Shell evolution and pairing in calcium isotopes with two- and three-body forces

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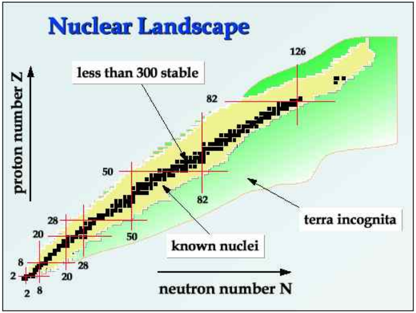
Computational and Theoretical Advances
for Exotic Isotopes in the Medium Mass Region

INT Seattle, 18 April 2013

Outline

1. Ca ground states: pairing, shell evolution
2. Ca excited states: shell evolution, spectra, transitions
3. Residual 3N forces: oxygen and calcium isotopes

The nuclear many-body approach



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

Exact (*ab initio*) calculations only possible in the lightest nuclei

Poses a hard many-body problem: design approximate methods valid in different regions

In the rest of the nuclear chart, pick only the (more) relevant degrees of freedom for observable to study: idea of the Interacting Shell Model

Medium-mass nuclei: standard view

Standard studies of medium-mass nuclei ($A \sim 20 - 80$) are performed with theoretical approaches based on phenomenology:

- Shell Model calculations
  use fitted interactions or modified G-matrices
- Energy Density Functional interactions
  use Skyrme, Gogny or Relativistic fitted interactions

Interactions are made to reproduce experiment for stable nuclei

- When extrapolated to exotic (neutron rich) regions results differ
  $\Rightarrow$ Need to guide (ideally avoid) fits!
- Why microscopic NN interactions have to be modified?
  $\Rightarrow$ Need to include 3N forces explicitly!

Towards microscopic medium-mass nuclei calculation

Microscopic calculation of medium-mass nuclei including 3N forces

- Use Chiral Effective Field Theory (chiral EFT) interactions, includes naturally NN and 3N forces.
- Perform a renormalization group evolution to V_{lowk} interaction to enhance convergence of the MBPT calculation
- Apply Many-Body Perturbation Theory (MBPT) to 3rd order to obtain interactions to be used in Shell Model (SM) calculations
- Full diagonalizations using codes ANTOINE and NATHAN
  Caurier et al. RMP77 427(2005)

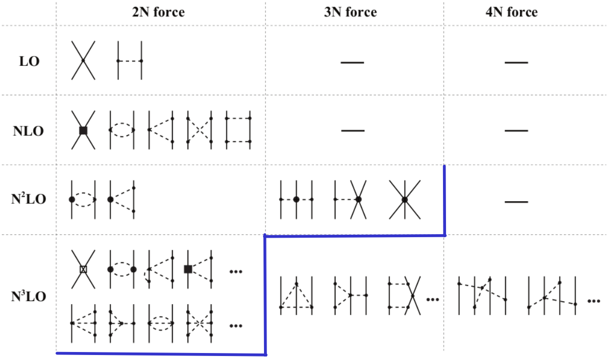
⇒ 3N forces are naturally included
Shown necessary to reproduce light nuclei spectra

⇒ All the parameters that appear in the SM hamiltonian calculated from the input of the microscopic interaction (no fits!)

Chiral EFT NN+3N Forces

Systematic expansion: state-of-the-art chiral EFT forces

- NN forces included up to N^3LO
- 3N forces included up to N^2LO



NN fitted to:

- NN scattering data
- π-N scattering data

3N fitted to:

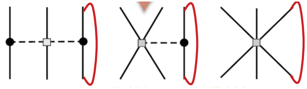
- ^3H Binding Energy
- ^4He radius

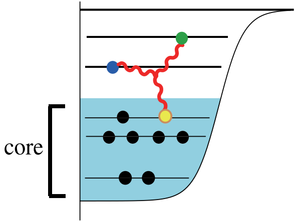
Weinberg, van Kolck, Kaplan, Savage, Wise, Epelbaum, Kaiser, Meißner...

Normal-ordered 3N Forces

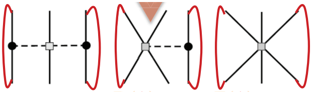
Approximate treatment of 3N forces:

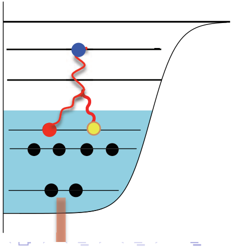
normal-ordered 2B: 2 valence, 1 core particle
$\Rightarrow$ (effective) Two-body Matrix Elements (TBME)





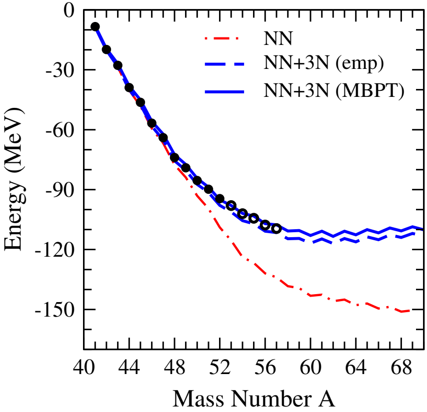
normal-ordered 1B: 1 valence, 2 core particles
$\Rightarrow$ (effective) Single particle energies (SPE)





residual 3B:
$\Rightarrow$ Estimated to be suppressed by $N_{valence}/N_{core}$

Ca isotopes: Ground-state energies



Ca calculations with respect to ^{40}Ca core

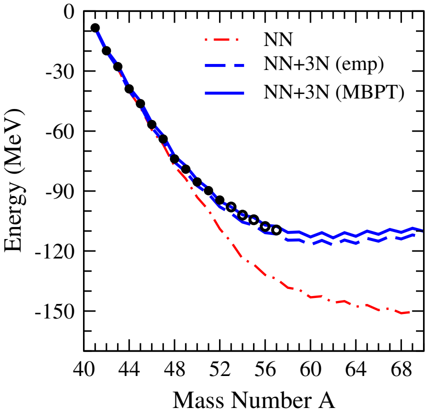
$\hbar\omega = 11.48$ MeV, appropriate for Ca radii

Normal-ordered 3N force contributions to TBMEs and SPEs

3N forces provide crucial repulsion (similar to O case)

NN+3N calculations nice agreement with experimental data

Ca isotopes: Ground-state energies

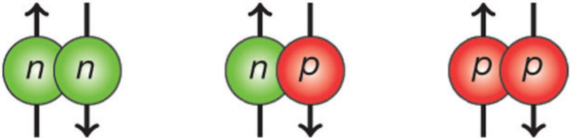


Results particularly sensitive to SPEs, especially more neutron-rich systems, consider two sets:
MBPT (calculated from NN+3N forces)
Empirical (from GXPF1 interaction)
to have an estimate of this uncertainty

Calculation performed in *pf* $g_{9/2}$ valence space

Flat behaviour towards ^{60}Ca does not allow clear prediction of the dripline:
enlarge valence space
include continuum degrees of freedom

Nuclear Pairing Gaps

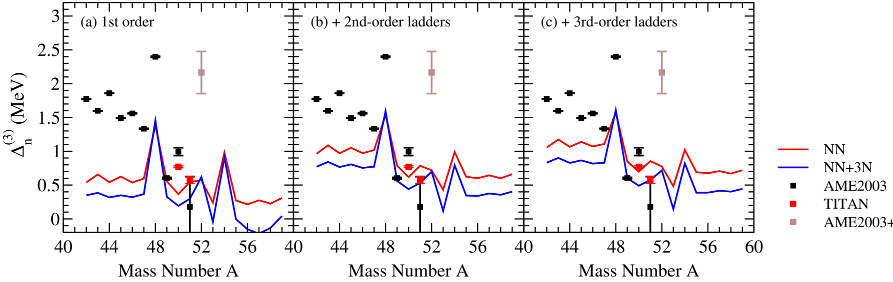


- Pairing correlations are important in nuclei
  - Odd-even mass staggering
  - Moments of Inertia
  - . . .
- Theoretical pairing gaps compared to experiment via the three point mass formula:

$$\Delta_N^3 = (-1)^N \frac{BE\,(N-1) + BE\,(N+1) - 2BE\,(N-1)}{2}$$

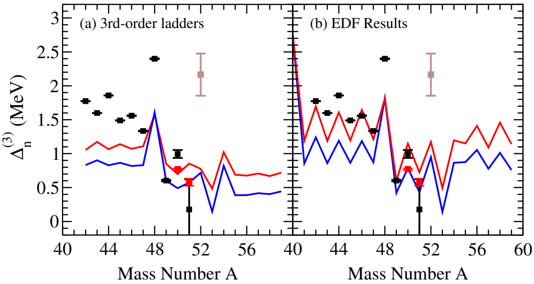
Holt, JM, Schwenk, arXiv:1304.0434

MBPT convergence



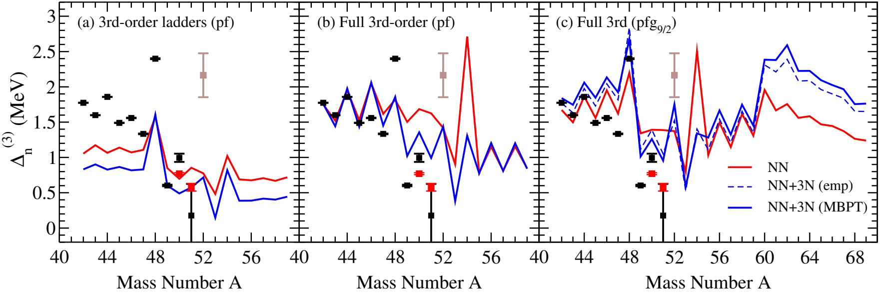
- Succesive orders *pp*, *hh* ladder diagrams build up pairing gaps
- At third order *pp*, *hh* ladders results seem to be converged
- Third order ladders results still away from experiment
  Incorrect even-odd staggering (too attractive mean-field)

Pairing, 3N forces and EDF



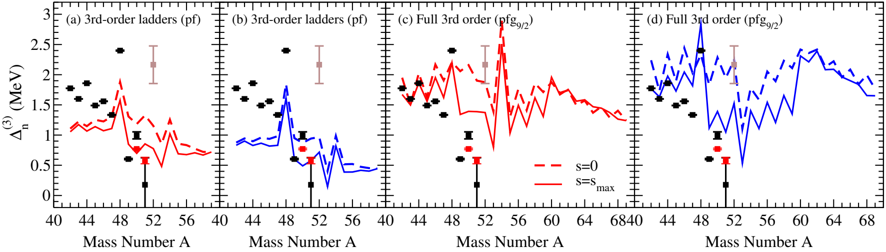
- At *pp-hh* level 3N forces reduce the pairing gaps in 200-500 keV first observed in EDF: Lesinski et al. JPhysG39 015108 (2012)
- EDF Δ_N^3 slightly closer to experiment, and more staggering
No indication of shell closures

Nuclear Pairing Gaps: NN vs NN+3N



- Full third order MBPT improves agreement with experiment
- Core-polarization effects significantly enhance pairing gaps
- Good agreement with experimental trends

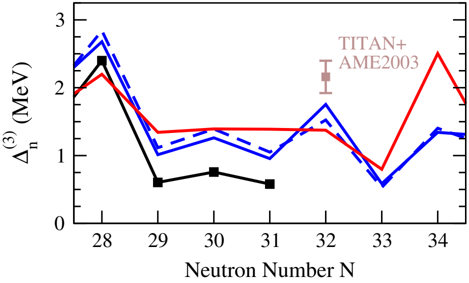
Pairing gaps and seniority



- Perform seniority truncation (limited number broken $J = 0$ pairs)
- Lowest order (no broken pairs) already good approximation apart from mid-shell nuclei
- 2 broken pairs needed in mid-shell, especially when including $g_{9/2}$ orbital

$\Delta_n^{(3)}$ and Shell Evolution

$\Delta_n^{(3)}$ can also tell us about shell evolution



A. T. Gallant et al. PRL109 032506 (2012)

The experimental trend is very well reproduced by NN+3N forces

Theoretical results systematically 0.5 MeV higher than experiment

Shell closure at $N = 28$, sub-shell closure $N = 32$ (moderate) and no apparent $N = 34$ closure

NN forces fail to reproduce $N = 28$ or $N = 32$ predict closed $N = 34$

Phenomenological interactions also describe data very well

$\Delta_n^{(3)}$ and Shell Evolution

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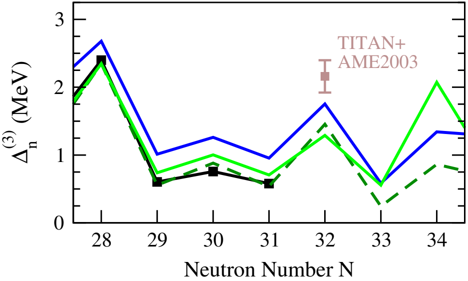

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predict closed $N = 34$

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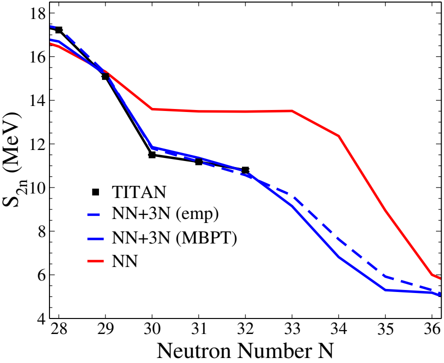
Two-neutron separation energies

Compare S_{2n} theoretical calculations with experimental results

$$S_{2n} = -[B(N,Z) - B(N-2,Z)]$$



A. T. Gallant et al. PRL109 032506 (2012)

NN S_{2n} too flat:
No $N = 28$ or $N = 32$ closures
Points to $N = 34$ closure

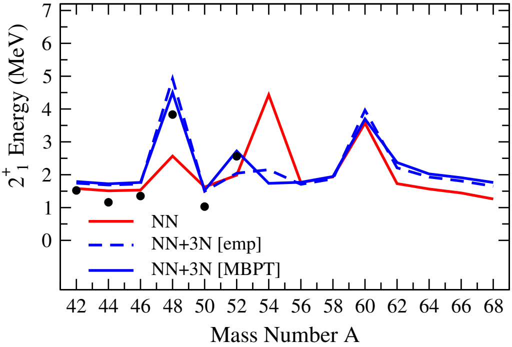
When NN+3N forces are included
Very good agreement with experiment

NN+3N point to $N = 28$ or $N = 32$ closures and no $N = 34$

^{53,54}Ca masses very recently measured at ISOLDE
Very good agreement with NN+3N
Nature, in print (2013)

Shell closures and 2_1^+ energies

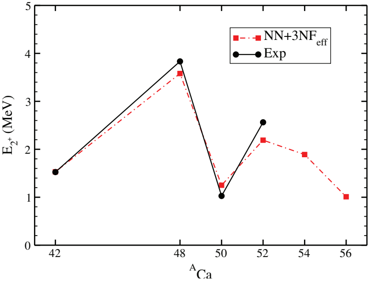
2_1^+ energies characterise shell closures of the neutron rich calcium isotopes



- Correct closure at $N = 28$ when 3N forces are included
- 3N forces enhance closure at $N = 32$
- 3N forces reduce strong closure at $N = 34$ (1.7-2.2 MeV)

Shell closures and 2_1^+ energies

Similar results from Coupled-Cluster

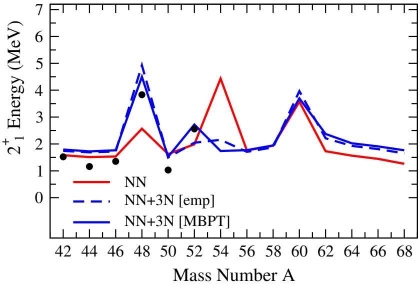


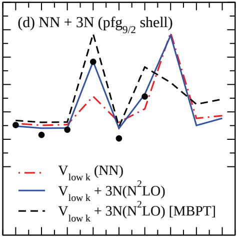
Hagen et al. PRL109 032502 (2012)

^{54}Ca sensitive to 3N interaction:

Difference 1st/3rd MBPT 3N forces

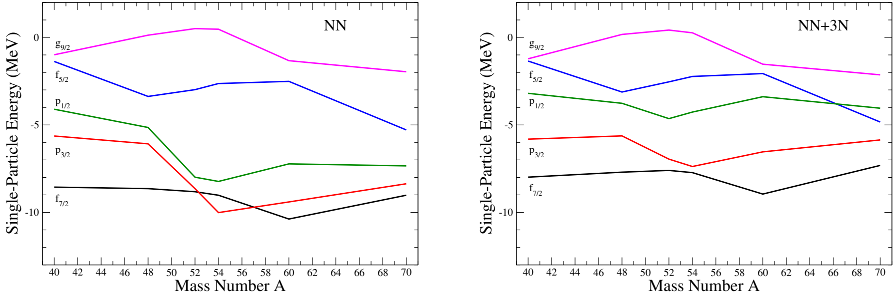
Holt et al. JPG39 085111(2012)





Effective SPEs and shell evolution

Calculate effective SPEs (monopoles)



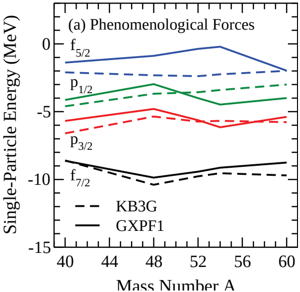
Closed-shells $N = 32$ and $N = 34$ with NN and NN+3N forces guided by ESPEs

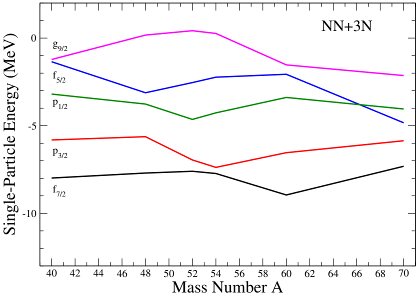
Neither ESPEs shows closed $N = 28$

Different behaviour as phenomenological interactions

Effective SPEs and shell evolution

Calculate effective SPEs (monopoles)





Closed-shells $N = 32$ and $N = 34$ with NN and NN+3N forces guided by ESPEs

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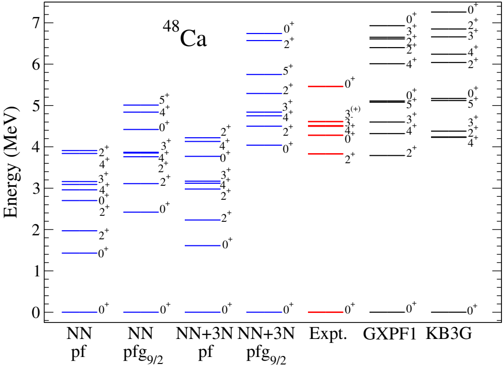
Different behaviour as phenomenological interactions

^{48}Ca spectra

Challenge: Doubly-closed nucleus ^{48}Ca



Spectra too compressed with NN forces only or *pf* space

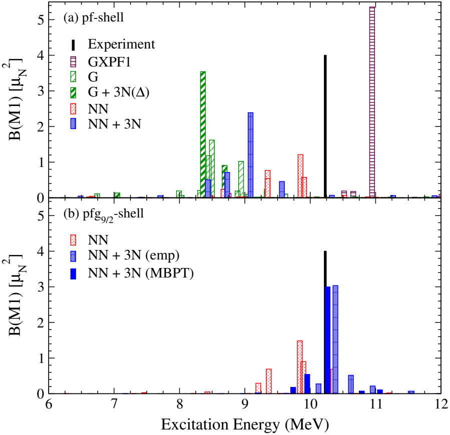
2_1^+ state only ∼appropriate energy in $pfg_{9/2}$ NN+3N calculation

0_1^+ state too low (1st excited state) especially compared to phenomenological interactions

Importance of 3N forces

Importance of including $g_{9/2}$ orbit

B(M1) Transition in ^{48}Ca



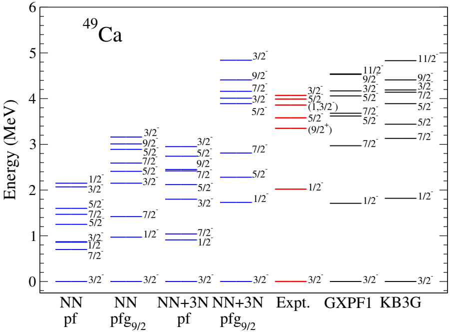
B(M1) strength in ^{48}Ca too fragmented in *pf* space

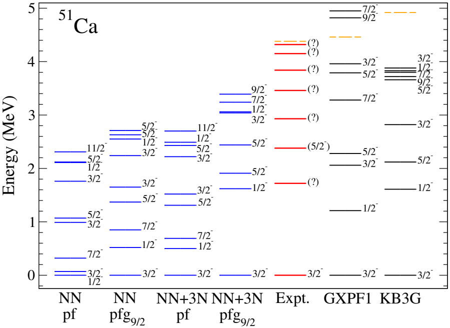
Phenomenological calculations reproduce experimental concentration

In the extended $pfg_{9/2}$ space NN forces also fragmented strength

NN+3N calculation in $pfg_{9/2}$ very good agreement with experiment

^{49}Ca, ^{51}Ca neutron rich spectra





Spectrum compressed unless *pfg*$_{9/2}$ NN+3N

Correct $(1/2)^-$ energy, (but too low $(5/2)^-$), possibility to assign experimental spins

Similar quality comparable to phenomenological interactions

Spectroscopic factors

Have a look at the spectroscopic factors (Shell Model calculation)

	$^{49}\mathrm{Ca}_{gs} \rightarrow {}^{48}\mathrm{Ca}$					SF $\frac{1}{2J_i+1}$				
			$\mathrm{p}_{3/2}$					$\mathrm{f}_{7/2}$		
	0^+_{gs}	1^+_1	2^+_1	3^+_1	sum	2^+_1	3^+_1	4^+_1	5^+_1	sum
GXPF1	0.95	0.00	0.00	0.01	0.96	1.19	1.64	2.11	2.63	**7.57**
(Sum Rule)	(0.96)	(0.01)	(0.03)	(0.04)	(1.04)	(1.25)	(1.72)	(2.23)	(2.69)	**(7.89)**
pf NN+3N	0.77	0.02	0.01	0.02	0.82	0.15	1.24	1.78	2.28	**5.45**
(SR)	(0.85)	(0.04)	(0.22)	(0.11)	(1.22)	(1.25)	(1.59)	(2.04)	(2.53)	**(7.41)**
$\mathrm{pfg}_{9/2}$ NN+3N MBPT spe's	0.91	0.01	0.00	0.01	0.93	0.71	1.15	1.57	1.99	**5.42**
(SR)	(0.93)	(0.02)	(0.09)	(0.04)	(1.08)	(1.00)	(1.32)	(1.70)	(2.10)	**(6.12)**

	$^{50}\mathrm{Ca}_{gs} \rightarrow {}^{49}\mathrm{Ca}$	SF $\frac{1}{2J_i+1}$
	$\mathrm{p}_{3/2}$ $\frac{3}{2}^-_{gs}$	$\mathrm{f}_{7/2}$ $\frac{7}{2}^-_1$
GXPF1	1.73	**7.71**
(SR)	(1.82)	**(7.90)**
pf NN+3N	1.57	**4.54**
(SR)	(1.95)	**(7.31)**
$\mathrm{pfg}_{9/2}$ NN+3N MBPT spe's	1.64	**4.54**
(SR)	(1.81)	**(6.09)**

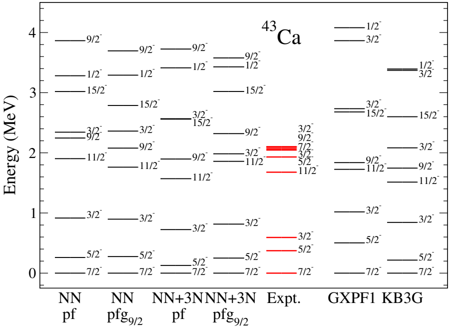
Occupancy of the $f_{7/2}$ orbital lower than phenomenological models (and naively expected)

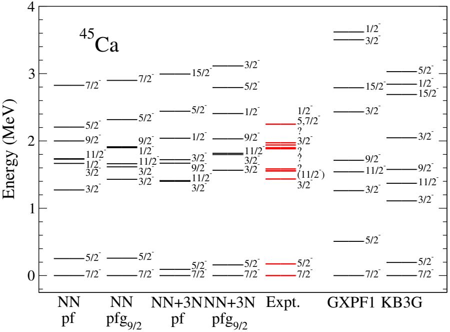
Extended $g_{9/2}$ orbital takes missing occupancy

^{45}Ca, ^{47}Ca light isotopes spectra

Test our interaction with light Ca isotopes

Results in *pf*–*pfg*$_{9/2}$ spaces and based on NN–NN+3N interactions compared to standard phenomenological interactions





Agreement with experiment similar to phenomenological interactions

sd degrees of freedom might still play a role for some excited states

B(E2) Transition Strengths

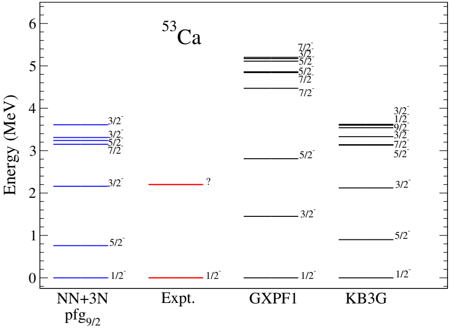
Isotope	Transition	KB3G	GXPF1A	MBPT	EXP.
^{46}Ca	$2^+ \to 0^+$	9.2	9.2	13.3	25.4±4.5 36.4±2.6
^{46}Ca	$6^+ \to 4^+$	3.6	3.6	4.8	5.38±0.29
^{47}Ca	$3/2^- \to 7/2^-$	0.84	3.6	1.0	4.0±0.2
^{48}Ca	$2^+ \to 0^+$	11.5	11.9	10.3	19±6.4
^{49}Ca	$7/2^- \to 3/2^-$	0.41	4.0	0.22	0.53±0.21
^{50}Ca	$2^+ \to 0^+$	8.9	9.1	11.2	7.4±0.2

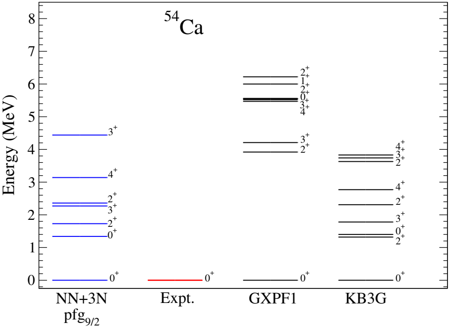
B(E2)s in reasonable agreement with experiment
(order of magnitude)

Similar quality as phenomenological interactions (very close to KB3G)

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

^{53}Ca, ^{54}Ca neutron rich spectra:





Phenomenological interactions different results in neutron rich nuclei

MBPT: prediction, more controlled

Explore sensitivity to theoretical uncertainties
(difference with respect to 3N 1st order results)

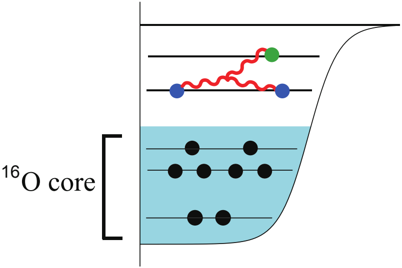
Residual 3N Forces

In the most neutron-rich isotopes,
3N forces between 3 valence neutrons
(suppressed by $N_{valence}/N_{core}$)
can give a relevant contribution

Exact treatment of residual 3N forces
would demand V^{3N} diagonalization

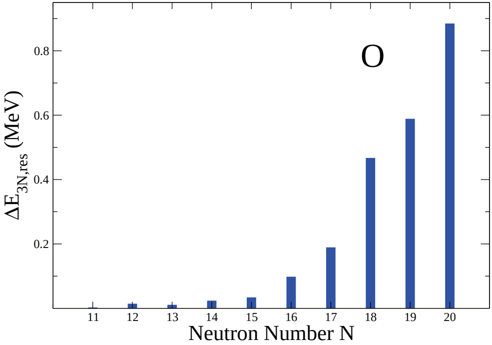
Expected small correction
compared to other 3N contributions
Evaluated 1st order perturbation theory:

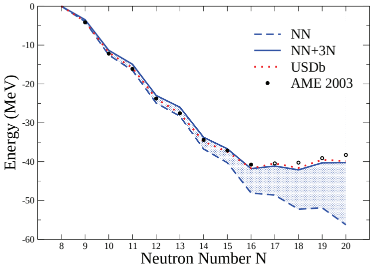
$$\langle\Psi|V^{3N}|\Psi\rangle$$



Residual 3N forces expected more
important in O isotopes

Residual 3N forces in O isotopes





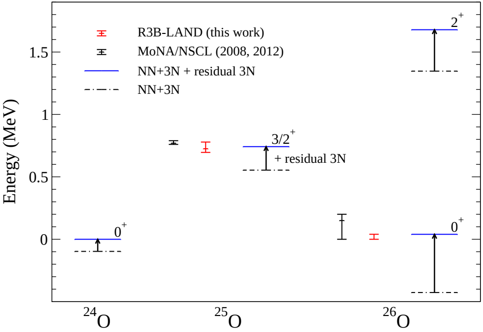
Residual 3N forces small and repulsive correction

Increase with the number of neutrons

Negligible up to ^{24}O, up to $\sim$1 MeV in ^{28}O

Important in the dripline region: flat energy behaviour

Residual 3N Forces around O dripline



Caesar, Simonis et al, arXiv:1209.0156

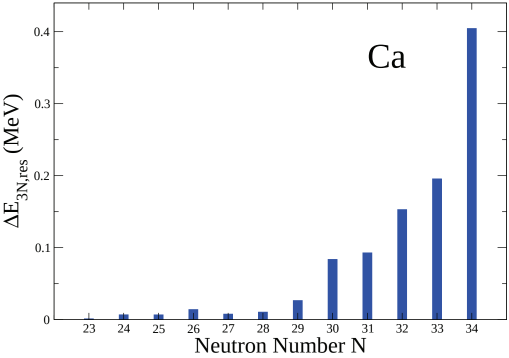
Compare to experimental energies of unbound ^{25}O and ^{26}O (relative to ^{24}O)

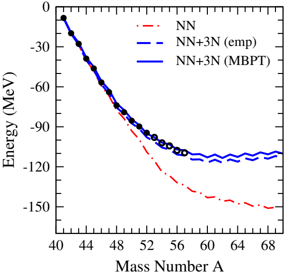
Without residual 3N forces
O dripline predicted at ^{26}O
by $\sim$ 300 keV
(3N forces to 3rd order in MBPT)

Residual 3N forces drive dripline to ^{24}O in agreement with experiment

Unbound ^{25}O and ^{26}O also in very good agreement with MSU and GSI measurements

Residual 3N forces in Ca isotopes





Residual 3N forces repulsive

Smaller that in the O case: 20 vs 8 core-neutrons

Negligible for the discussion of S_{2n}, Δ_n or spectra

Summary and Outlook

Microscopic calculation based on chiral EFT (NN+3N forces) and MBPT gives good agreement with experimental two-neutron separation energies, pairing gaps and excitation spectra for calcium isotopes:

- Experimental trends in S_{2n}'s and $\Delta_n^{(3)}$'s nicely reproduced
- S_{2n}'s and $\Delta_n^{(3)}$ together with 2_1^+ energies establish shell closures: $N = 28$ appears, $N = 32/34$ enhanced/reduced by 3N forces
- Predicted spectra for Ca neutron rich isotopes
- Residual 3N forces included and found relevant in O isotopes

Outlook:

Explore uncertainties in the theoretical calculation

Lee-Suzuki transformation from $pf\, g_{9/2}$ to pf space