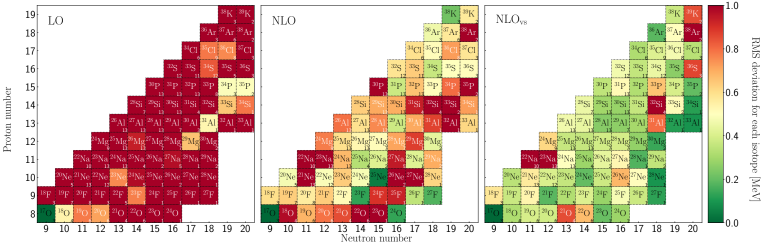
Shell-model interactions from chiral effective field theory

Lukas Huth, 04.10.2017



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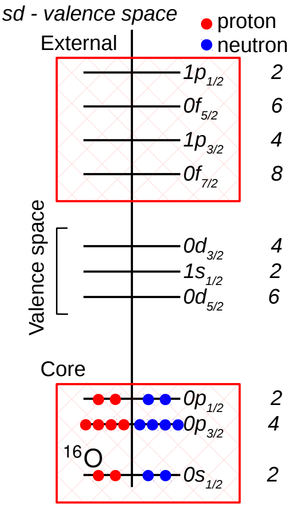
Outline

- Introduction
  - Nuclear shell model
  - Chiral effective field theory
  - Motivation
- Valence-shell interactions
- Results
  - Ground-state energies and spectra
  - Predictions
- Summary & outlook

Nuclear shell model

- Define a core
- Space above the core forms the valence space
  Valence space is filled with valence nucleons that interact with each other in a valence shell
  $\Rightarrow$ particle-hole excitations
- External space
  assumption: effects of external space and core can be included in effective Hamiltonian



Effective Hamiltonian usually consists of single-particle energies (SPEs) and two-body matrix elements (TBMEs)

SPEs taken, e.g., from core+1 spectrum

TBMEs two-body interaction among valence nucleons

Effective Hamiltonians

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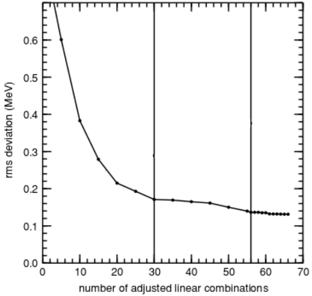
Traditional shell-model interactions:

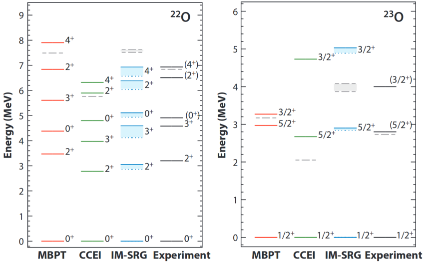
- fitted to ground-state and excitation energies in a valence space
- very successful reproduction of experimental data ($\sim$ 100 keV RMS)



Brown and Richter, PRC (2006)

Ab initio approaches:

- NCSM, IM-SRG, ... (see Vobig)
- based on two- and three-body forces
- modern approaches use chiral effective field theory (EFT)



Hebeler et al., Ann. Rev. Nucl. and Part. Sci. (2015)

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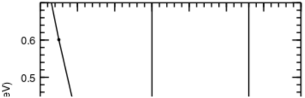

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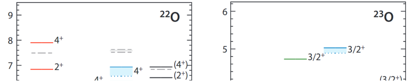
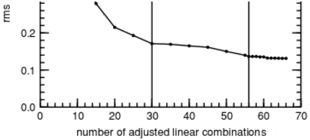


derive shell-model interactions based on chiral EFT



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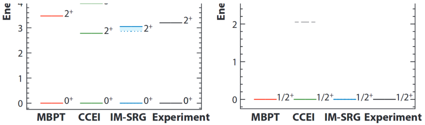

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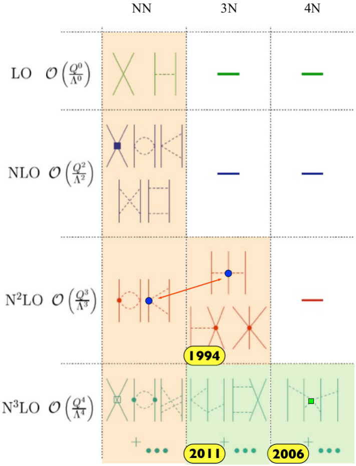
Chiral effective field theory



Hebeler et al. Eur. Phys. J. (2014)

- diagrams are ordered in $(Q/\Lambda)^\nu$, with:
  Q = typical momentum scale
  Λ = breakdown scale of the theory
- nucleon-nucleon contacts:
  low-energy constants (LECs)
  $\Rightarrow$ adjusted to data
- pion exchanges: dashed lines
  (long-range part of interactions)
- three- and many-body interactions
  arise naturally

Operators from chiral EFT contacts

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For a free-space interaction:

- at any given order ν, we obtain operators proportional to momentum$^\nu$ (momentum transfer: $\mathbf{q} = \mathbf{p} - \mathbf{p}'$ and average momentum : $\mathbf{k} = \frac{1}{2}\left(\mathbf{p} + \mathbf{p}'\right)$ with final and initial relative momenta $\mathbf{p}$ and $\mathbf{p}'$)
- according to the spin part, interactions can be central, vector, and tensor

$$V_{\text{cont}}^{\text{NLO}}(\mathbf{p}, \mathbf{p}') = C_S + C_T\,(\sigma_1 \cdot \sigma_2) + C_1\mathbf{q}^2 + C_2\mathbf{k}^2 + C_3\mathbf{q}^2\,(\sigma_1 \cdot \sigma_2) + C_4\mathbf{k}^2\,(\sigma_1 \cdot \sigma_2)$$
$$+ C_5\,\mathrm{i}\,(\mathbf{q} \times \mathbf{k}) \cdot (\sigma_1 + \sigma_2) + C_6\,(\mathbf{q} \cdot \sigma_1)\,(\mathbf{q} \cdot \sigma_2) + C_7\,(\mathbf{k} \cdot \sigma_1)\,(\mathbf{k} \cdot \sigma_2)$$

In the valence space:

- presence of a core defines a reference frame for the system
  $\Rightarrow$ Galilean invariance gets broken
- interaction may depend explicitly on the center-of-mass momentum **P**
  $\Rightarrow$ new operator structures

Schwenk, Friman, PRL (2004)

Valence-space specifics

- valence-space (vs) operators, e.g.:

$$V_{\text{cont}}^{\text{NLO}_{\text{vs}}}(\mathbf{p},\mathbf{p}',\mathbf{P}) = V_{\text{cont}}^{\text{NLO}}(\mathbf{p},\mathbf{p}') + P_1\,\mathbf{P}^2 + P_2\,\mathbf{P}^2(\sigma_1\cdot\sigma_2) + P_3\,\mathrm{i}\,(\mathbf{q}\times\mathbf{P})\cdot(\sigma_1-\sigma_2)$$
$$+ P_4\,(\mathbf{k}\times\mathbf{P})\cdot(\sigma_1\times\sigma_2) + P_5\,(\mathbf{P}\cdot\sigma_1)\,(\mathbf{P}\cdot\sigma_2)$$

- regulators:
  valence-space limits the maximal momenta $\sim \Lambda_{\text{HO}} = \sqrt{2N+7} \approx 375$ MeV

  König et al., PRC (2014)

  no need for additional regulators
- fit to 441 states in the *sd* shell with χ^2 minimization (for now: $\sigma_k^{\text{theo}} = 100$ keV)

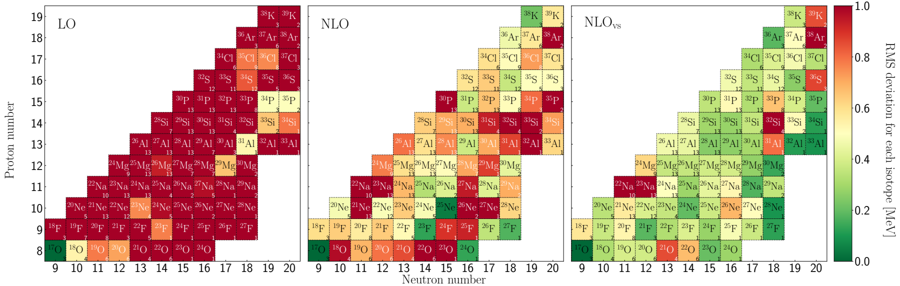
$$\chi^2 = \sum_{k=1}^{441} \frac{\left(\mathrm{E}_k^{\text{exp}} - \mathrm{E}_k^{\text{theo}}\right)^2}{(\sigma_k^{\text{exp}})^2 + (\sigma_k^{\text{theo}})^2}$$

- shell-model diagonalizations with ANTOINE

Nowacki, Caurier, Acta Phys. Pol. (1999)

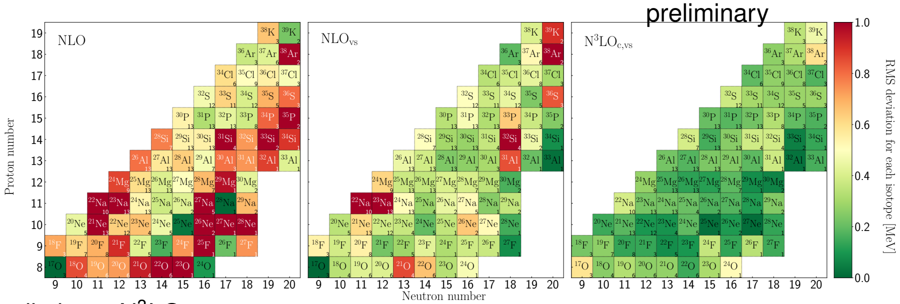
Caurier et al., Rev. Mod. Phys. (2005)

Fit performance



- striking improvement from LO to NLO to NLO$_{vs}$
- LO interaction has too few parameters to handle this data set
- overall: small RMS deviation at NLO$_{vs}$ with few statistical outliers (^{21}O,^{22,23}Na, ^{32}Si and ^{36}S)

Preliminary N^{3}LO results

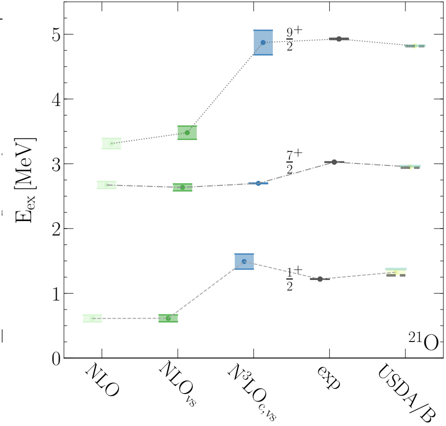


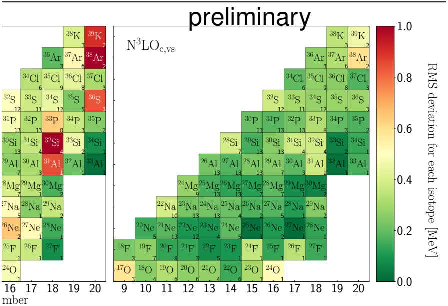
Preliminary N^{3}LO$_{c,vs}$:

- determined by 24 free-space LECs + 5 NLO vs LECs + NLO pion exchange + 10 Central N^{3}LO vs LECs + 3 SPE
- NLO outliers (^{21}O,^{22,23}Na, ^{32}Si and ^{36}S) improve drastically at N^{3}LO$_{vs}$

$\Rightarrow$ Promising behavior of preliminary results

Preliminary N^3LO results





P… 5 NLO vs LECs + NLO pion exchange

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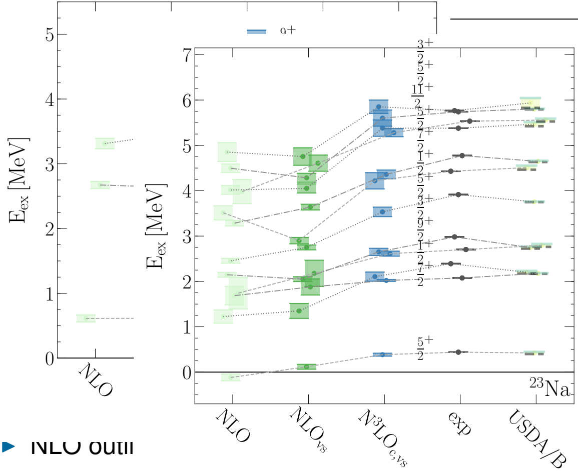
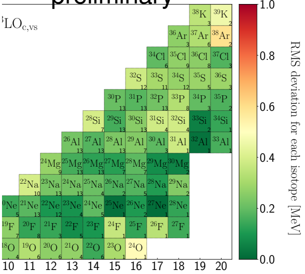
⇒ Promising behavior of preliminary results

Preliminary N^{3}LO results

preliminary





P

Cs + NLO pion exchange

- NLO outl

astically at N^{3}LO$_{vs}$

⇒ Promising behavior of preliminary results

Preliminary N^{3}LO results

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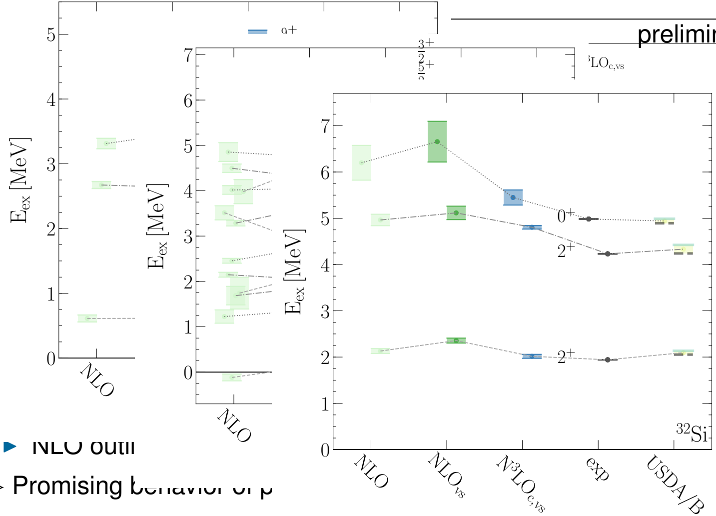
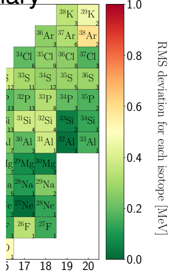
preliminary





P|

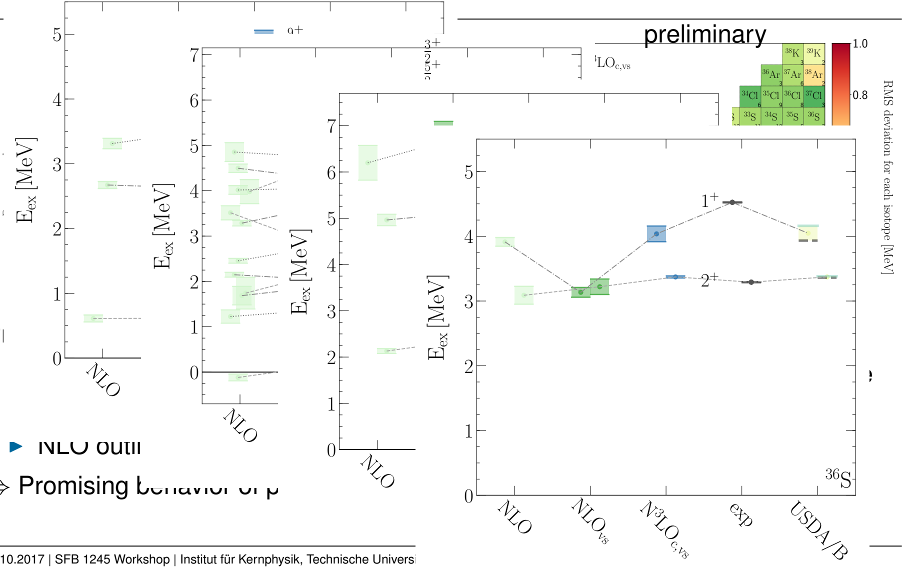
on exchange

- NLO outl

N^{3}LO$_{vs}$

⇒ Promising behavior of p

Preliminary N^3LO results



Pl

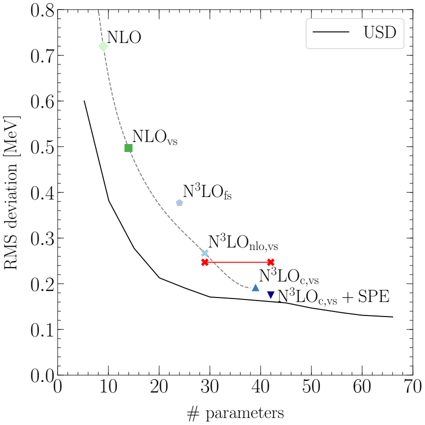
► NLO outl

⇒ Promising behavior of p

Fit performance

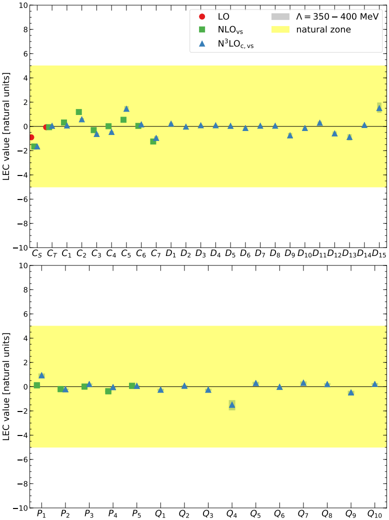
Interaction	#LECs	RMS [MeV]	USD RMS [MeV]
LO	2	1.77	-
NLO	9	0.72	0.43
$\mathrm{NLO_{vs}}$	14	0.50	0.30
$\mathrm{N^3LO^{nat}_{c,vs}}$+SPE	29	0.25	0.17
$\mathrm{N^3LO_{c,vs}}$+SPE	42	0.17	0.16

- systematics comparable to USD type interactions
- best RMS fit: close to USD, but unnatural LECs
- natural fit: only adjusts 29 linear combinations of the parameter set due to properties of the fit algorithm



Brown and Richter, PRC(2006)

LECs



Natural values at different orders can be calculated as follows:

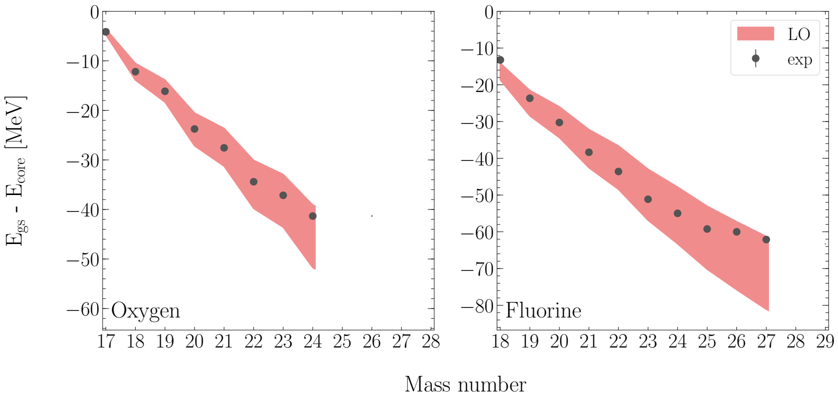
$$C^{\text{nat}}_{\text{LO}} = C_{\text{LO}} \cdot F_\pi^2$$

$$C/P^{\text{nat}}_{\text{NLO}} = C/P_{\text{NLO}} \cdot F_\pi^2 \Lambda^2_{\text{H.O.}}$$

$$D/Q^{\text{nat}}_{\text{N}^3\text{LO}} = D/Q_{\text{N}^3\text{LO}} \cdot F_\pi^2 \Lambda^4_{\text{H.O.}}$$

- LECs up to NLO$_{\text{vs}}$ are of natural size
- N^{3}LO$_{\text{c,vs}}$:
  - For now, we only use NLO pion exchange
  - Only central vs contributions at N^{3}LO
- Cutoff Λ = 375 MeV is only an estimate, (large) bands for variation of 25 MeV

Ground-state energies



- LO slightly too attractive in the neutron-rich region

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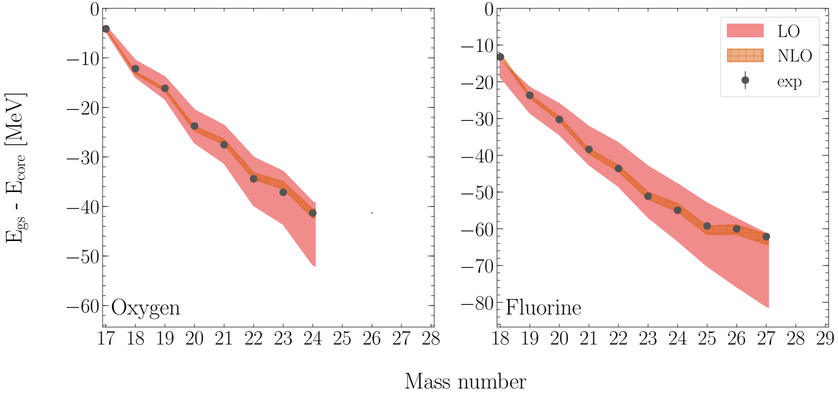

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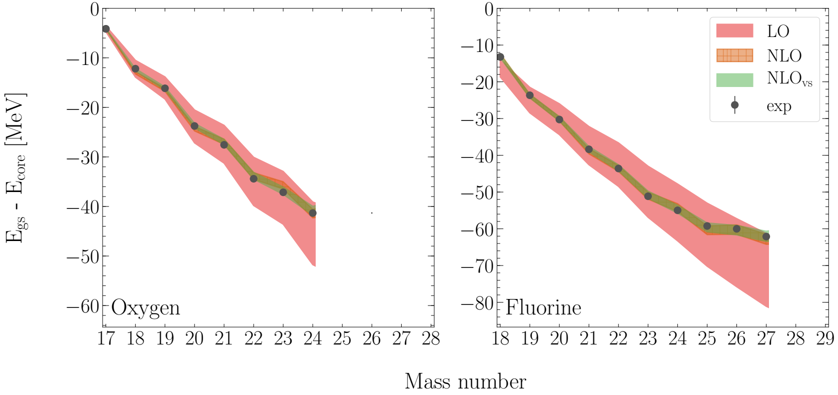

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- NLO and NLO_{vs} ground states overlap most of the time

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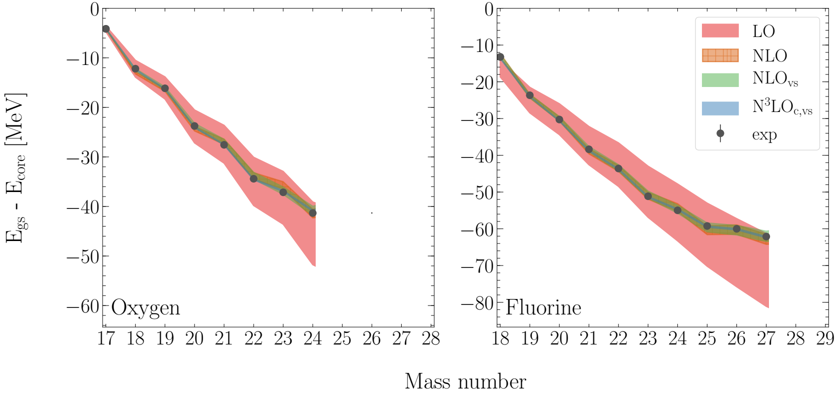

- LO slightly too attractive in the neutron-rich region
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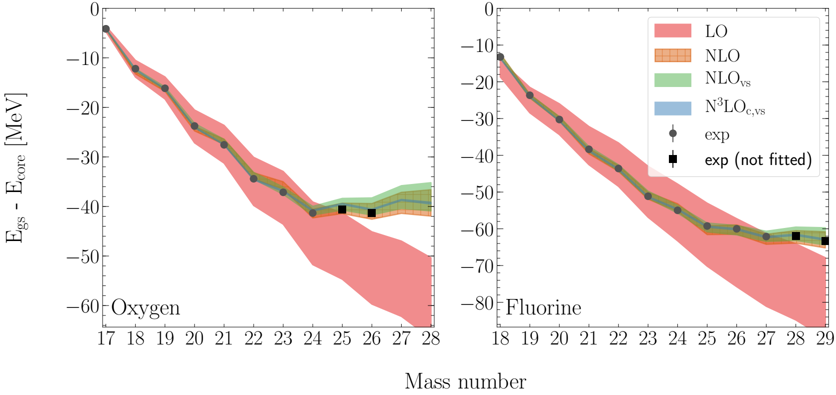
- Preliminary N^3LO interaction shows good agreement with experiment

Ground-state energies: Predictions



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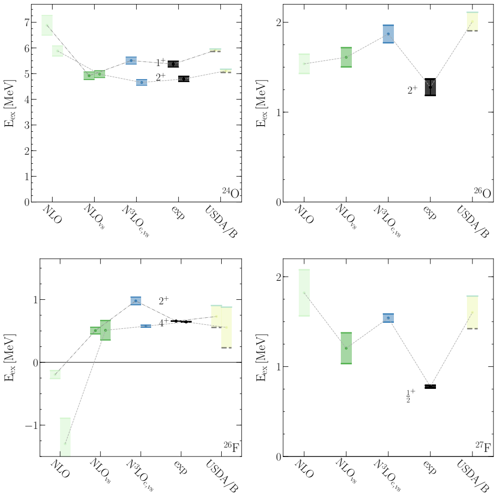
Spectra: Predictions



^{24}O:

- 2^+ and 1^+ reproduced at N^3LO

^{26}O:

- almost reproduced at NLO and NLO_{vs}
- N^3LO is too high in energy

^{26}F:

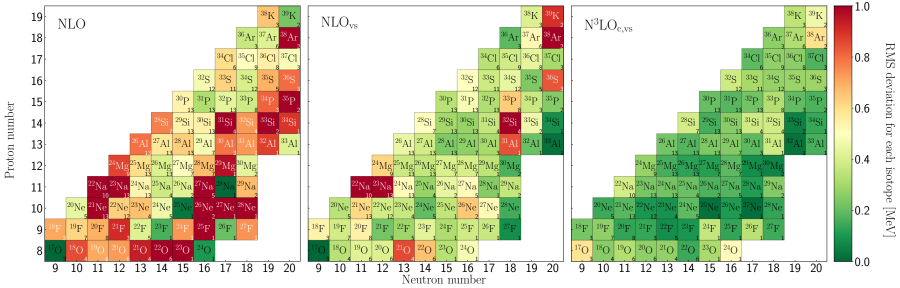
- reproduced within uncertainties at NLO_{vs}
- corrrect splitting but energies too low at N^3LO

^{27}F:

- trend towards right direction compared to NLO

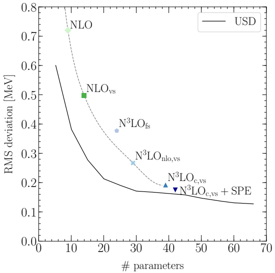
Summary

- shell-model interactions based on chiral EFT operators show promising results and order-by-oder improvement
- Galilean invariance breaking operators that depend on CM momentum
  $\Rightarrow$ vastly improve reproduction of experiment at NLO
- preliminary N^{3}LO results show promising improvement



Outlook

- include all cm operators at N^3LO
- calculations beyond the sd-shell and for cross-shell interactions
- need to better understand uncertainty estimates



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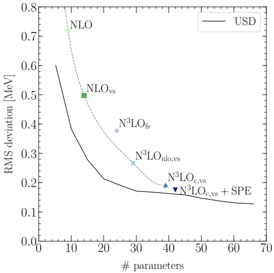
Thank you for your attention!

Collaborators: **V. Durant**, J. Simonis and A. Schwenk



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Uncertainty estimates

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In subsequent plots we show chiral EFT uncertainty estimates with $Q = \frac{m_\pi}{\Lambda_b} \approx 0.4$:

Epelbaum et al., EPJA (2015)

- Uncertainties (usual approach)

$$\Delta E_{\mathrm{LO}} = |E_{\mathrm{LO}}|Q^2 \,,$$

$$\Delta E_{\mathrm{NLO}} = \max\left(|E_{\mathrm{LO}}|Q^3 \,, |E_{\mathrm{LO}} - E_{\mathrm{NLO}}|Q\right) \,,$$

$$\Delta E_{\mathrm{N^2LO}} = \max\left(|E_{\mathrm{LO}}|Q^4 \,, |E_{\mathrm{LO}} - E_{\mathrm{NLO}}|Q^2 \,, |E_{\mathrm{NLO}} - E_{\mathrm{N^2LO}}|Q\right) \,,$$

$$\Delta E_{\mathrm{N^3LO}} = \max\left(|E_{\mathrm{LO}}|Q^5 \,, |E_{\mathrm{LO}} - E_{\mathrm{NLO}}|Q^3 \,, |E_{\mathrm{NLO}} - E_{\mathrm{N^2LO}}|Q^2 \,, |E_{\mathrm{N^2LO}} - E_{\mathrm{N^3LO}}|Q\right) \,.$$

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- **Uncertainties here** (preliminary) Epelbaum et al., EPJA (2015)

$$\Delta E_{\mathrm{LO}} = \max\left(|E_{\mathrm{LO}}|, E_{\mathrm{sd}}^{\mathrm{av}}\right) Q^2 \,,$$

$$\Delta E_{\mathrm{NLO}} = \max\left(\max\left(|E_{\mathrm{LO}}|, E_{\mathrm{sd}}^{\mathrm{av}}\right) Q^4 \,, |E_{\mathrm{LO}} - E_{\mathrm{NLO}}| Q^2\right) \,,$$

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- Include average SPE spacing $E_{\mathrm{sd}}^{\mathrm{av}} \approx 3$ MeV to assign more conservative values to low-lying excitations
- $\frac{q}{2m_\pi}$ expansion in TPE: contributions beyond OPE are absorbed by LECs $\Rightarrow$ no Q^3
- Consequently NLO uncertainty estimates corrections from $N^3LO \Rightarrow Q^x \rightarrow Q^{x+1}$ (same thing happens at N^3LO with corrections from Q^6)

Truncations

Full calculations provide all states of interest but reach computational limit quickly

Example:

$^{16}O \longrightarrow 8\text{ n} + 8\text{ p}$
$0s, 0p, 1s0d, 1p0f \longrightarrow$ 40 places each (n and p)

Resulting matrix dimension:

$$d = \binom{40}{8}^2 \sim 10^{15}$$

technical limit is at $d \sim 10^9 - 10^{10}$

$\Rightarrow$ **Truncations are necessary in large nuclei**

Truncations:

- State maximum orbit
  (See example)
  $\Rightarrow$ Full configuration
- Limit p-h excitations
  $\Rightarrow$ Configuration interaction
- Energy truncation in $N\hbar\Omega$
  $\Rightarrow$ No core shell model
- Effective Hilbert space
  with respect to a given core
  So called **valence space**
  $\Rightarrow$ Standard shell model

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- Galilean invariance breaking operators that depend on CM momentum $\Rightarrow$ vastly improve reproduction of experiment at NLO
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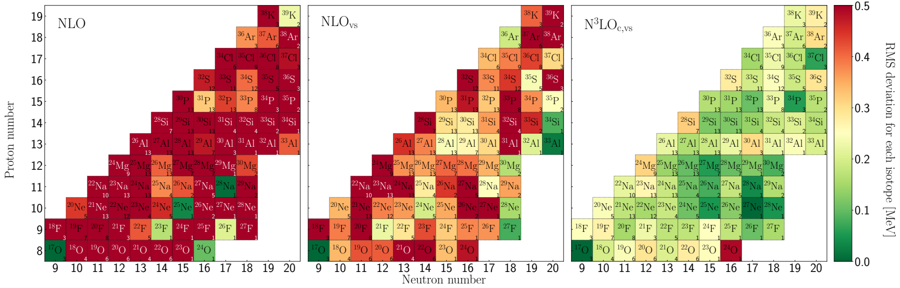

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N^3LO_{fs}	24	0.38	0.20
$N^3LO_{nlo,vs}$	29	0.27	0.17
$N^3LO_{c,vs}$	39	0.19	0.17

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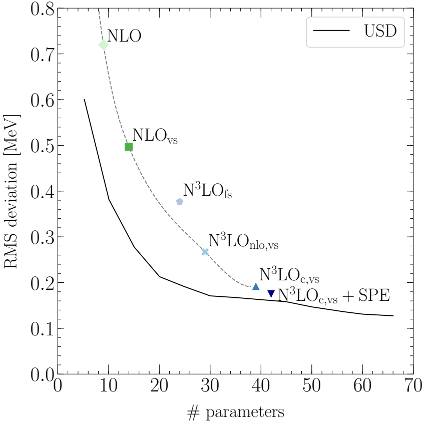
- largest source of improvement from central **P** operators
- Preliminary N^3LO results fit into systematics



Brown and Richter, PRC(2006)

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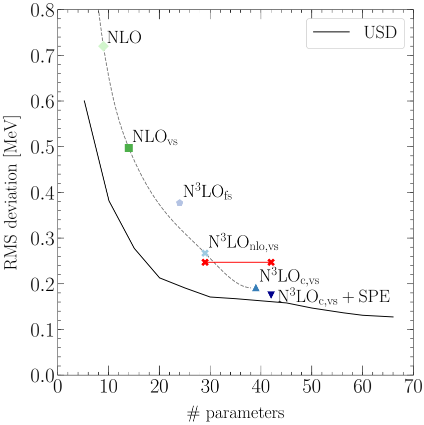

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