Chiral three-body forces and the monopole component of effective shell-model Hamiltonians

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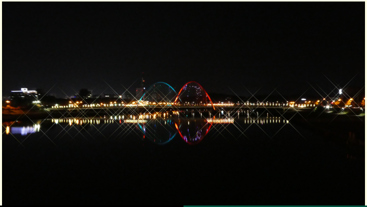

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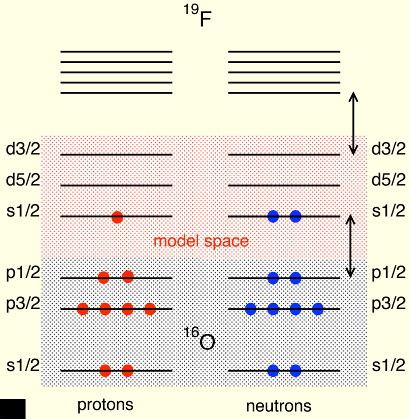
Outline

- Introduction to the realistic nuclear shell model
- The derivation of the effective shell-model Hamiltonian from nuclear potentials derived from EFT
- Testing the many-body theoretical framework: calculations for *p*-shell nuclei and comparison with *ab initio* methods (NCSM)
- Shell-model calculations for *fp*-shell nuclei: a paradigm to study the contribution of effective Hamiltonians to the shell evolution
- Conclusions and outlook

The nuclear shell model

The nucleons are subjected to the action of a mean field, that takes into account most of the interaction of the nucleus constituents.

Only valence nucleons interact by way of a residual two-body potential, within a reduced model space.



- Advantage → It is a microscopic model, the degrees of freedom of the valence nucleons are explicitly taken into account.
- Shortcoming → High-degree computational complexity.

Effective shell-model Hamiltonian

The shell-model Hamiltonian has to take into account in an effective way all the degrees of freedom not explicitly considered

Two alternative approaches

- phenomenological
- microscopic

$$V_{NN} \ \ (+V_{NNN}) \Rightarrow \text{many-body theory} \Rightarrow H_{\text{eff}}$$

Definition

The eigenvalues of H_{eff} belong to the set of eigenvalues of the full nuclear Hamiltonian

The realistic shell model

- The derivation of the shell-model Hamiltonian using the many-body theory provides an advantageous approach to nuclear structure investigations
- The model space may be “shaped” according to the computational needs of the diagonalization of the shell-model Hamiltonian
- In such a case, the effects of the neglected degrees of freedom are taken into account by the effective Hamiltonian H_{eff} theoretically

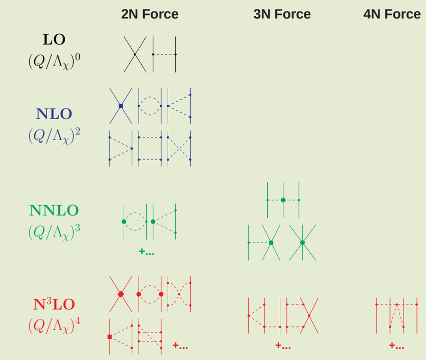
Workflow of our realistic shell-model calculation

1. Start from a nuclear potential based on chiral perturbation theory (*NN* plus *NNN*)
2. Set the model space *P* that is better tailored to study the system under investigation
3. Derive the effective shell-model Hamiltonian $H_{\rm eff}$ and transition operators $\Theta_{\rm eff}$ by way of the many-body perturbation theory
4. Diagonalize $H_{\rm eff}$ and then calculate the physical observables (energies, e.m. transition probabilities, ...)

The chiral perturbative expansion

Why nuclear potentials from chiral EFT are so appealing?

- Chiral EFT Lagrangians symmetries and symmetry breakings are consistent with those of low-energy QCD ⇒ a direct link to the underlying theory
- Soft and hard scales of the EFT identify the relevant degrees of freedom for low-energy nuclear physics (nucleons, pions, deltas)
- EFT provides an organizational scheme for a low-momentum expansion of the chiral lagrangian
- The power counting allows to evaluate the approximation due to the truncation of the perturbative expansion
- Two- and many-body forces are introduced on an equal footing within the perturbative expansion



The shell-model effective Hamiltonian

We start from the many-body Hamiltonian H defined in the full Hilbert space:

$$H = H_0 + H_1 = \sum_{i=1}^{A}(T_i + U_i) + \sum_{i<j}(V_{ij}^{NN} - U_i)$$

Then, introducing a similarity transformation X:

$$\left(\begin{array}{c|c} PHP & PHQ \\ \hline QHP & QHQ \end{array}\right) \quad \begin{array}{c} \mathcal{H} = X^{-1}HX \\ \Longrightarrow \\ Q\mathcal{H}P = 0 \end{array} \quad \left(\begin{array}{c|c} P\mathcal{H}P & P\mathcal{H}Q \\ \hline 0 & Q\mathcal{H}Q \end{array}\right)$$

$$H_{\rm eff} = P\mathcal{H}P$$

Suzuki & Lee $\Rightarrow X = e^{\omega}$ with $\omega = \left(\begin{array}{c|c} 0 & 0 \\ \hline Q\omega P & 0 \end{array}\right)$

$$H_1^{\rm eff}(\omega) = PH_1P + PH_1Q\frac{1}{\epsilon - QHQ}QH_1P -$$
$$-PH_1Q\frac{1}{\epsilon - QHQ}\omega H_1^{\rm eff}(\omega)$$

The shell-model effective Hamiltonian

Folded-diagram expansion

This recursive equation for $H_{\rm eff}$ may be solved using iterative techniques (Krenciglowa-Kuo, Lee-Suzuki, ...)

$$H_{\rm eff} = \hat{Q} - \hat{Q}' \int \hat{Q} + \hat{Q}' \int \hat{Q} \int \hat{Q} - \hat{Q}' \int \hat{Q} \int \hat{Q} \int \hat{Q} \cdots ,$$

$\hat{Q}$-box vertex function

$$\hat{Q}(\epsilon) = PH_1P + PH_1Q \frac{1}{\epsilon - QHQ} QH_1P$$

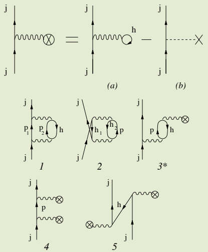
The perturbative approach to the shell-model $H^{2b}_{\rm eff}$

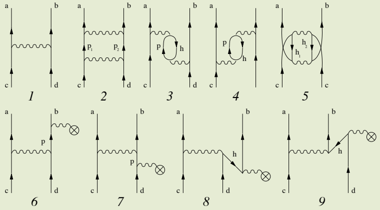
$$\hat{Q}(\epsilon) = PH_1P + PH_1Q\frac{1}{\epsilon - QHQ}QH_1P$$

Exact calculation of the $\hat{Q}$-box is computationally prohibitive for many-body system $\Rightarrow$ we perform a perturbative expansion

$$\frac{1}{\epsilon - QHQ} = \sum_{n=0}^{\infty}\frac{(QH_1Q)^n}{(\epsilon - QH_0Q)^{n+1}}$$

The diagrammatic expansion of the $\hat{Q}$-box

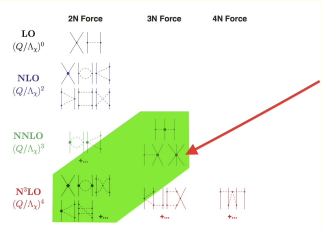


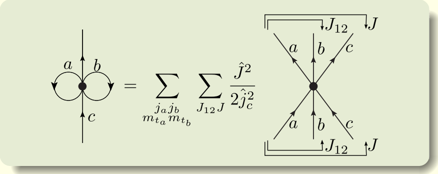


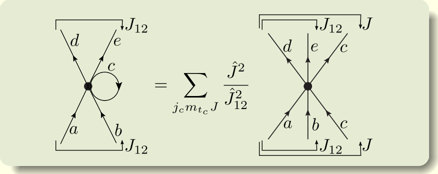
Introducing 3-body force in RSM, $H_{\rm eff}^{2b+3b}$

The next step is to include the effects of three-body forces

At present, we include in the effective shell-model Hamiltonian $H_{\rm eff}^{2b+3b}$ diagrams only at first order in perturbation theory with N^2LO three-body vertices







This is the well-known normal-ordering approximation that is employed in many *ab initio* calculations

The shell-model effective operators

Consistently, any effective shell-model transition operator may be calculated

It has been demonstrated that, for any bare operator Θ, a non-Hermitian effective operator $\Theta_{\rm eff}$ can be written in the following form:

$$\begin{aligned}\Theta_{\rm eff} &= (P + \hat{Q}_1 + \hat{Q}_1\hat{Q}_1 + \hat{Q}_2\hat{Q} + \hat{Q}\hat{Q}_2 + \cdots)(\chi_0 + \\ &\quad + \chi_1 + \chi_2 + \cdots) = \\ &= (P + \hat{Q}_1 + \hat{Q}_1\hat{Q}_1 + \hat{Q}_2\hat{Q} + \hat{Q}\hat{Q}_2 + \cdots)\hat{Q}\hat{Q}^{-1} \\ &\quad \times(\chi_0 + \chi_1 + \chi_2 + \cdots) = \\ &= H_{\rm eff}\hat{Q}^{-1}(\chi_0 + \chi_1 + \chi_2 + \cdots) \ ,\end{aligned}$$

where

$$\hat{Q}_m = \frac{1}{m!} \frac{d^m \hat{Q}(\epsilon)}{d\epsilon^m}\Big|_{\epsilon=\epsilon_0} \ ,$$

ϵ_0 being the model-space eigenvalue of the unperturbed Hamiltonian H_0

K. Suzuki and R. Okamoto, Prog. Theor. Phys. **93** *, 905 (1995)*

The shell-model effective operators

The χ_n operators are defined in terms of the bare operator Θ:

$$\begin{aligned}
\chi_0 &= (\hat{\Theta}_0 + h.c.) + \Theta_{00} \ , \\
\chi_1 &= (\hat{\Theta}_1 \hat{Q} + h.c.) + (\hat{\Theta}_{01} \hat{Q} + h.c.) \ , \\
\chi_2 &= (\hat{\Theta}_1 \hat{Q}_1 \hat{Q} + h.c.) + (\hat{\Theta}_2 \hat{Q}\hat{Q} + h.c.) + \\
& (\hat{\Theta}_{02} \hat{Q}\hat{Q} + h.c.) + \hat{Q}\hat{\Theta}_{11} \hat{Q} \ , \\
& \ldots
\end{aligned}$$

and

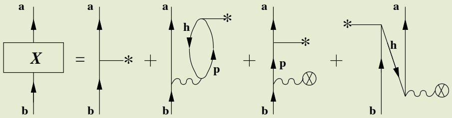
$$\begin{aligned}
\hat{\Theta}(\epsilon) &= P\Theta P + P\Theta Q \frac{1}{\epsilon - QHQ} QH_1 P \ , \\
\hat{\Theta}(\epsilon_1; \epsilon_2) &= PH_1 Q \frac{1}{\epsilon_1 - QHQ} Q\Theta Q \frac{1}{\epsilon_2 - QHQ} QH_1 P \ ,
\end{aligned}$$

$$\hat{\Theta}_m = \frac{1}{m!} \frac{d^m \hat{\Theta}(\epsilon)}{d\epsilon^m} \Big|_{\epsilon=\epsilon_0} \ , \quad \hat{\Theta}_{nm} = \frac{1}{n!m!} \frac{d^n}{d\epsilon_1^n} \frac{d^m}{d\epsilon_2^m} \hat{\Theta}(\epsilon_1; \epsilon_2) \Big|_{\epsilon_1=\epsilon_0, \epsilon_2=\epsilon_0}$$

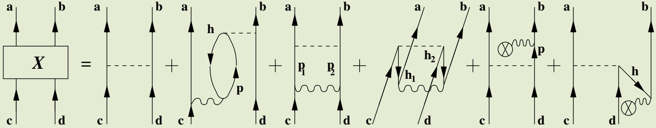
The effective shell-model transition operators

We arrest the χ series at the leading term χ_0, and then expand it perturbatively:

One-body operator

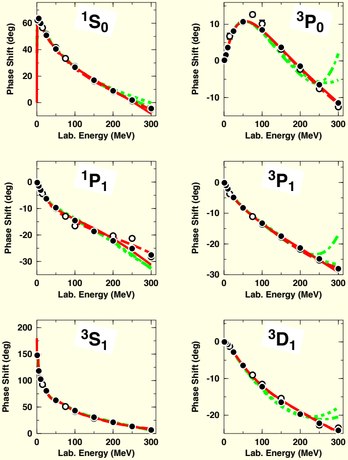


Two-body operator



Test case: *p*-shell nuclei

- H_{eff} for two valence nucleons outside ^{4}He
- $V_{NN} \Rightarrow$ chiral N^{3}LO potential by Entem & Machleidt (smooth cutoff $\simeq 2.5$ fm^{-1})
- $V_{NNN} \Rightarrow$ chiral N^{2}LO potential, one-pion-exchange LEC $c_D = -1$, contact-term LEC $c_E = -0.35$
- Single-particle energies and residual two-body interaction are derived from the theory.
  No empirical input



First, benchmark calculations!

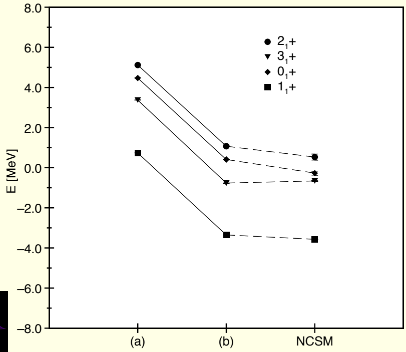
L.C., A. Covello, A. Gargano, N. Itaco, and T. T. S. Kuo, Ann. Phys. ***327*** *, 2125-2151 (2012)*
T. Fukui, L. De Angelis, Y. Z. Ma, L. C., A. Gargano, N. Itaco, and F. R. Xu, Phys. Rev. C ***98****, 044305 (2018)*

Benchmark calculation

We start from a translationally invariant Hamiltonian to compare our results with NCSM

$$H_{int} = \left(1-\frac{1}{A}\right)\sum_{i=1}^{A}\frac{p_i^2}{2m} + \sum_{i<j=1}^{A}\left(V_{ij}^{NN} - \frac{\mathbf{p_i}\cdot\mathbf{p_j}}{mA}\right) =$$

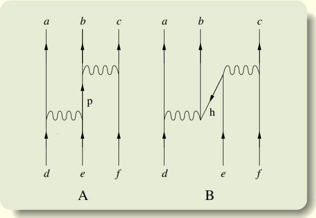
$$= \left[\sum_{i=1}^{A}\left(\frac{p_i^2}{2m}+U_i\right)\right] + \left[\sum_{i<j=1}^{A}\left(V_{ij}^{NN} - U_i - \frac{p_i^2}{2mA} - \frac{\mathbf{p_i}\cdot\mathbf{p_j}}{mA}\right)\right]$$

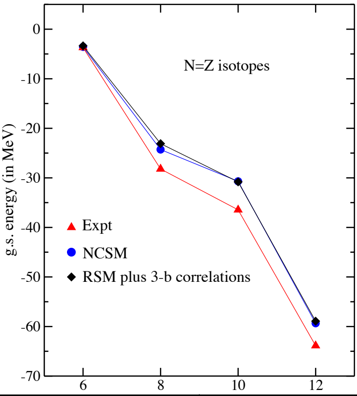


^{6}Li low-energy spectrum with two-body-force Hamiltonian $H_{\mathrm{eff}}^{\mathrm{2b}}$:

- (a) not translationally invariant Hamiltonian
- (b) purely intrinsic Hamiltonian

Ground-state energies with respect to ^{4}He, $H_{\rm eff}^{2b}$



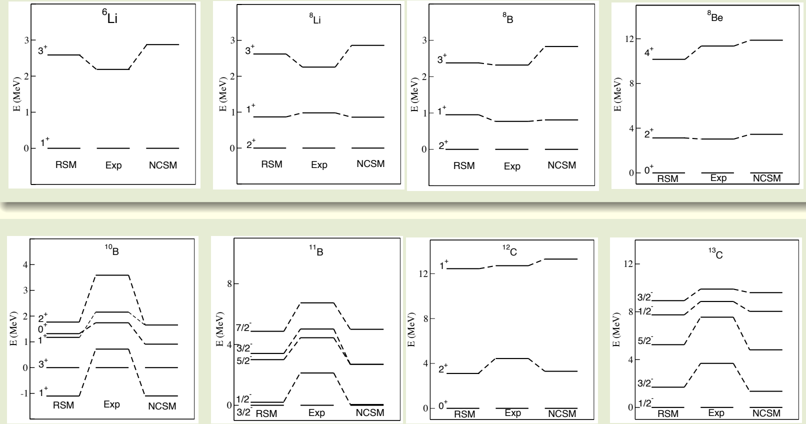


To calculate the g. s. energies with respect to the ^{4}He core, we also include the contributions of three-body correlations diagrams on the g. s. wavefunctions. This improves the agreement of $H_{\rm eff}^{2b}$ with NCSM

The largest discrepancy is about 1.1 MeV for ^{8}Be, all other results differ less than 0.6 MeV

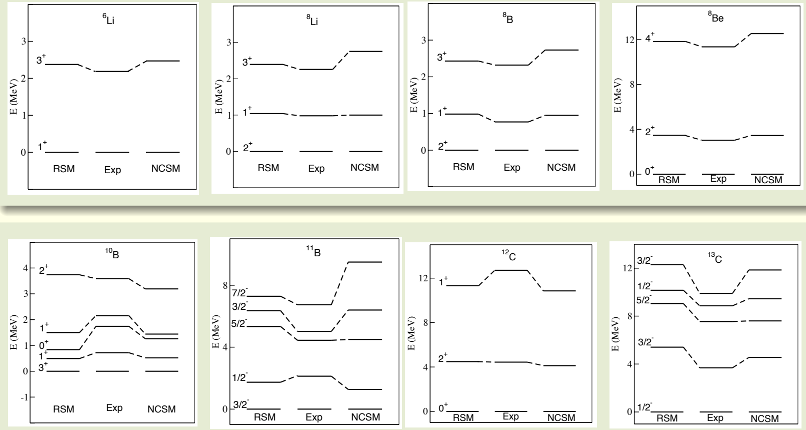
Benchmark calculation - low-lying excitation spectra with H_{eff}^{2b}

Results with two-body-force Hamiltonian H_{eff}^{2b}



Benchmark calculation - low-lying excitation spectra with H_{eff}^{2b+3b}

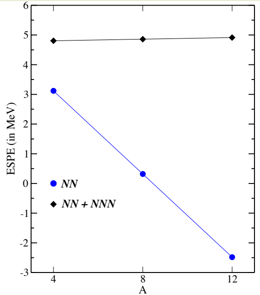
Results with two-body-force Hamiltonian H_{eff}^{2b+3b}

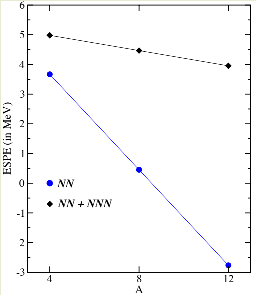


Effective single-particle energies

Proton and neutron ESPE $0p_{1/2} - 0p_{3/2}$ as a function of A

$$\mathrm{ESPE}(j) = \epsilon_j + \sum_J (2J+1) \langle jj' | V | jj' \rangle_J / \sum_J (2J+1)$$

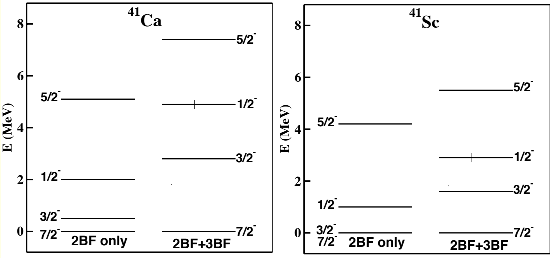




- Two-body potential **only**: $0p_{1/2} - 0p_{3/2}$ spacings reduce with A
- Two-body plus **three-body potential**: $0p_{1/2} - 0p_{3/2}$ spacings are constant ⇒ better closure properties!

fp-shell single-particle nuclei

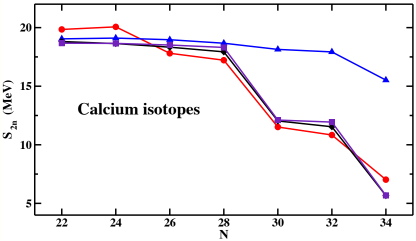
- The study of *fp*-shell nuclei provides a unique opportunity to investigate the monopole properties of $H_{\rm eff}$
- The observed spin-orbit and $l(l+1)$ splitting of the *fp* orbitals in ^{41}Ca and ^{41}Sc is responsible of $N, Z = 28$ shell closure

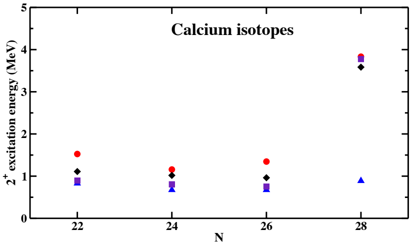


- **Two-body force alone** is not enough to produce enough $l(l+1)$ splitting $\Rightarrow$ the **three-body force** is crucial to reproduce the correct shell evolution and closures

The calcium isotopes chain

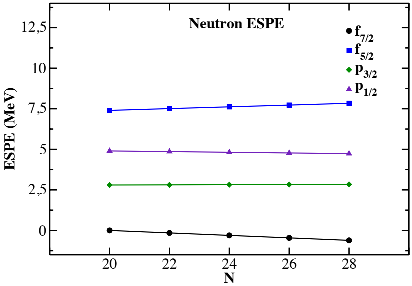
As a matter of fact, the shell evolution of the two-neutron separation energies S_{2n} and $J = 2^+_1$ excitation energies can be reproduced introducing $3NF$ effects employing $H^{2b+3b}_{\rm eff}$, or "transplanting" the $H^{2b+3b}_{\rm eff}$ monopole component to $H^{2b}_{\rm eff}$.



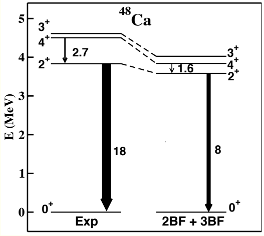


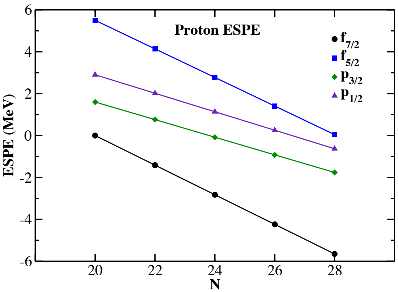
- Red dots: experimental values
- Blue triangles: $H^{2b}_{\rm eff}$
- Black diamonds: $H^{2b+3b}_{\rm eff}$
- Indigo squares: $H^{2b}_{\rm eff}$ monopole corrected

fp-shell effective single-particle energies with H_{eff}^{2b+3b}

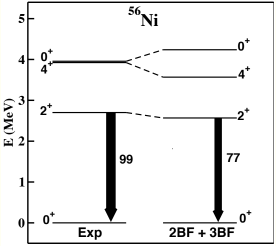


Doubly-closed ^{48}Ca

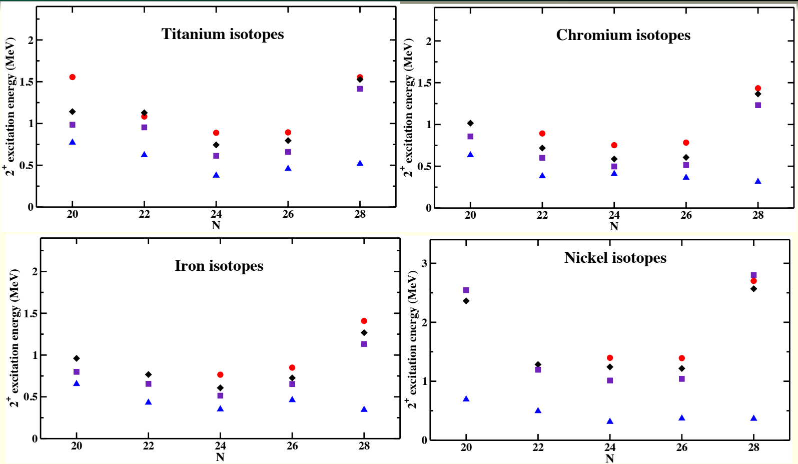




Doubly-closed ^{56}Ni



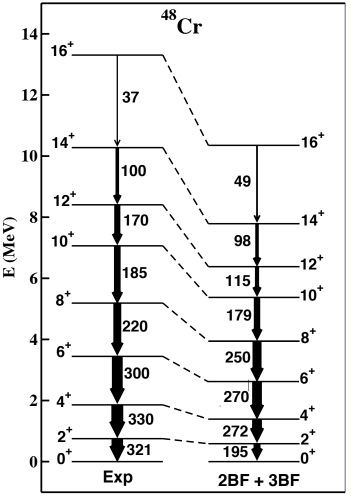
fp-shell isotopic chains



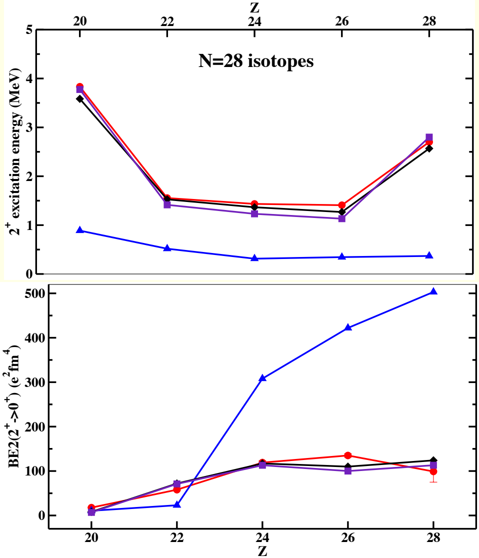
- Red dots: experimental values
- Blue triangles: $H_{\rm eff}^{\rm 2b}$
- Black diamonds: $H_{\rm eff}^{\rm 2b+3b}$
- Indigo squares: $H_{\rm eff}^{\rm 2b}$ monopole corrected

Collective features in *fp* shell

Deformed yrast band in ^{48}Cr



Evolution of collectivity at $N = 28$



Conclusions

- Realistic shell model provides a reasonable comparison with *ab initio* methods, with and without three-body contributions
- For nuclear potentials from chiral EFT three-body contributions are relevant for a satisfactory reproduction of the observed shell evolution and closures

Outlook

- We plan to include higher-order contributions of the three-body potential in the perturbative expansion of $H_{\rm eff}^{\rm 2b+3b}$
- An extensive study of heavier systems is underway
- This is a valuable approach to perform fully consistent studies of β-decay properties