Nuclear structure studies with chiral EFT and many body perturbation theory

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Progress in Ab Initio Techniques in Nuclear Physics
TRIUMF, 20th February 2015

日本学術振興会
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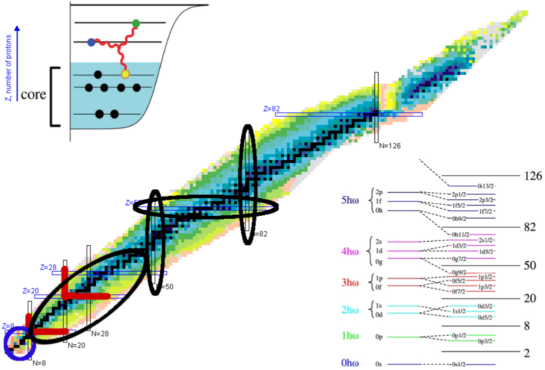
Nuclear landscape



Big variety of nuclei in the nuclear chart, $A \sim 2...300$

Systematic *ab initio* calculations only possible in the lightest nuclei

Hard many-body problem: approximate methods suited for different regions

Shell Model: Choose relevant degrees of freedom (valence space)

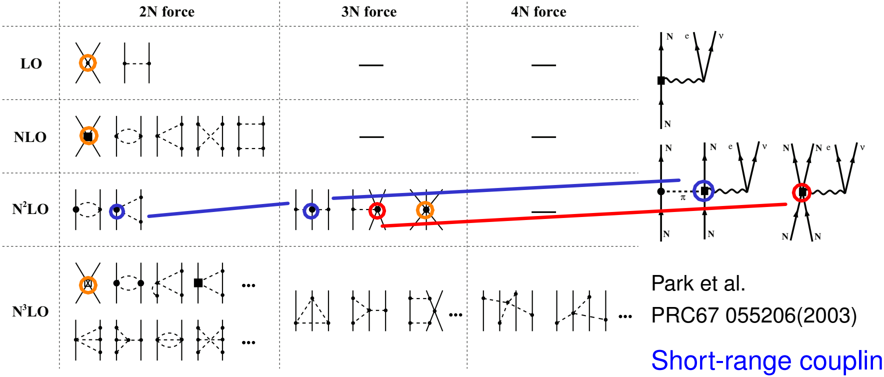
Interactions based on realistic nucleon-nucleon (NN) potentials
phenomenological modifications $\Rightarrow$ three-nucleon (3N) interactions

Chiral Effective Field Theory

Chiral EFT: low energy approach to QCD, nuclear structure energies

Approximate chiral symmetry: pion exchanges, contact interactions

Systematic expansion: nuclear forces and electroweak currents



Weinberg, van Kolck, Kaplan, Savage, Weise, Epelbaum, Meißner...

Park et al.
PRC67 055206(2003)

Short-range couplings
fitted to experiment once

Shell model interactions based on chiral EFT

Different approaches based on chiral EFT forces
can provide shell model interactions for wide range of medium-mass nuclei

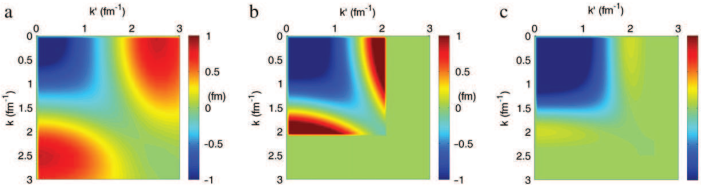
- Many-body perturbation theory
  Otsuka et al. PRL105 032501 (2010); Holt et al. JPG39 085111 (2012)
- In-medium similarity renormalization group
  Bogner et al. PRL113, 142501 (2014)
- Coupled-cluster effective interaction
  Jansen et al. PRL113, 142502 (2014)
- No-core shell model
  Dikmen et al. arXiv:1502.00700 (2015)

Effective Hamiltonian in valence space:

$$H\,|\Psi\rangle = E\,|\Psi\rangle \rightarrow H_{eff}\,|\Psi\rangle_{eff} = E\,|\Psi\rangle_{eff}$$

Many Body Perturbation Theory

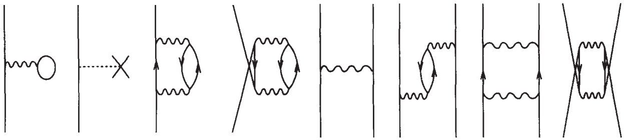
Better convergence of chiral forces after RG transformation



Many-body perturbation theory to third order: obtain effective Shell Model interaction in the valence space

Single Particle Energies

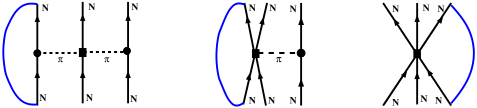
Two-Body Matrix Elements

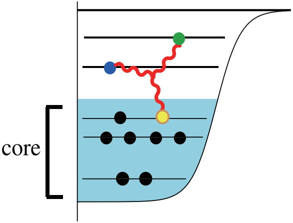


3N couplings c_D, c_E fitted with evolved NN forces (induced + initial 3N forces)

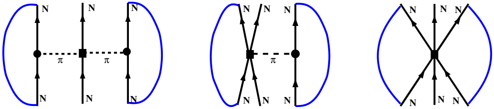
3N forces in normal-ordering approximation:

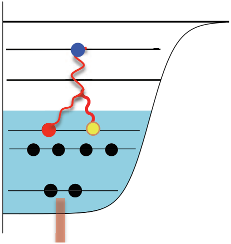
normal-ordered 2B: 2 valence, 1 core particle
⇒ Two-body Matrix Elements





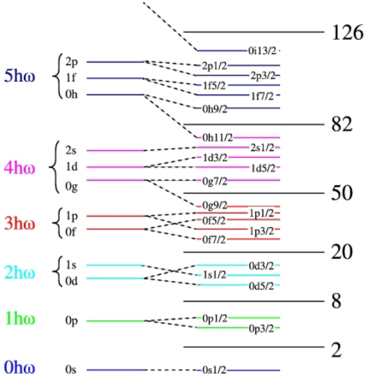
normal-ordered 1B: 1 valence, 2 core particles
⇒ Single particle energies





3N forces in H_{eff} treated to third order in MBPT

Shell model calculations with 3N forces



To keep the problem feasible, the configuration space is separated into

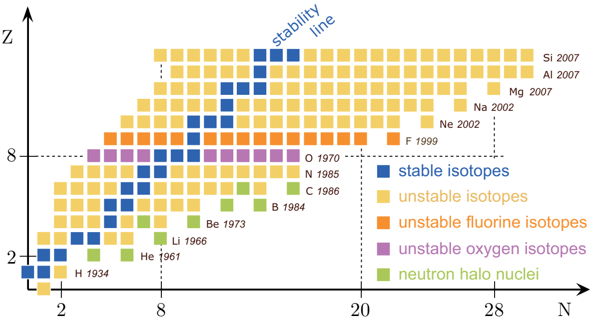
- Outer orbits:
  orbits that are always empty
- Valence space:
  obtis where we explicitly solve the problem
- Inner core:
  orbits that are always filled

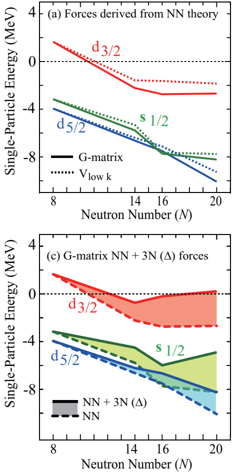
Solve many-body problem with ISM codes ANTOINE/NATHAN
Diagonalize up to 10^{10} Slater determinants Caurier *et al.* RMP 77 (2005)

$$H_{eff} \left|\Psi\right\rangle_{eff} = E \left|\Psi\right\rangle_{eff}$$

$$\left|\Psi\right\rangle_{eff} = \sum_{\alpha} c_\alpha \left|\phi_\alpha\right\rangle \qquad \left|\phi_\alpha\right\rangle = a^+_{i1} a^+_{i2} ... a^+_{iA} \left|0\right\rangle$$

O isotopes: 'anomaly' in the dripline at ^{24}O, doubly magic nucleus





Calculations based on chiral NN+3N forces
and MBPT correctly predict dripline at ^{24}O

Otsuka et al. PRL105 032501 (2010)

Oxygen dripline in ab-initio calculations

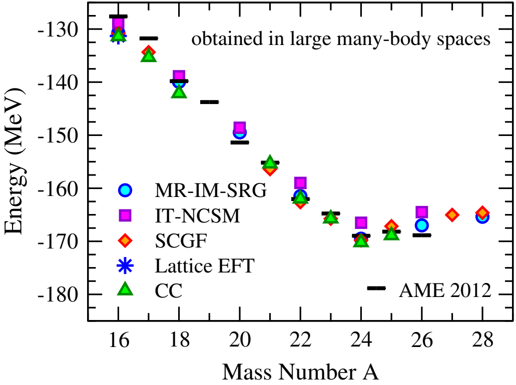
Oxygen dripline including chiral NN+3N forces correctly reproduced
confirmed in ab-initio calculations by different approaches,
treating explicitly all nucleons as degrees of freedom

No-core shell model
(Importance-truncated)

In-medium SRG
Hergert et al. PRL110 242501 (2013)

Self-consistent Green's function
Cipollone et al. PRL111 062501 (2013)

Coupled-cluster
Jansen et al. PRL113 142502 (2014)

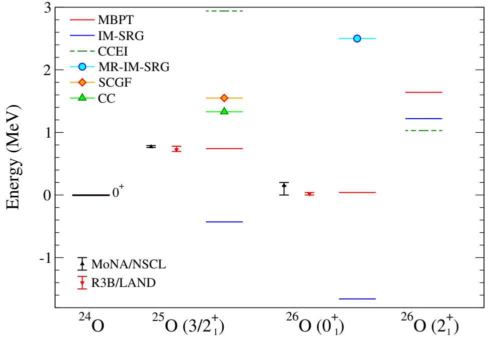


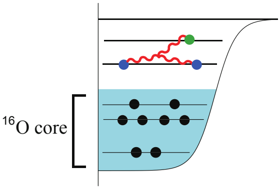
Benchmark with the same initial Hamiltonian
Sensitivity to the chiral interaction not systematically explored

Residual 3N Forces

In extreme neutron-rich oxygen isotopes, 3N forces between 3 valence neutrons can give a relevant contribution

Evaluated perturbatively: $\langle \Psi | V^{3N} | \Psi \rangle$





Repulsive residual 3N contributions

Small compared to normal-ordered 3N force, but increase with N

Very good agreement with resonances in ^{25}O and ^{26}O

Caesar, Simonis et al. PRC88 034313 (2013)

Hergert et al. PRL110 242501 (2013)

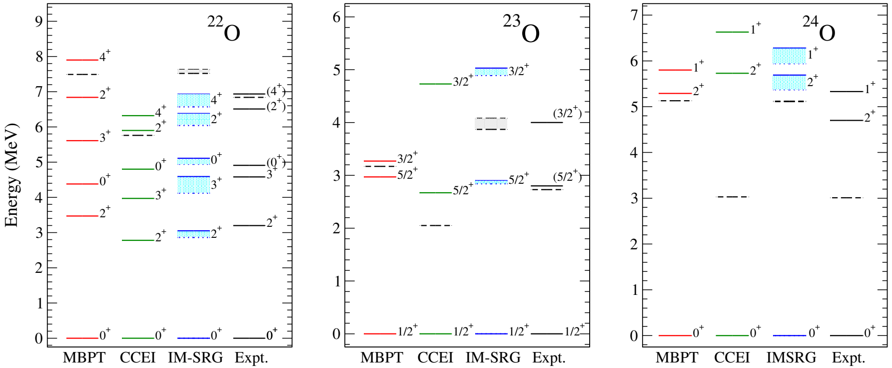
Cipollone et al. PRL111 062501 (2013)

Jansen et al. PRL113 142502 (2014)

Challenge: include continuum

O isotopes: excitation spectra

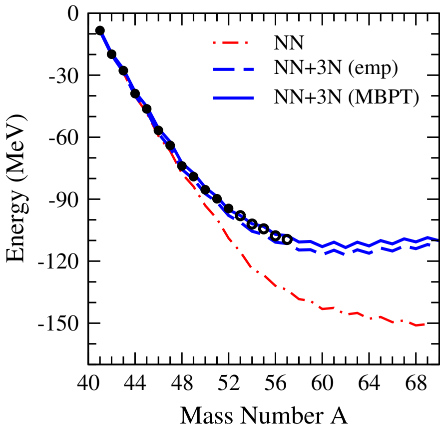
Shell model interactions obtained with MBPT, CCEI, IM-SRG
in good agreement with experiment on excitation spectra



Holt, JM, Schwenk EPJA49 39 (2013)

Bogner et al. PRL113, 142501 (2014), Jansen et al. PRL113, 142502 (2014)

Ca isotopes: explore nuclear shell evolution $N = 20, 28, 32?, 34?$



Ca measured from ^{40}Ca core in pfg$_{9/2}$ valence space

3N forces repulsive contribution, chiral NN-only forces too attractive

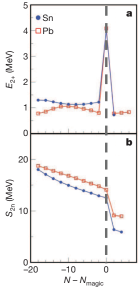
Probe shell evolution:

Mass-differences

2_1^+ energies

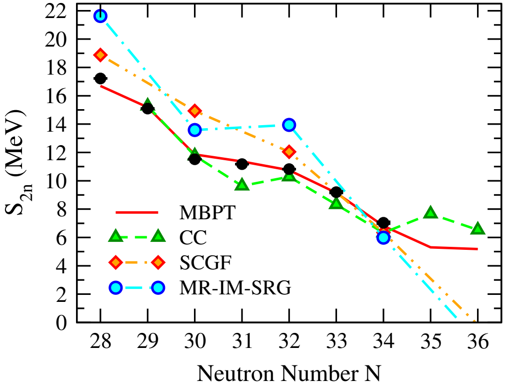
Jones et al.

Nature 465 454 (2010)



Calcium two-neutron separation energies

Measurement of ^{51,52}Ca at TRIUMF and ^{53,54}Ca at ISOLDE



Excellent agreement of MBPT prediction with experiment

Coupled-cluster, SCGF, IM-SRG also in good agreement with experiment

S_{2n} evolution:
^{52}Ca–^{54}Ca decrease similar to ^{48}Ca–^{50}Ca unambiguously establishes $N = 32$ shell closure

Gallant et al. PRL 109 032506 (2012)
Wienholtz et al. Nature 498 346 (2013)
Hagen et al. PRL 109 032502 (2012)
Somà et al. PRC 89 061301 (2014)
Hergert et al. PRC 90 041302 (2014)

Calcium 2_1^+ energies

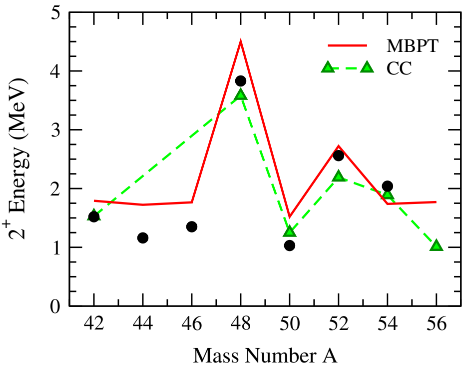
2_1^+ energies characterize shell closures

Correct closure at $N = 28$ when 3N forces are included

Holt et al. JPG39 085111 (2012)

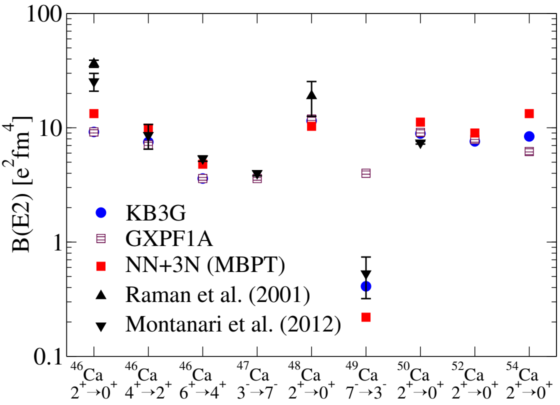
Holt, JM, Schwenk, JPG40 075105 (2013)

Hagen et al. PRL 109 032502 (2012)



- High 2^+ in ^{32}Ca related to closure at $N = 32$
- Relatively high 2^+ in ^{32}Ca measured at RIBF indicate closure at $N = 34$ to be confirmed in mass, B(E2) measurements
  Steppenbeck et al. Nature 502 207 (2013)

Calcium B(E2) transition strengths



B(E2)s in reasonable agreement with experiment, spread two over orders of magnitude

Similar quality as phenomenological interactions

^{46}Ca: *sd* degrees of freedom?

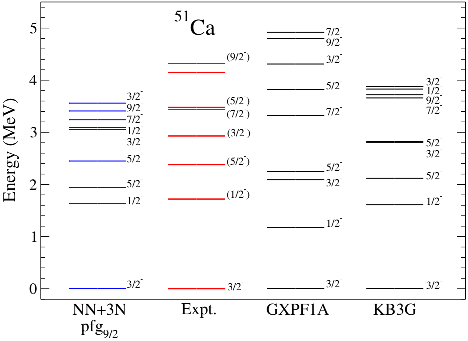
No clear signature for closed-shells

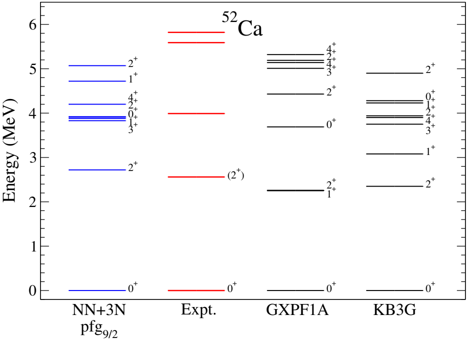
At $N = 34$, MBPT prediction deviates from phenomenological interactions

Phenomenological effective charges

Excitation spectra

Spectra for neutron-rich calcium isotopes



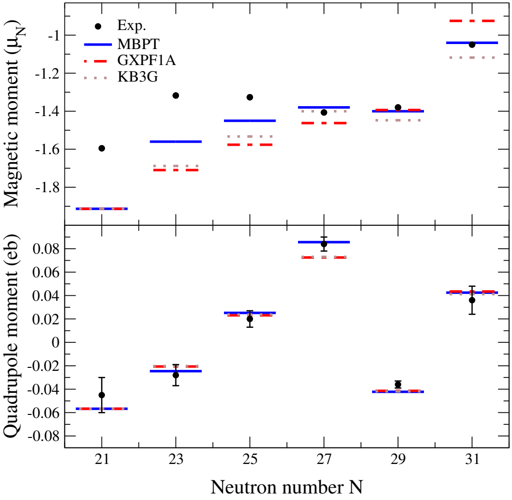


Good agreement with experiment, comparable to phenomenological interactions, and predictions given for heavier systems

Holt, JM, Simonis, Schwenk PRC90 024312 (2014)

Calcium magnetic and quadrupole moments

Electric quadrupole moments and magnetic momentss
in ground states of calcium isotopes measured by COLLAPS at ISOLDE



Consistent description of
ground-state masses
and spectroscopy

Very good agreement to
experiment,
up to neutron-rich systems

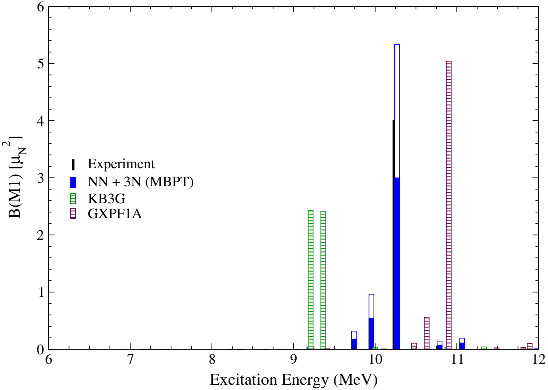
Comparable to
phenomenological interactions

Phenomenological effective
charges $q_n = 0.5e$,
and bare g-factor g_s(bare)

Garcia Ruiz et al., submitted

B(M1) Transition in ^{48}Ca

B(M1) strength in ^{48}Ca with NN+3N in very good agreement with experimental strength and energy, but need a quenched g-factor



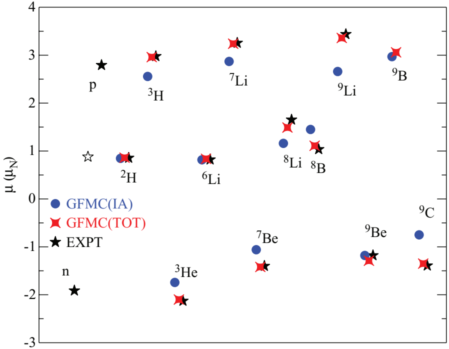
$g_s = 0.9 g_s$(bare), phenomenological interactions need $g_s = 0.75 g_s$(bare).

Currents and operators

Good agreement with ground-states, spectroscopy and electromagnetic transitions but with effective charges and g-factors

Origin of the need of this phenomenological input?

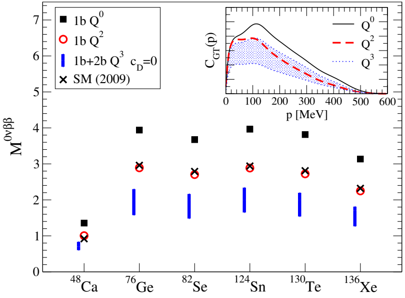
- Shell-model calculation in limited valence space: Appropriate effective operators to be obtained perturbatively or non-perturbatively
- Transition operators non-evolved
- Operators are not complete: Need of two-body currents well known from light nuclei



Pastore et al. PRC87 035503 (2013)

2b currents in medium-mass nuclei

First applications in medium-mass nuclei for Gamow-Teller transitions



JM, Gazit, Schwenk PRL107 062501 (2011)

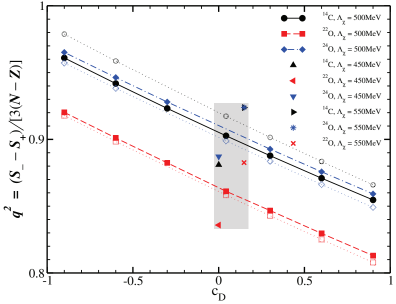
Normal-ordered 2b currents, assuming Fermi gas

Prediction for sizeable β-decay quenching ($q \sim 0.8$) from long-range, smaller for neutrinoless $\beta\beta$ decay (momentum transfer $p \sim 200$ MeV)

Coupled-cluster calculations
p, low-sd nuclei ^{14}C, ^{22}O and ^{24}O

Dominant effect normal-ordered 1b part with respect to Hartree-Fock state

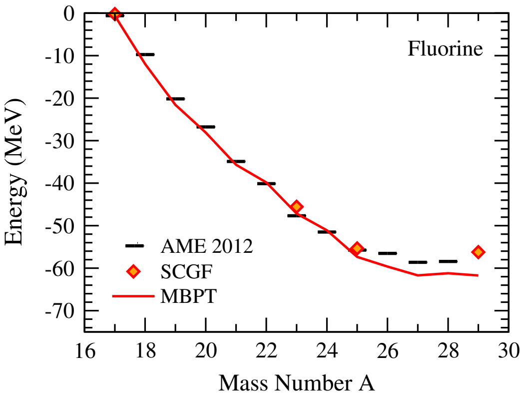
Predict small quenching $q = 0.96 ... 0.92$



Ekström et al. PRL113 262504 (2014)

Fluorine isotopes

In the shell model, sd-shell beyond oxygen, pf-shell beyond calcium, involve proton-neutron interactions:
these are stronger than neutron-neutron, proton-proton interactions



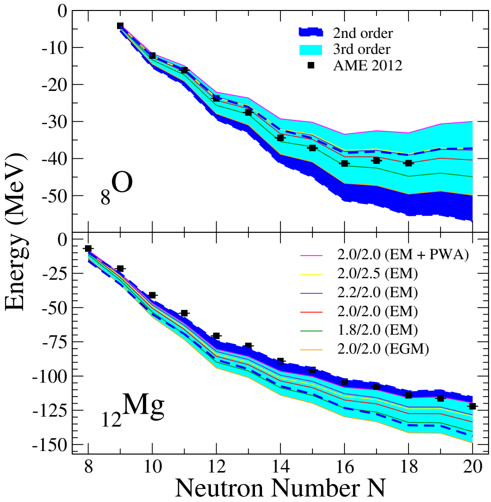
Ground-state of F isotopes good agreement to experiment, also for SCGF calculations

MBPT results somewhat overbound
towards fluorine dripline

SCGF:
Cipollone et al. PRL111 062501 (2013)

Nuclei in *sd* shell and theoretical uncertainties

Extend the study to *sd*-shell nuclei, proton-neutron interaction included



For nuclear forces with good saturation properties

Explore the theoretical sensitivity:

Initial chiral Hamiltonian

RG evolution of NN, 3N forces

Convergence in MBPT

Oxygen ground-state energies good agreement to experiment

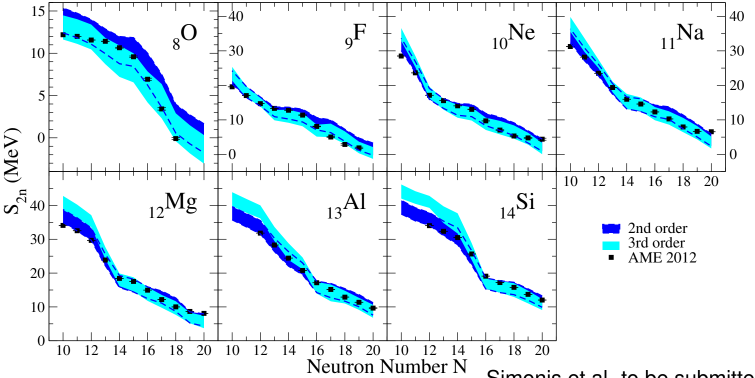
Magnesium ground-state energies tend to be overbound

Uncertainties dominated by initial nuclear Hamiltonian

Simonis et al. to be submitted

Two-neutron separation energies in *sd*-shell nuclei

Study of the sensitivity to initial chiral Hamiltonian,
evolution of NN and 3N forces and convergence in MBPT



Simonis et al. to be submitted

Experimental trends well reproduced with ΔS_{2n}'s $\sim$ 5 MeV
dominated by initial Hamiltonian uncertainty,
but in $N \sim Z$ (pn interaction), ΔS_{2n}'s $\sim$ 10 MeV due to MBPT convergence

Summary

Shell Model calculation based on chiral effective field theory
including NN+3N forces and many-body perturbation theory

- Shell structure: very good agreement with neutron-rich nuclei:
  S_{2n}'s and 2^+_1 ($N = 32, 34$), excitation spectra
- Electromagnetic and weak transitions: good agreement to experiment
  unclear effective charges, g-factors, g_A coupling:
  use consistent operators including predicted chiral 2b currents
- First calculations involving valence neutrons and protons show
  somewhat too strong pn interaction for the Hamiltonians used:
  full sd shell covered, extend to all medium-mass nuclei
- Towards theoretical uncertainty quantification of calculations in
  medium-mass nuclei: (some) uncertainties associated to the
  Hamiltonian and to many-body perturbation theory