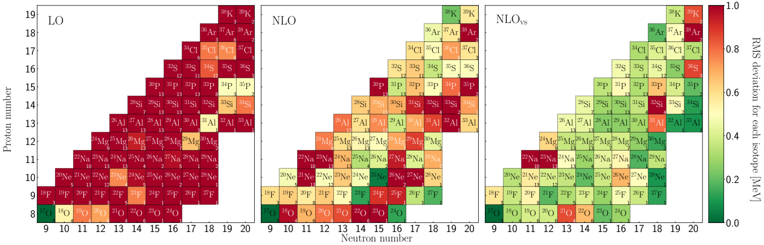
# Shell-model interactions from chiral effective field theory

TECHNISCHE UNIVERSITÄT DARMSTADT

Lukas Huth, 06.11.2017

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# Outline

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

# Nuclear shell model

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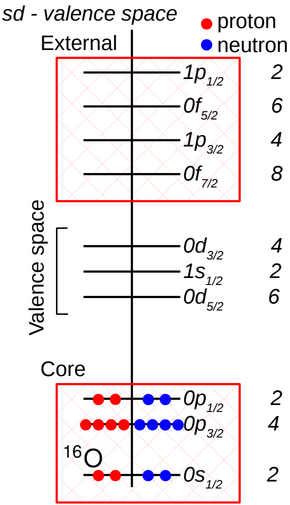
- Define a core
- Valence space above core
  Valence nucleons interact through effective interactions
- External space
  Assumption: effects of external space and core can be included in effective Hamiltonian



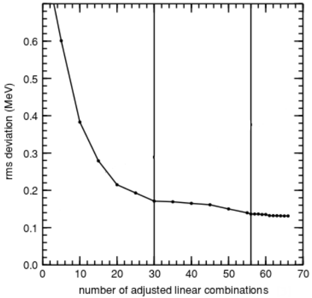

Effective Hamiltonian usually consists of single-particle energies (SPEs) and two-body matrix elements (TBMEs)

**SPEs** taken, e.g., from core+1 spectrum
**TBMEs** two-body interaction among valence nucleons

# Effective Hamiltonians

Traditional shell-model interactions:

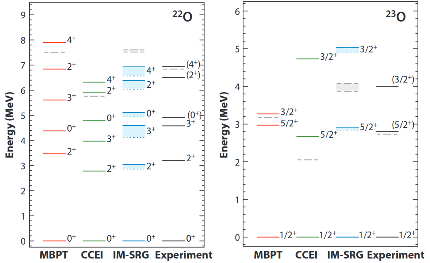
- Fitted to ground-state and excitation energies in a valence space
- Very successful reproduction of experimental data ($\sim$ 100 keV RMS)




Brown and Richter, PRC (2006)

Ab initio approaches:

- NCSM, CC, IM-SRG, ...
- Based on few-body forces
- Modern approaches use chiral effective field theory (EFT)




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

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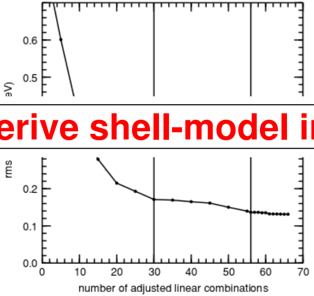


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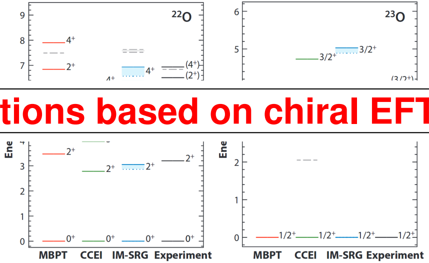



Hebeler et al., Annu. Rev. Nucl. and Part. Sci. (2015)

**derive shell-model interactions based on chiral EFT**

# Chiral EFT contact interactions

For a free-space interaction:

- According to the spin part, interactions can be central, vector, and tensor

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

- Fit low-energy constants (LECs) to ground-state and excitation energies

In the valence space:

- Valence-space limits the maximal momenta (here HO length $b \approx 1.7$ fm)

$$\Lambda_{\text{HO}} = \sqrt{2N+7}/b \overset{sd}{\approx} 375\ \text{MeV}$$

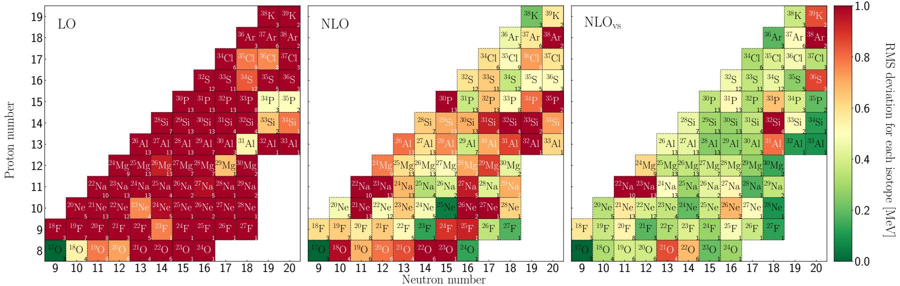
König et al., PRC (2014)

- Presence of a core defines a reference frame for the system
  $\Rightarrow$ core breaks Galilean invariance
  (explicit dependence on center-of-mass momentum **P**)

Schwenk, Friman, PRL (2004)

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

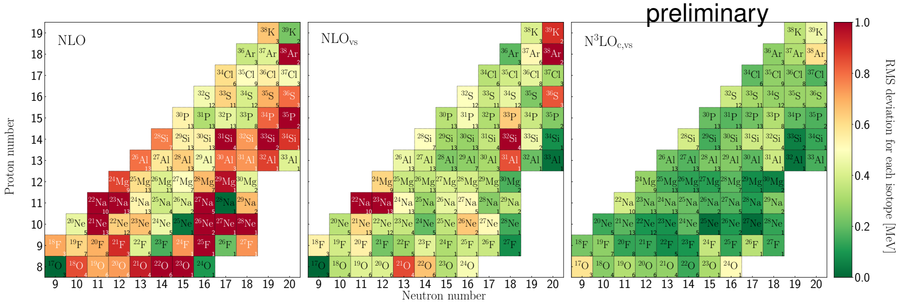
# Fit performance




- Striking improvement from LO to NLO to NLO$_{\text{vs}}$
- LO errors larger than present $\sigma_{\text{th}}$
- Overall: small RMS deviation at NLO$_{\text{vs}}$ with few statistical outliers ($^{21}$O,$^{22,23}$Na, $^{32}$Si and $^{36}$S)

LH, V. Durant, J. Simonis, and A. Schwenk, in prep.

# Preliminary $N^3LO$ results




Preliminary $N^3LO_{c,vs}$:

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

$\Rightarrow$ Promising behavior of preliminary results

# Uncertainty estimates

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- Start with EKM uncertainties

Epelbaum et al., EPJA (2015)

$$\Delta X^{(\mathrm{LO})}_{\nu=0} = |X_{\nu=0}| Q^2 \,,$$
$$\Delta X^{(\mathrm{NLO})}_{\nu=2} = \max\left(\Delta X_{\nu=0}\,, |X_{\nu=2} - X_{\nu=0}|\right) Q \,,$$
$$\Delta X_{\nu} = \max\left(\Delta X_{\nu-1}, |X_{\nu} - X_{\nu-1}|\right) Q \,.$$

with $Q = \max\left(\cancel{\frac{p}{\Lambda}}, \frac{m_\pi}{\Lambda}\right)$

and $\Lambda = \Lambda_{\mathrm{HO}} \approx 375$ MeV

here: $X$ can be a ground-state energy or excitation energy

- Calculate LO uncertainty in reference to mean-field (mf) effects

$$\Delta X^{(\mathrm{LO})}_{\nu=0} \to |X_{\nu=0} - X_{\mathrm{mf}}| Q^2 \,.$$

- For now: study uncertainties after fit, next step include while fitting

# Uncertainty estimates

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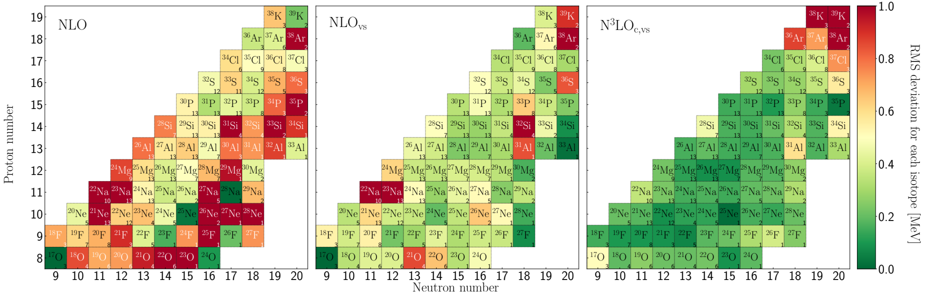
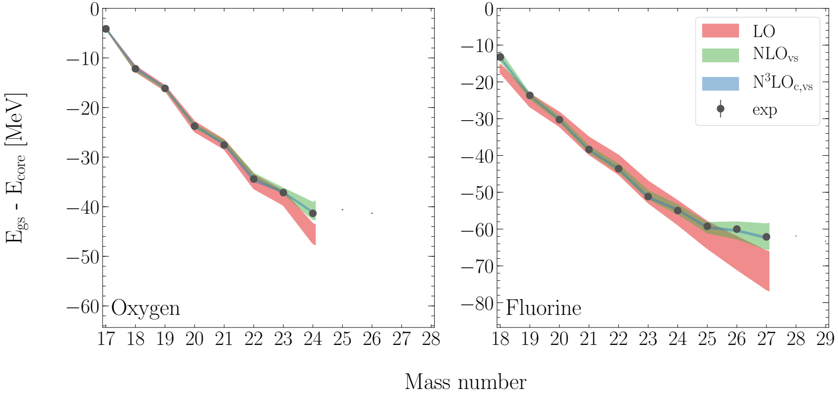



- For now: study uncertainties after fit, next step include while fitting
  Very preliminary $N^3LO$ includes those uncertainties (iteratively)
  Potassium gs uncertainty is dominated by LO uncertainty

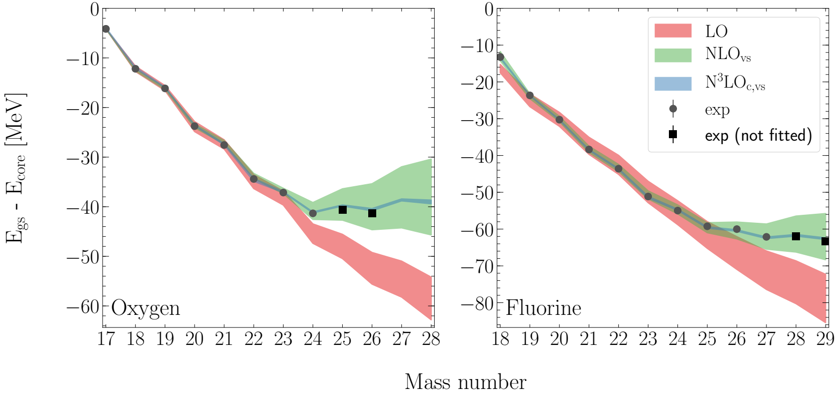
$$\Delta E \sim 200 \cdot Q^5 \text{ MeV} \approx 1.5 \text{ MeV}$$

# Ground-state energies




- LO slightly too attractive in the neutron-rich region
- $NLO_{vs}$ corrects this LO behavior (uncertainty dominated by difference to LO)
- Preliminary $N^3LO$ follows this trend

# Ground-state energies: Predictions

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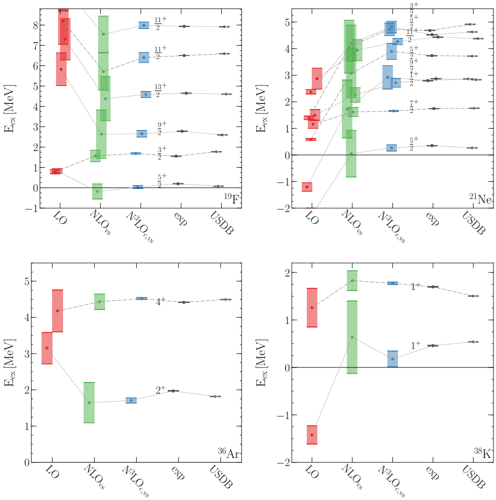
# Spectra



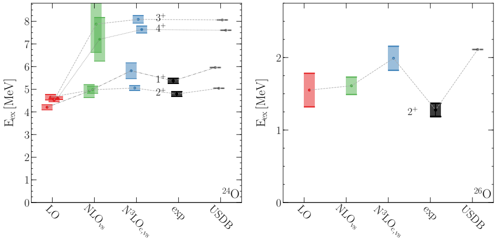

$^{19}$F and $^{21}$Ne:

- Order by order improvement
- Most uncertainties dominated by $|E_{LO} - E_{NLO}|$

$^{36}$Ar and $^{38}$K:

- Outliers of very preliminary N$^3$LO must be due to deviations in the gs
- Also here, order by order improvement

# Spectra: Predictions




$^{19}$F and $^{21}$Ne:

- Order by order improvement
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$^{36}$Ar and $^{38}$K:

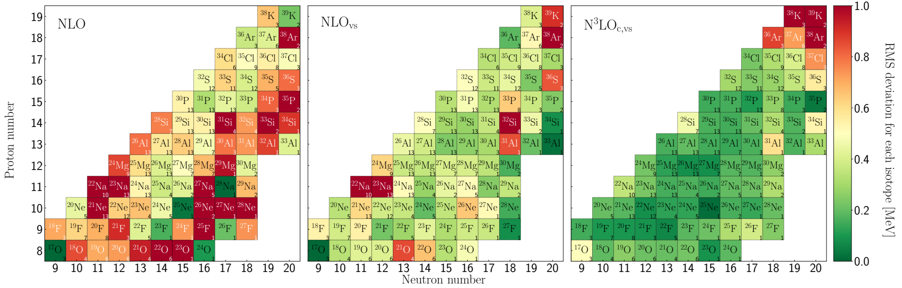
- Outliers of very preliminary N$^3$LO must be due to deviations in the gs
- Also here, order by order improvement

$^{24}$O and $^{26}$O:

- Very good agreement for $^{24}$O
- $^{26}$O prediction gets a bit worse at N$^3$LO

# Summary

- Shell-model interactions based on chiral EFT operators show promising results and order-by-oder improvement
- With (for now) post-processing EKM uncertainties
- Very preliminary: fit with EKM uncertainties for $N^3LO$



# Outlook

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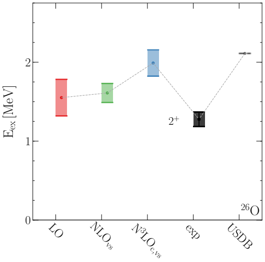
Valence-space interaction:

- Include all cm operators at $N^3LO$
- Investigate $q/(2m_\pi)$ expansion of TPE
- Calculations beyond the sd-shell and for cross-shell interactions




Uncertainties:

- LO is insufficient to describe the dataset:
  Most uncertainties are either dominated by the LO uncertainty or the difference between LO and NLO (investigate Bayesian methods)
- Include EFT uncertainties in all fits

# Outlook

Valence-space interaction:

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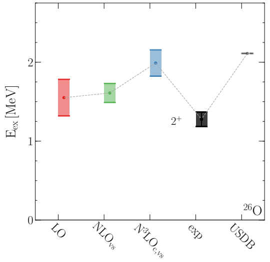


**Thank you for your attention!**

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

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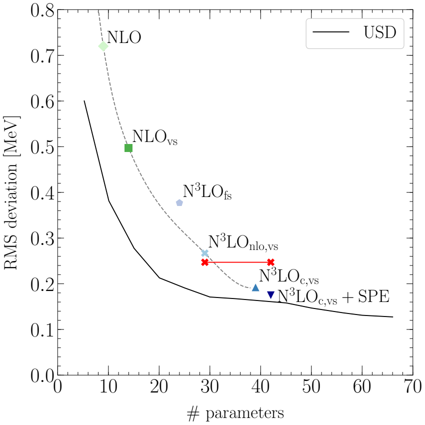
# Fit performance

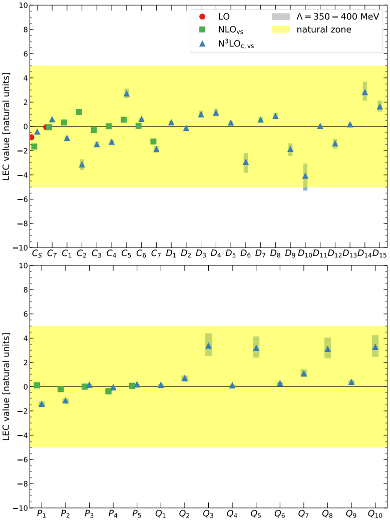
| Interaction | #LECs | RMS [MeV] | USD RMS [MeV] |
|---|---|---|---|
| LO | 2 | 1.77 | - |
| NLO | 9 | 0.72 | 0.43 |
| $NLO_{vs}$ | 14 | 0.50 | 0.30 |
| $N^3LO^{nat}_{c,vs}$+SPE | 29 | 0.25 | 0.17 |
| $N^3LO_{c,vs}$+SPE | 42 | 0.17 | 0.16 |

- 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:

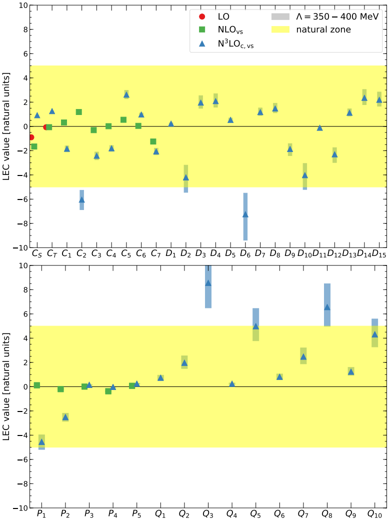
$$C^{\text{nat}}_{\text{LO}} = C_{\text{LO}} \cdot F_\pi^2$$

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

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

- 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

# LECs

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

- 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
- Relaxed fit constrains lead to unnatural values

# Chiral EFT contact interactions

For a free-space interaction:

- At any given order $\nu$, 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

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

In the valence space:

- Presence of a core defines a reference frame for the system
  $\Rightarrow$ core breaks Galilean invariance
- Interaction may depend explicitly on the center-of-mass momentum **P**
  $\Rightarrow$ new operator structures

Schwenk, Friman, PRL (2004)

# New valence-space contact interactions

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

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

- Valence-space limits the maximal momenta (here HO length $b \approx 1.7$ fm)

$$\Lambda_{\text{HO}} = \sqrt{2N+7}/b \overset{sd}{\approx} 375\ \text{MeV}$$

König et al., PRC (2014)

no need for additional regulators ( + possible $q/2m_\pi$ expansion of TPE)

- Fit to 441 states in the *sd* shell with $\chi^2$ minimization (for now: $\sigma_k^{\text{th}} = 100$ keV )

$$\chi^2 = \sum_{k=1}^{441} \frac{\left(E_k^{\text{exp}} - E_k^{\text{th}}\right)^2}{(\sigma_k^{\text{exp}})^2 + (\sigma_k^{\text{th}})^2}$$

- Shell-model diagonalizations with ANTOINE

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

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