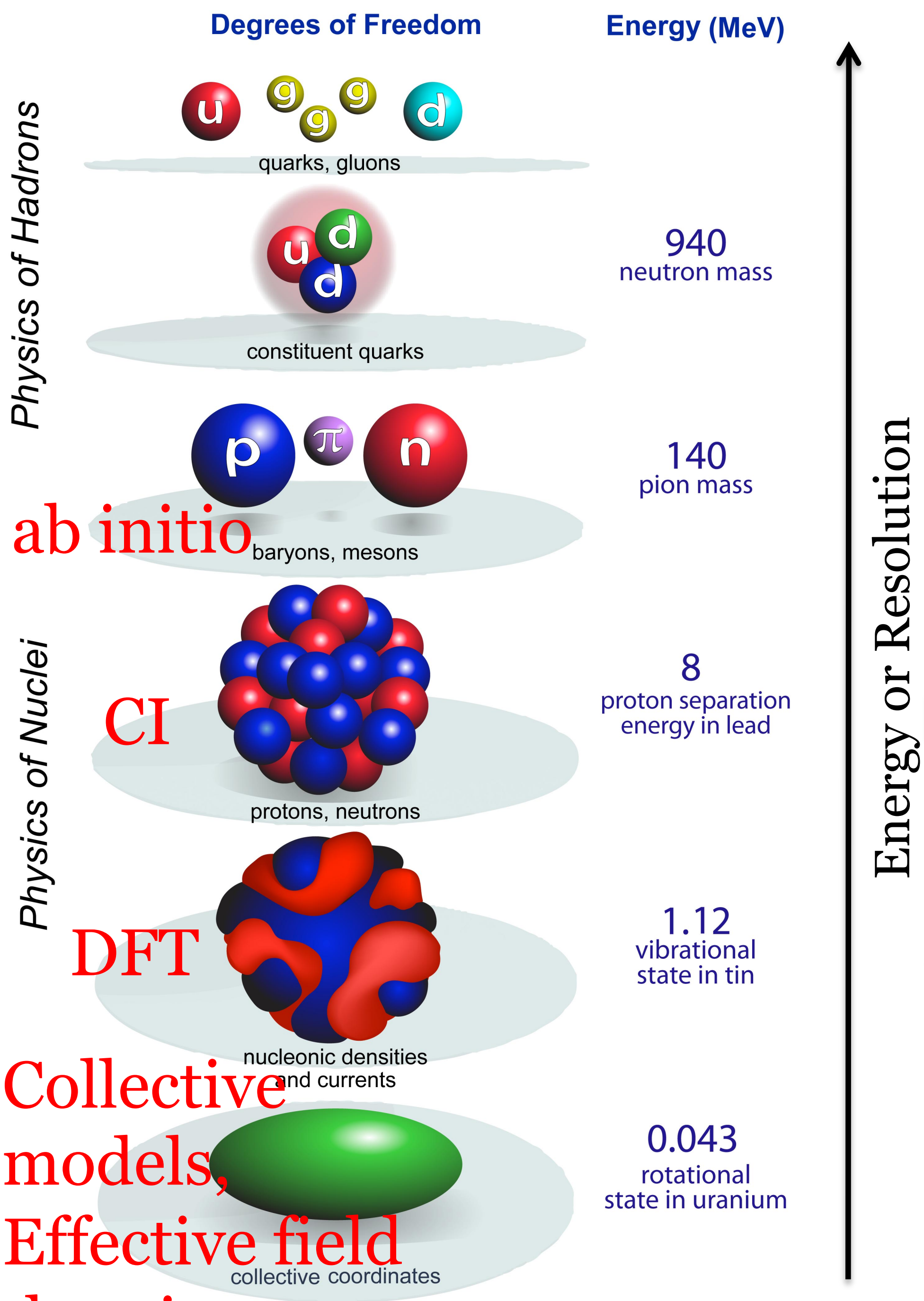


Fig.: Bertsch, Dean, Nazarewicz (2007)

Chiral symmetry is broken

Pion is Nambu-Goldstone boson

Tool: Chiral EFT [Epelbaum, Kaiser, Krebs, Machleidt, Meissner, Weise, van Kolck, …]

EFT for nuclear vibrations

EFT for deformed nuclei

Other EFTs:
Pion-less EFT [Bedaque, Hammer, Kaplan, Phillips, Savage, v. Kolck,…];
Halo EFT [Bertulani, Hammer, Higa, Phillips, Platter, van Kolck, …]

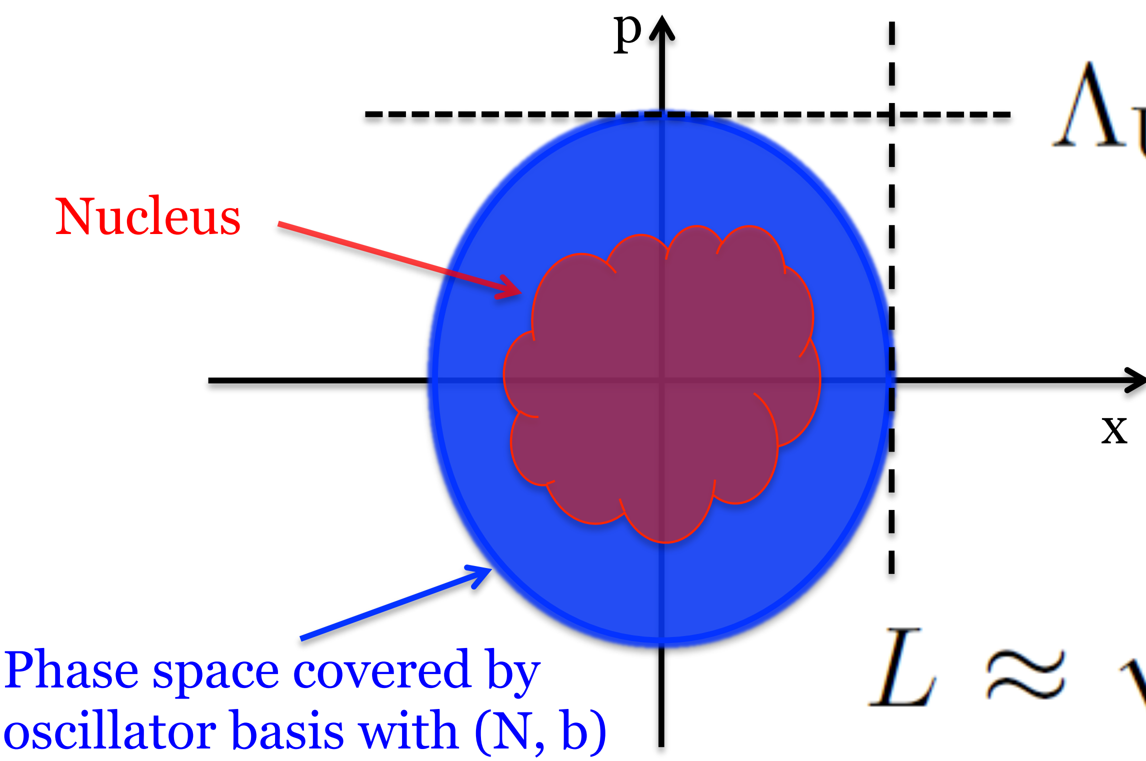
A key question of this INT program

In each of the three subdisciplines [Lattice QCD, nuclear EFTs, *ab initio* methods] ultraviolet and infrared cutoffs are imposed to limit the model spaces where explicit calculations are performed. Can the errors due to these truncations be estimated, and reliable extrapolation methods be developed?

Convergence in finite oscillator spaces

What is the equivalent of Lüscher's formula for the harmonic oscillator basis?
[Lüscher, Comm. Math. Phys. 104, 177 (1986)]

Convergence in momentum space (UV) and in position space (IR) needed
[Stetcu *et al.*, PLB (2007); Hagen *et al.*, PRC (2010); Jurgenson *et al.*, PRC (2011); Coon *et al.*, PRC (2012); König *et al.*, PRC (2014)]



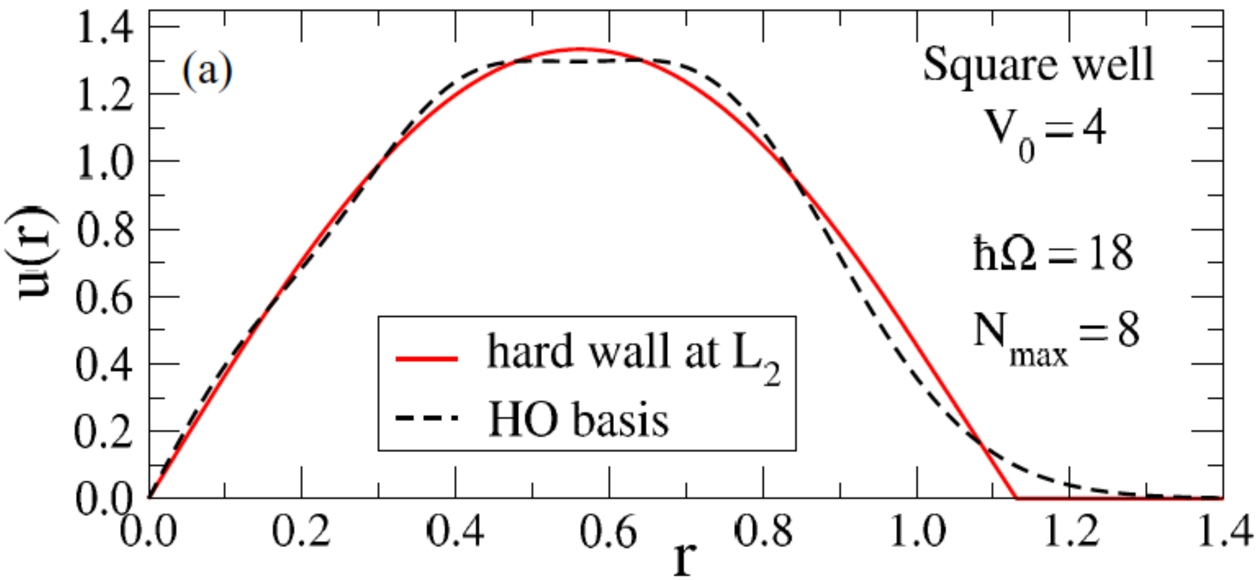
$$\Lambda_{\mathrm{UV}} \approx \sqrt{2N}/b$$

$$L \approx \sqrt{2N}b$$

Nucleus needs to "fit" into basis:

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

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



Ground-state wave functions in position space

[Coon *et al.* (2012); Furnstahl, Hagen TP (2012); More, Ekström, Furnstahl, Hagen, TP (2013); Furnstahl, More, TP (2014)]

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

$$E_L = E_\infty + a_0 e^{-2k_\infty L} \qquad \langle r^2 \rangle_L \approx \langle r^2 \rangle_\infty [1 - (c_0 \beta^3 + c_1 \beta) e^{-\beta}]$$

$$\beta \equiv 2k_\infty L$$

Notes:

- Leading asymptotic formulas for $k_\infty L >> 1$
- Algebraic corrections for partial waves with nonzero angular momentum
- Choose regime (N, $\hbar\omega$) with negligible UV corrections
- Length scales L depends on nature of Hilbert space

What (precisely) is the IR length L?

Key idea: compute eigenvalues of kinetic energy and compare with *corresponding* (hyper)spherical cavity to find L.

What is the corresponding cavity?

Single particle	**A particles (product space)**	**A particles in No-core shell model**
Diagonalize $T_{kin}=p^2$	Diagonalize A-body T_{kin}	Diagonalize A-body T_{kin}
3D spherical cavity	A fermions in 3D cavity	3(A-1) hyper-radial cavity

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

$$L_{\rm eff} = \left(\frac{\sum_{nl}\nu_{nl}a_{l,n}^2}{\sum_{nl}\nu_{nl}\kappa_{l,n}^2}\right)^{1/2}$$

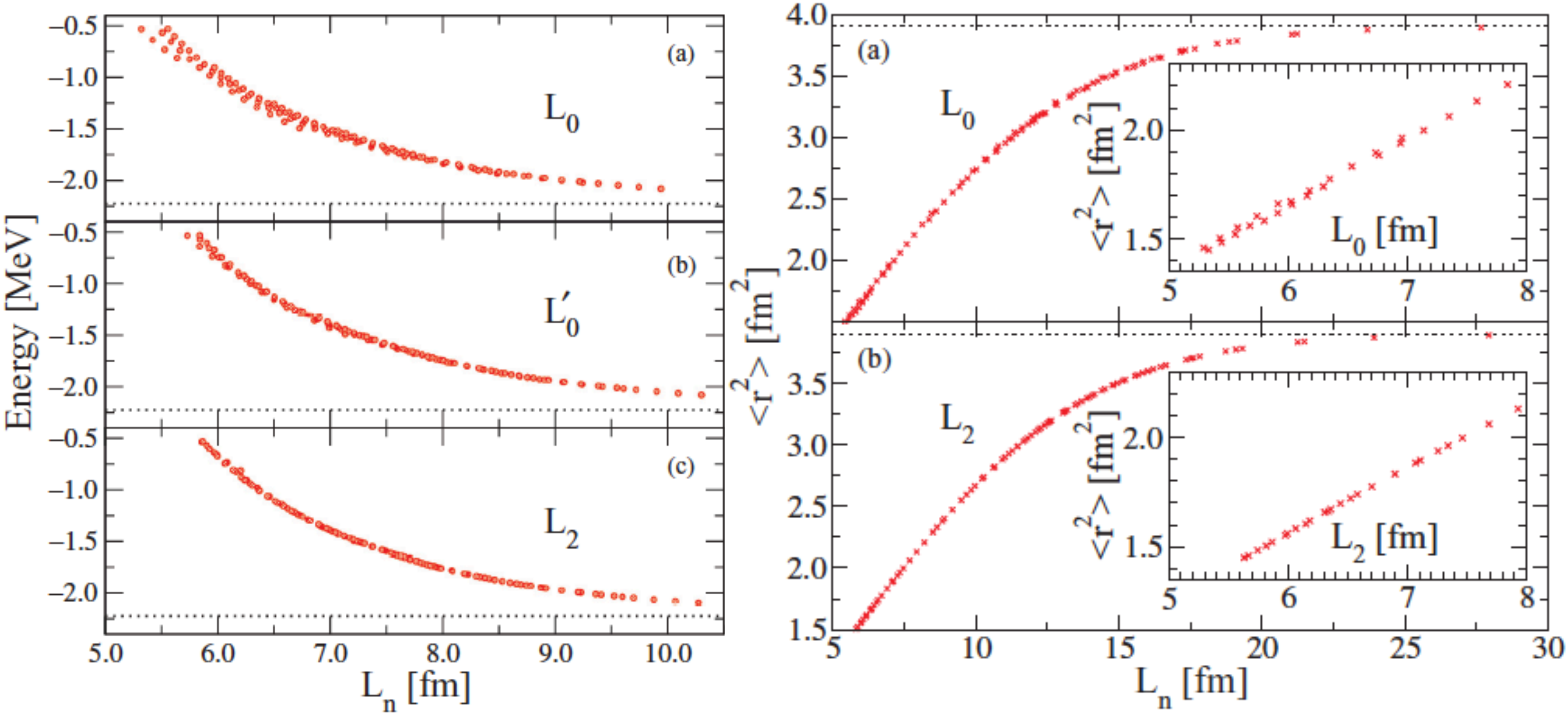
$$L_{\rm eff} = b\frac{X_{1,\mathcal{L}}}{\sqrt{T_{1,\mathcal{L}}(N_{\rm max}^{\rm tot})}}$$

More, Ekström, Furnstahl, Hagen, TP, PRC 87, 044326 (2013)

Furnstahl, Hagen, TP, Wendt, J. Phys. G 42, 034032 (2015)

Wendt, Forssén, TP, Sääf, PRC 91, 061301(R) (2015)

IR length for deuteron



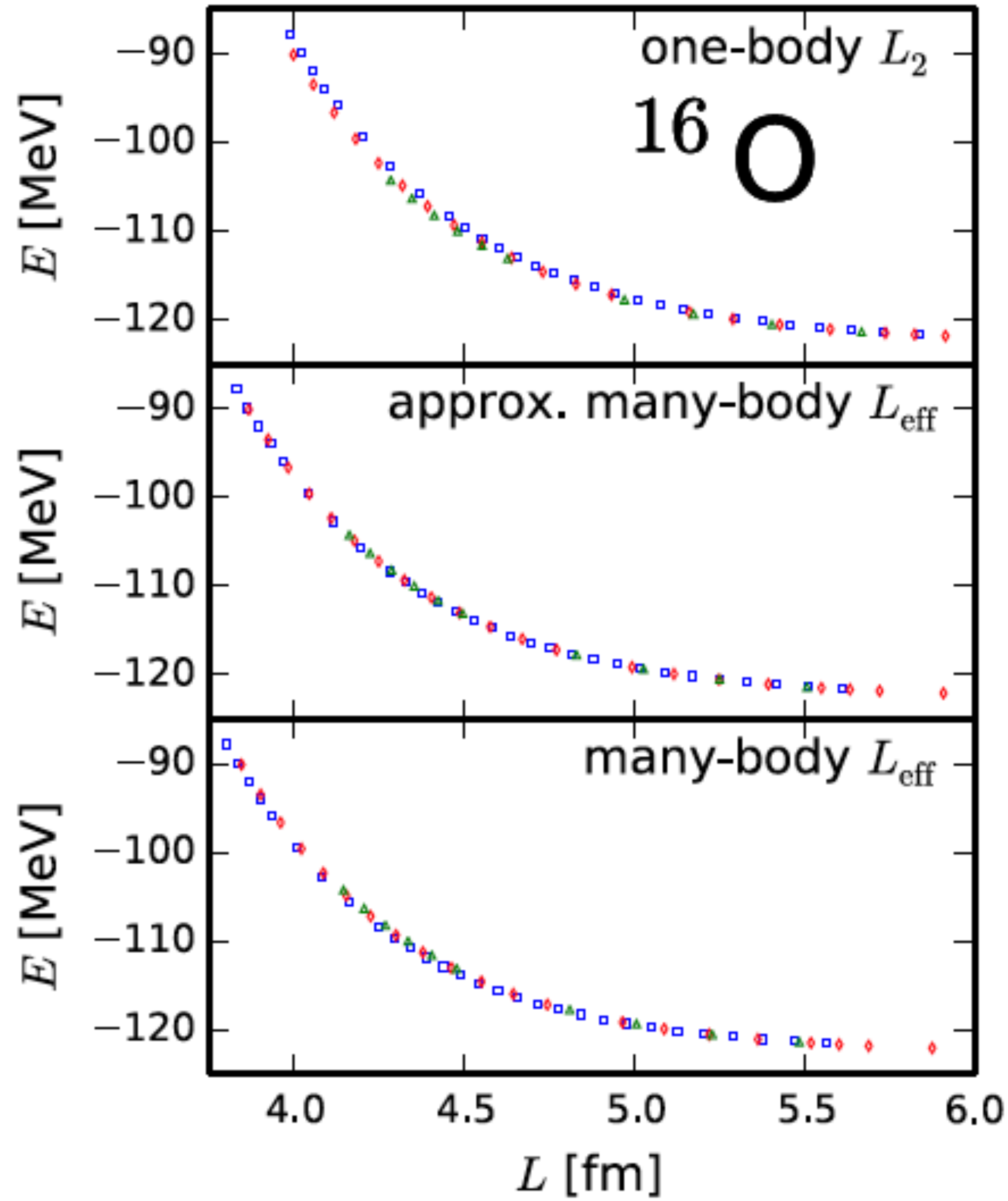
Diagonalize p^2 in harmonic oscillator and equate to kinetic energy of single particle in a cavity of radius L.

More, Ekström, Furnstahl, Hagen, TP (2013)

IR length in many-body product space

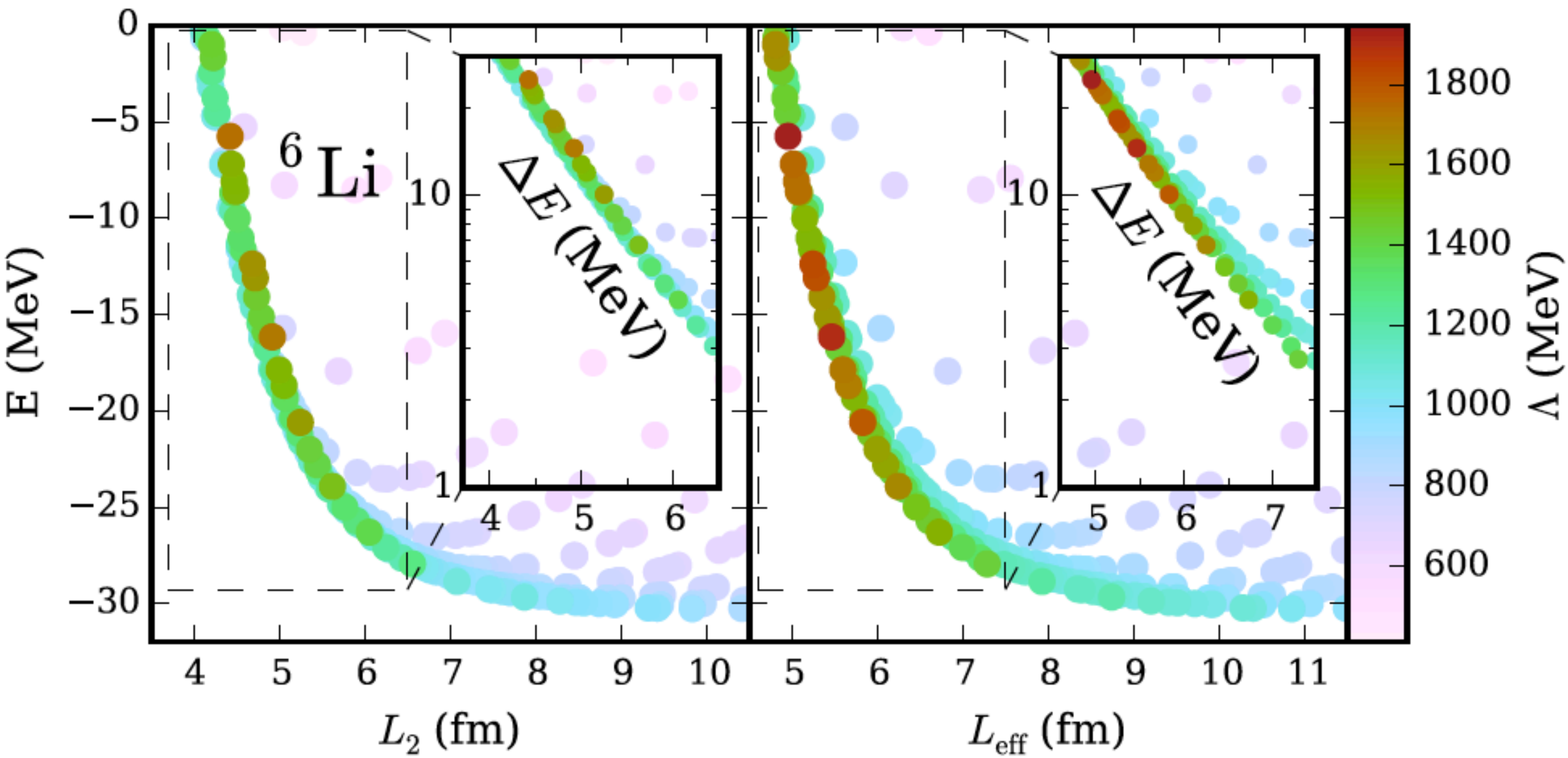
Diagonalize kinetic energy of A fermions in HO basis and equate to kinetic energy of A fermions in spherical cavity of radius L_{eff}.

$$L_{\text{eff}} = \left(\frac{\sum_{nl} \nu_{nl} a_{l,n}^2}{\sum_{nl} \nu_{nl} \kappa_{l,n}^2} \right)^{1/2}$$



Furnstahl, Hagen, TP, Wendt, J. Phys. G 42, 034032 (2015)

IR length in NCSM spaces



Diagonalize kinetic energy in 3(A-1) dimensional harmonic oscillator; seek lowest antisymmetric state and equate to hyperspherical cavity with radius L_{eff}.

Wendt, Forssén, TP, Sääf, PRC 91, 061301(R) (2015)

Extrapolations in finite Hilbert spaces

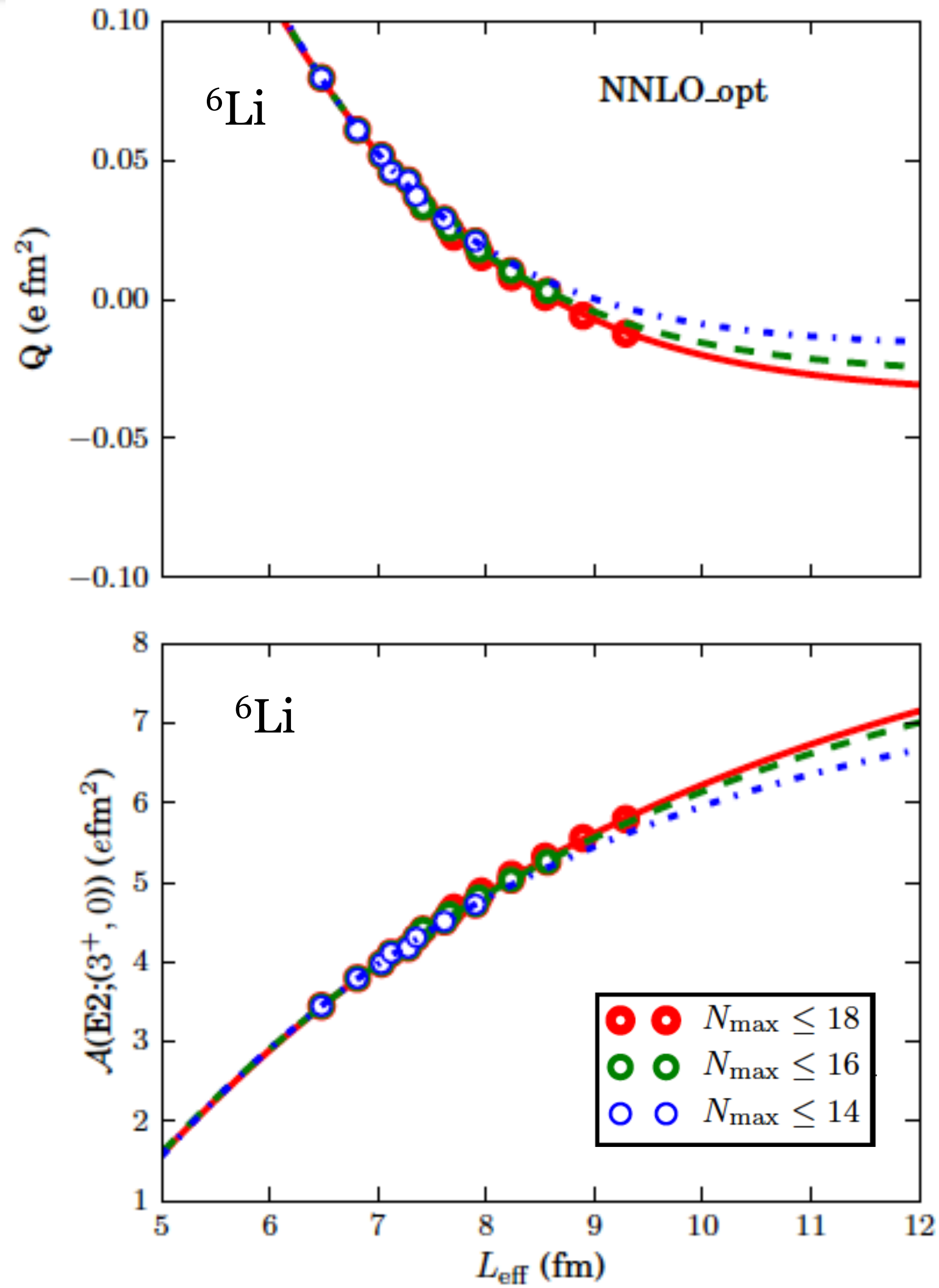
Quadrupole moment

$$Q_L = Q_\infty - a(k_\infty L)^3 e^{-2k_\infty L}$$

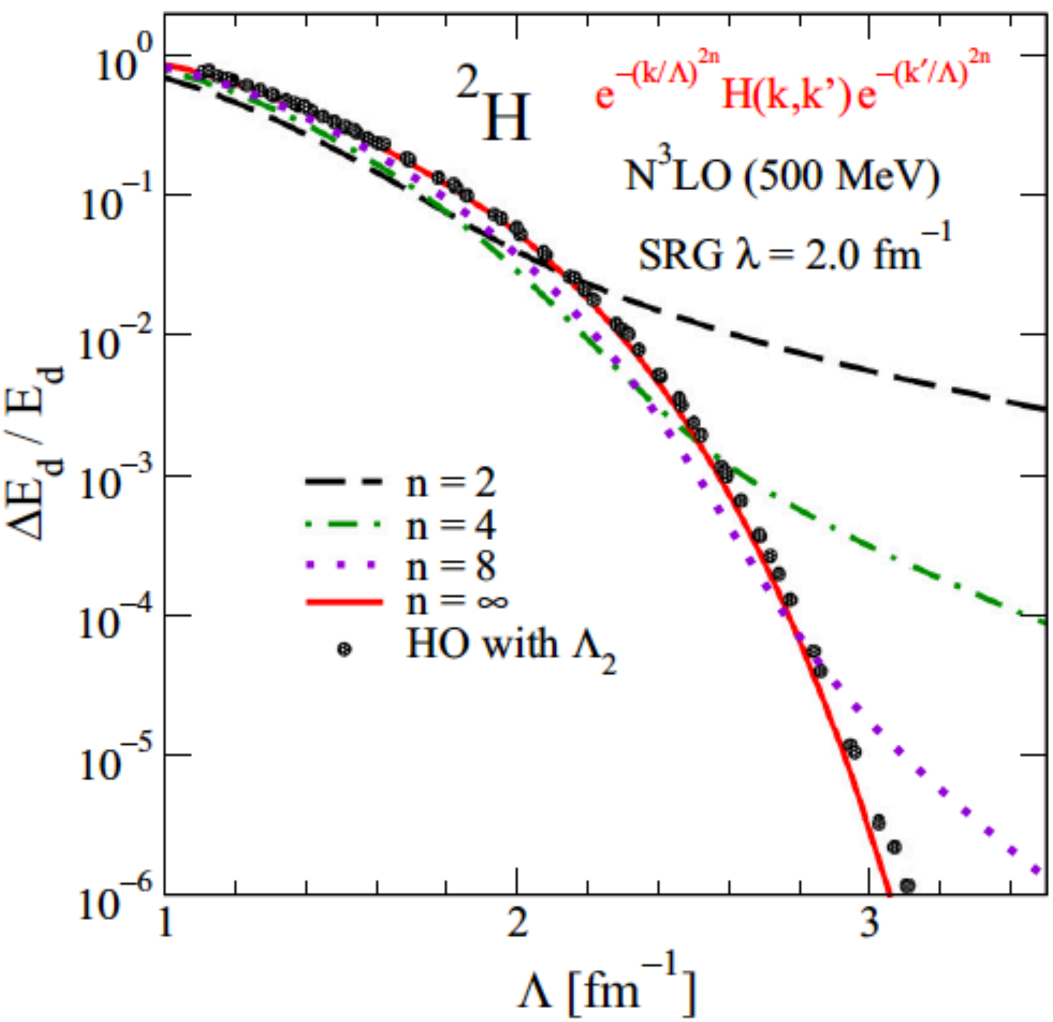
E2 transition amplitude

$$\mathcal{A}_L = \mathcal{A}_\infty + a_0 e^{-2k_< L}$$

Derivation: Odell, TP, Platter, PRC (2016).
Application: Ik Jae Shin *et al.*, 1605.02819.



UV extrapolation depends on the interaction (cutoff)



UV cutoff imposed by HO basis resembles a sharp cutoff; cutoff dual to IR length

Analytical extrapolation formulas for separable potentials (or separable approximations of other potentials

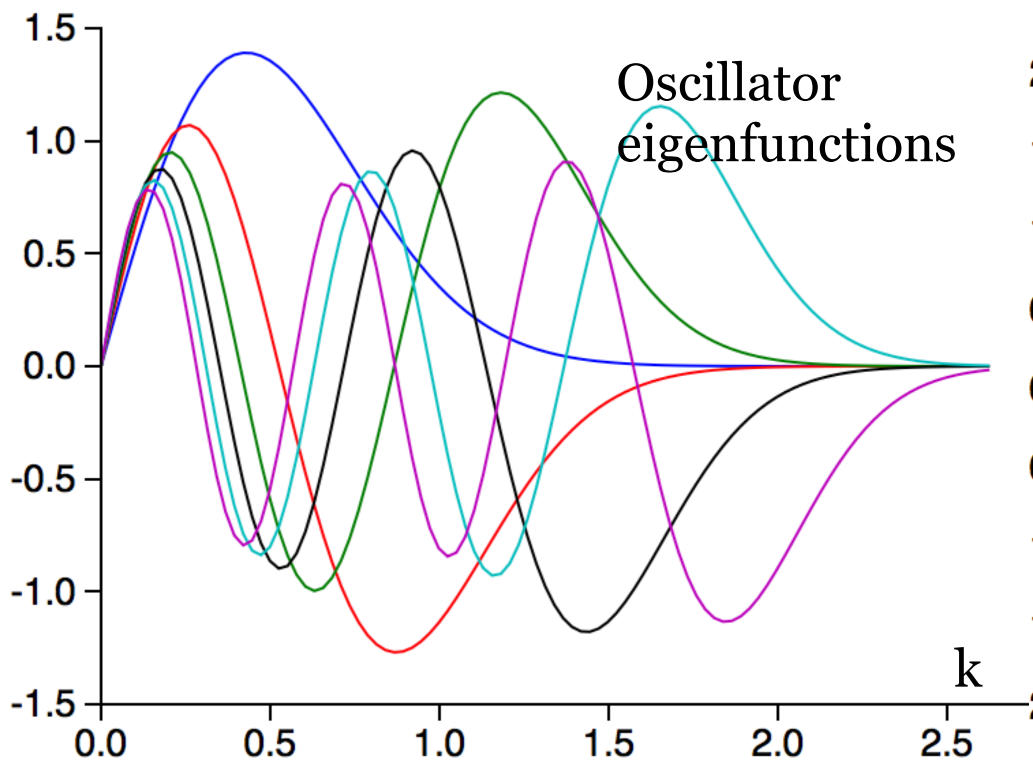
→ optimize interaction directly in HO basis:
EFT in HO basis is DVR

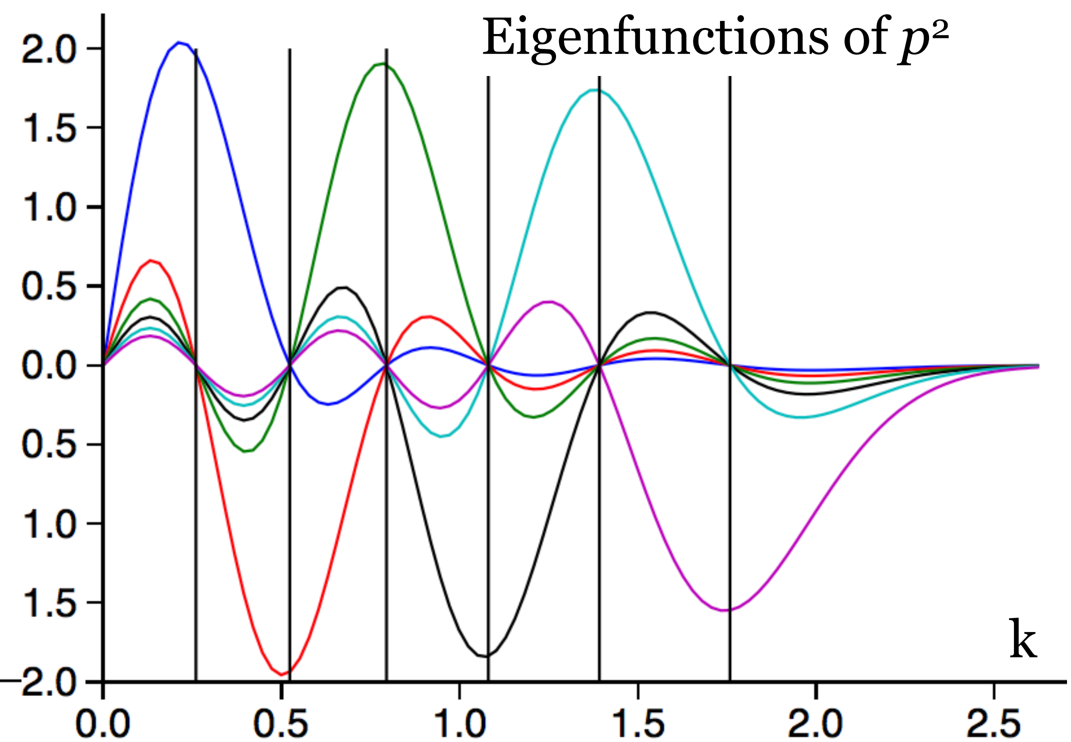
König, Bogner, Furnstahl, More, TP C 90, 064007 (2014)

EFT in harmonic oscillator basis is a DVR

Motivation: optimize and generate interactions in basis of computation

- Formulate EFT directly in the oscillator basis [Haxton & Song (2000); Stetcu, Barrett & van Kolck (2007); Tölle, Hammer & Metsch (2011)]
- A finite harmonic oscillator basis exhibits IR and UV cutoffs [Stetcu, Barrett & van Kolck (2007); Coon *et al.* (2012); Furnstahl, Hagen & TP (2012)]
- Discrete momentum eigenstates from diagonalization of p^2 for DVR in oscillator basis [Binder *et al.*, PRC 93, 044332 (2016)]

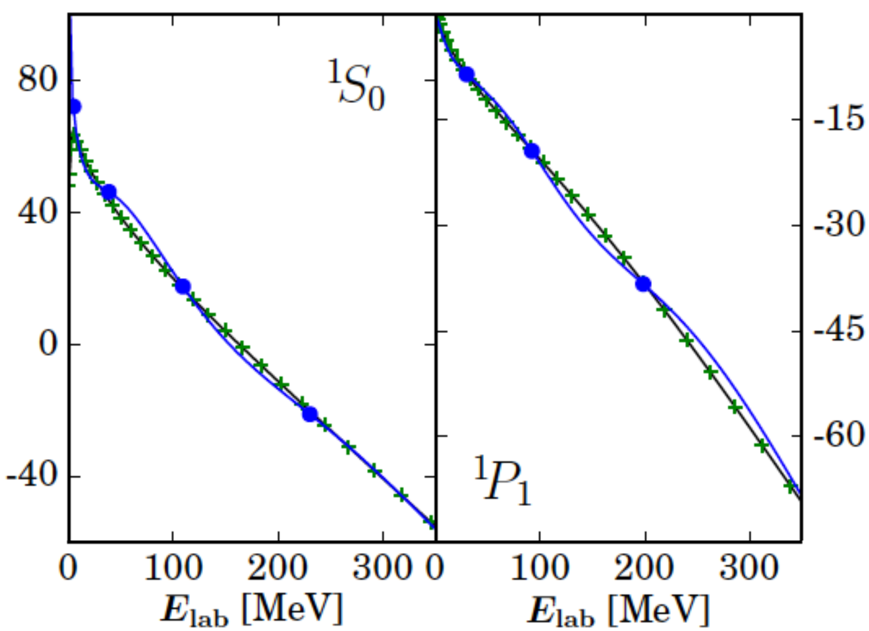




Chiral interaction at NLO in the oscillator basis

- Construct and optimize interaction in oscillator basis (→ JISP16)
- UV convergence by construction
- NLO interaction constructed with E_{max}=10ħω at ħω=22 MeV
- Rapid convergence of ground-state energies even for heavy nuclei

Phase shifts compared to NLO_{sim}



Convergence of ground-state energies

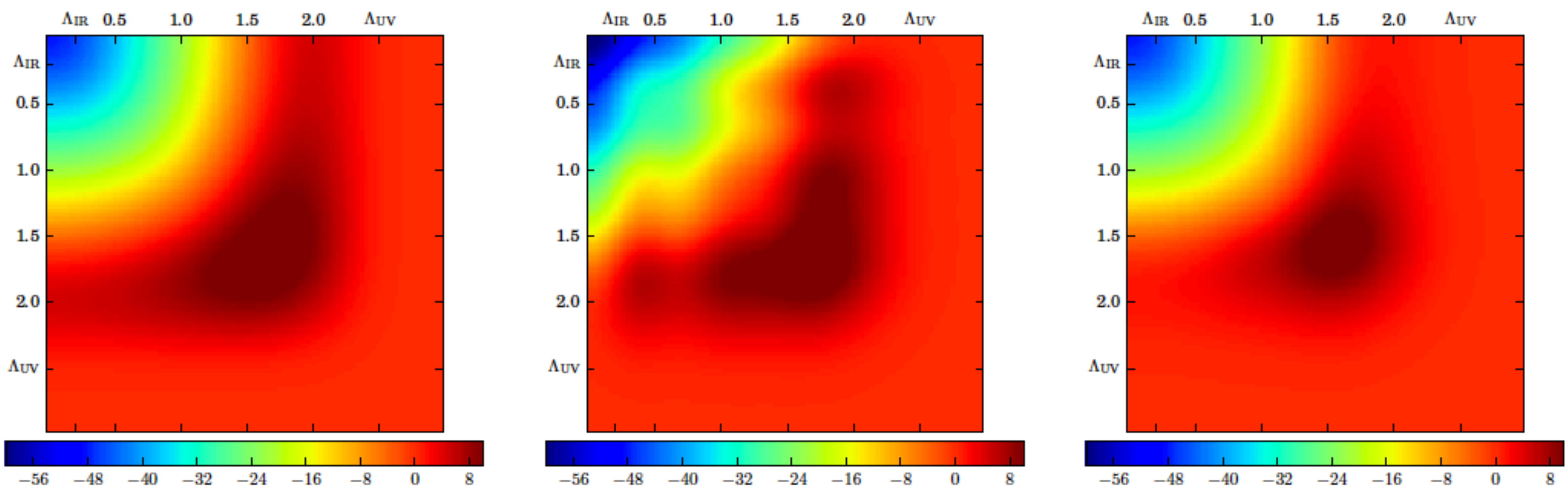
N_{max}	^{4}He	^{16}O	^{40}Ca	^{90}Zr	^{132}Sn
	E_{CCSD} [MeV]				
10	-31.57	-142.89	-402.0	-918.4	-1230.0
12	-31.57	-142.92	-402.4	-923.1	-1249.3
14	-31.57	-142.93	-402.5	-924.6	-1255.6
16	-31.57	-142.93	-402.5	-925.1	-1258.3
∞	-31.57	-142.93	-402.5	-925.4	-1260.1
exp	-28.30	-127.62	-342.1	-783.9	-1102.9

Binder *et al.* PRC 93, 044332 (2016)

Matrix elements in a finite oscillator basis

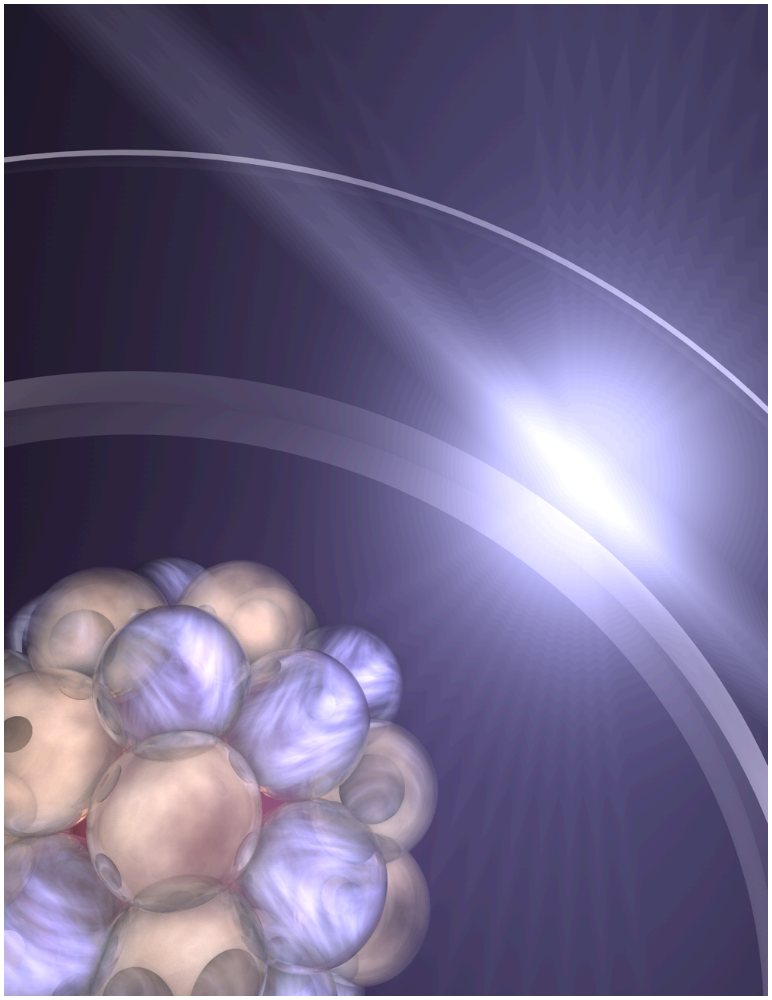
Momentum-space matrix elements
$^1S_0$ channel of $NNLO_{sim}$ with Λ_χ = 400 MeV
E_{max}=10ħω in harmonic oscillator (6 *s* states)

$V(k',k)$ | DVR: $V_{HO}(k',k)$ | IR improved $V_{HO}(k',k)$



IR improvement in oscillator EFT:
Modify matrix elements at high discrete momenta to improve low-momentum physics

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



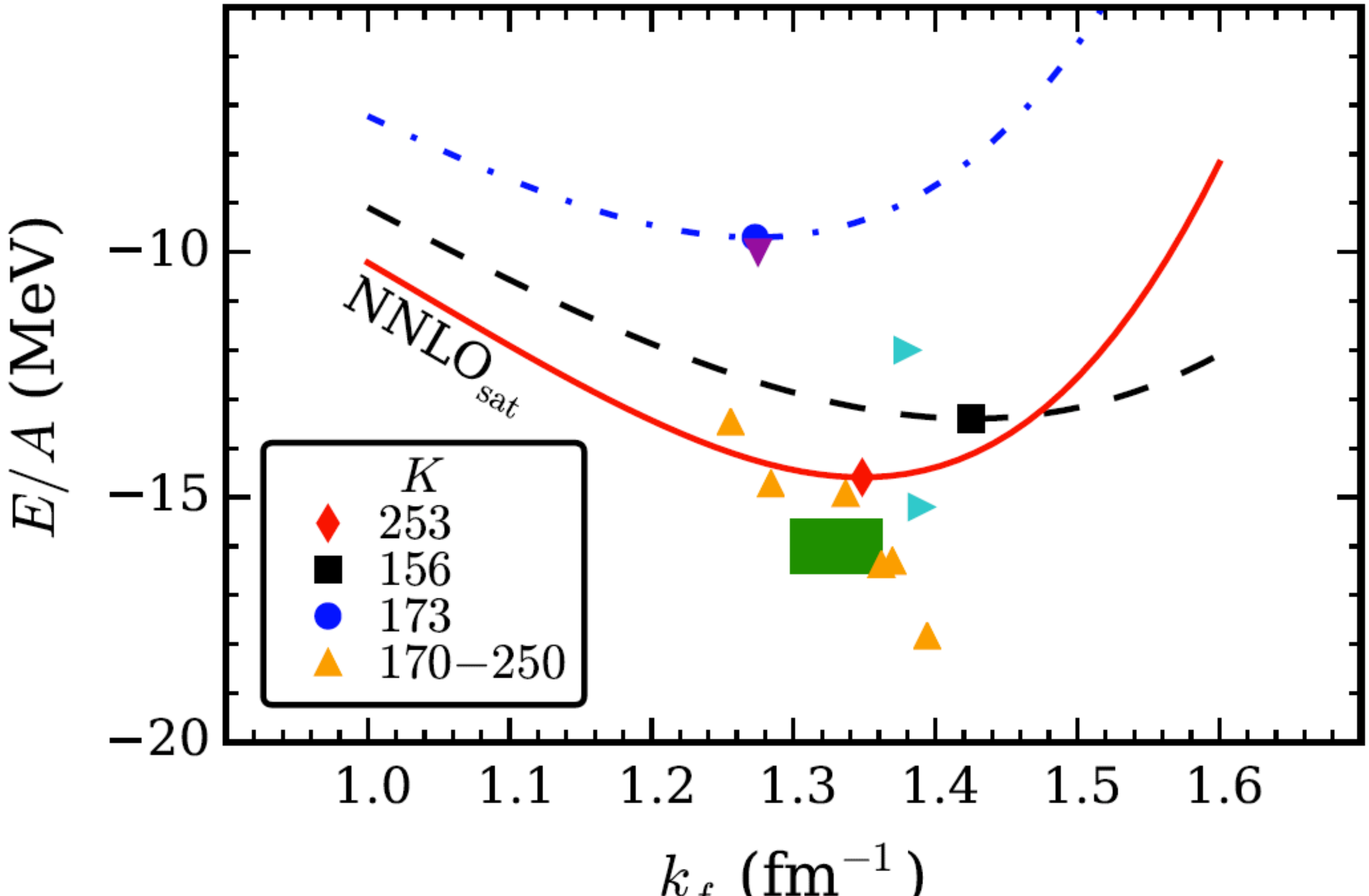
Neutron skin = Difference between radii of neutron and proton distributions

Relates atomic nuclei to neutron stars via neutron EOS

Correlated quantity: dipole polarizability

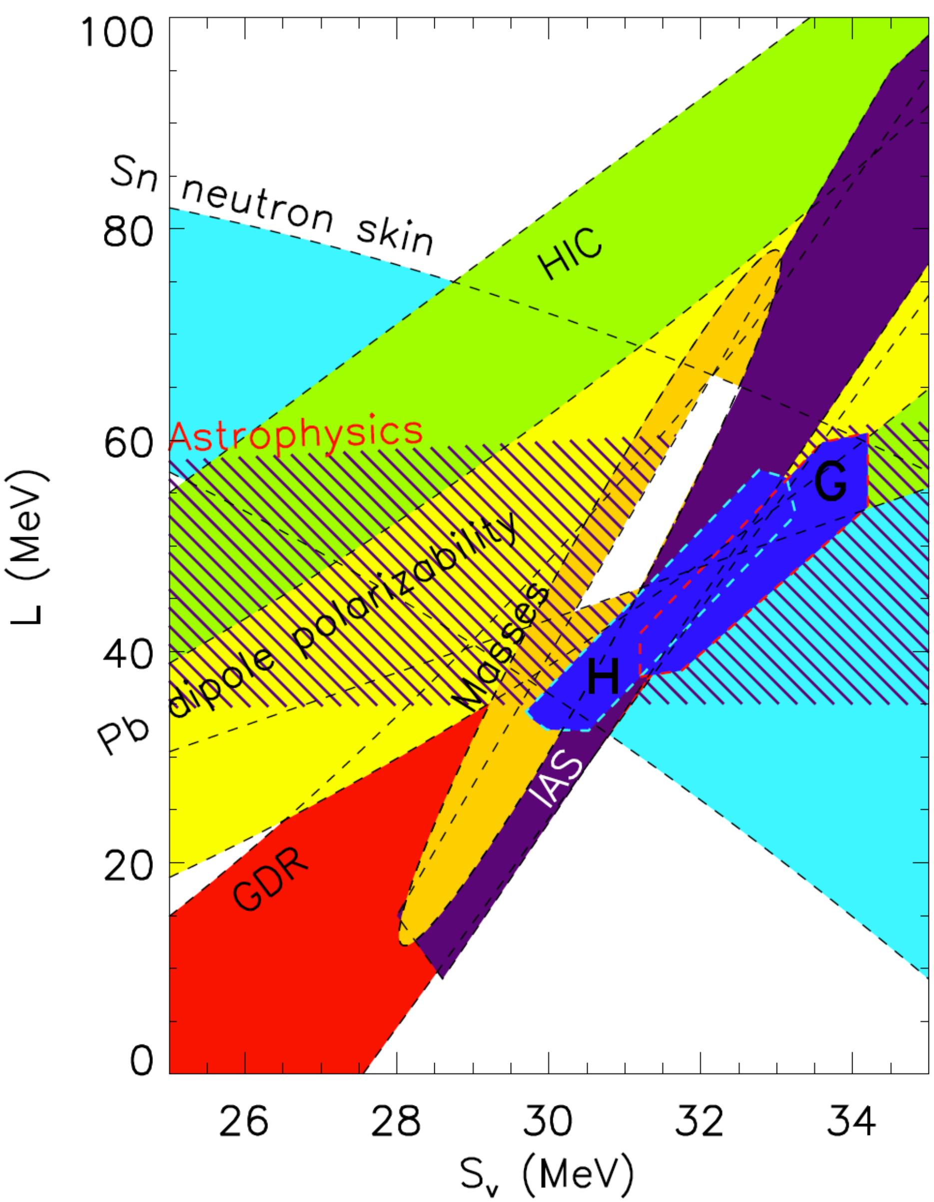
Model-independent measurement possible via parity-violating electron scattering

Nuclear matter from chiral interactions



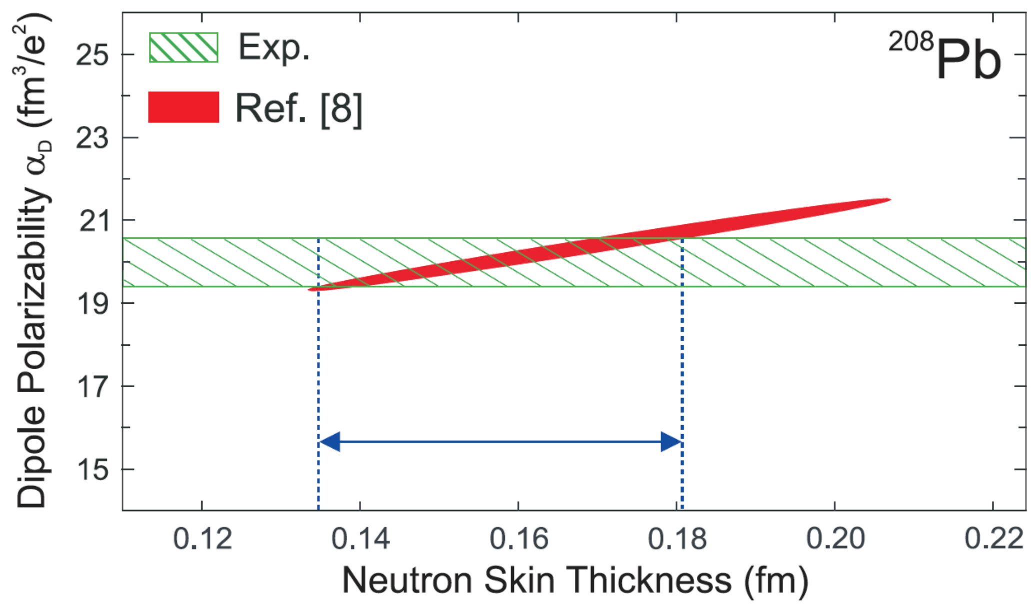
Interactions: (orange triangles) Hebeler *et al.* (2011); (red diamond) Ekström et al (2015); others: Hagen *et al.* (2014); Carbone *et al.* (2013); Coraggio *et al.* (2014).

Neutron radii and dipole polarizabilities



Lattimer & Lim 2013; Lattimer & Steiner 2014

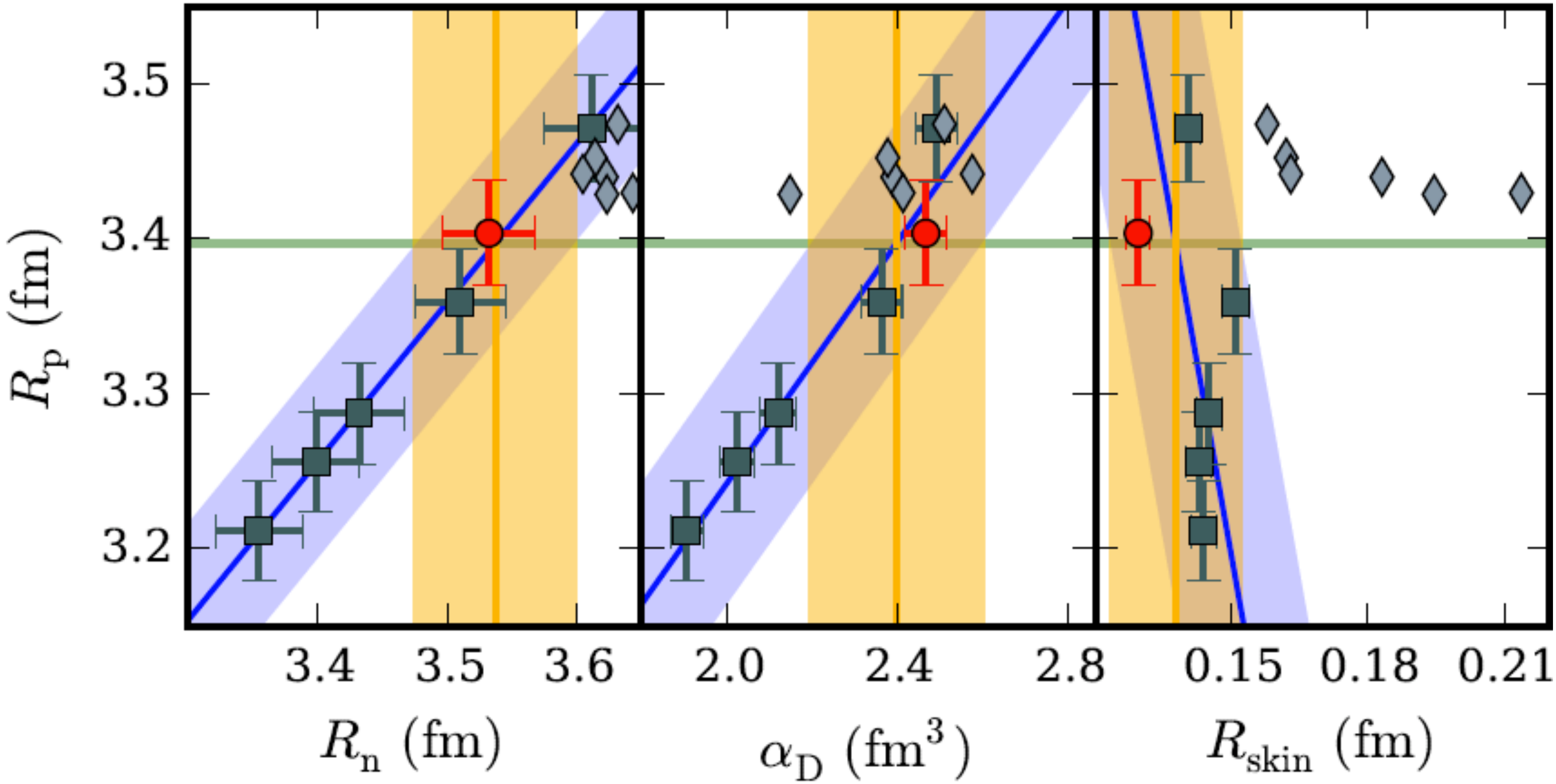
Brown, PRL 2000, Piekarewicz & Horowitz, PRL 2001; Furnstahl, NPA 2002; Reinhard & Nazarewicz, PRC 2010; Piekarewicz et al., PRC 2012; Horowitz et al, PRC 2012; …



$\boldsymbol{\alpha_D}$: ^{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 …

$\mathbf{R_n}$: ^{208}Pb by Abrahamyan et al, PRL 2012; Tarbert et al, PRL 2013; ^{48}Ca planned …

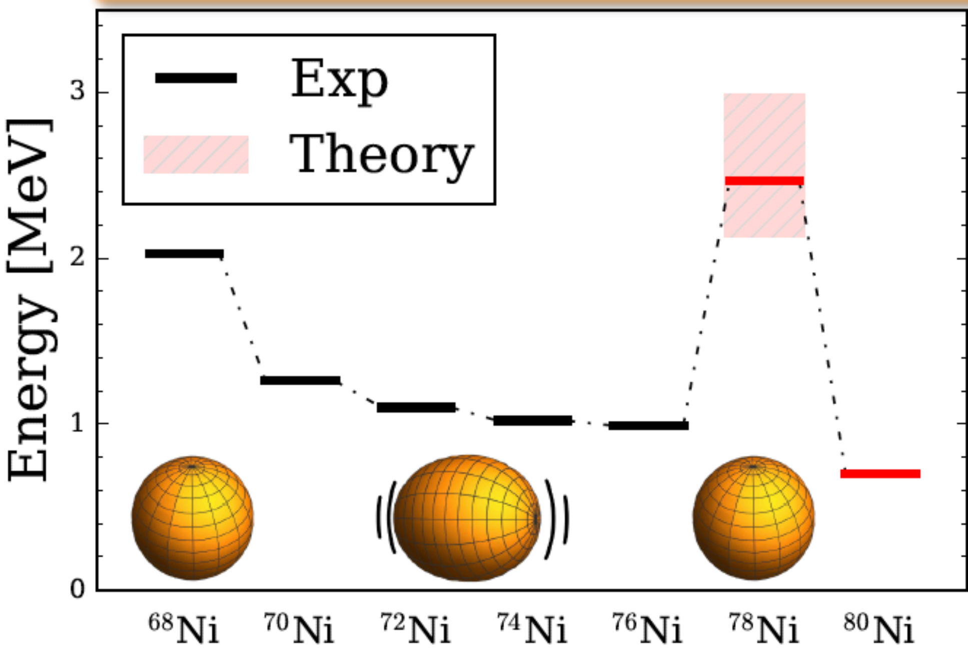
Correlations of critical observables

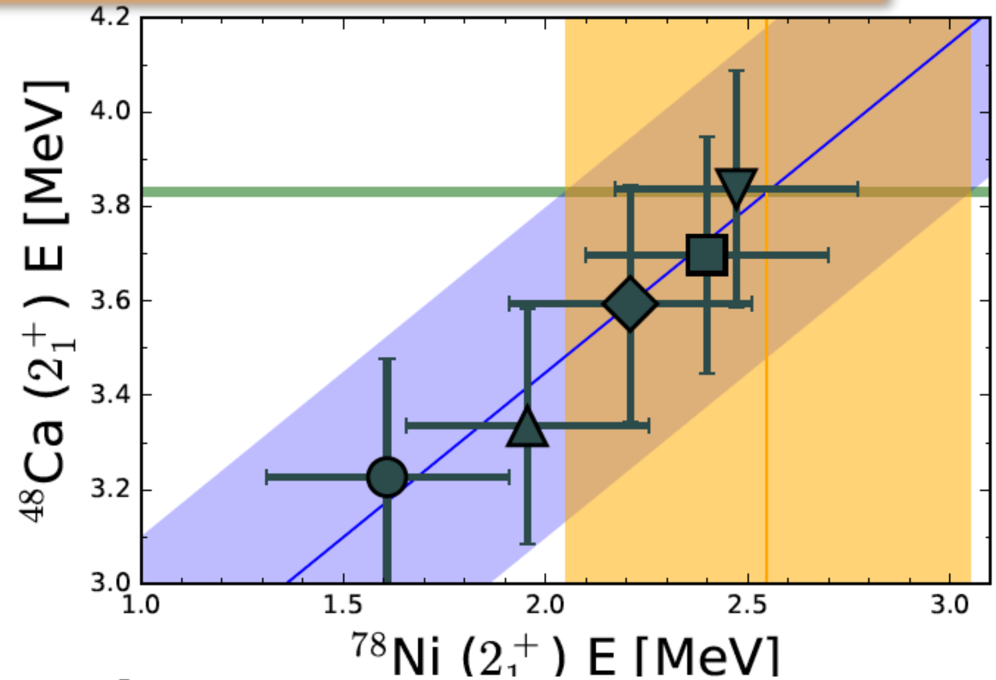


Uncertainty estimates from family of chiral interactions [NNLO_{sat}, potentials by Hebeler *et al.* (2011), and DFT].

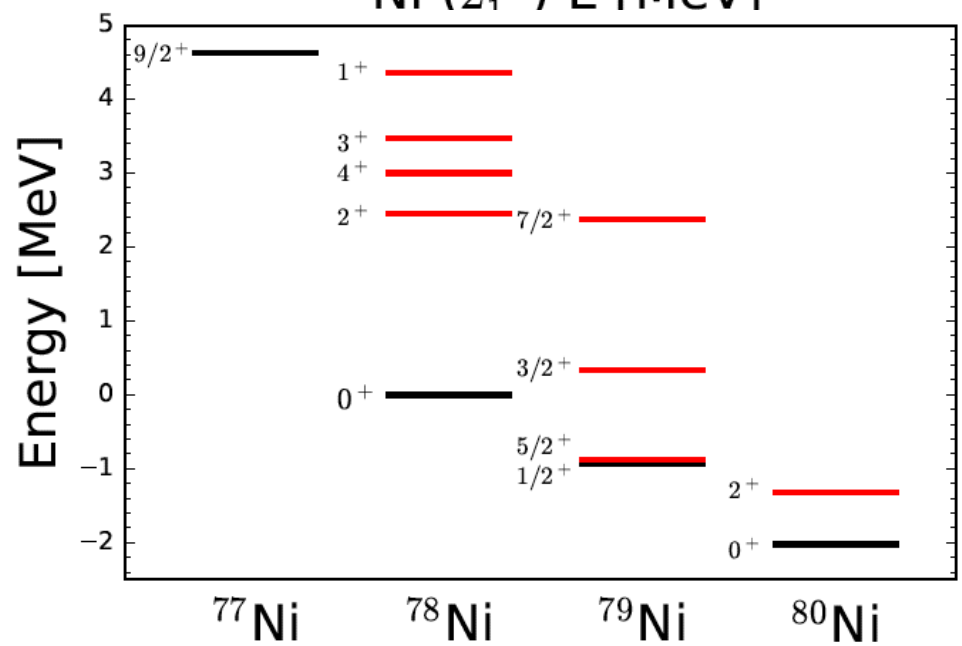
G. Hagen *et al.*, Nature Physics 12, 186 (2016)

What is the structure of ^{78}Ni?





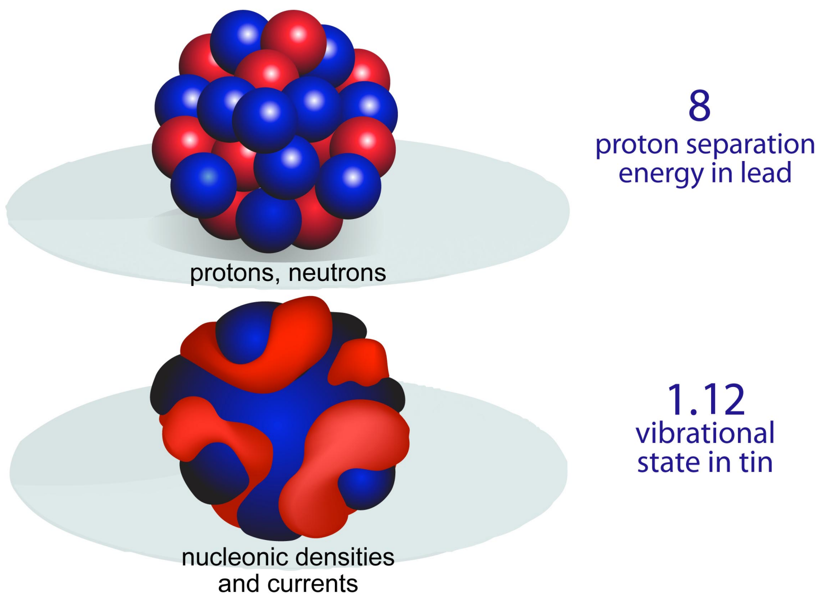
- Shell closure in ^{78}Ni
- Continuum effects relevant beyond neutron number N=50



(NNLOsat [circle], 2.0/2.0 (PWA) [square], 2.0/2.0 (EM) [diamond], 2.2/2.0 (EM) [triangle up], 1.8/2.0 (EM) [triangle down])

Hagen, Jansen, TP, arXiv:1605.01477.

EFT for nuclear vibrations

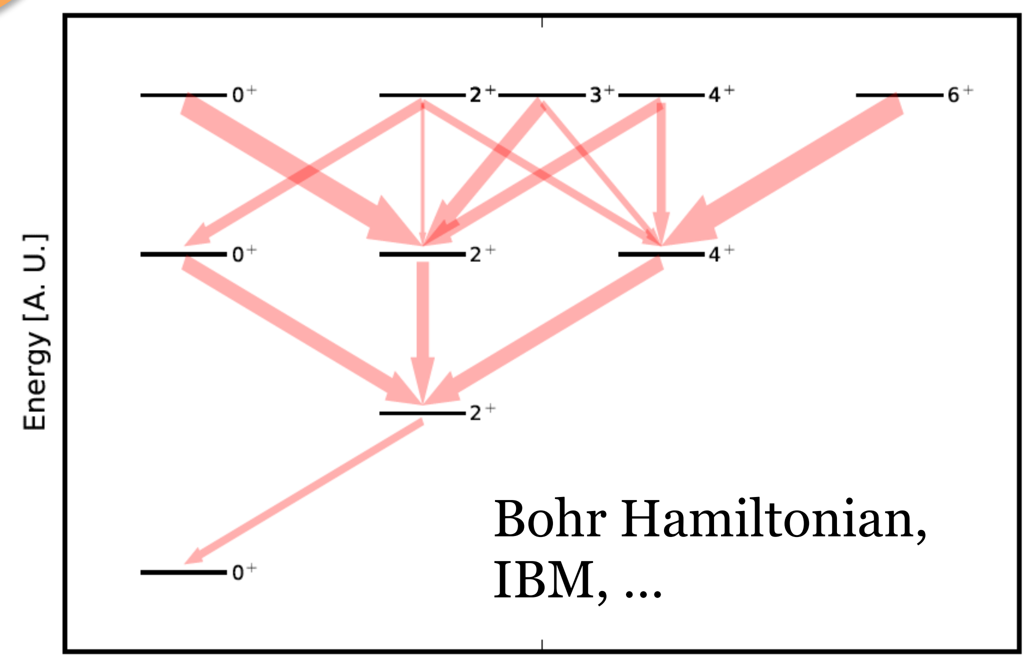


EFT for nuclear vibrations

[Coello Pérez & TP, PRC (2015)]

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?"

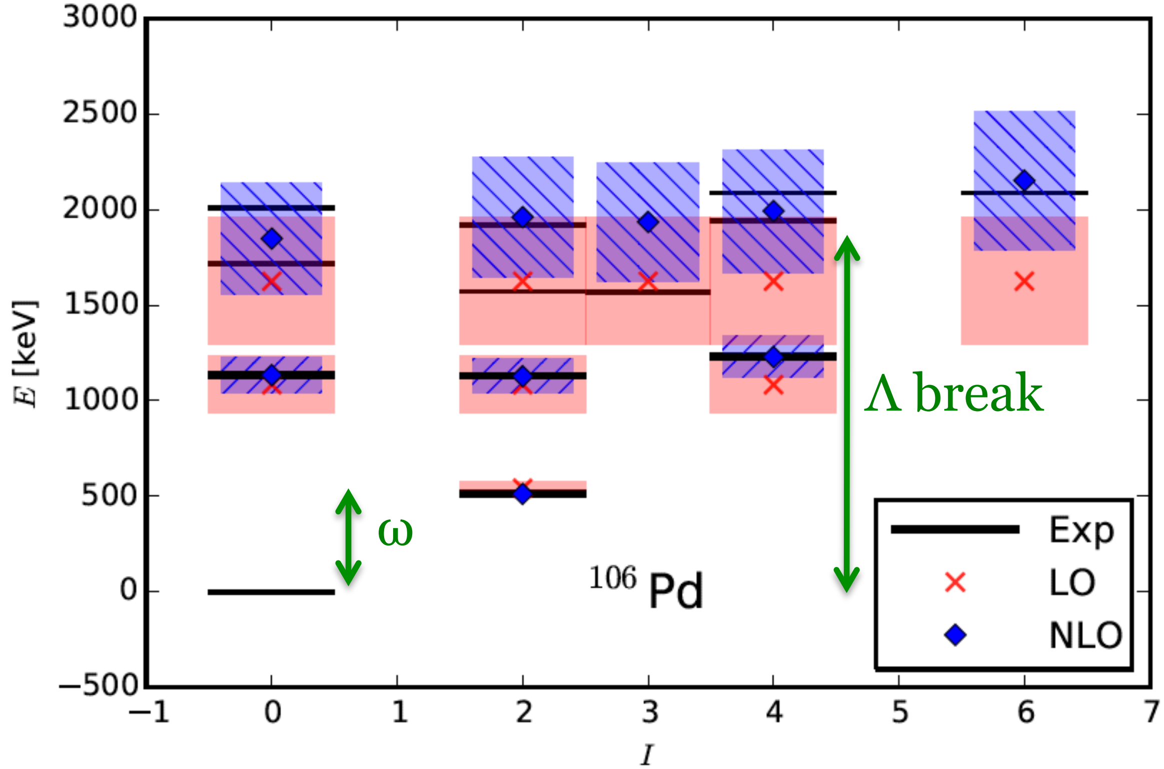


Spectrum and B(E2) transitions of the *harmonic* quadrupole oscillator

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.

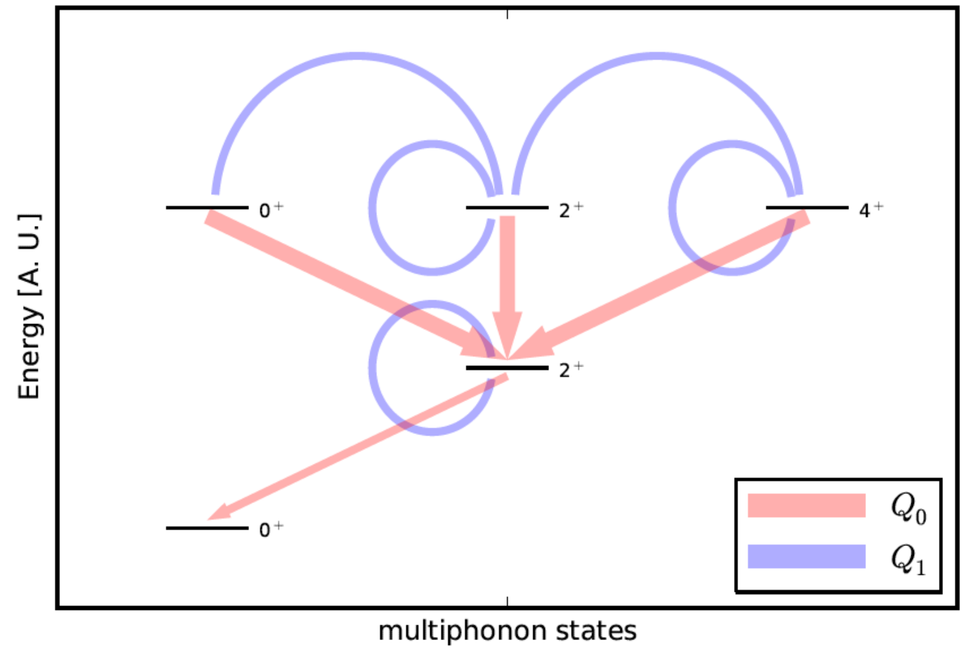
EFT result: sizeable quadrupole matrix elements are natural in size

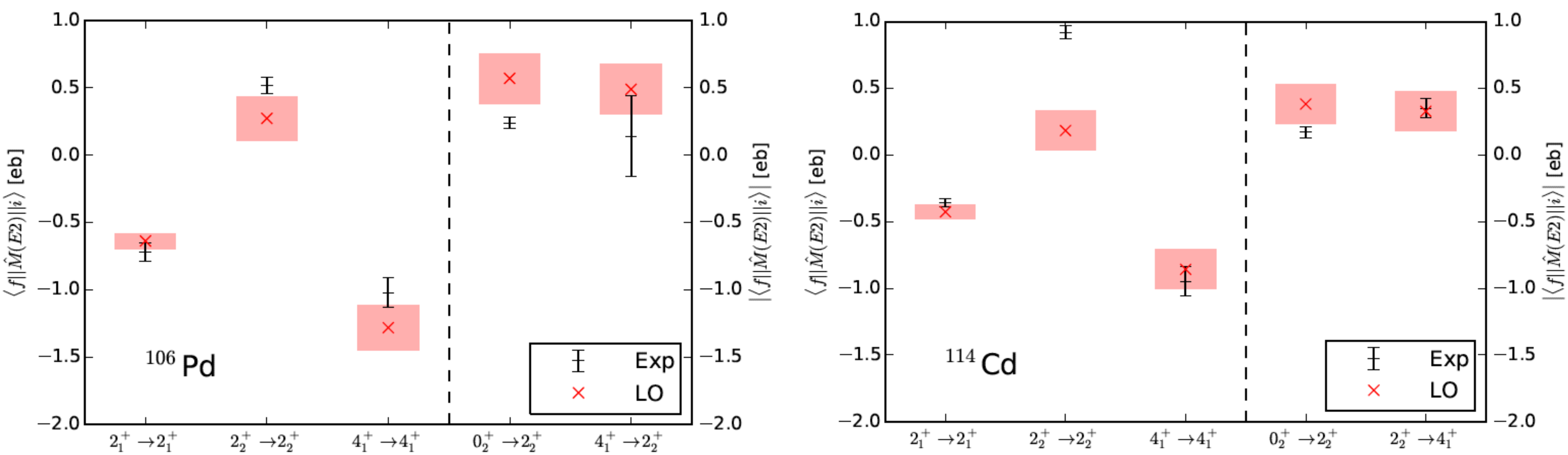
In the EFT, the quadrupole operator is also expanded:

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

Subleading corrections are sizable:

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

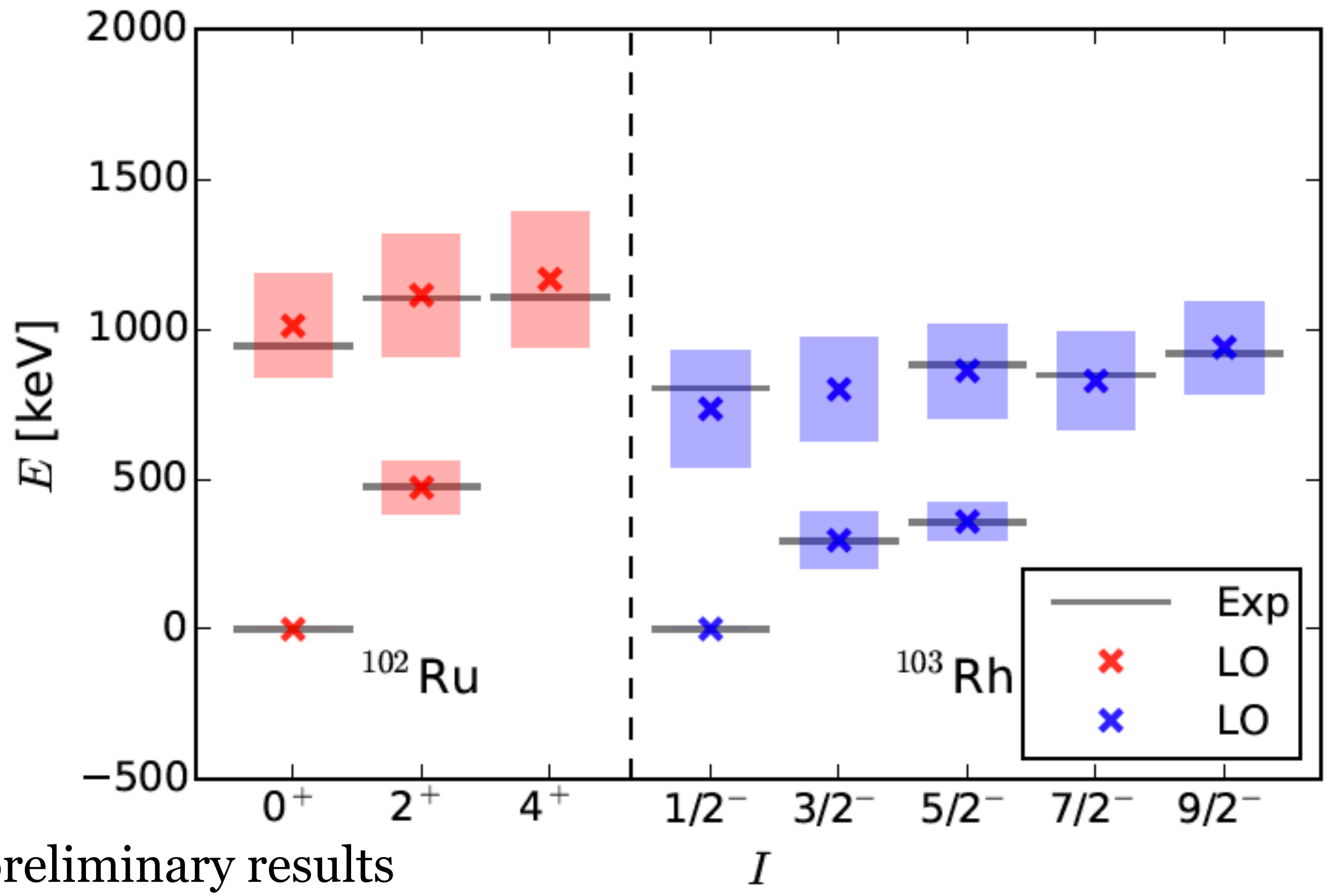




Work in progress: Fermion coupled to vibrating nucleus

Approach: Follow Halo EFT [Bertulani, Hammer, van Kolck (2002); Higa, Hammer, van Kolck (2008); Hammer & Phillips (2011); Ryberg et al. (2014)], and couple a fermion to describe odd-mass neighbors; particle-vibrator models [de Shalit (1961); Iachello & Scholten (1981); Vervier (1982);...]

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(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)

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

E. A. Coello Pérez & TP, preliminary results

Summary

- From EFTs to nuclei: Exploit separation of scales
- UV and IR cutoffs of HO basis understood for single particle, NCSM, and many-body product spaces
- Construct EFT directly in HO basis → DVR in momentum space
- Chiral interactions available with improved radii and binding
- Predictions of relevant nuclei and observables
    - Neutron radius, and dipole polarizability in ^{48}Ca
    - Shell structure of ^{78}Ni
    - 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
    - Picture of anharmonic vibrations consistent with data within uncertainties

(Some) open problems

- IR and UV length scales understood for a few relevant model spaces; leading order extrapolation formulas (derived in two-body systems) also seem to be applicable to many-body problems.
    - Understanding of momentum scale is lacking in many-body spaces
    - Higher-order corrections?
    - From bound states to resonances / continuum states?

- Relation between saturation properties and LECs of interactions?