

EFTs for Nuclei

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NUCLEI
Nuclear Computational Low-Energy Initiative

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Menu

1. IR extrapolations

1. Using data that is not yet fully UV converged
2. Quadrupole operators, radiative capture

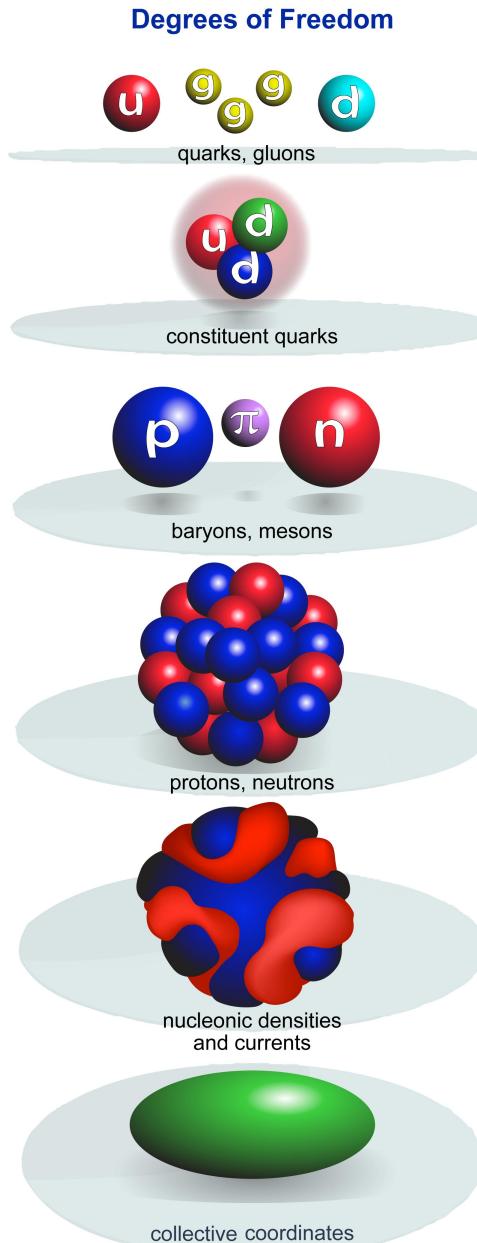
2. Pion-less EFT for ^{16}O and ^{40}Ca

1. DVR in the oscillator basis
2. Bound nuclei at non-perturbative NLO

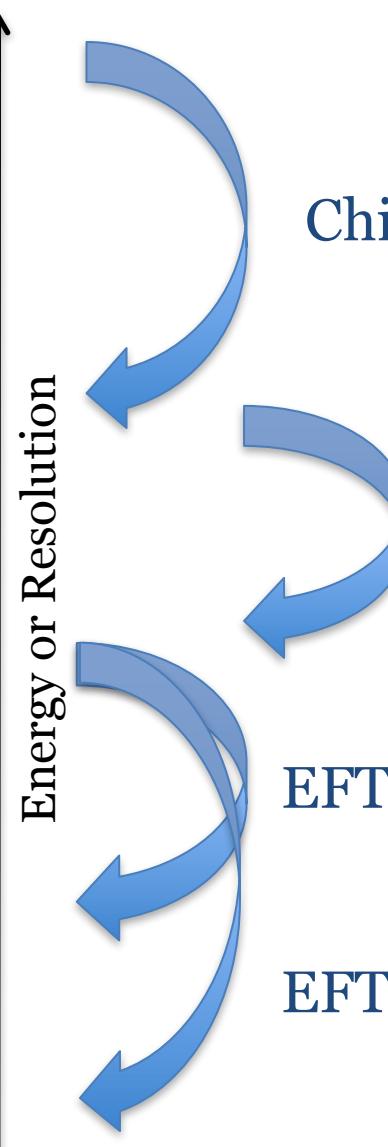
3. EFT for vibrations in odd-mass nuclei

Energy scales and relevant degrees of freedom

Physics of Hadrons



Energy or Resolution



Chiral EFT

Pion-less EFT

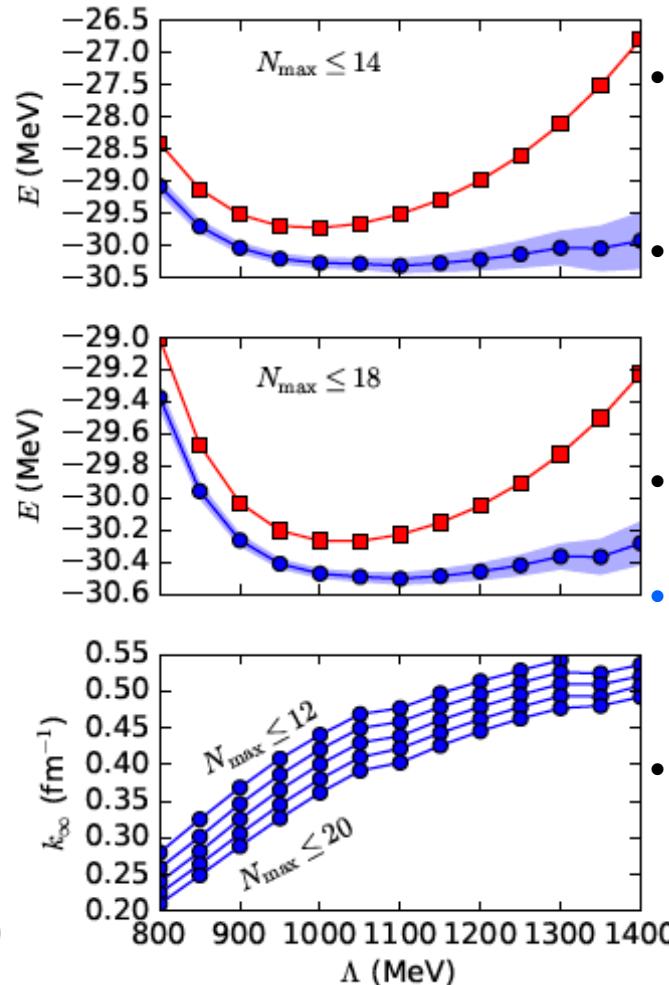
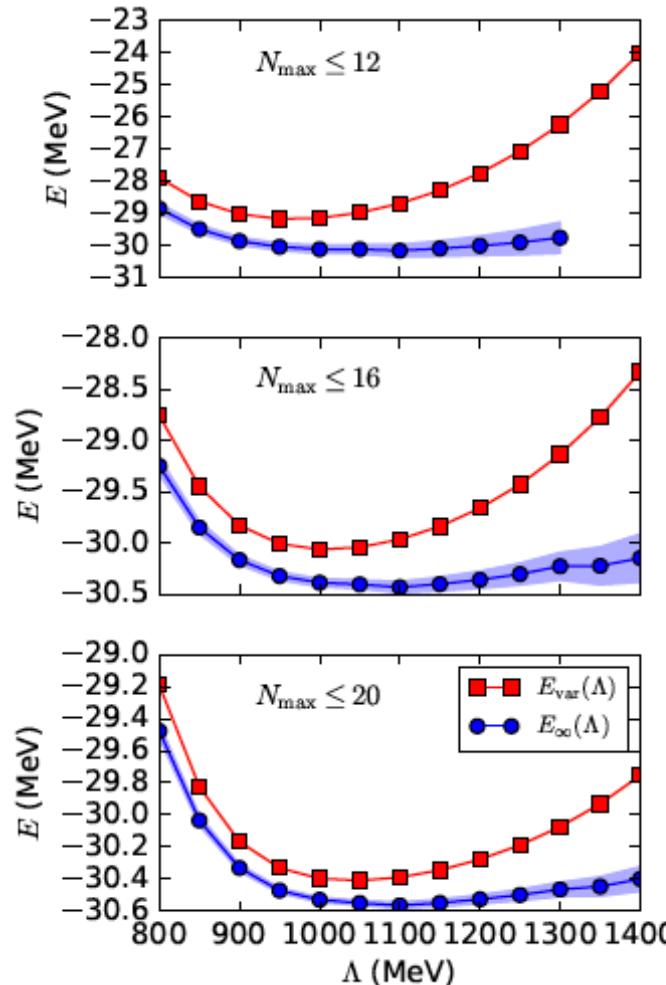
EFT for nuclear vibrations

EFT for deformed nuclei

IR extrapolation for ${}^6\text{Li}$ with NCSM

Use IR extrapolation formula [Coon et al. 2012 ; Furnstahl, Hagen & TP 2012]
at fixed UV cutoff Λ

$$E(L, \Lambda) = E_\infty(\Lambda) + a(\Lambda) \exp [-2k_\infty(\Lambda)L]$$



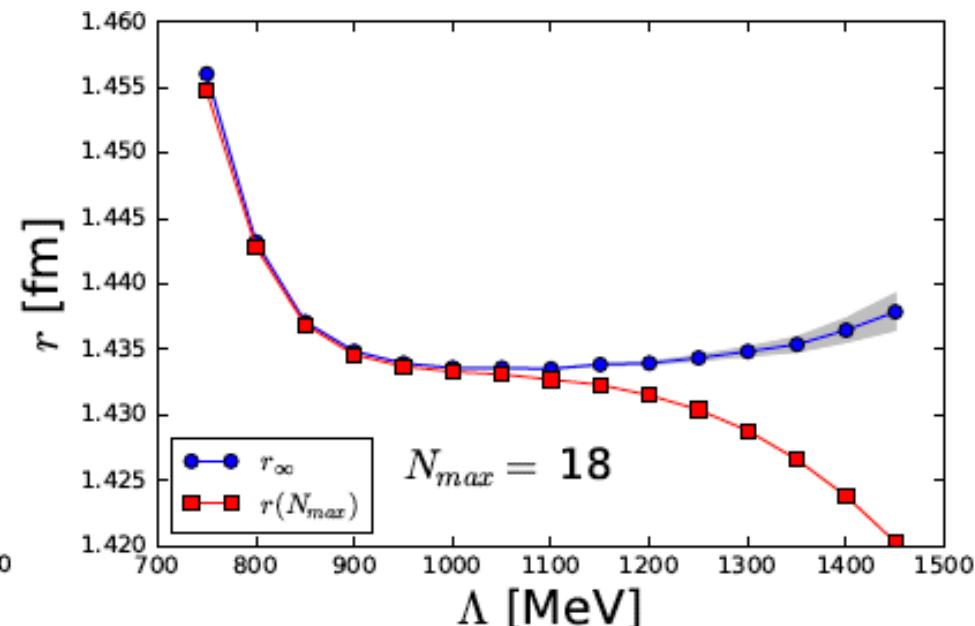
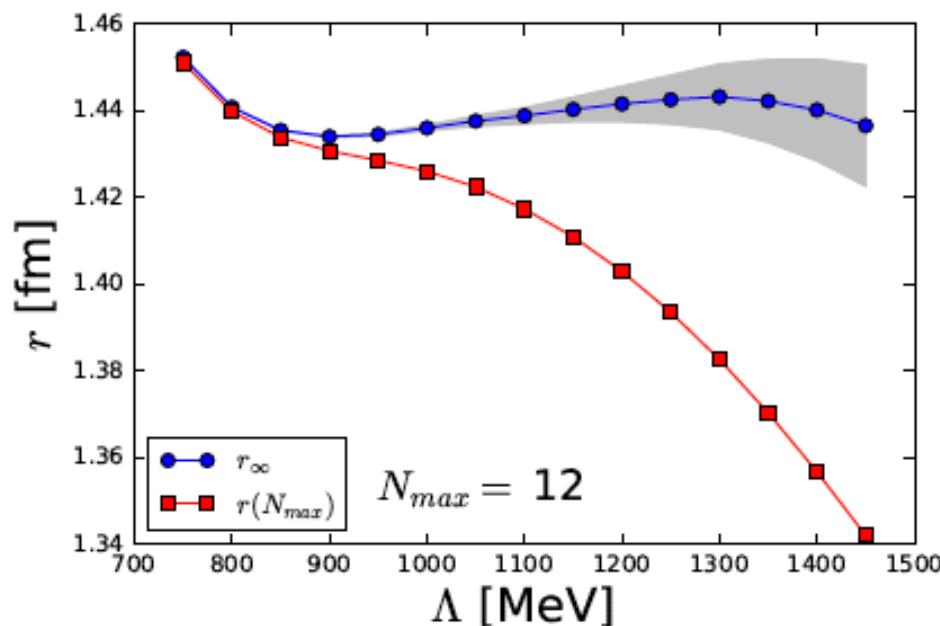
Rationale:

- At high Λ , UV converged, but NLO IR corrections enter
- IR extrapolations profitable as long as UV correction smaller than IR correction
- Improve on **variational minimum**
- **Uncertainty estimates** from IR extrapolation only
- k_∞ stabilizes

IR extrapolation for ${}^6\text{Li}$ with NCSM

Modified approach: Use IR extrapolation formula at fixed UV cutoff Λ

$$r^2(L, \Lambda) = r_\infty^2(\Lambda) - \alpha(\Lambda) [k_\infty(\Lambda)L]^3 \exp [-2k_\infty(\Lambda)L]$$

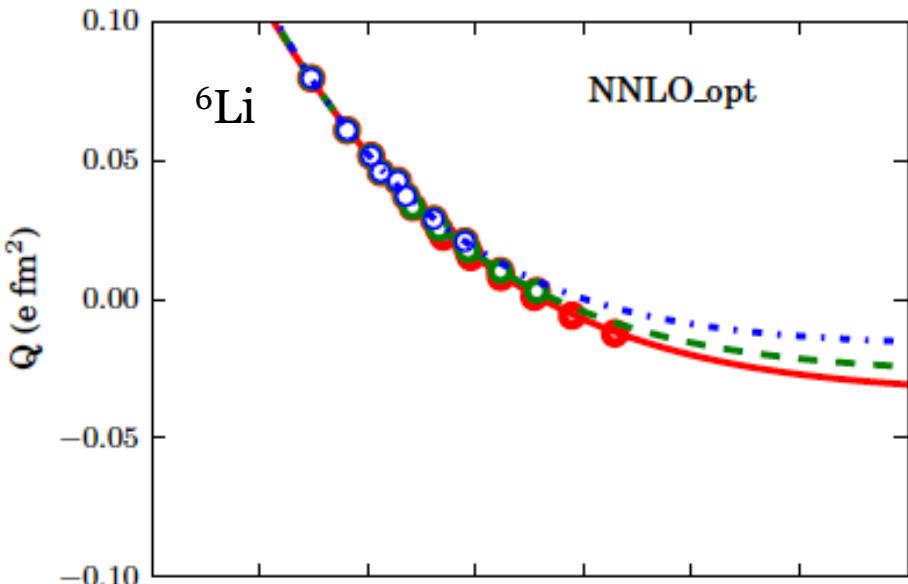


- Uncertainty estimates from IR extrapolation
- k_∞ stabilizes at higher cutoffs; consistent with energy extrapolation

Extrapolations in finite Hilbert spaces

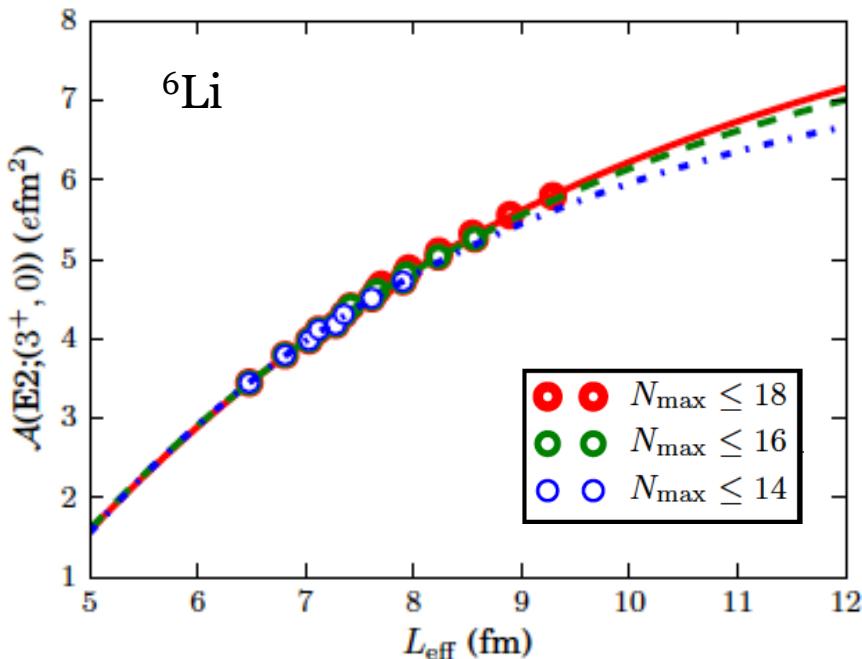
Quadrupole moment

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



E2 transition amplitude

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



Derivation: Odell, TP, Platter, PRC (2016).

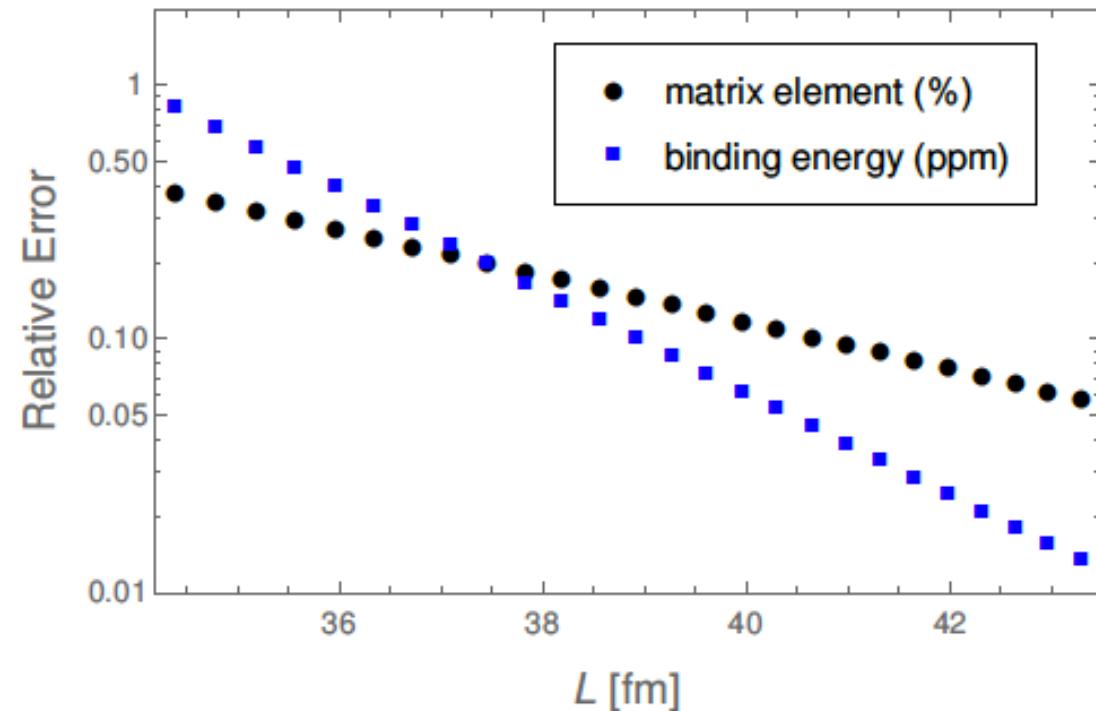
Application: Ik Jae Shin *et al.*, 1605.02819.

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 $\sim 1\%$, even when integrating out to 30 fm.

[Girlanda *et al.* PRL 2010]

Acharya *et al.*, arXiv:1608.04699
→ PRC Rapid 2017

EFT in harmonic oscillator via discrete variable representation (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)]

Useful tool: Computation of scattering phase shifts directly in the finite oscillator basis [Heller & Yamani (1974); Bang *et al.* (2000); Shirokov *et al.* (2004)]

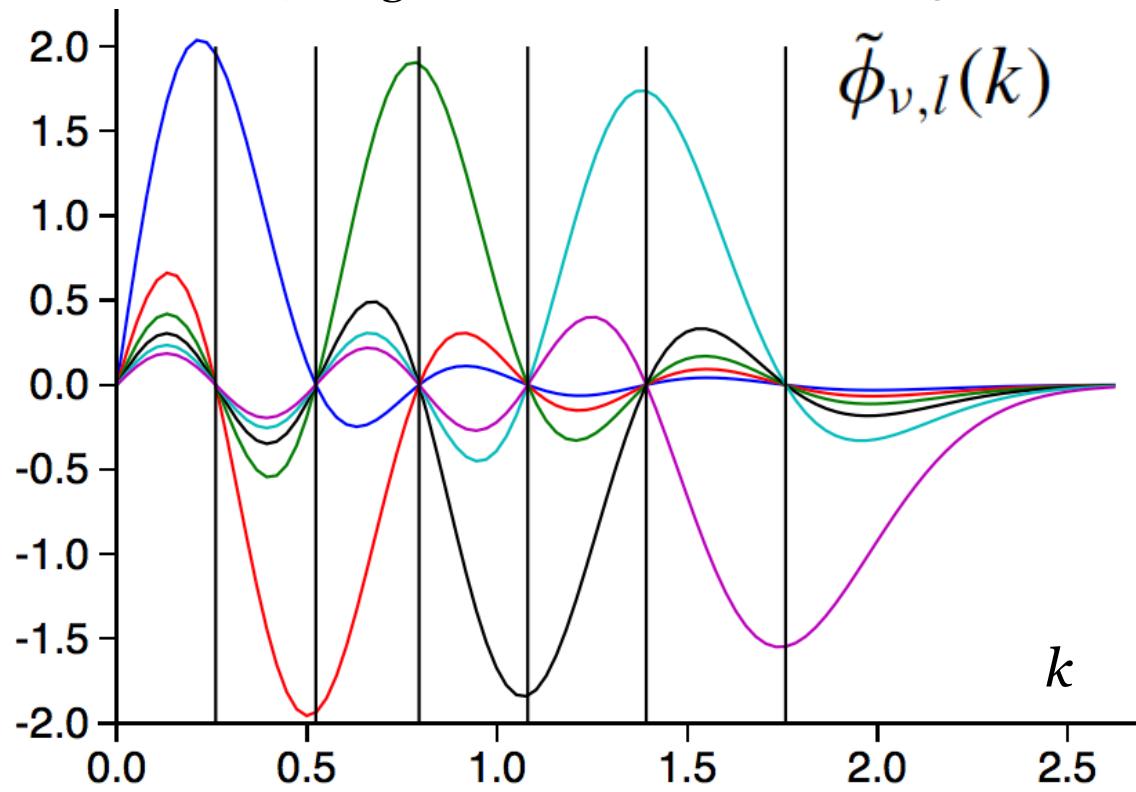
Eigenfunctions and eigenvalues of p^2

For a partial wave l in a Hilbert space with energies up to $(2N+l)\hbar\omega$, 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
 $\hbar\omega = 10$ MeV.
Vertical lines are
eigenvalues $k_{\mu l}$.



DVR yields simple matrix elements

1. Matrix elements in the DVR are just rescaled ME from continuum, evaluated at discrete momenta

$$\langle \phi_{\nu,l'} | \hat{V} | \phi_{\mu,l} \rangle = c_{\nu,l'} c_{\mu,l} \langle k_{\nu,l'}, l' | \hat{V} | k_{\mu,l}, l \rangle$$

2. Exact overlap between a Cartesian and a spherical oscillator state

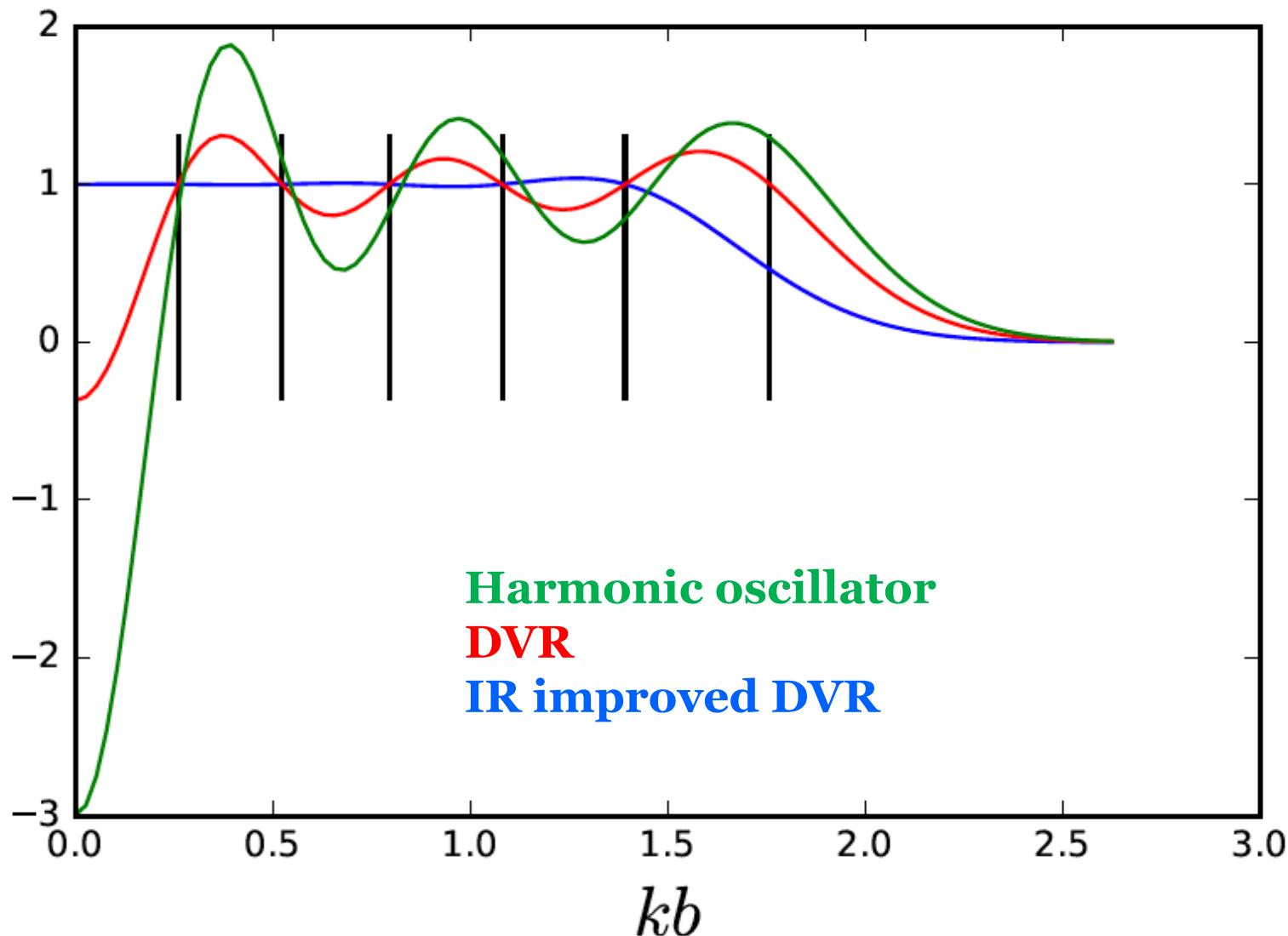
$$\langle \phi_{\mathbf{a}} | nlm \rangle = c_{\mathbf{a}} \tilde{\psi}_{n,l}(|\mathbf{k}_{\mathbf{a}}|) Y_{lm}(\hat{\mathbf{k}}_{\mathbf{a}})$$

3. Partial-wave decomposition made easy:

$$\begin{aligned} \langle n'l'm' | V_M^{(L)} | nlm \rangle_o &= C_{lmLM}^{l'm'} \frac{(-1)^l}{\sqrt{(2l'+1)(2L+1)}} \\ &\times \sum_{\mathbf{ab}} c_{\mathbf{a}}^2 c_{\mathbf{b}}^2 \tilde{\psi}_{n',l'}(|\mathbf{k}_{\mathbf{a}}|) \tilde{\psi}_{n,l}(|\mathbf{k}_{\mathbf{b}}|) \langle \mathbf{k}_{\mathbf{a}} | V^{(L)} | \mathbf{k}_{\mathbf{b}} \rangle \cdot \left\{ Y_l(\hat{\mathbf{k}}_{\mathbf{b}}) \times Y_{l'}(\hat{\mathbf{k}}_{\mathbf{a}}) \right\}^{(L)} \end{aligned}$$

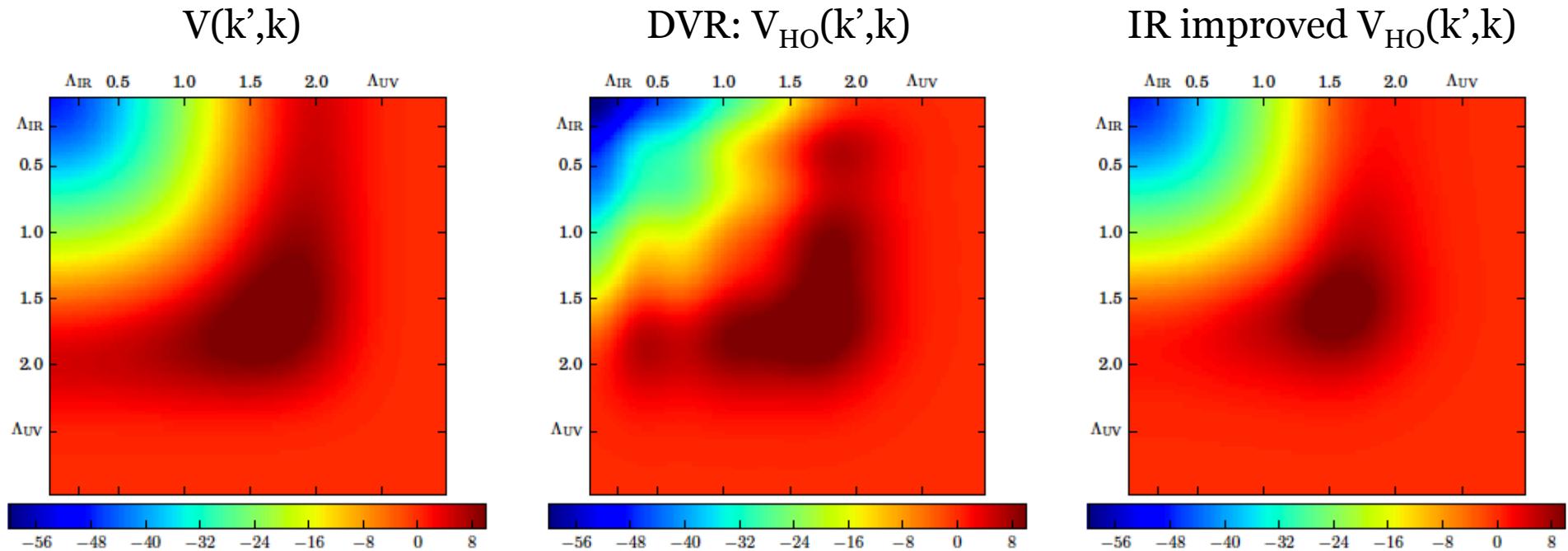
Restoring spherical symmetry à la [Bing-Nan Lu et al., PRD 92, 014506 (2015)]

Contact interactions, transformed back to momentum space



Matrix elements in a finite oscillator basis

Momentum-space matrix elements
 1S_0 channel of NNLO_{sim} with $\Lambda_\chi = 400$ MeV
 $E_{\max} = 10\hbar\omega$ in harmonic oscillator (6 s states)



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

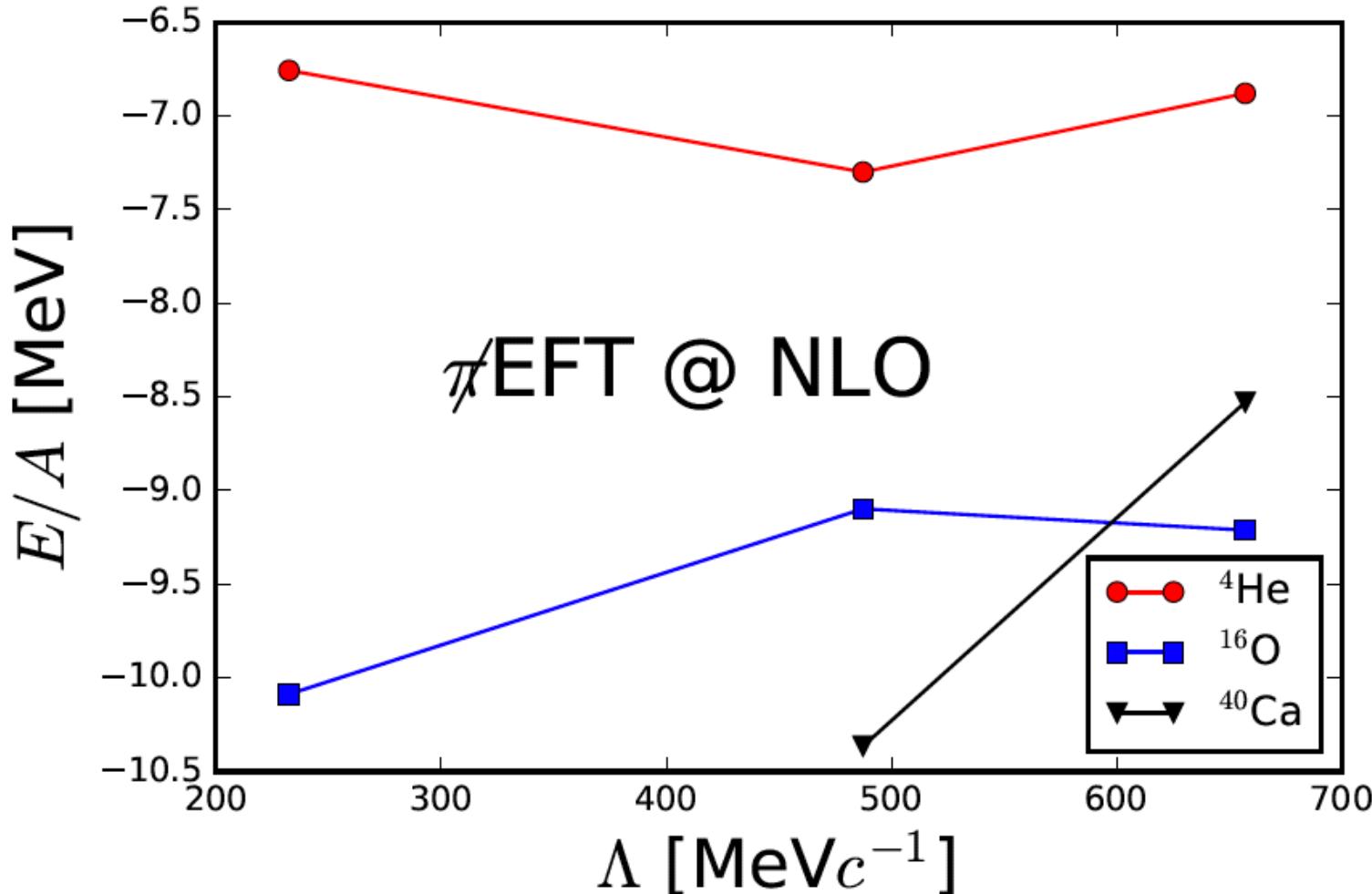
Pionless EFT for A>4

- 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]

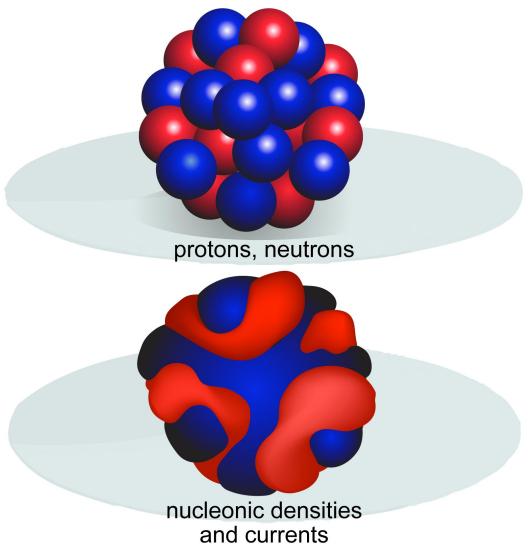
Here:

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

Preliminary results



EFT for nuclear vibrations



8
proton separation
energy in lead

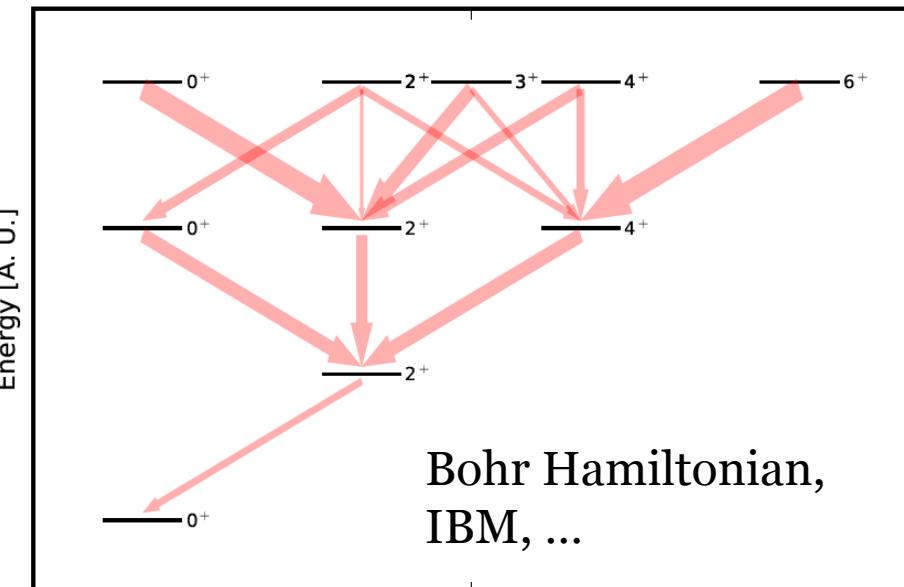
1.12
vibrational state in tin

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?”



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

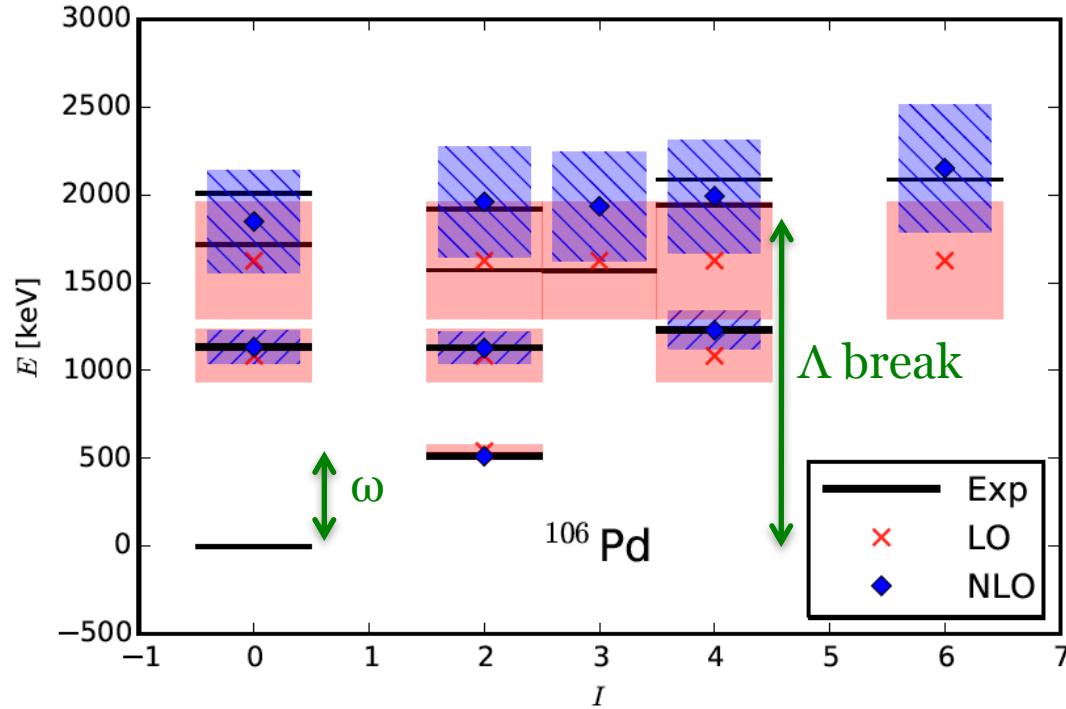


Spectrum and $B(E2)$ transitions of the *harmonic quadrupole oscillator*

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.

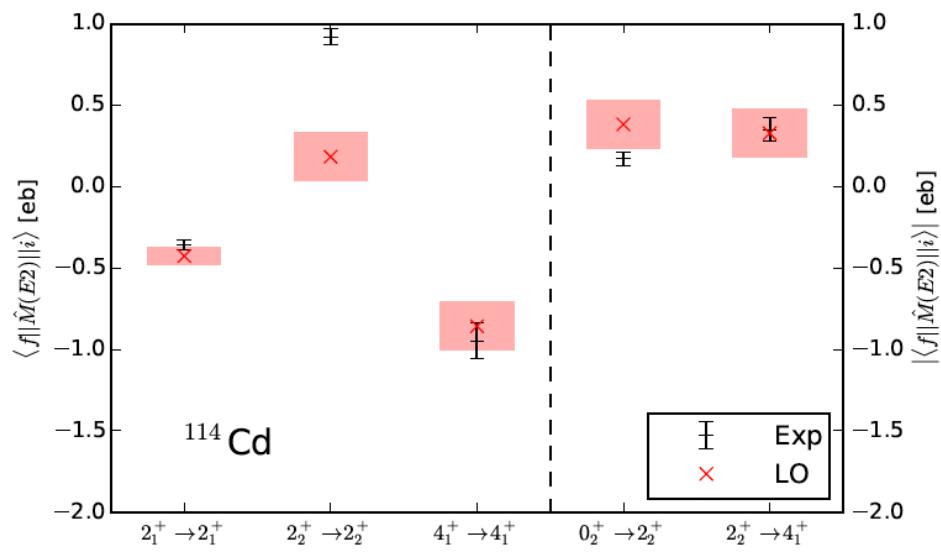
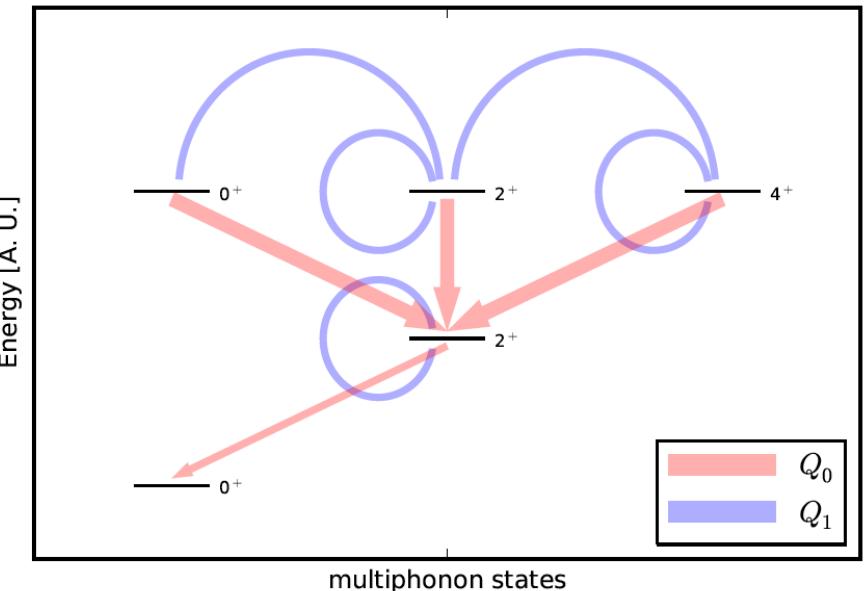
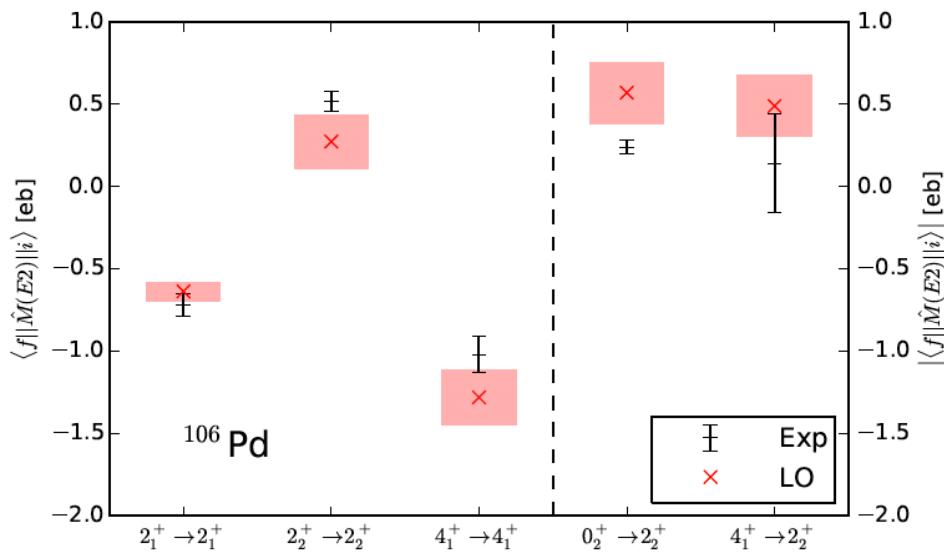
EFT result: sizeable quadrupole matrix elements are natural in size

In the EFT, the quadrupole operator is also expanded:

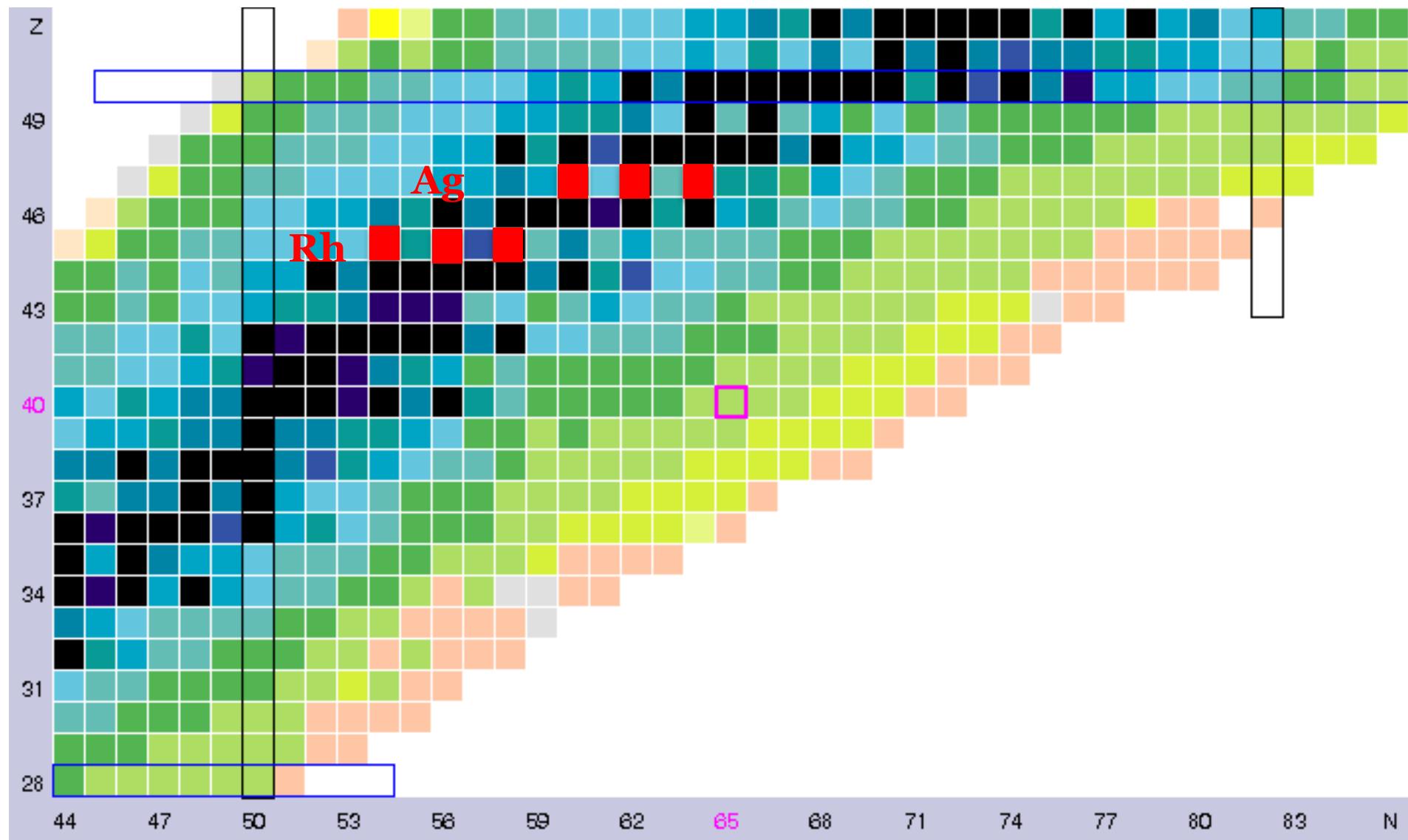
$$\hat{Q}_\mu = Q_0 \left(d_\mu^\dagger + \tilde{d}_\mu \right) + Q_1 \left(d^\dagger \times d^\dagger + \tilde{d} \times \tilde{d} + 2d^\dagger \times \tilde{d} \right)_\mu^{(2)}$$

Subleading corrections are sizable:

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



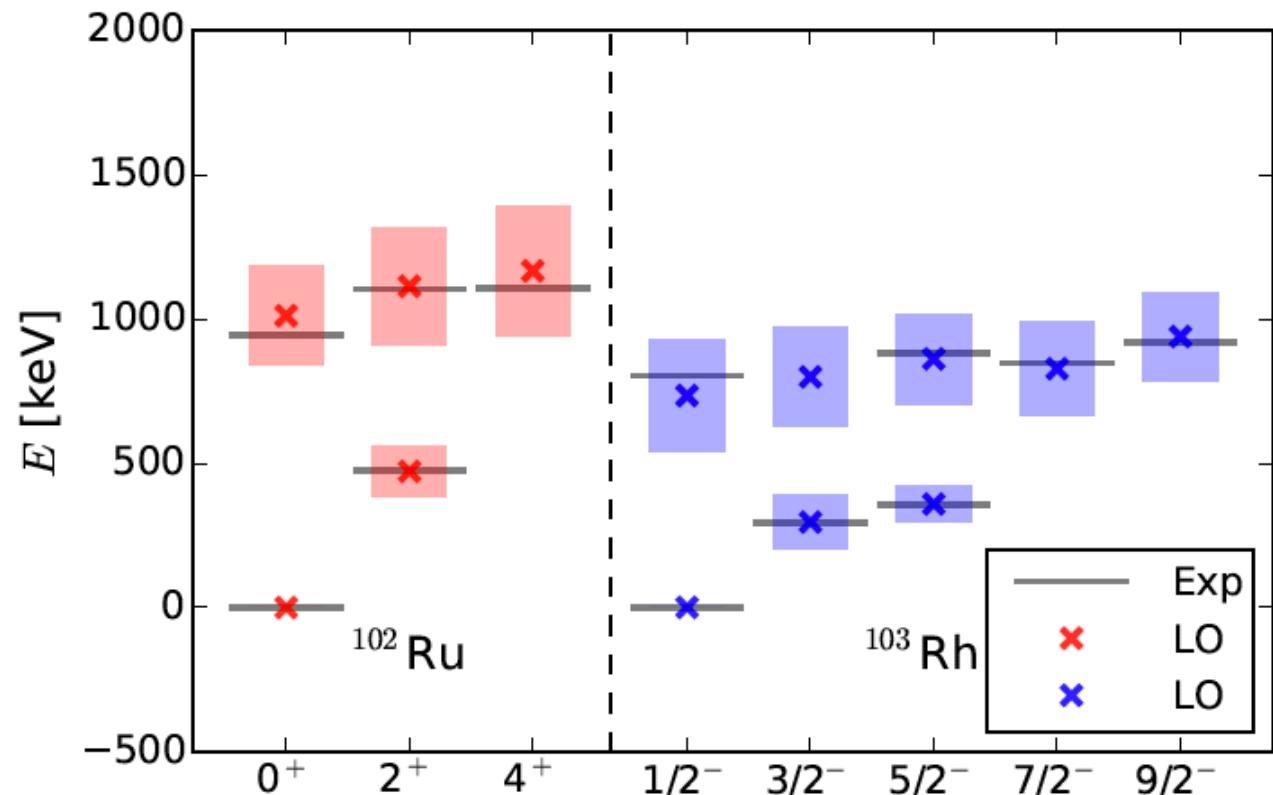
$^{99,101,103}\text{Rh}$ and $^{105,107,109,111}\text{Ag}$ as a proton coupled to $^{98,100,102}\text{Ru}$ and $^{104,106,108,110}\text{Pd}$, respectively, or $^{107,109,111}\text{Ag}$ as a proton-hole in $^{108,110,112}\text{Cd}$



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



Static E2 moments (in eb)

Nucleus	I_i^π	Q_{exp}	Q_{EFT}	Nucleus	I_i^π	Q_{exp}	Q_{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 fit to all data with EFT weighting.

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

Nucleus	I_i^π	$\mu_{\text{exp}}(I_i^\pi)$	$\mu_{\text{EFT}}(I_i^\pi)$	Nucleus	I_i^π	$\mu_{\text{exp}}(I_i^\pi)$	$\mu_{\text{EFT}}(I_i^\pi)$
^{102}Ru	2_1^+	0.85(3)*	0.85(5)	^{106}Pd	2_1^+	0.79(2)*	0.79(5)
	2_2^+		0.85(10)		2_2^+	0.71(10)	0.79(10)
	4_1^+		1.70(8)		4_1^+	1.8(4)	1.58(8)
	$\frac{1}{2}_1$	-0.088*	-0.088		$\frac{1}{2}_1$	-0.11*	-0.11
	$\frac{3}{2}_1$	0.77(7)	0.81(5)		$\frac{3}{2}_1$	0.98(9)	0.78(5)
	$\frac{5}{2}_1$	1.08(4)	0.76(5)		$\frac{5}{2}_1$	1.02(9)	0.68(4)
	$\frac{7}{2}_1$	2.0(6)	1.7(1)		$\frac{7}{2}_1$		1.6(1)
^{103}Rh	$\frac{9}{2}_1$	2.8(5)	1.6(1)		$\frac{9}{2}_1$		1.5(1)

At LO, one new LEC enters to describe the magnetic moments in the odd-mass neighbor

Summary

- IR extrapolations
 - Lüscher-like formulas for energies, radii, quadrupole moments, transitions, radiative capture reactions
 - Compute at fixed Λ and IR extrapolate on all data.
- DVR in HO basis economical implementation of EFT
 - DVR in momentum space
 - fast convergence of many-body calculations
- Pion-less EFT
 - bound ^{16}O , ^{40}Ca at nonperturbative NLO for cutoffs $200 < \Lambda < 700$ MeV
- EFT for nuclear vibrations
 - Picture of anharmonic vibrations consistent with data within uncertainties

Hamiltonian

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

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

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

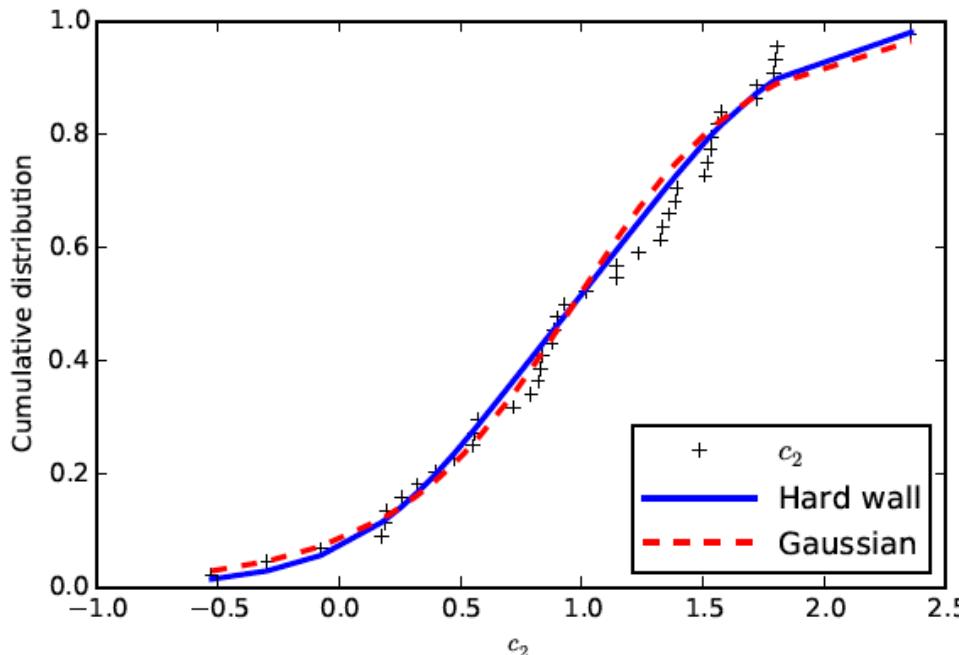
Uncertainty quantification

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

$$c_2 \equiv c_2(N, v, I)$$

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

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



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.

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

$$p_M(\Delta|c_0, \dots, c_k) = \frac{\int_0^\infty dc \, \text{pr}(c) p_M(\Delta|c) \prod_{m=0}^k \text{pr}(c_m|c)}{\int_0^\infty dc \, \text{pr}(c) \prod_{m=0}^k \text{pr}(c_m|c)}$$

Lüscher formulas for many-body systems

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 $T_{\text{kin}} = p^2$	Diagonalize A-body T_{kin}	Diagonalize A-body T_{kin}
3D spherical cavity	A fermions in 3D cavity	3(A-1) hyper-radial cavity

$$L_2 = \sqrt{2(N + 3/2 + 2)}b \quad L_{\text{eff}} = \left(\frac{\sum_{nl} \nu_{nl} a_{l,n}^2}{\sum_{nl} \nu_{nl} \kappa_{l,n}^2} \right)^{1/2} \quad L_{\text{eff}} = b \frac{X_{1,\mathcal{L}}}{\sqrt{T_{1,\mathcal{L}}(N_{\max}^{\text{tot}})}}$$

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

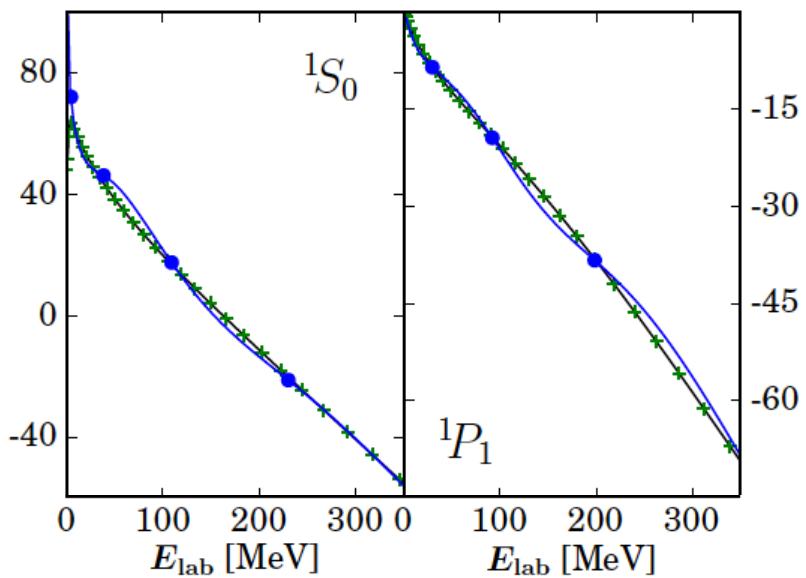
Furnstahl, Hagen, TP,
Wendt, J. Phys. G 42,
034032 (2015)

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

Chiral interaction at NLO in the oscillator basis

- Construct and optimize interaction in oscillator basis
- UV convergence by construction
- NLO interaction constructed with $E_{\max} = 10\hbar\omega$ at $\hbar\omega = 22$ MeV
- Rapid convergence of ground-state energies even for heavy nuclei

Phase shifts compared to NLO_{sim}



Convergence of ground-state energies

N_{\max}	^4He	^{16}O	^{40}Ca	^{90}Zr	^{132}Sn
	$E_{\text{CCSD}} [\text{MeV}]$				
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