Nuclear structure and reactions from coupled-cluster theory

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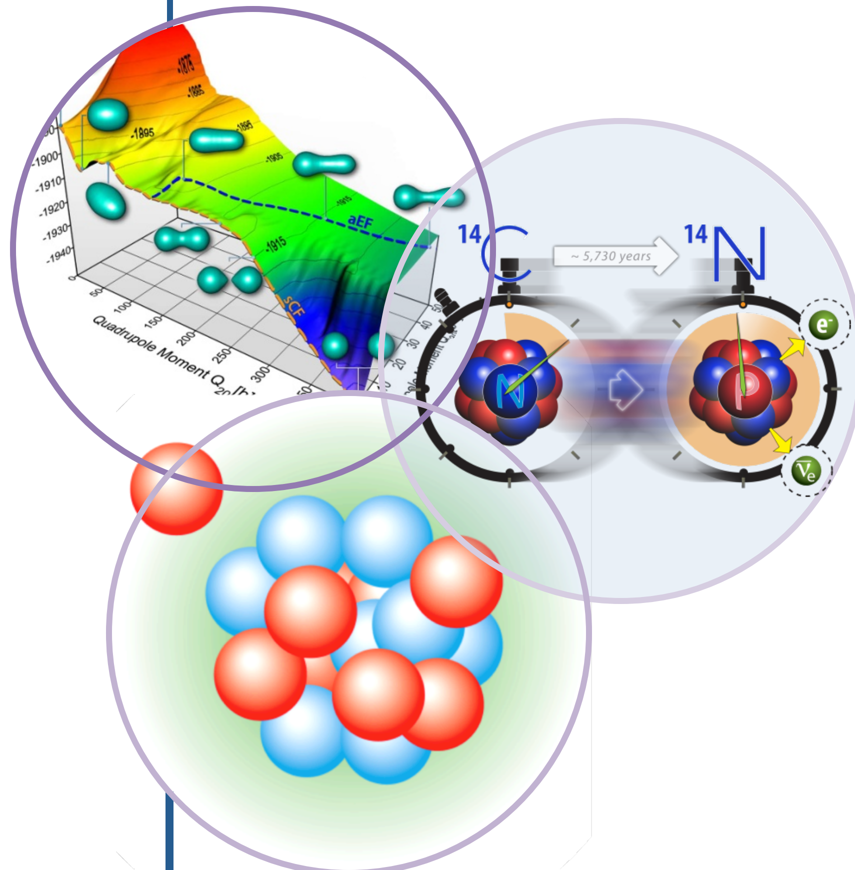


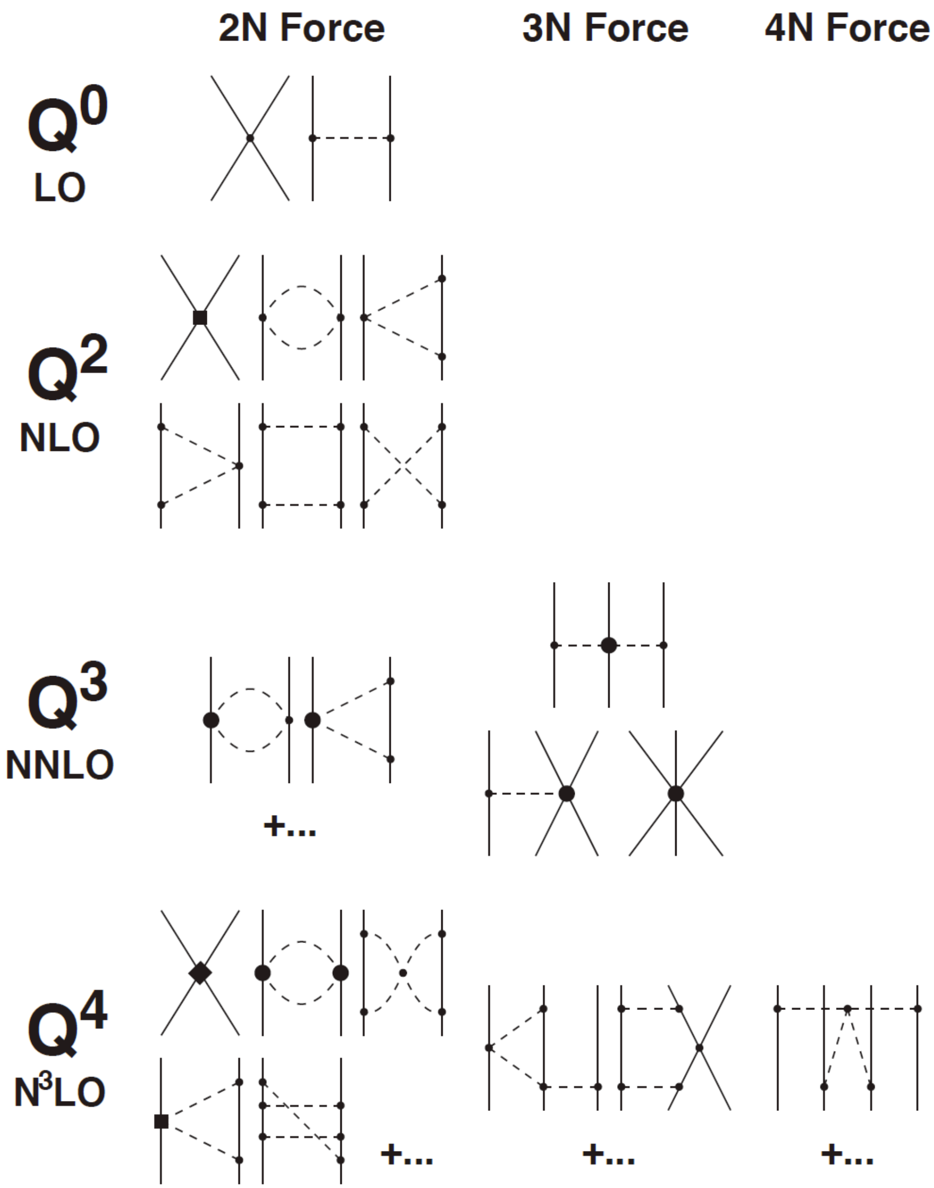
ECT, Trento, June 13 2013

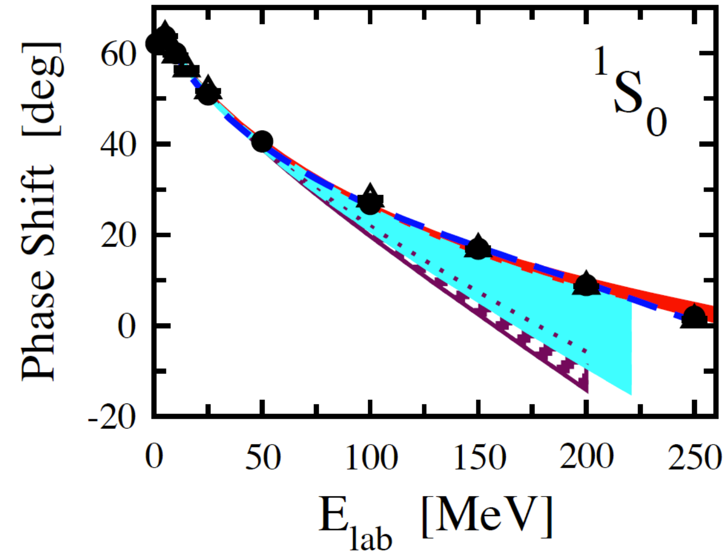
Outline

1. Optimization of interactions from Chiral Effective Field Theory.
2. Physics of nuclei at the limits of stability and Coupled-Cluster theory
3. Structure of neutron rich oxygen and fluorine isotopes from optimized chiral interactions
4. Shell evolution in neutron rich calcium isotopes: Is ^{54}Ca (N=34) a magic nucleus?
5. Coupled-cluster approach to nucleon-nucleus scattering: *p*-^{40}Ca elastic scattering
6. Merging coupled-cluster with halo EFT: Efimov physics around the neutron rich ^{60}Ca

Nuclear forces from chiral effective field theory

[Weinberg; van Kolck; Epelbaum *et al*.; Entem & Machleidt; …]





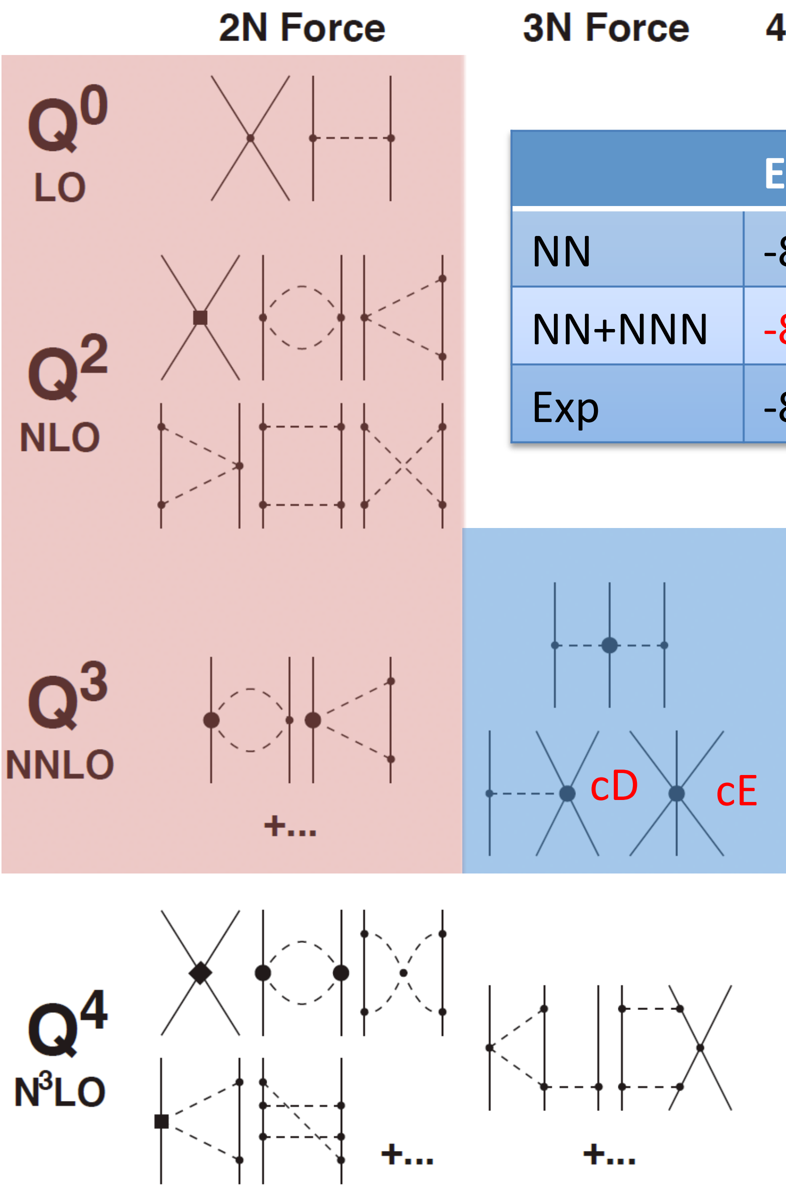
[Epelbaum, Hammer, Meissner RMP 81, 1773 (2009)]

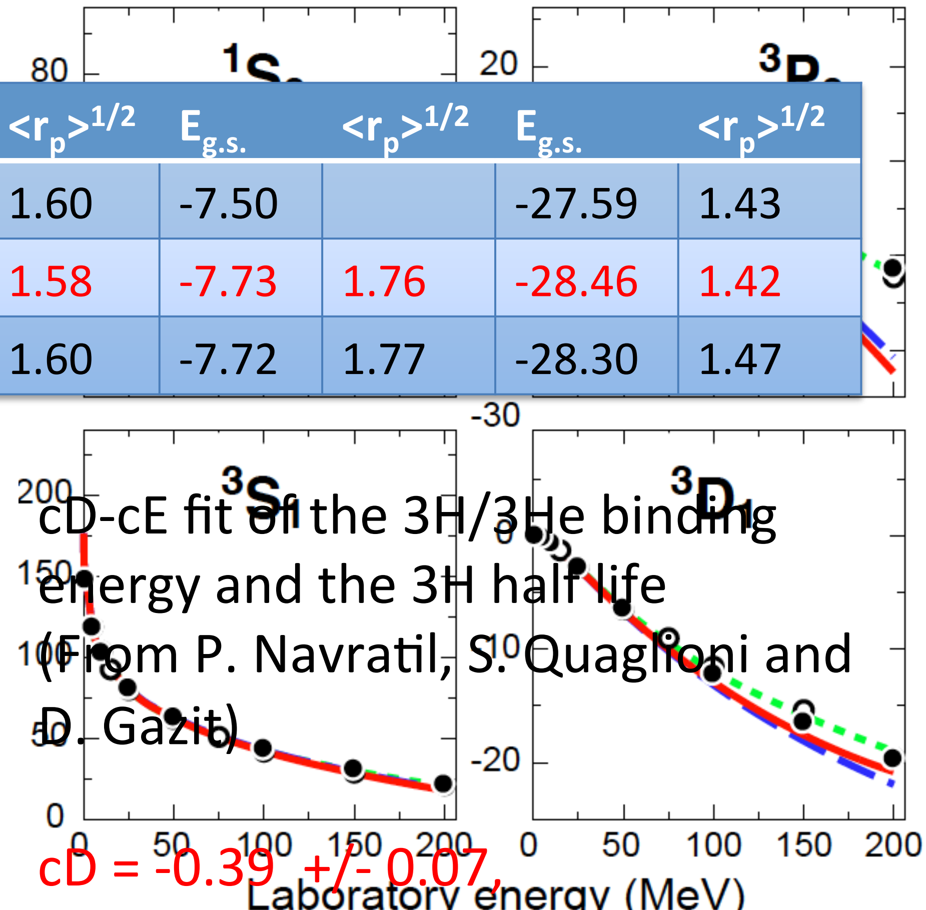
Low energy constants from fit of NN data, A=3,4 nuclei, or light nuclei.

- Model inadequacy: optimization of the parameters order-by-order
- Parameter uncertainties: Covariance and sensitivity analysis of parameters in few- AND many-body systems
- What is the right power counting?

Optimization of Chiral interactions at NNLO

A. Ekström et al, Phys. Rev. Lett. 110, 192502 (2013)





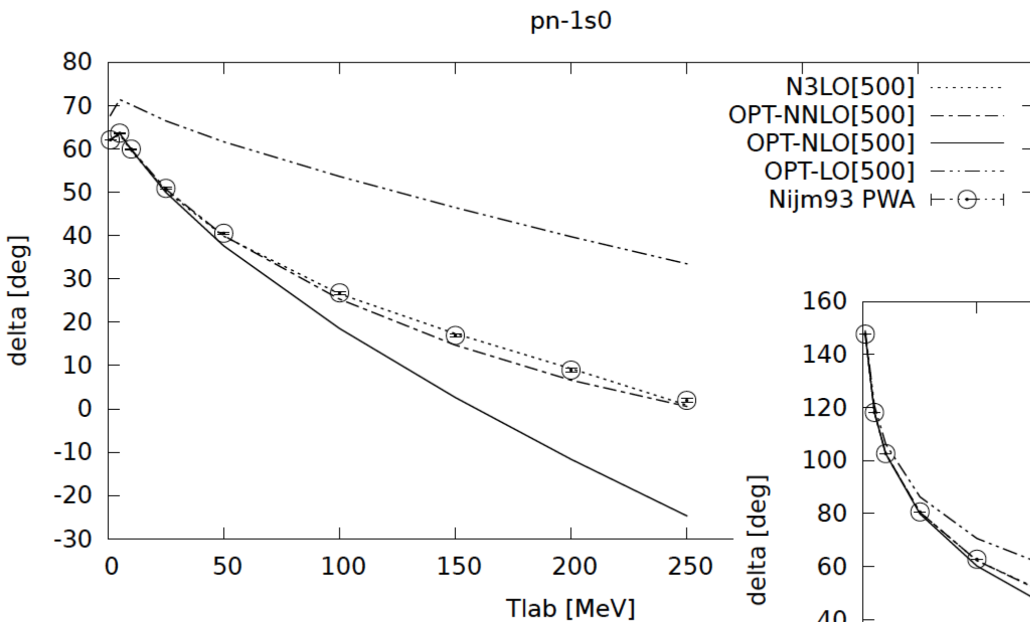
	$E_{g.s.}$	$\langle r_p \rangle^{1/2}$	$E_{g.s.}$	$\langle r_p \rangle^{1/2}$	$E_{g.s.}$	$\langle r_p \rangle^{1/2}$
NN	-8.25	1.60	-7.50		-27.59	1.43
NN+NNN	-8.48	1.58	-7.73	1.76	-28.46	1.42
Exp	-8.48	1.60	-7.72	1.77	-28.30	1.47

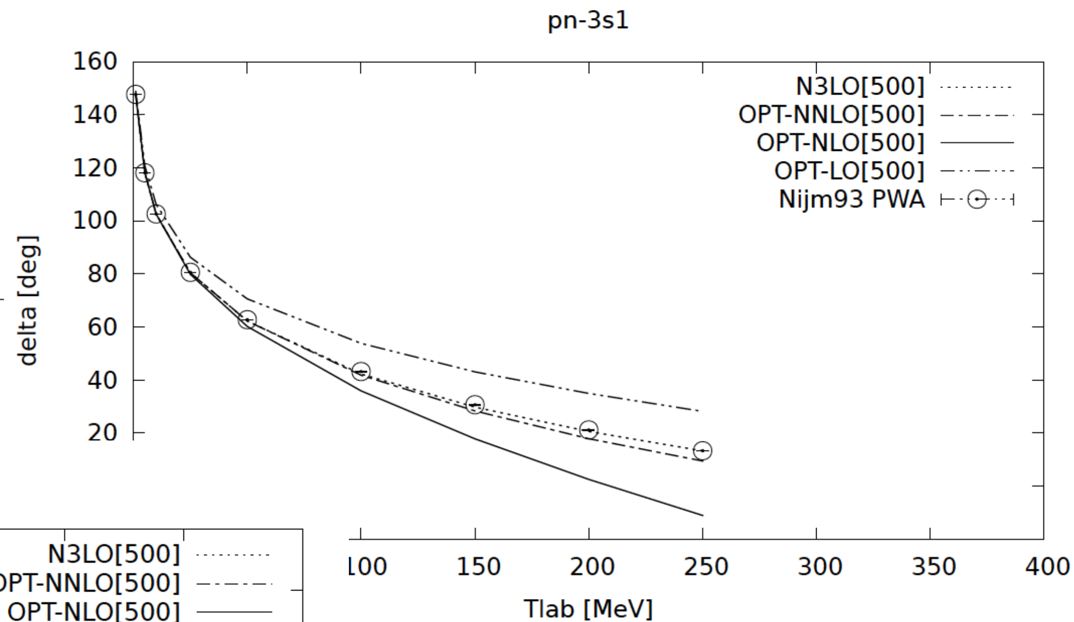
cD-cE fit of the 3H/3He binding energy and the 3H half life (From P. Navratil, S. Quaglioni and D. Gazit)

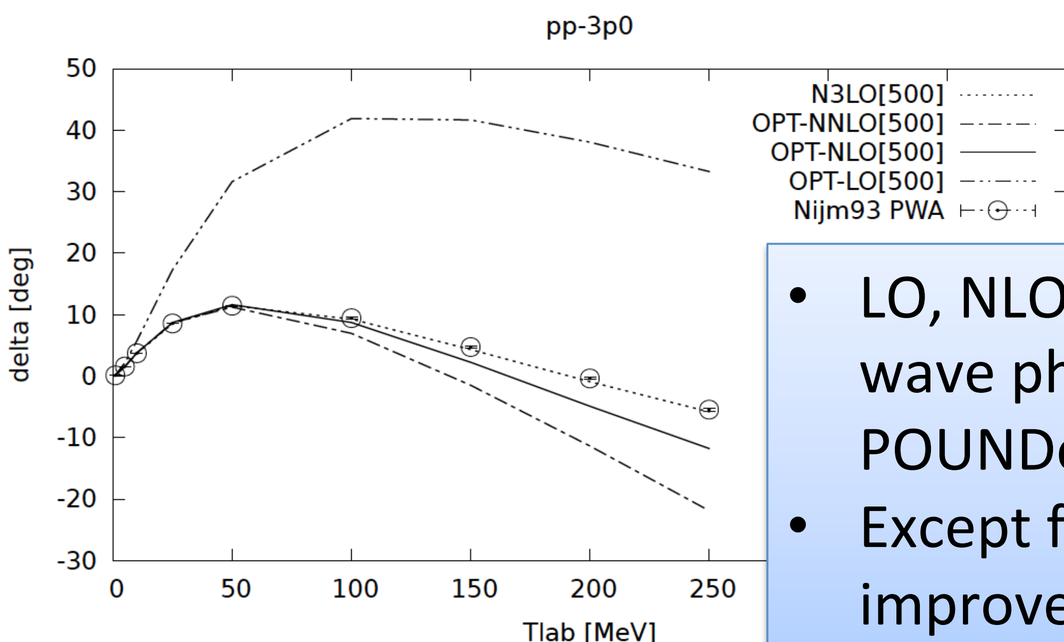
cD = -0.39 +/- 0.07,

cE = -0.398 +0.015/-0.016

T_{lab} (MeV)	0–35	35–125	125–183	183–290	0–290
$pp\ \chi^2$/datum	1.11	1.56	23.95 4.35^a	29.26	17.10 14.03^a
$np\ \chi^2$/datum	0.85	1.17	1.87	6.09	2.95







- LO, NLO and NLO selected partial wave phaseshifts obtained with POUNDerS.go
- Except for 3P0 we see a systematic improvement in phase shifts.

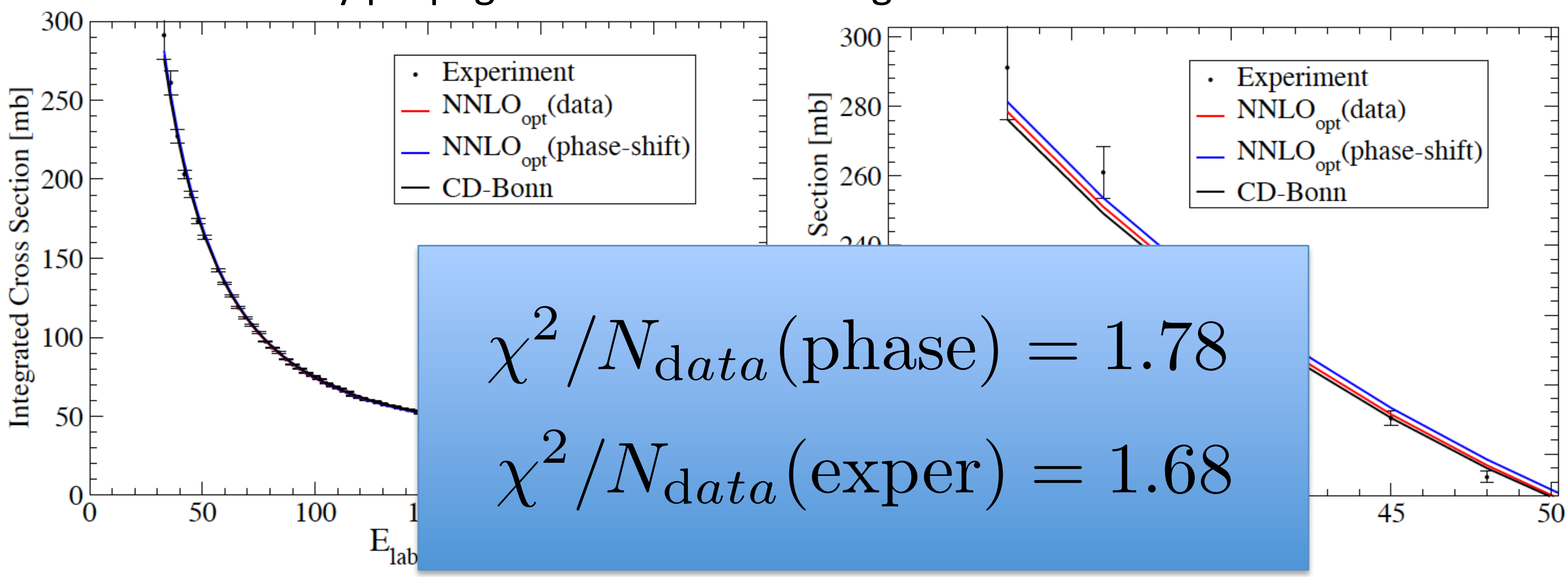
Optimization strategy of chiral interactions

Sources of error:

1. Experimental error – how does this propagate from light to medium mass nuclei?
2. Error from truncation at a given order in chiral EFT:
   - ➢ Establish the correct power counting and placement of counter terms

$$\chi^2 = \sum \frac{(\text{Theory} - \text{Exp.})}{\text{Error}}$$

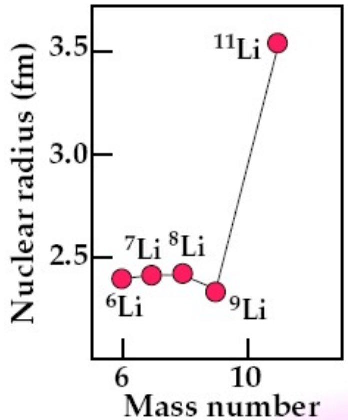
- Minimize the objective function with respect to pool of data
- Compute the co-variance matrix and perform sensitivity analysis
- Study propagation of error from light to medium mass



$$\chi^2/N_{data}(\text{phase}) = 1.78$$

$$\chi^2/N_{data}(\text{exper}) = 1.68$$

Physics of nuclei at the edges of stability



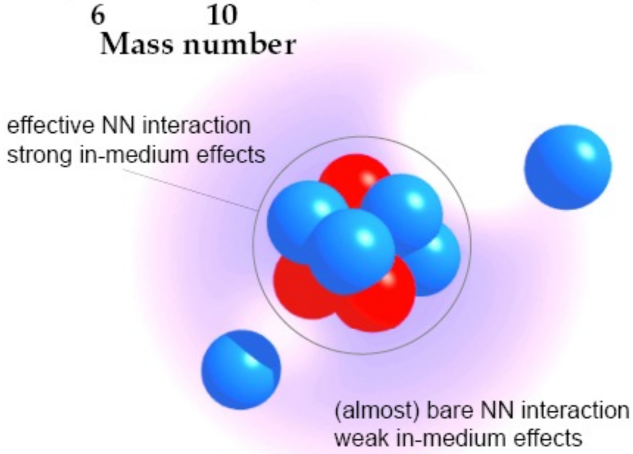
I. Tanihata et al.
Phys. Rev. Lett. 55, 2676 (1985)

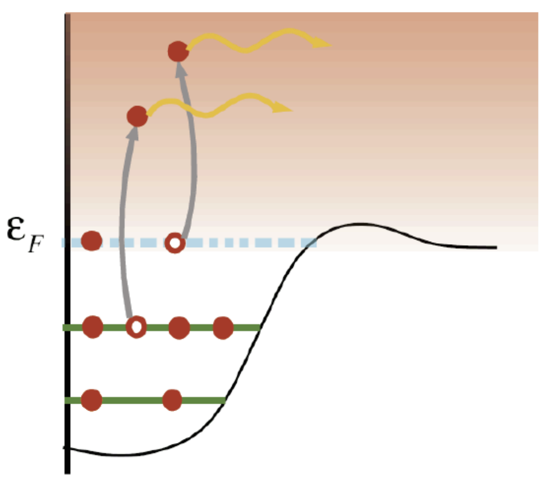
Interaction cross section
measurements at Bevalac
(790 MeV/u)

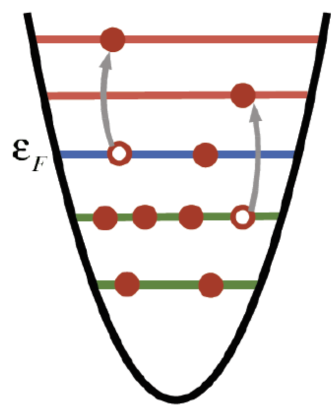
The Berggren completeness treats bound, resonant and scattering states on equal footing.

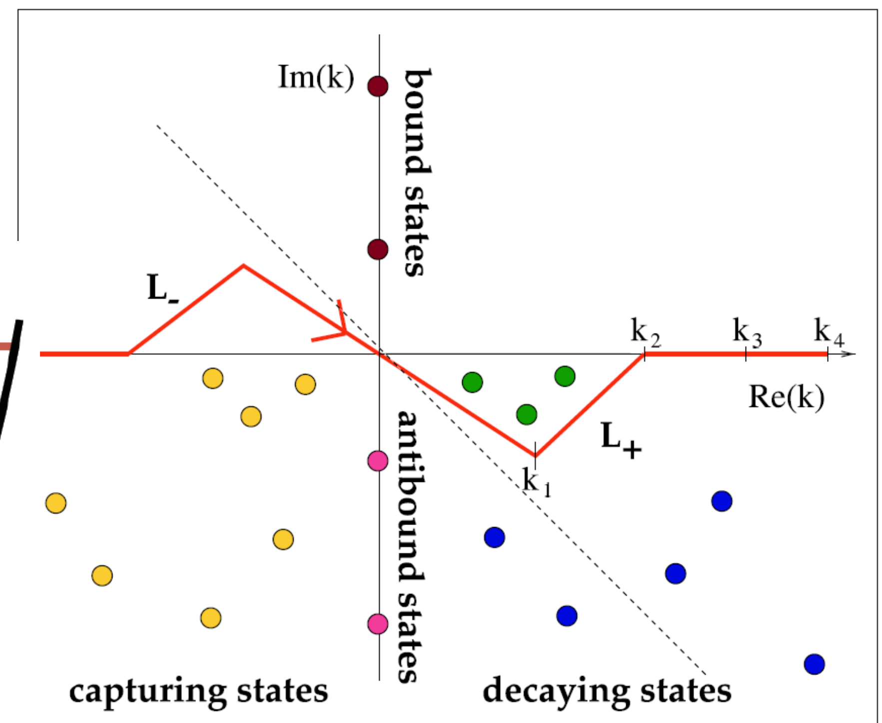
Has been successfully applied in the shell model in the complex energy plane to light nuclei. For a review see

N. Michel et al J. Phys. G 36, 013101 (2009).









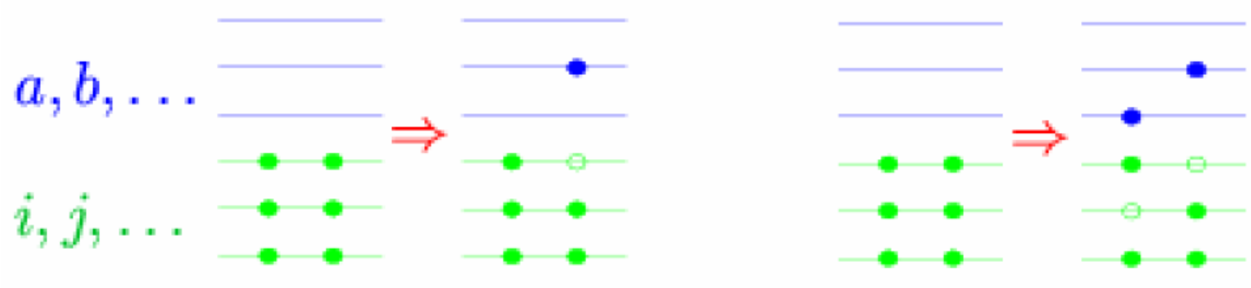
Coupled-cluster method (in CCSD approximation)

Ansatz:

$$
\begin{aligned}
|\Psi\rangle &= e^{T}|\Phi\rangle \\
T &= T_1 + T_2 + \ldots \\
T_1 &= \sum_{ia} t_i^a a_a^\dagger a_i \\
T_2 &= \sum_{ijab} t_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i
\end{aligned}
$$

- ☺ Scales gently (polynomial) with increasing problem size o^2u^4 .
- ☺ Truncation is the only approximation.
- ☺ Size extensive (error scales with A)
- ☹ Most efficient for doubly magic nuclei

Correlations are *exponentiated* 1p-1h and 2p-2h excitations. Part of np-nh excitations included!



Coupled cluster equations

$$
\begin{aligned}
E &= \langle\Phi|\overline{H}|\Phi\rangle \\
0 &= \langle\Phi_i^a|\overline{H}|\Phi\rangle \\
0 &= \langle\Phi_{ij}^{ab}|\overline{H}|\Phi\rangle
\end{aligned}
$$

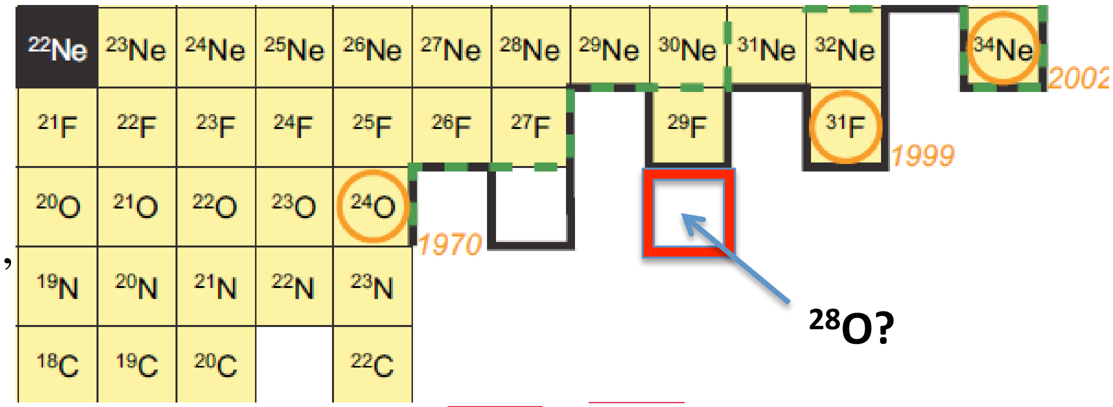
Alternative view: CCSD generates similarity transformed Hamiltonian with no 1p-1h and no 2p-2h excitations.

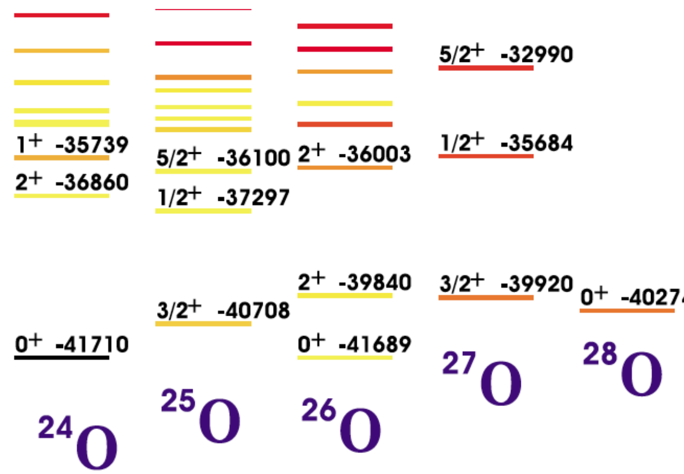
$$
\overline{H} \equiv e^{-T}He^{T} = \left(He^{T}\right)_c = \left(H + HT_1 + HT_2 + \frac{1}{2}HT_1^2 + \ldots\right)_c
$$

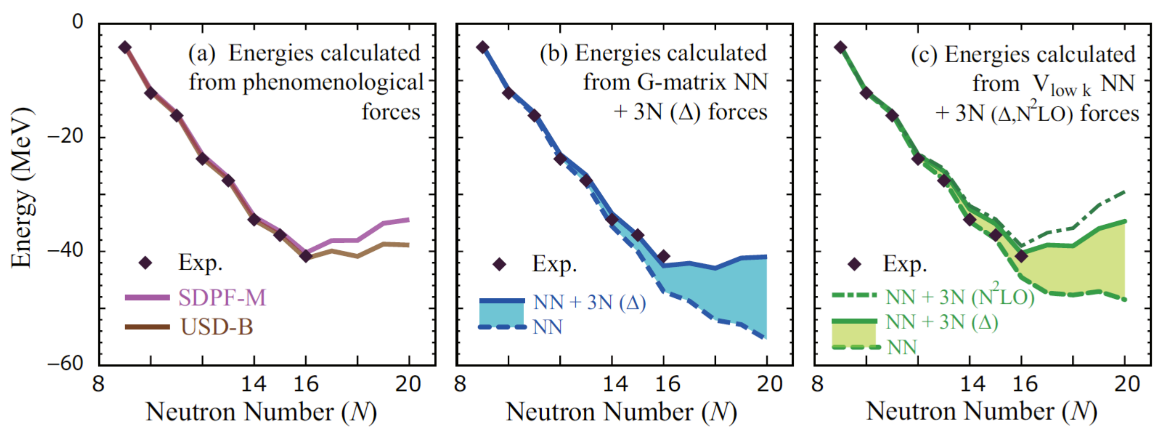
Structure of neutron rich oxygen isotopes

Experimental situation

- “Last” stable oxygen isotope ^{24}O
- ^{25,26}O unstable (Hoffman et al 2008, Lunderberg et al 2012)
- ^{28}O not seen in experiments
- ^{31}F exists (adding on proton shifts drip line by 6 neutrons)



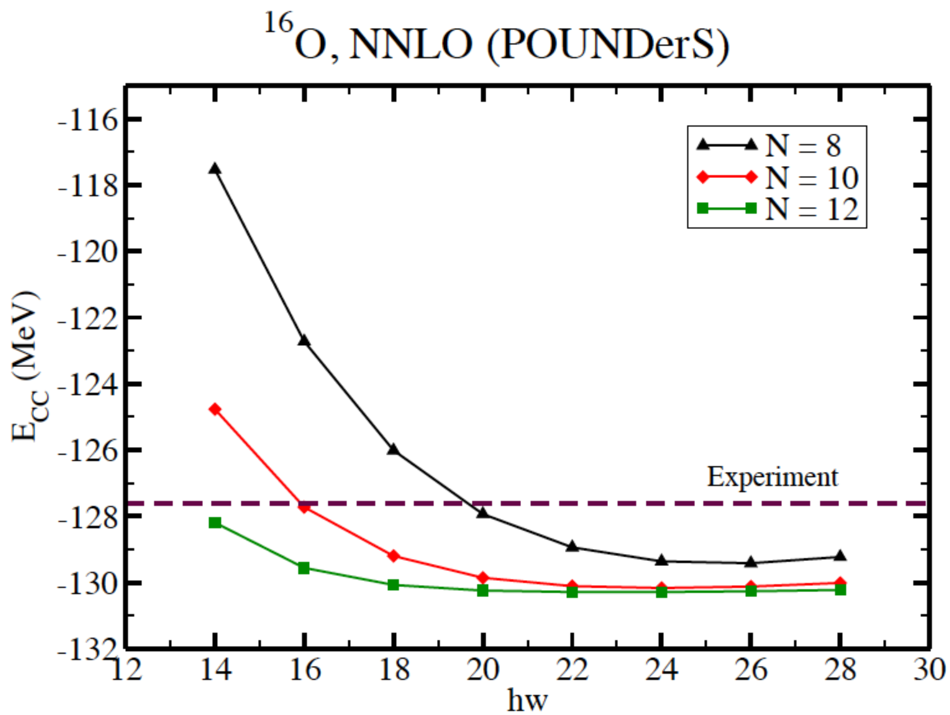




Continuum shell model with HBUSD interaction predict ^{28}O unbound. A. Volya and V. Zelevinsky PRL (2005)

Shell model (sd shell) with monopole corrections based on three-nucleon force predicts 2nd O as last stable isotope of oxygen. [Otsuka, Suzuki, Holt, Schwenk, Akaishi, PRL (2010), arXiv:0908.2607]

Light nuclei from NNLO-POUNDerS

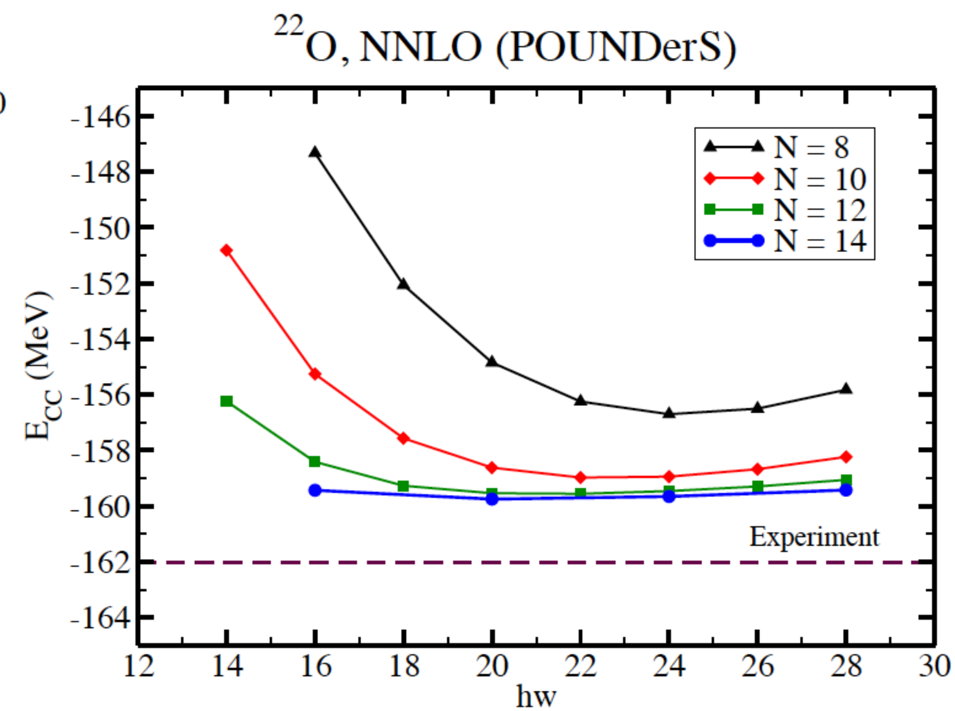


- Rapid Convergence for ground states of oxygen isotopes with NNLO-POUNDerS.
- Already with N =12-14 major harmonic oscillator shells results are well converged.

A. Ekström et al, Phys. Rev. Lett. 110, 192502 (2013)

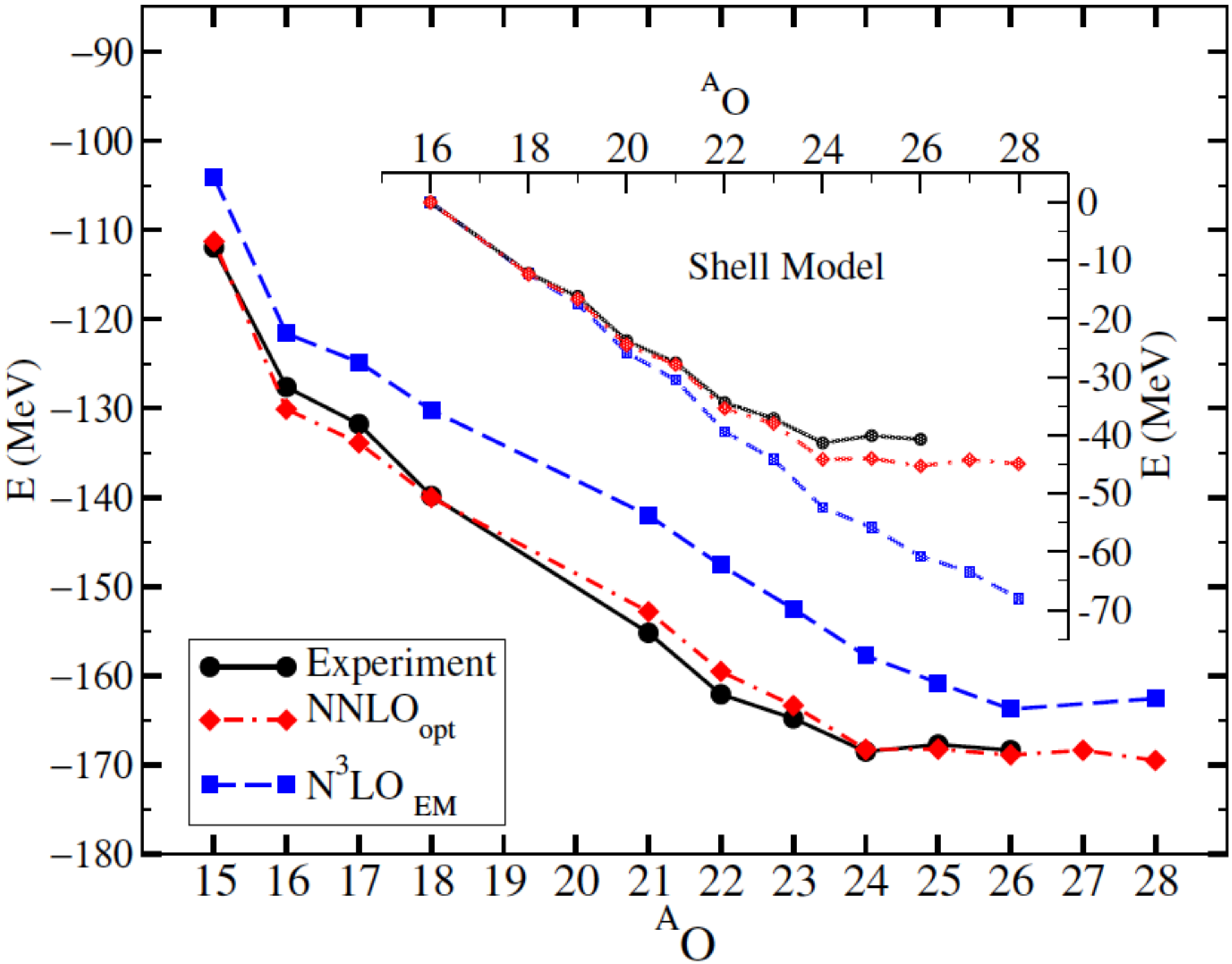
- NNLO-POUNDerS is a “soft” potential
- No dramatic overbinding is found for light nuclei

	$E(^3\mathrm{H})$	$E(^3\mathrm{He})$	$E(^4\mathrm{He})$	$r_p(^4\mathrm{He})$
NNLO	-8.249	-7.501	-27.759	1.43(8)
NNLO+NNN	-8.469	-7.722	-28.417	1.43(8)
Experiment	-8.482	-7.717	-28.296	1.467(13)



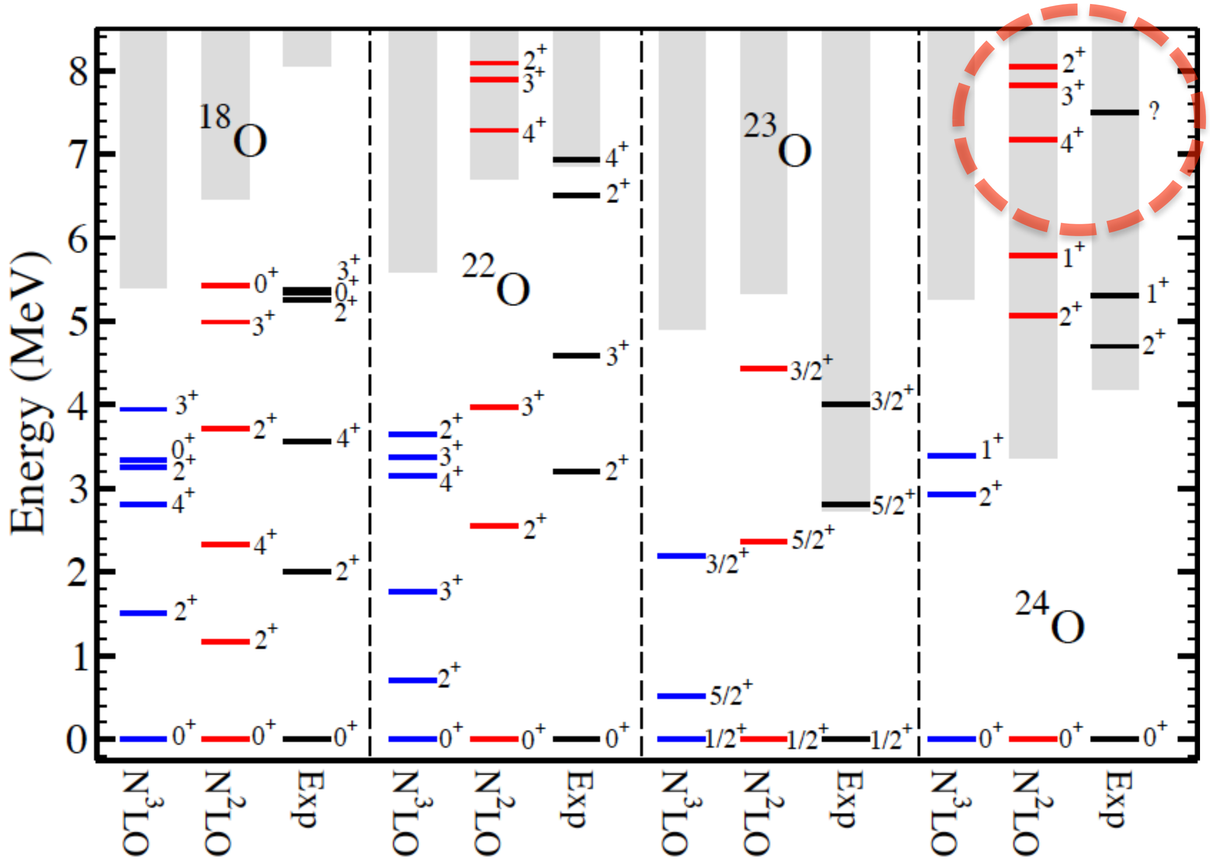
Oxygen isotopes from NNLO(POUNDerS)

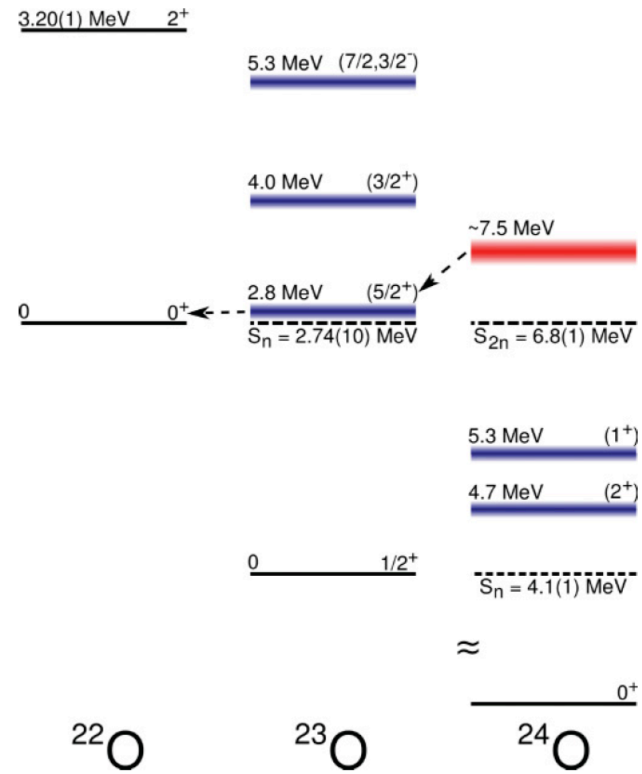
A. Ekström et al, Phys. Rev. Lett. 110, 192502 (2013)



Excited states in neutron rich oxygen isotopes

Coupled-cluster calculations of excited states in neutron rich oxygen isotopes from NNLO(POUNDerS)





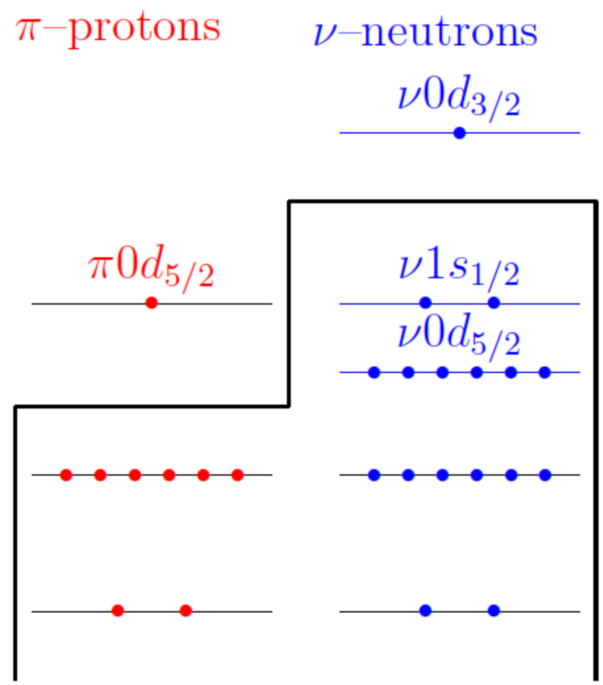
Experiment

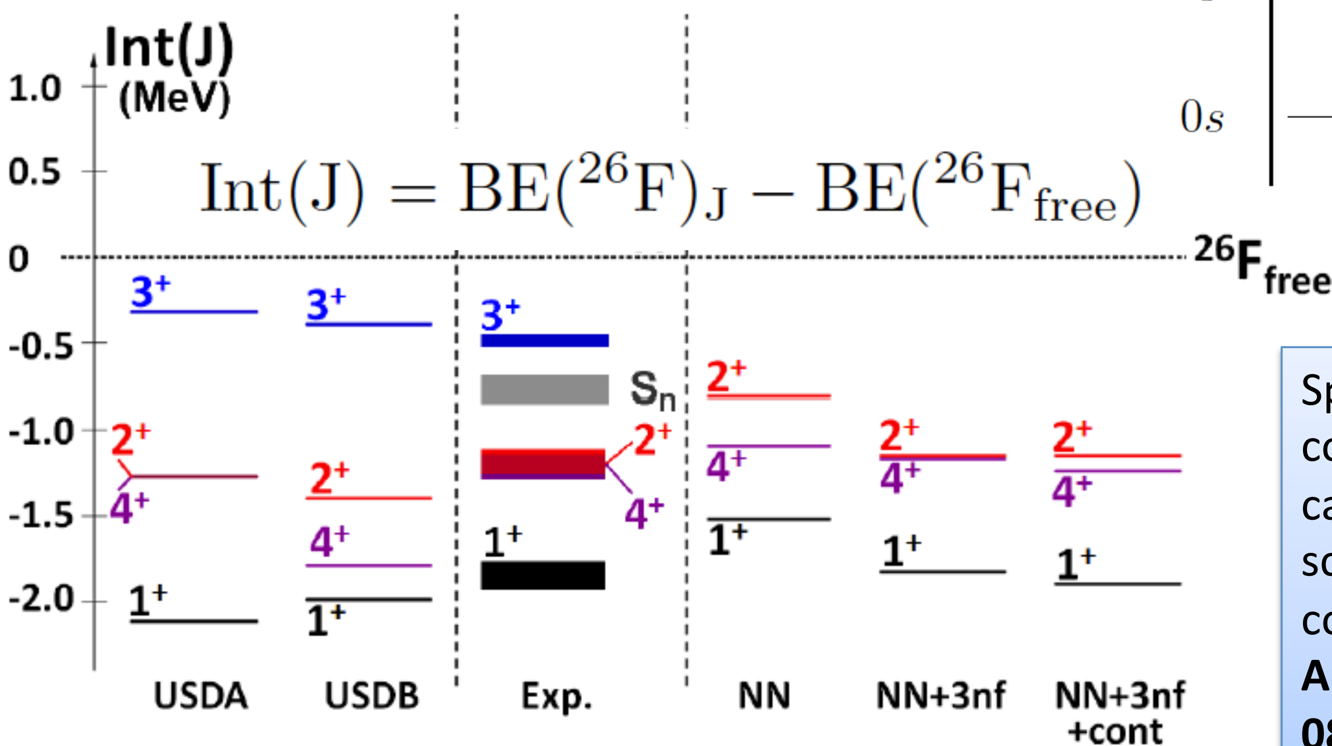
[Hoffman et al., PRC 83, 031303 (2011)] Unbound states in ^{24}O populated by knockout from ^{26}F. Observation of ^{22}O and two-neutron cascade. Speculation: single resonance or superposition of states with $J^{\pi} = 1^+$ to 4^+.

Long-lived 4^+ isomer in Fluorine-26

$$(\bar{H}\hat{R}_\mu^{(A\pm2)})_C|\Phi_0\rangle = \omega_\mu \hat{R}_\mu^{(A\pm2)}|\Phi_0\rangle$$

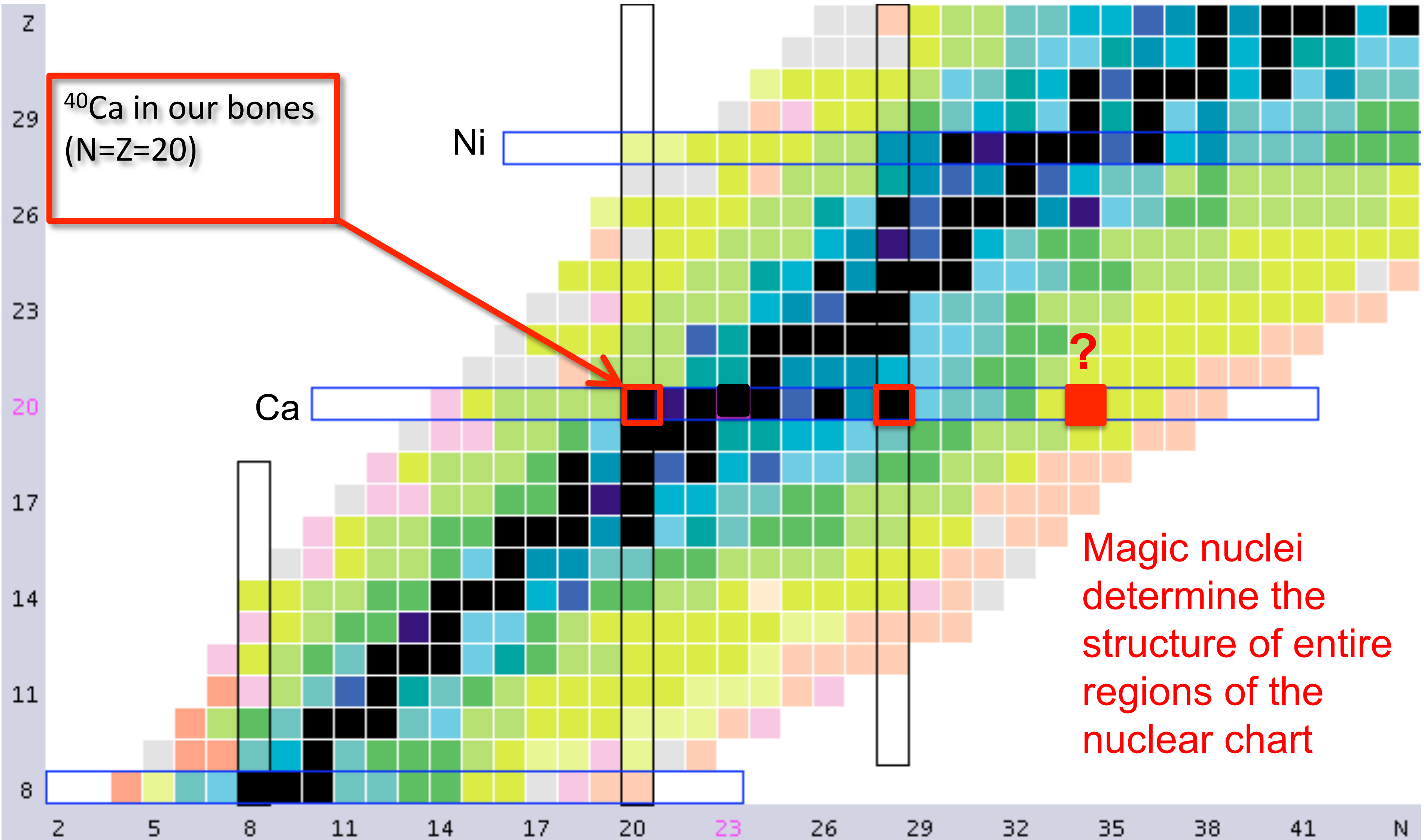
$$\hat{R}^{(A+2)} = \frac{1}{2}\sum_{ba} r^{ab} a_a^\dagger a_b^\dagger + \frac{1}{6}\sum_{iabc} r_i^{abc} a_a^\dagger a_b^\dagger a_c^\dagger a_i + \ldots$$





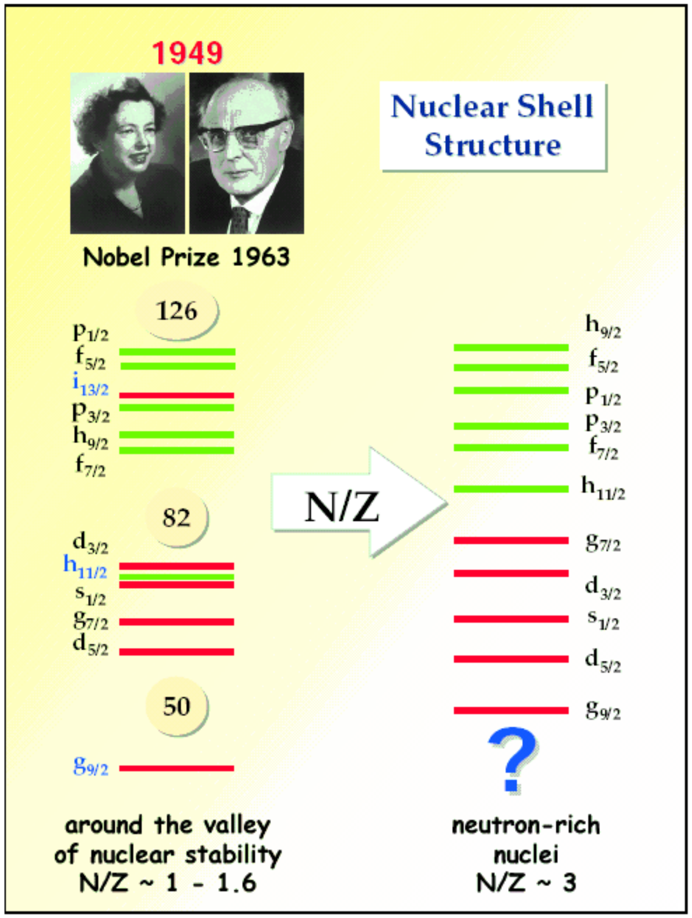
Spectra in ^{26}F compared to coupled-cluster calculations with inclusion of schematic 3NFs and continuum
A. Lepailleur et al, PRL 110 082502 (2013)

Is ^{54}Ca a magic nucleus?

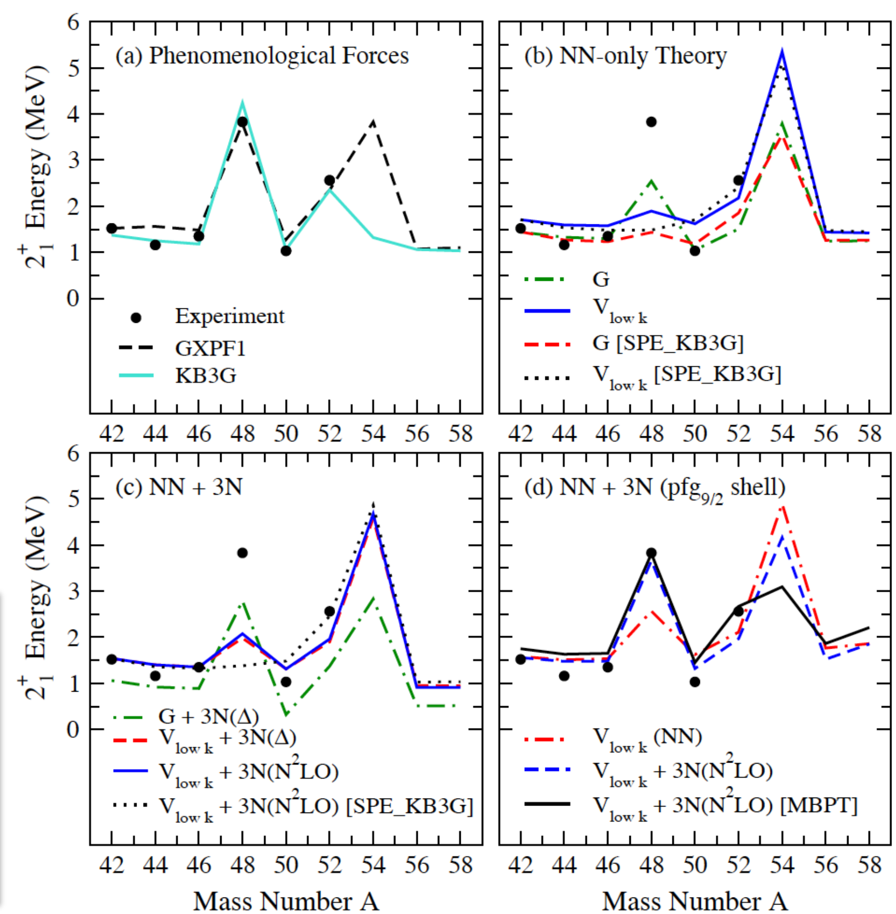


Magic nuclei determine the structure of entire regions of the nuclear chart

Evolution of shell structure in neutron rich Calcium



- How do shell closures and magic numbers evolve towards the dripline?
- Is the naïve shell model picture valid at the neutron dripline?



- What are the mechanisms responsible for shell closure in ^{48}Ca?
- Different models give conflicting result for shell closure in ^{54}Ca.

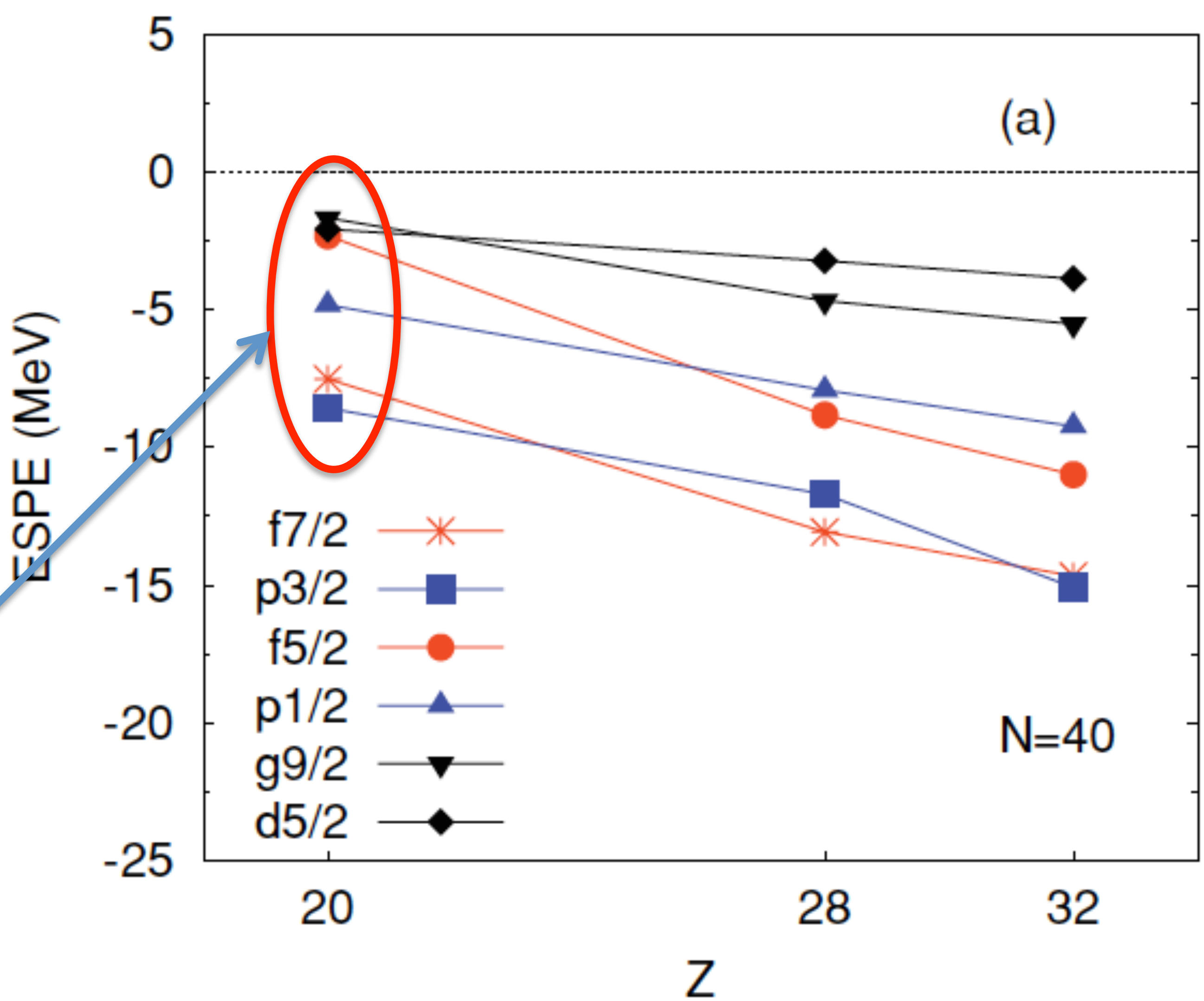
J. D. Holt et al, J. Phys. G **39**, 085111 (2012)

Evolution of shell structure in neutron rich Calcium

Inversion of shell order in ^{60}Ca

S. M. Lenzi, F. Nowacki, A. Poves, and K. Sieja Phys. Rev. C 82, 054301 (2010)

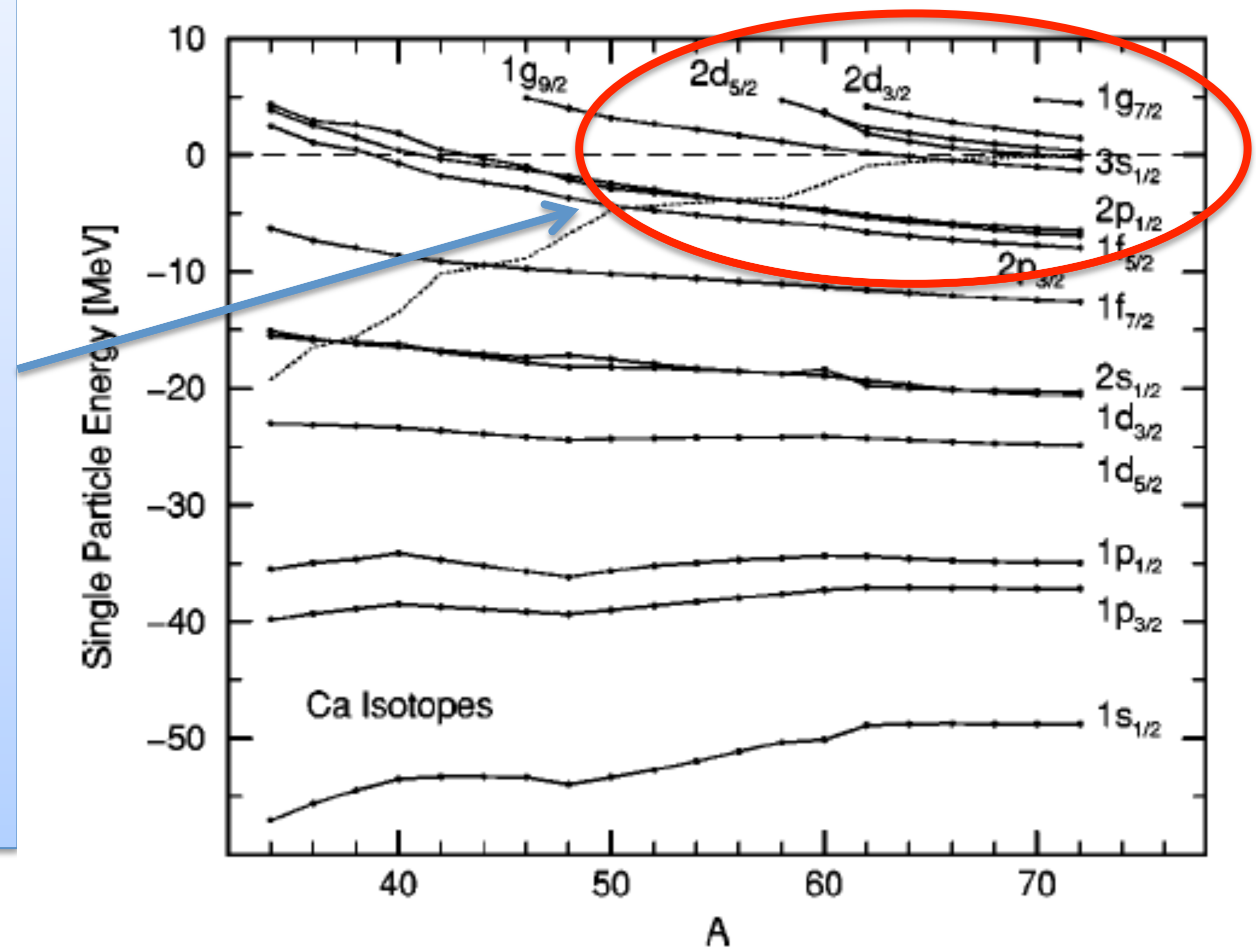
- Inversion of d5/2 and g9/2 in ^{60}Ca.
- Bunching of levels pointing to no shell-closure.



Evolution of shell structure in neutron rich Calcium

- Relativistic mean-field show no shell gap in $^{60-70}Ca$
- Bunching of single-particle orbitals
- large deformations and no shell closure

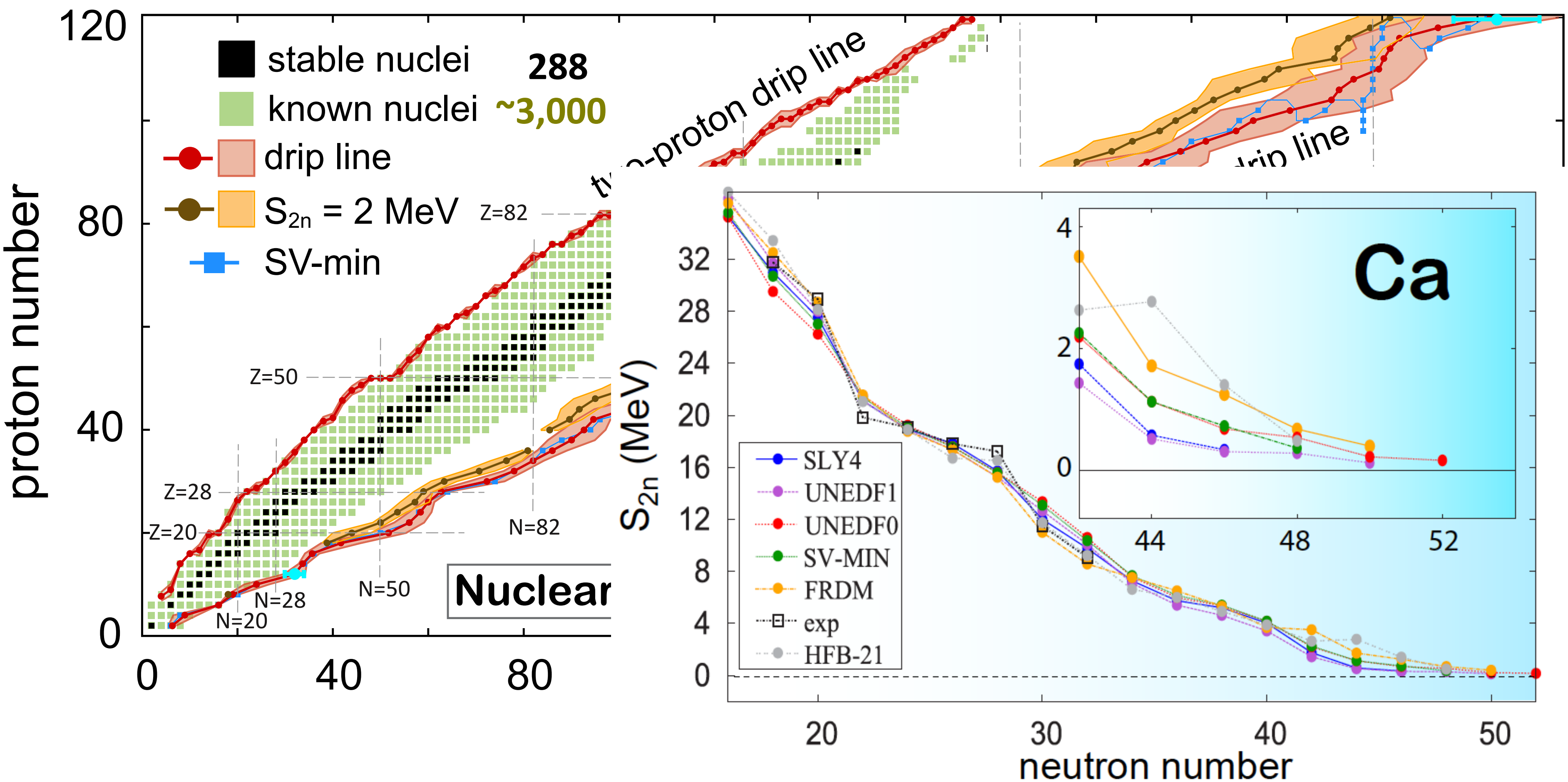
J. Meng et al, Phys. Rev. C 65, 041302(R) (2002)



How many protons and neutrons can be bound in a nucleus?

Literature: 5,000-12,000

Skyrme-DFT: 6,900±500$_{syst}$



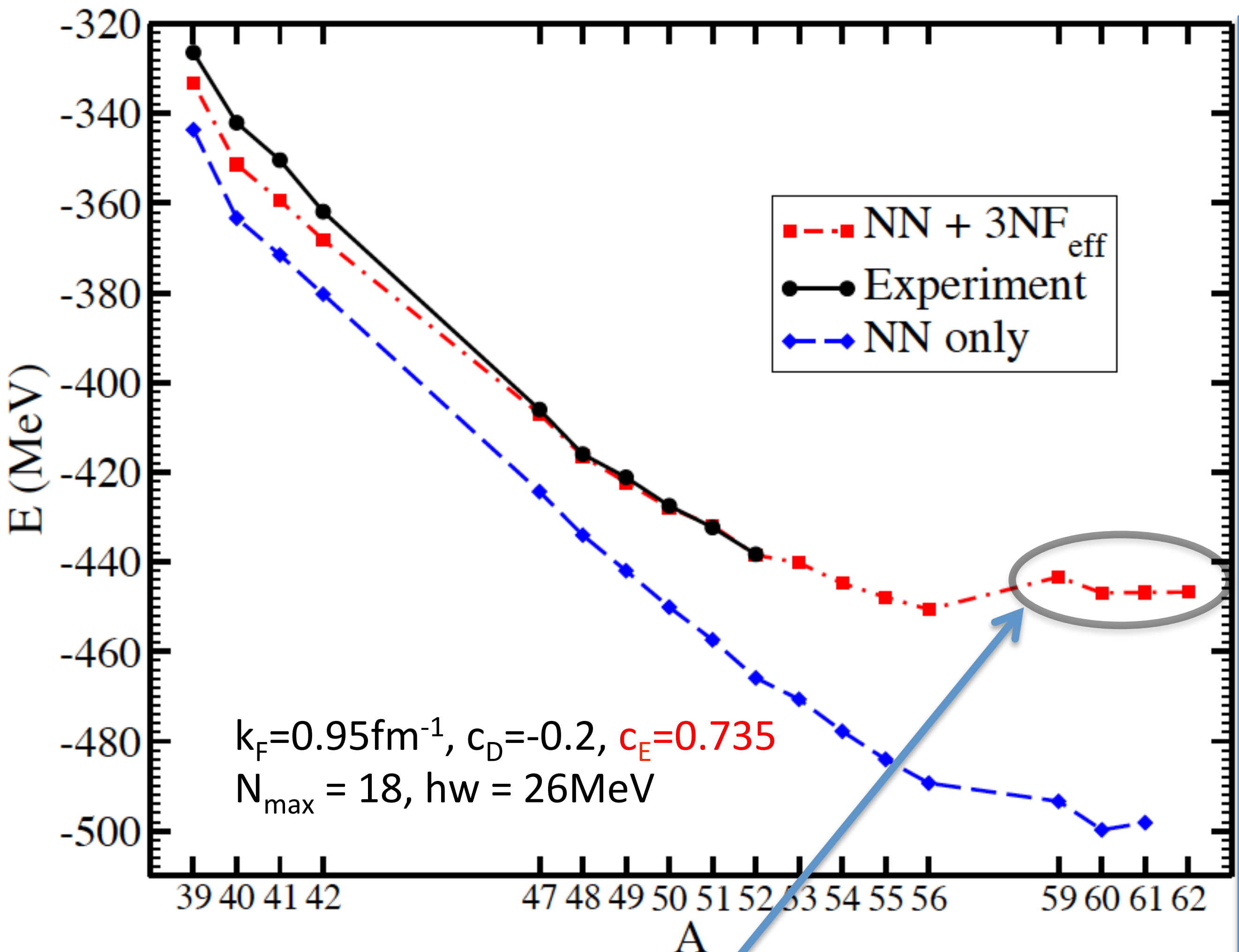
Description of observables and model-based extrapolation

- Systematic errors (due to incorrect assumptions/poor modeling)
- Statistical errors (optimization and numerical errors)

Erler et al., Nature 486, 509 (2012)

Calcium isotopes from chiral interactions

Hagen, Hjorth-Jensen, Jansen, Machleidt, Papenbrock, Phys. Rev. Lett. 109, 032502 (2012).



A peninsula of weak stability?

NN forces from chiral EFT and in-medium schematic 3NF: k_F=0.95 fm^{-1}, c_E=0.735, c_D=-0.2

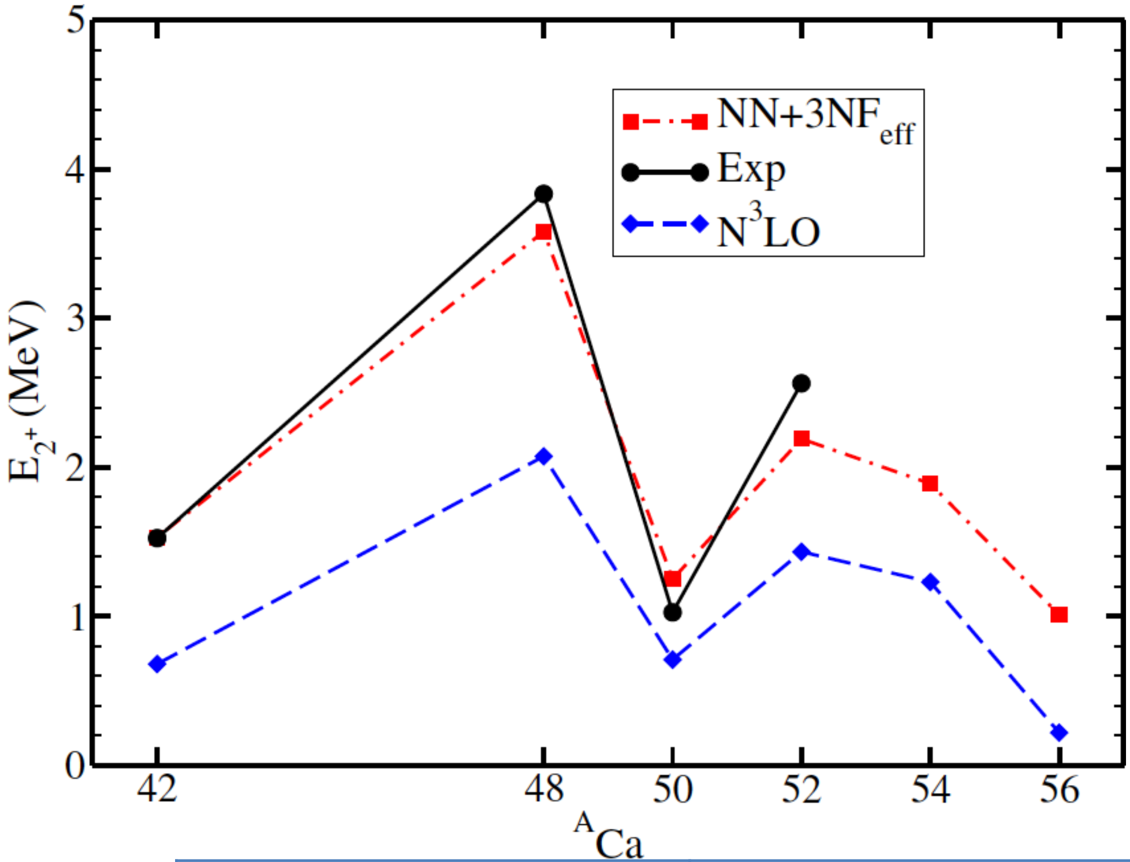
Main Features:

1. NN + schematic 3NFs: good agreement with experiment.
2. NN forces alone overbinds calcium
3. $^{61-62}$Ca are located right at threshold

<u>See also:</u>
Meng et al PRC 65, 041302 (2002), Lenzi et al PRC 82, 054301 (2010) and Erler et al, Nature 486, 509 (2012)

Is ^{54}Ca a magic nucleus? (Is N=34 a magic number?)

Hagen, Hjorth-Jensen, Jansen, Machleidt, Papenbrock, Phys. Rev. Lett. 109, 032502 (2012).

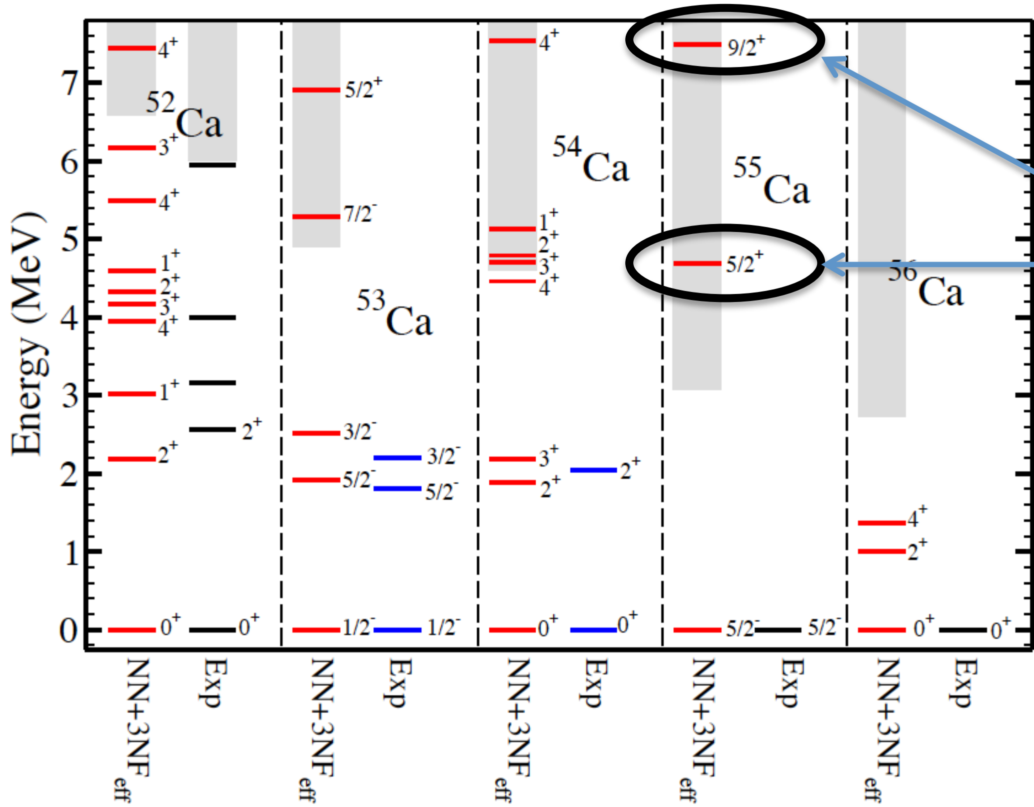


Main Features:

1. Good agreement between theory and experiment.
2. Shell closure in ^{48}Ca due to effects of 3NFs
3. Predict weak (sub-)shell closure in ^{54}Ca.

	^{48}Ca			^{52}Ca			^{54}Ca		
	2^+	4^+	$4^+/2^+$	2^+	4^+	$4^+/2^+$	2^+	4^+	$4^+/2^+$
CC	3.58	4.20	1.17	2.19	3.95	1.80	1.89	4.46	2.36
Exp	3.83	4.50	1.17	2.56	?	?	?	?	?

Spectra and shell evolution in Calcium isotopes



1. Our prediction for excited 5/2- and ½- states in 53Ca recently verified by RIKEN
2. We find inversion of 9/2+ and 5/2+ states in neutron rich calciums
3. Harmonic oscillator basis gives the naïve shell model ordering of states

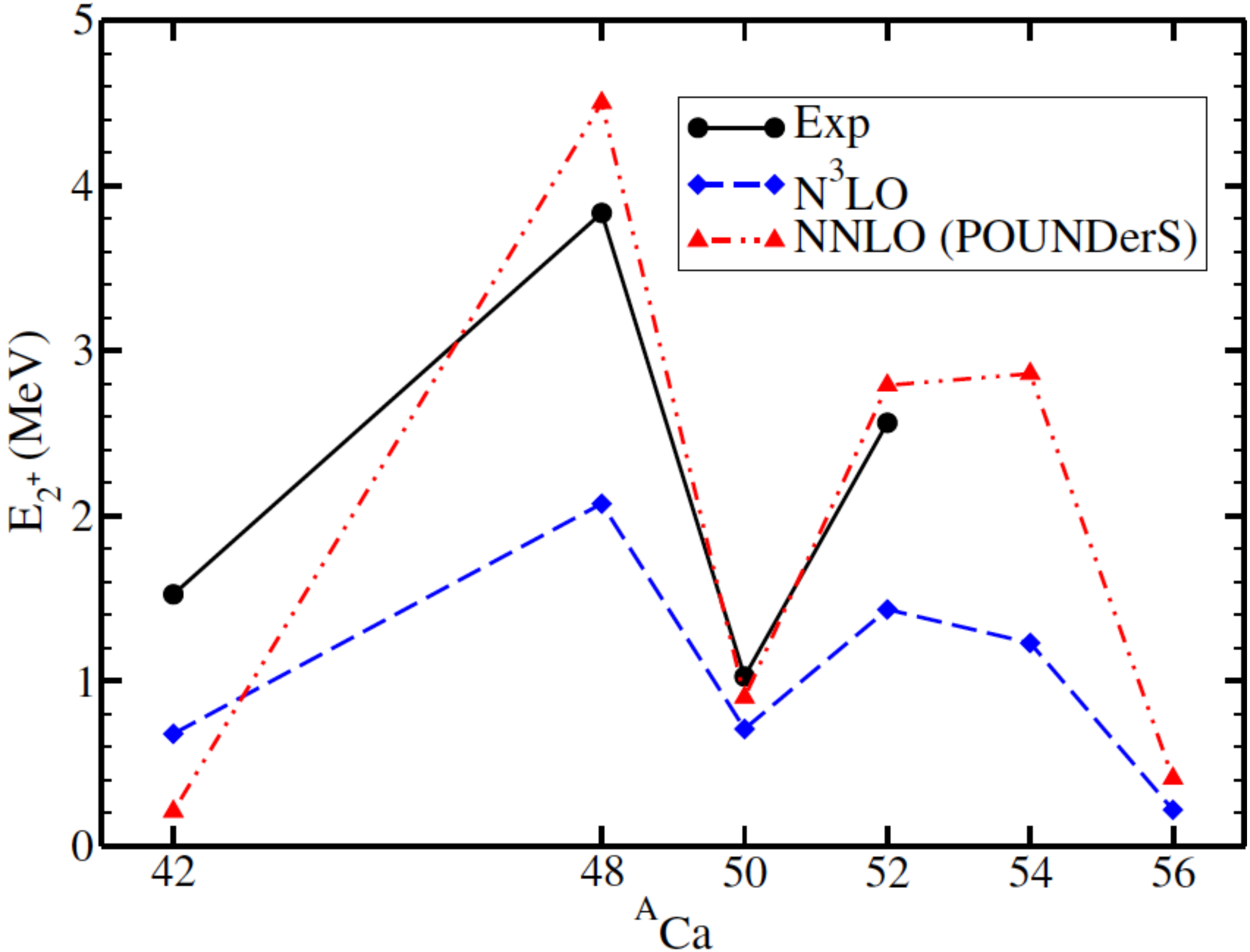
Continuum coupling is crucial!

	^{48}Ca	^{52}Ca	^{54}Ca
E_{2^+}(CC)	3.58	2.19	1.89
E_{2^+}(Exp)	3.83	2.56	n.a.
E_{4^+}/E_{2^+}(CC)	1.17	1.80	2.36
E_{4^+}/E_{2^+}(Exp)	1.17	n.a.	n.a.
S_n(CC)	9.45	6.59	4.59
S_n(Exp)	9.95	6.0*	4.0†

New penning trap measurement of masses of ^{51,52}Ca
A. T. Gallant et al Phys. Rev. Lett. **109**, 032506 (2012)

	^{53}Ca		^{55}Ca		^{61}Ca	
J^π	Re[E]	Γ	Re[E]	Γ	Re[E]	Γ
$5/2^+$	1.99	1.97	1.63	1.33	1.14	0.62
$9/2^+$	4.75	0.28	4.43	0.23	2.19	0.02

Calcium isotopes from NNLO-POUNDerS



Treatment of long-range Coulomb effects

We write the Coulomb interaction

$$V_{\mathrm{Coul}} = U_{\mathrm{Coul}}(r) + [V_{\mathrm{Coul}} - U_{\mathrm{Coul}}(r)]$$

Demanding

$$U_{\mathrm{Coul}}(r) \longrightarrow (Z-1)e^2/r \text{ for } r \rightarrow +\infty$$

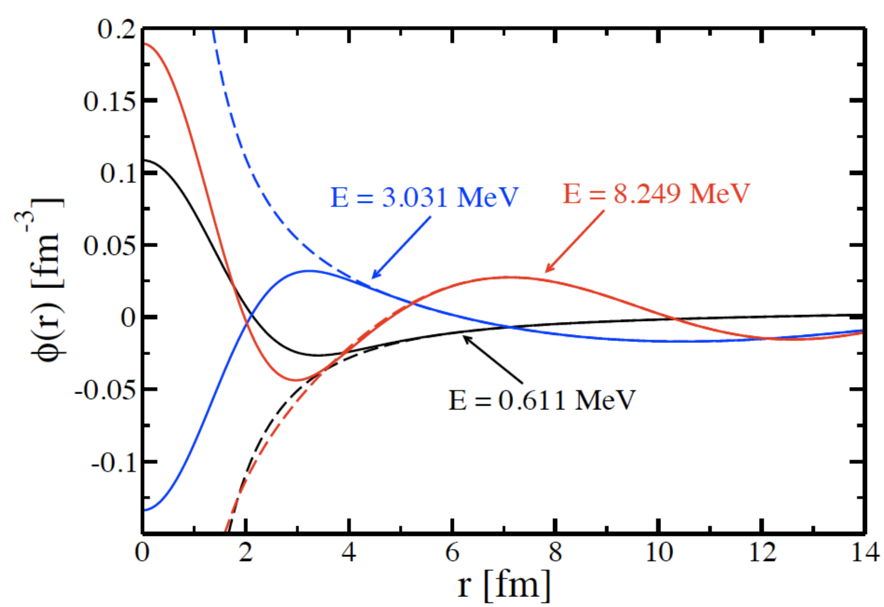
The second term is short range and can be Expanded in Harmonic Oscillator basis. The first term contain the long range Coulomb part:

$$U_{\mathrm{Coul}}(k,k') = \langle k|U_{\mathrm{Coul}}(r) - \frac{(Z-1)e^2}{r}|k'\rangle + \frac{(Z-1)e^2}{\pi} Q_\ell\left(\frac{k^2+k'^2}{2kk'}\right)$$

We diagonalize the one-body shcrodinger equation in momentum space using the off-diagonal method

N. Michel Phys. Rev. C 83, 034325 (2011)

		$s_{1/2}$		$d_{3/2}$		$d_{5/2}$	
N_R	N_T	Re[E]	Γ	Re[E]	Γ	Re[E]	Γ
5	15	1.1054	0.1446	5.0832	1.3519	1.4923	0.0038
5	20	1.1033	0.1483	5.0785	1.3525	1.4873	0.0079
10	25	1.0989	0.1360	5.0765	1.3525	1.4858	0.0093
10	30	1.0986	0.1366	5.0757	1.3529	1.4849	0.0103
15	40	1.0978	0.1351	5.0749	1.3531	1.4842	0.0111
15	50	1.0978	0.1353	5.0746	1.3533	1.4838	0.0114
20	60	1.0976	0.1349	5.0745	1.3533	1.4837	0.0116
30	70	1.0975	0.1346	5.0744	1.3534	1.4837	0.0117
(Michel 2011)		1.0975	0.1346	5.0744	1.3535	1.4836	0.0119



Elastic proton/neutron scattering on 40Ca

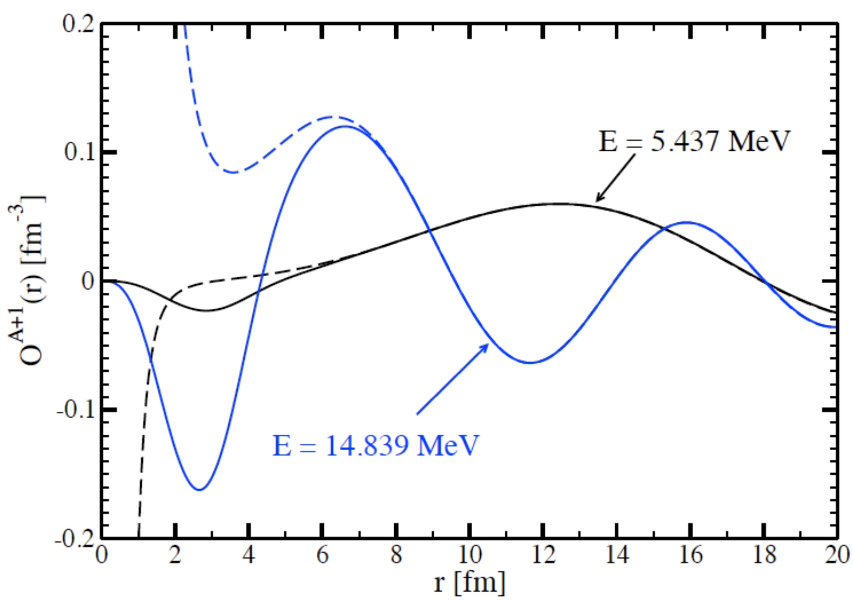
G. Hagen and N. Michel, Phys. Rev. C 86, 021602(R) (2012).

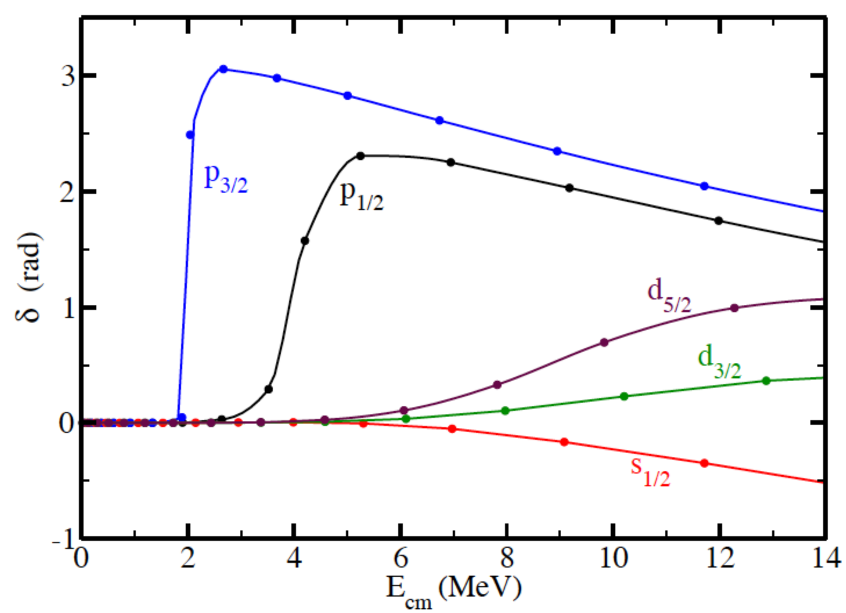
The one-nucleon overlap function: $O_A^{A+1}(lj;kr) = \sum_n \left\langle A+1 \left\| \tilde{a}^\dagger_{nlj} \right\| A \right\rangle \phi_{nlj}(r).$

Beyond the range of the nuclear interaction the overlap functions take the form:

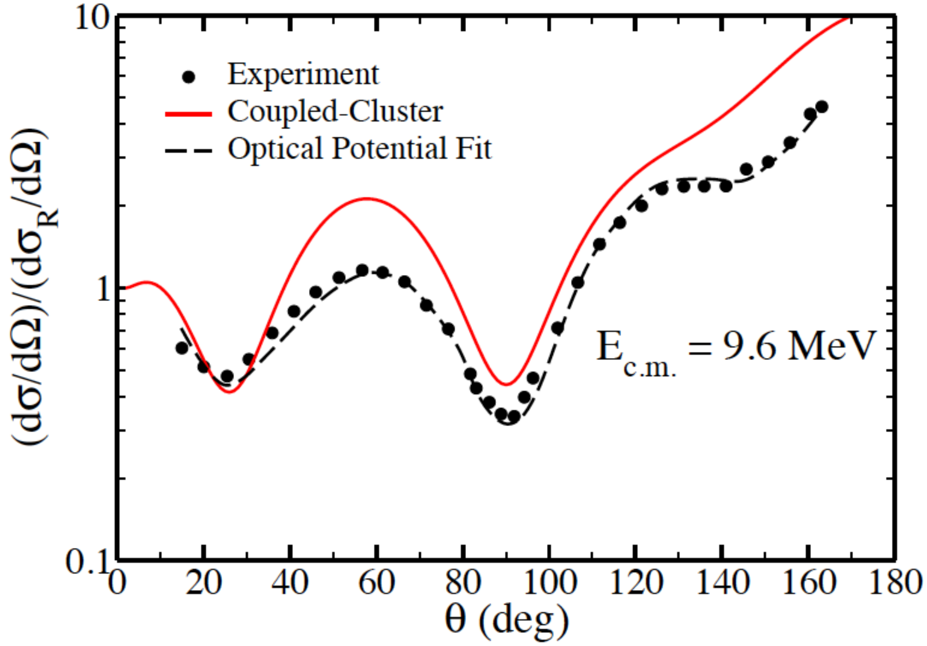
$$O_A^{A+1}(lj;kr) \;=\; C_{lj}\frac{W_{-\eta,l+1/2}(kr)}{r}, \;\; k = i\kappa$$

$$O_A^{A+1}(lj;kr) \;=\; C_{lj}\left[F_{\ell,\eta}(kr) - \tan\delta_l(k) G_{\ell,\eta}(kr)\right]$$





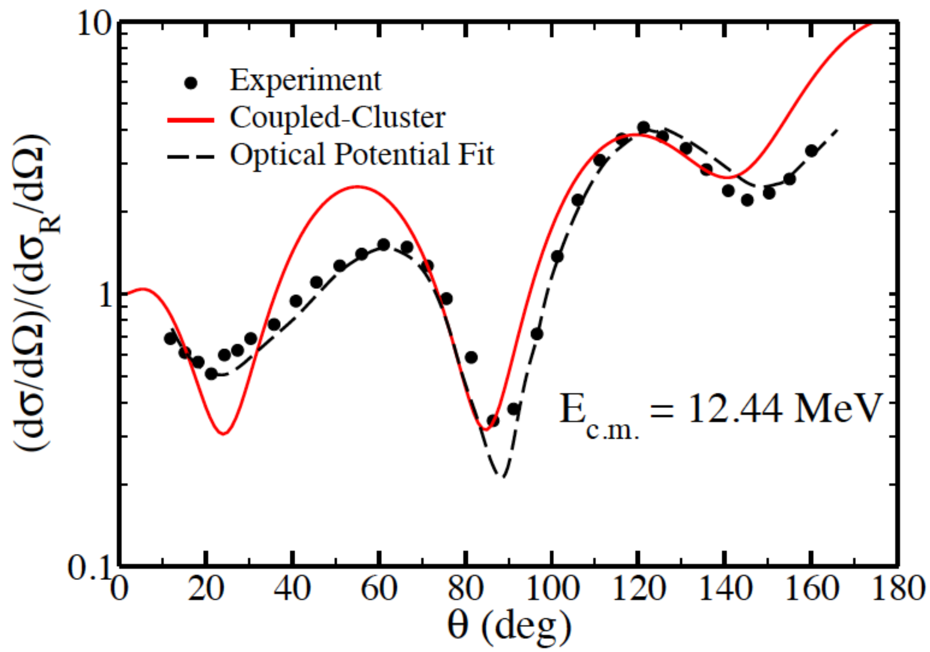
Elastic proton/neutron scattering on 40Ca



Differential cross section for elastic proton scattering on ^{40}Ca.

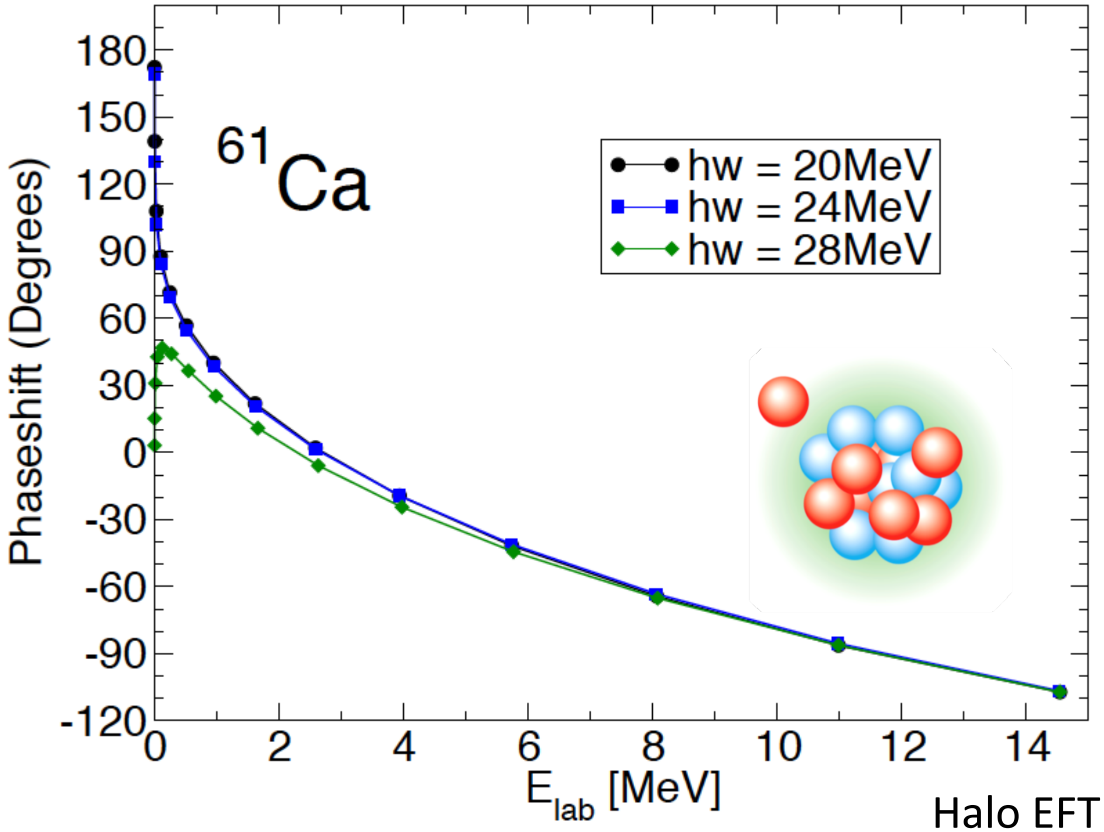
Fair agreement between theory and experiment for low-energy scattering.

G. Hagen and N. Michel
Phys. Rev. C **86**, 021602(R) (2012).



Efimov physics around neutron rich 60Ca

G. Hagen, P. Hagen, H.-W. Hammer, and L. Platter, in preparation (2013).



- Phase shifts from CC overlap functions
- Large S-wave scattering length in ^{61}Ca implies Halo phenomena
- Novel Approach: Merge halo-EFT and input from CC to study properties of ^{62}Ca

Halo EFT breakdown scale

$\hbar\omega$ [MeV]	a_{cn} [fm]	r_{cn} [fm]	S_n [keV]	S_{deep} [keV]
20	55.0	8.8	8.4	544
24	53.2	9.1	5.3	509
28	-26.1	10.8	-	361

	^{53}Ca		^{55}Ca		^{61}Ca	
J^π	Re[E]	Γ	Re[E]	Γ	Re[E]	Γ
$5/2^+$	1.99	1.97	1.63	1.33	1.14	0.62
$9/2^+$	4.75	0.28	4.43	0.23	2.19	0.02

Efimov physics around neutron rich 60Ca

- Halo EFT provides a model-independent description of halo nuclei
- Core + valence nucleons are effective degrees of freedom
- The coupling constants from the *n*-*n* and core-*n* effective range
- The expansion is given in powers of R/a with R ~ effective range

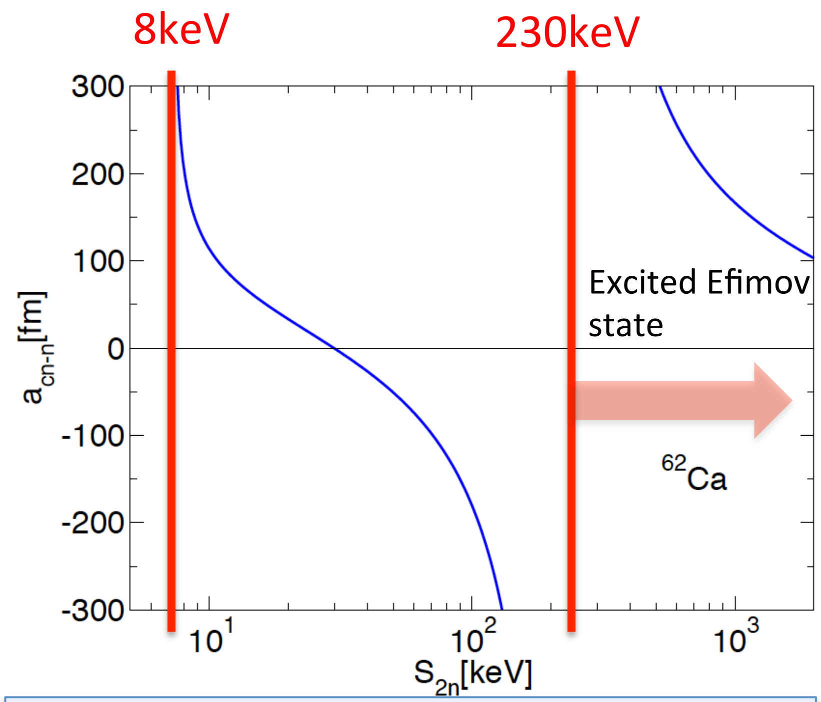
The Halo EFT core *n*-*n* Lagrangian to leading order:

$$\begin{aligned}\mathcal{L} \;=\; & \psi_c^\dagger \left(i\partial_0 + \frac{\vec{\nabla}^2}{2M} \right) \psi_c + \vec{\psi}_n^\dagger \left(i\partial_0 + \frac{\vec{\nabla}^2}{2m} \right) \vec{\psi}_n \\ & + \Delta_{nn} d_{nn}^\dagger d_{nn} + \Delta_{cn} \vec{d}_{cn}^\dagger \vec{d}_{cn} + h\, d_{nn}^\dagger \psi_c^\dagger \psi_c\, d_{nn} \\ & - \left[g_{cn} \vec{d}_{cn}^\dagger \vec{\psi}_n \psi_c + \frac{g_{nn}}{2} d_{nn}^\dagger \left(\vec{\psi}_n^{\,\mathrm{T}} P\, \vec{\psi}_n \right) + \mathrm{h.c} \right] + \ldots\; .\end{aligned}$$

Coupling constants given by *n*-*n* and core-*n* effective ranges

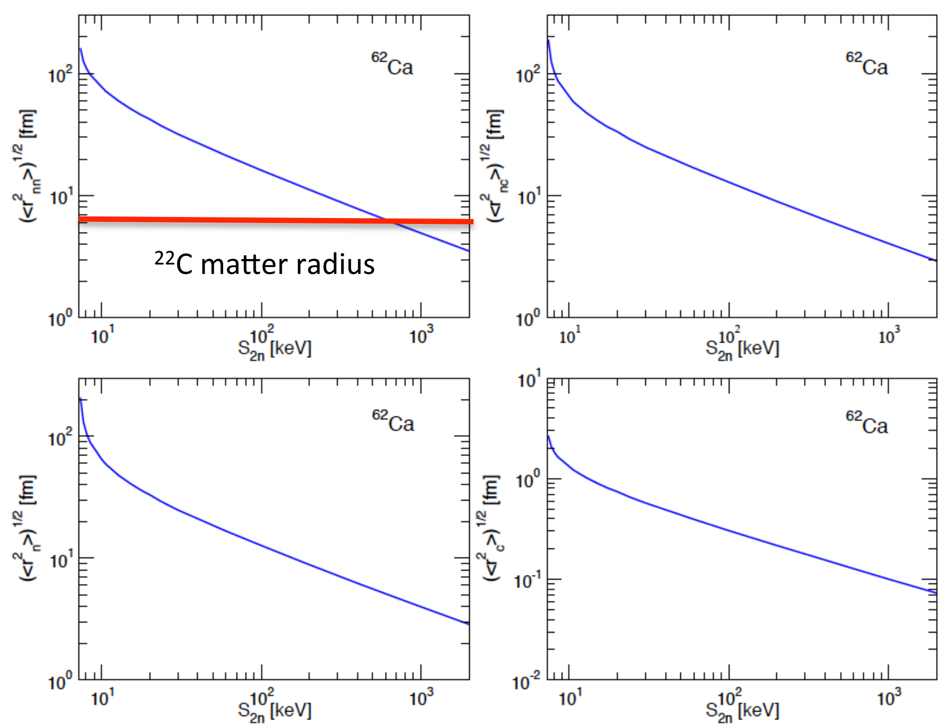
Three-body coupling

Efimov physics around neutron rich 60Ca



- For S_{2n} larger than ~ 230keV another state appears in the spectrum
- ^{62}Ca is likely to have an Efimov state (large halo)
- It is conceivable that ^{62}Ca displays an excited Efimov state

- ^{22}C is the largest known two-neutron halo R_{rms} ~5.4fm (Tanaka PRL 2010)
- Computed matter radii for ^{62}Ca imply that it has the potential to be the largest and heaviest halo in the chart of nuclei



Summary

1. Optimized interactions from Chiral EFT probed in nuclei
2. NNLO (POUNDerS) captures key aspects of nuclear structure, what is the role of 3NF?
3. Predict spin and parity of observed resonance peak in ^{24}O.
4. Prediction of weak sub-shell closure in ^{54}Ca and excited states in ^{53}Ca recently verified by RIKEN.
5. Inversion of *gds* levels in neutron rich calcium
6. Merging CC and Halo EFT to describe universal properties in systems dominated by large scattering length
7. ^{62}Ca displays Efimov phsyics: Excited Efimov states? Largest two-neutron halo?