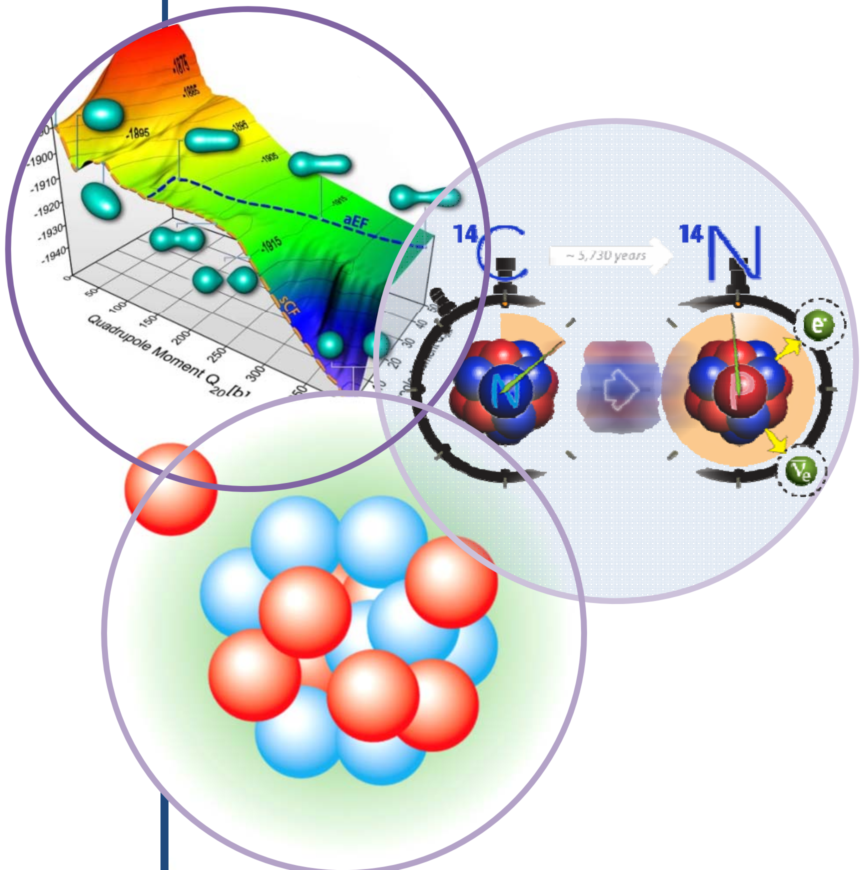
Coupled cluster calculations of nuclear structure and reactions

Gaute Hagen (ORNL)



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U.S. DEPARTMENT OF ENERGY
NUCLEI Nuclear Computational Low-Energy Initiative
BSF United States – Israel Binational Science Foundation
OAK RIDGE NATIONAL LABORATORY MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

Outline

- Optimization of interactions and currents from chiral EFT
- Beta decays and quenching of Gamow-Teller strengths in ^{14}C and $^{22,24}O$.
- Predictions for the weak charge form factor and neutron radius in ^{48}Ca with NNLOsat
- Correlations between neutron radius and other observables in ^{48}Ca

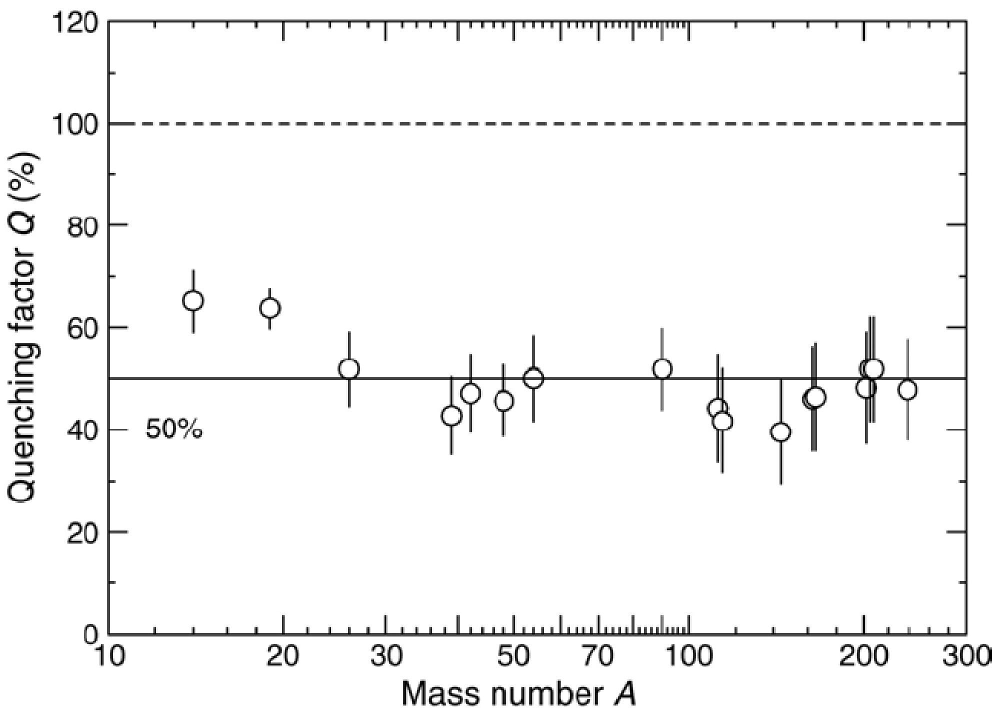
- Continuum coupling and level ordering in odd neutron rich calcium isotopes
- Elastic scattering from Coupled-cluster theory
- Ab-initio input to Halo EFT study of Efimov physics in ^{62}Ca

Quenching of Gamow-Teller strength in nuclei

The Ikeda sum-rule $$S^{\mathrm{N}}(\mathrm{GT}) = S^{\mathrm{N}}(\mathrm{GT}^-) - S^{\mathrm{N}}(\mathrm{GT}^+) = 3(N-Z)$$

Long-standing problem: Experimental beta-decay strengths quenched compared to theoretical results.

$$Q = \frac{S^-_{\mathrm{GT}}(\omega^-_{\mathrm{top}}) - S^+_{\mathrm{GT}}(\omega^+_{\mathrm{top}})}{3(N-Z)}$$



Surprisingly large quenching *Q* (50%) obtained from (*p,n*) experiments. The excitation energies were just above the giant Gamow-Teller resonance ~10-15MeV (Gaarde 1983).

- Charge exchange reactions on ^{90}Zr was used to extract GT strengths to high energies (Sasano et al 2009, Yako et al 2005) and deduced a smaller quenching *Q* =0.88-0.92

- Renormalizations of the Gamow-Teller operator?
- Missing correlations in nuclear wave functions?
- Model-space truncations?

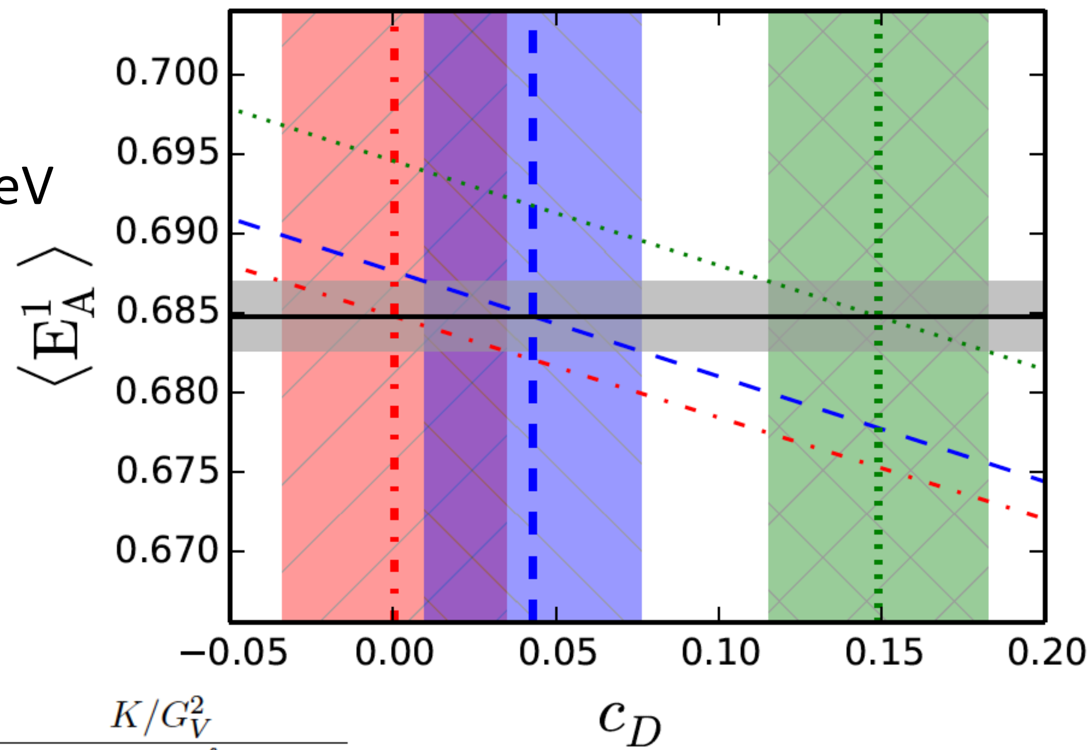
- **What does two-body currents and three-nucleon forces add to this long-standing problem?**

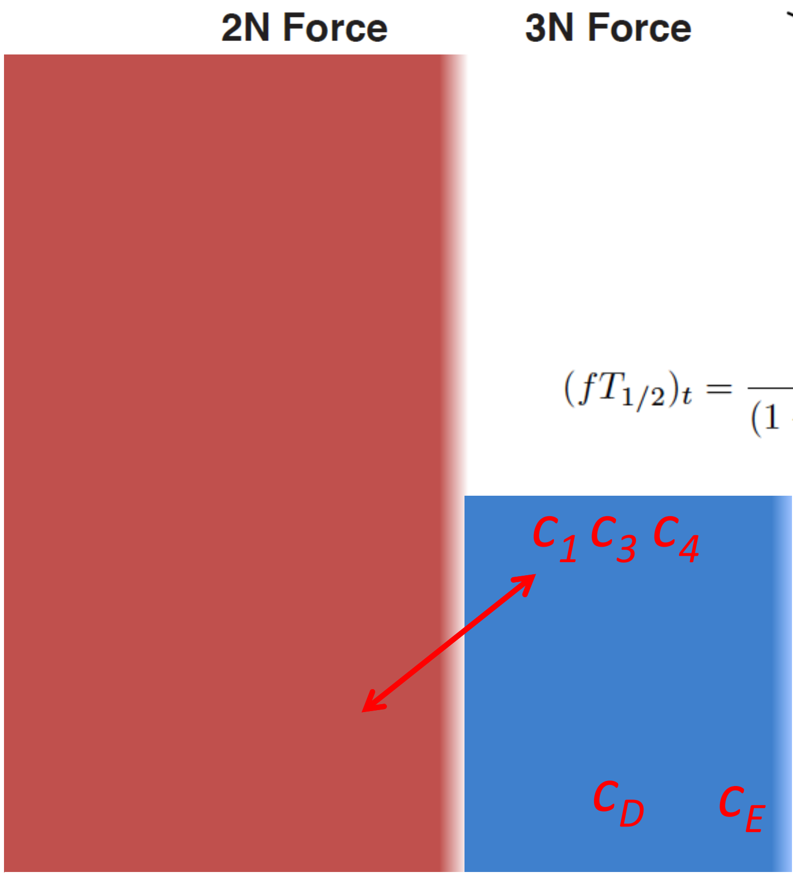
Optimization of chiral interactions currents at NNLO

A. Ekström, G. Jansen, K. Wendt et al, PRL 113 262504 (2014)

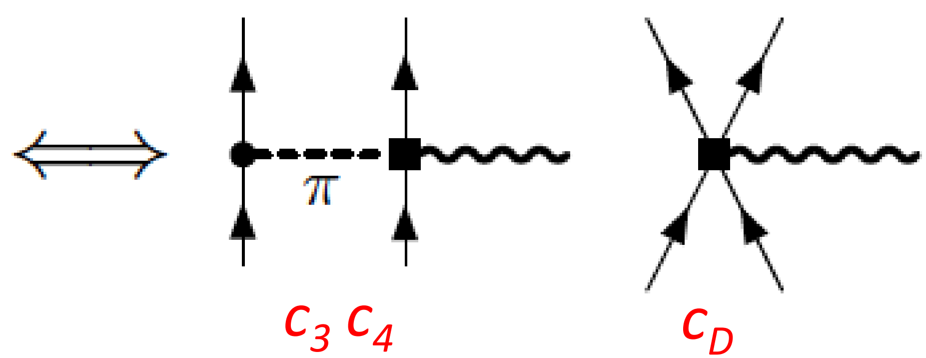
c_D - c_E fit of A=3 binding energies and the ^{3}H half life at NNLO for chiral cutoffs Λ = 450,500,550 MeV

$[c_D, c_E] = [0.043, -0.501]$





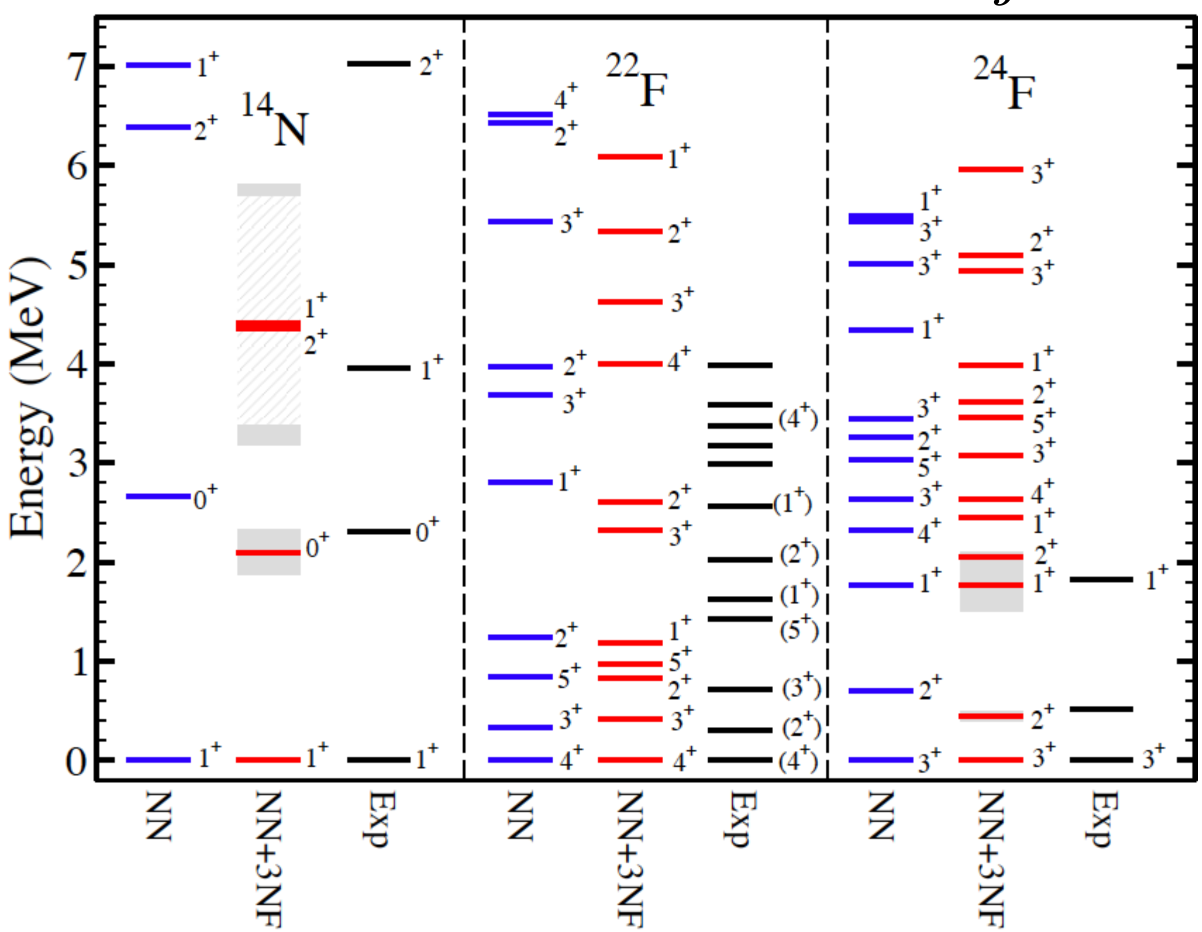
$$(fT_{1/2})_t = \frac{K/G_V^2}{(1-\delta_c) + 3\pi \frac{f_A}{f_V} \langle E_1^A \rangle^2}$$



Coupled cluster calculations of odd-odd nuclei

Diagonalize $\overline{H} = e^{-T} H_N e^{T}$ via a novel equation-of-motion technique:

$$R \equiv \sum_{ia} r_i^a p_a^\dagger n_i + \frac{1}{4} \sum_{ijab} r_{ij}^{ab} p_a^\dagger N_b^\dagger N_j n_i$$

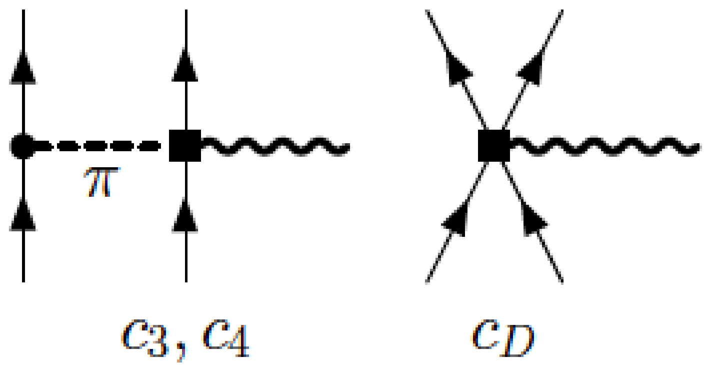


- Compute spectra of daughter nuclei as beta decays of mother nuclei
- Level densities in daughter nuclei increase slightly with 3NF
- Predict several states in neutron rich Fluorine

Normal ordered one- and two-body current

Gamow-Teller matrix element:

$$\hat{O}_{\rm GT} \equiv \hat{O}^{(1)}_{\rm GT} + \hat{O}^{(2)}_{\rm GT} \equiv g_A^{-1}\sqrt{3\pi}E_1^A$$



Normal ordered operator:

$$\hat{O}_{\rm GT} = O_N^0 + O_N^1 + O_N^2$$

$$O_N^0 = \sum_{i\le E_f} \langle i|O^{(1)}|i\rangle + \frac{1}{2}\sum_{i,j\le E_f}\langle ij|O^{(2)}|ij\rangle$$

$$O_N^1 = \sum_{pq}\langle p|O^{(1)}|q\rangle\{p^\dagger q\} + \sum_{pq}\sum_{i\le E_f}\langle pi|O^{(2)}|qi\rangle\{p^\dagger q\}$$

$$O_N^2 = \frac{1}{4}\sum_{pqrs}\langle pq|O^{(2)}|rs\rangle\{p^\dagger q^\dagger sr\}$$

One- and two-body currents and normal ordering in Coupled-Cluster

CCSD similarity transformed normal-ordered current operator: $T = T_1 + T_2$

3-body terms

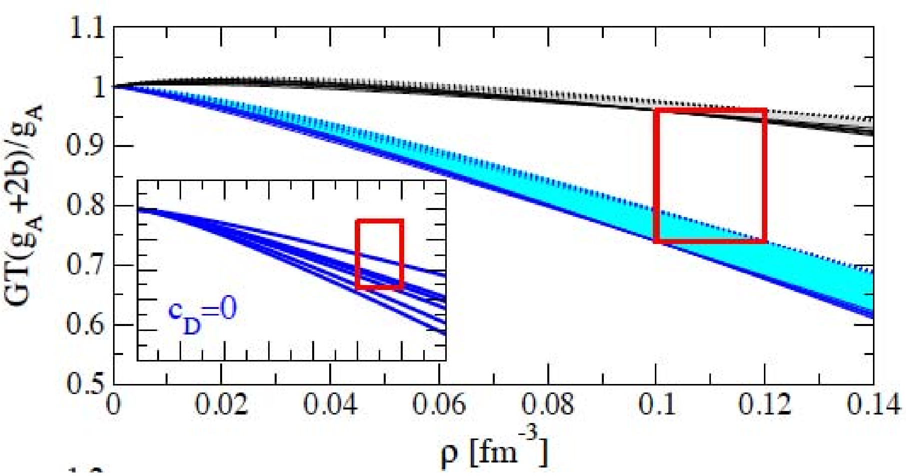
6-body terms

$$\overline{O_{\rm GT}} = e^{-T} O_N e^T = e^{-T} O_N^1 e^T + e^{-T} O_N^2 e^T$$

Normal ordered 1-body with Leading-Order (LO) two-body contribution

Normal-ordering 1-body Approximation

$$e^{-T} O_N^2 e^T \approx \quad O_N^2 = \frac{1}{4} \sum_{pqrs} \langle pq | O^{(2)} | rs \rangle \{ p^\dagger q^\dagger s r \}$$



J. Menéndez, D. Gazit, A. Schwenk
PRL 107, 062501 (2011)

Normal order with respect to free Fermi gas. One-body normal ordered approximation gives quenching of g_A by a factor q = 0.74…0.96 for different set of couplings constants

Quenching of Gamow-Teller strength in nuclei

A. Ekström, G. Jansen, K. Wendt et al, PRL 113 262504 (2014)

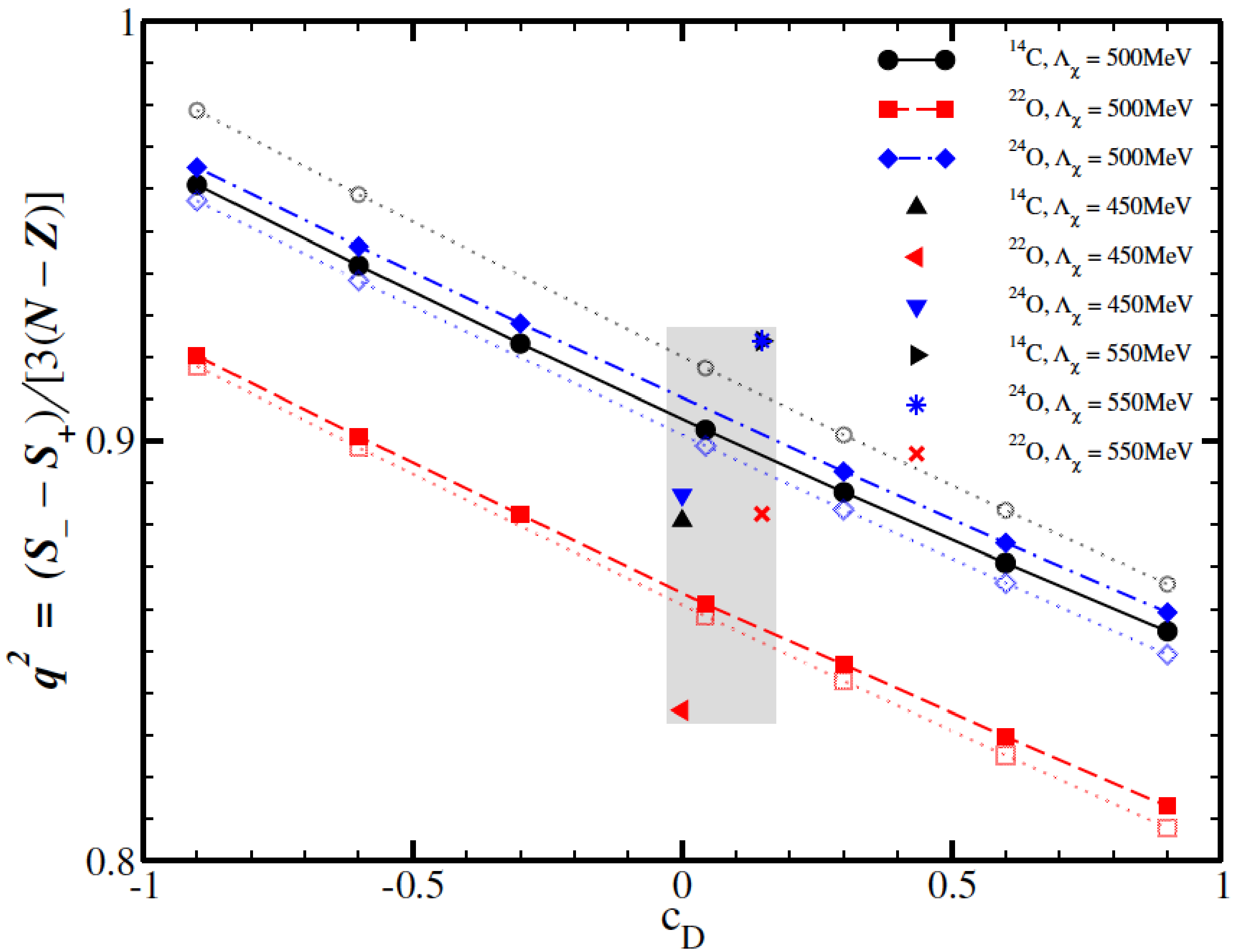
Gamow-Teller matrix element:

$$\hat{O}_{\mathrm{GT}} \equiv \hat{O}_{\mathrm{GT}}^{(1)} + \hat{O}_{\mathrm{GT}}^{(2)} \equiv g_A^{-1}\sqrt{3\pi}E_1^A$$

The Gamow-Teller strength functions:

$$S_- = \langle \Lambda | \overline{\hat{O}_{\mathrm{GT}}^\dagger} \cdot \overline{\hat{O}_{\mathrm{GT}}} | \mathrm{HF} \rangle$$

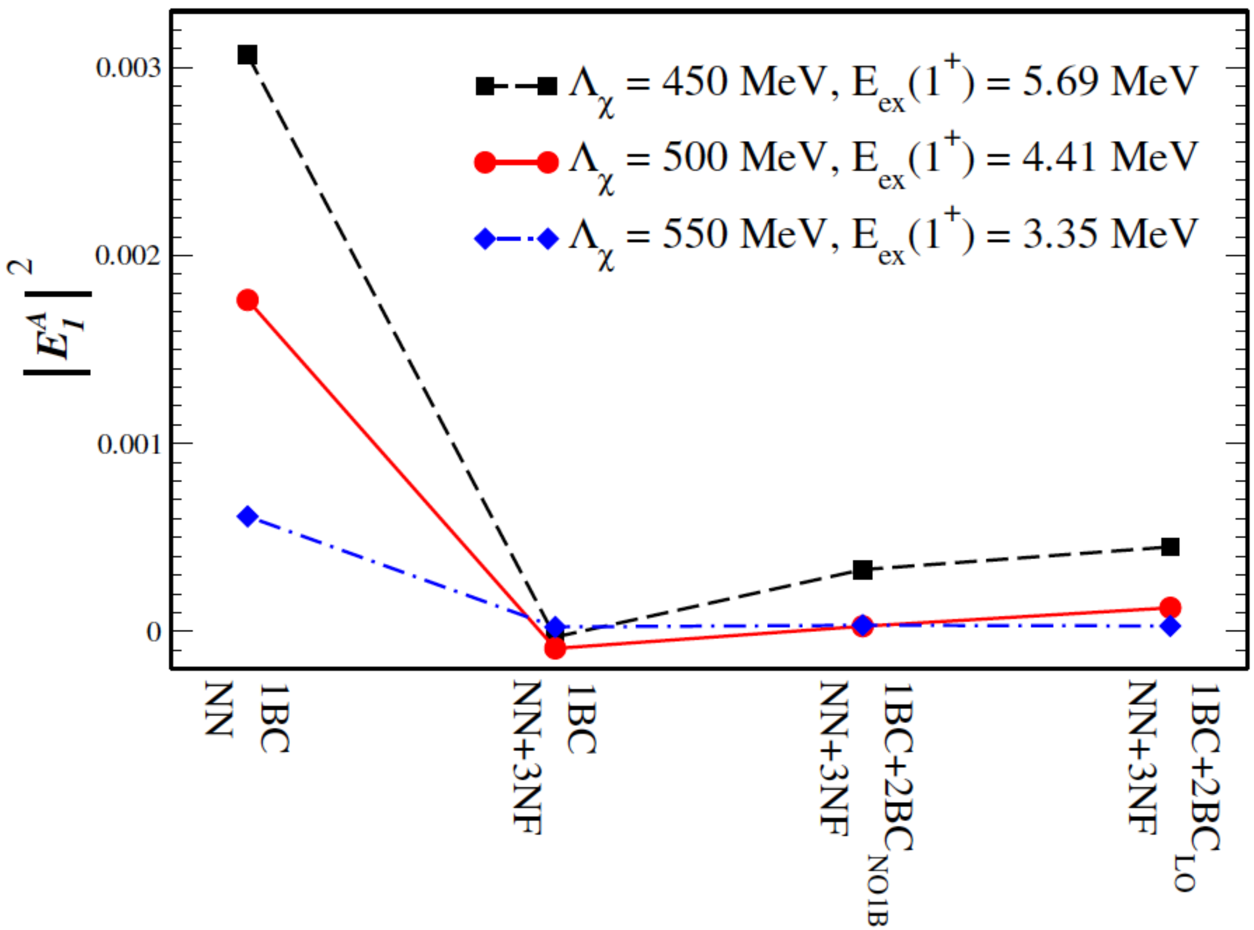
$$S_+ = \langle \Lambda | \overline{\hat{O}_{\mathrm{GT}}} \cdot \overline{\hat{O}_{\mathrm{GT}}^\dagger} | \mathrm{HF} \rangle$$



- Quenching of the Ikeda sum rule in ^{14}C and ^{22,24}O for different cutoffs. q = 0.92…0.96
- Grey area is region which reproduce triton half-life
- The quenching q^2 is about 8-16% and agrees with estimates in ^{90}Zr

Anomalous life-time of ^{14}C revisited

A. Ekström, G. Jansen, K. Wendt et al, PRL 113 262504 (2014)

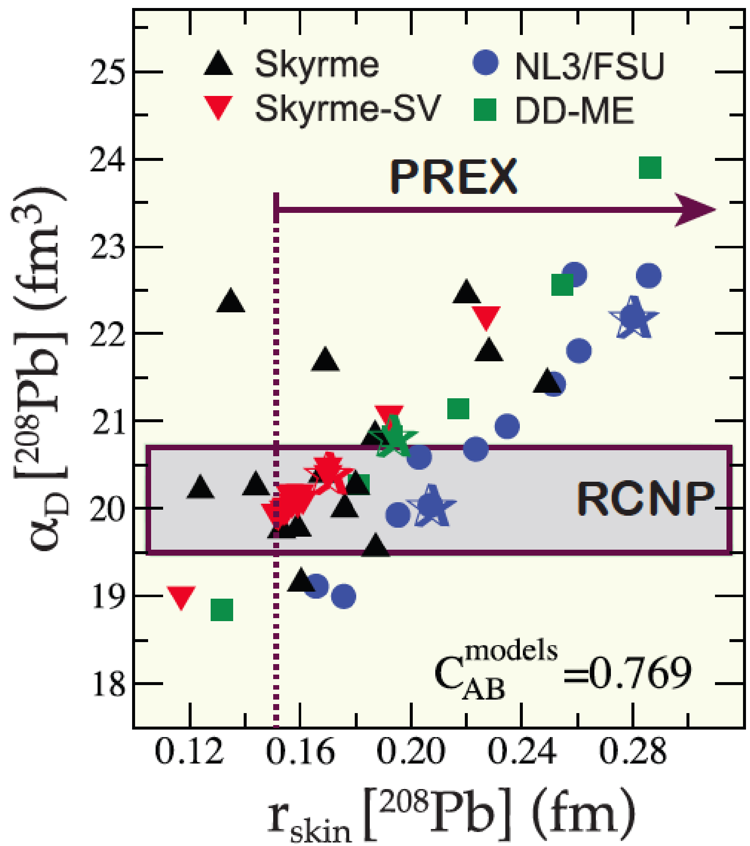


E_1^A varies between $5x10^{-3}$ to $2x10^{-2}$ which is more than one order of magnitude larger than the empirical value ~$6x10^{-4}$ extracted from the 5700 a half life of ^{14}C

The life time of ^{14}C depends in a complicated way on 3NFs, 2BCs and the energy of the first excited 1^+ state in ^{14}N.

- 3NFs decrease the transition matrix element significantly
- 2BC counter the effect of 3NFs to some degree.
- Note that 2BCs increases the strength to the first 1^+ state in ^{14}N but overall quenches the Ikeda sum rule.

The neutron radius of ^{48}Ca



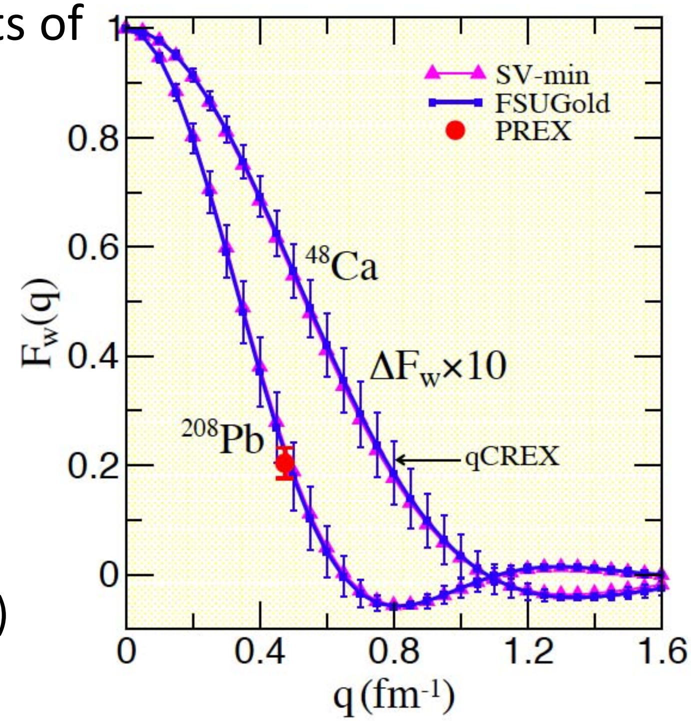
Relevance:

- C-REX will measure the weak charge distribution at a 0.02fm precision from parity violating electron scattering at JLab
- Darmstadt is currently analyzing data on α_D

Significance:

- Sets the size of neutron rich nuclei
- Impacts equation-of-state of neutron stars
- Constrains density dependence in DFT
- Determines limits of stability
- Pin down role of 3NFs in neutron rich matter

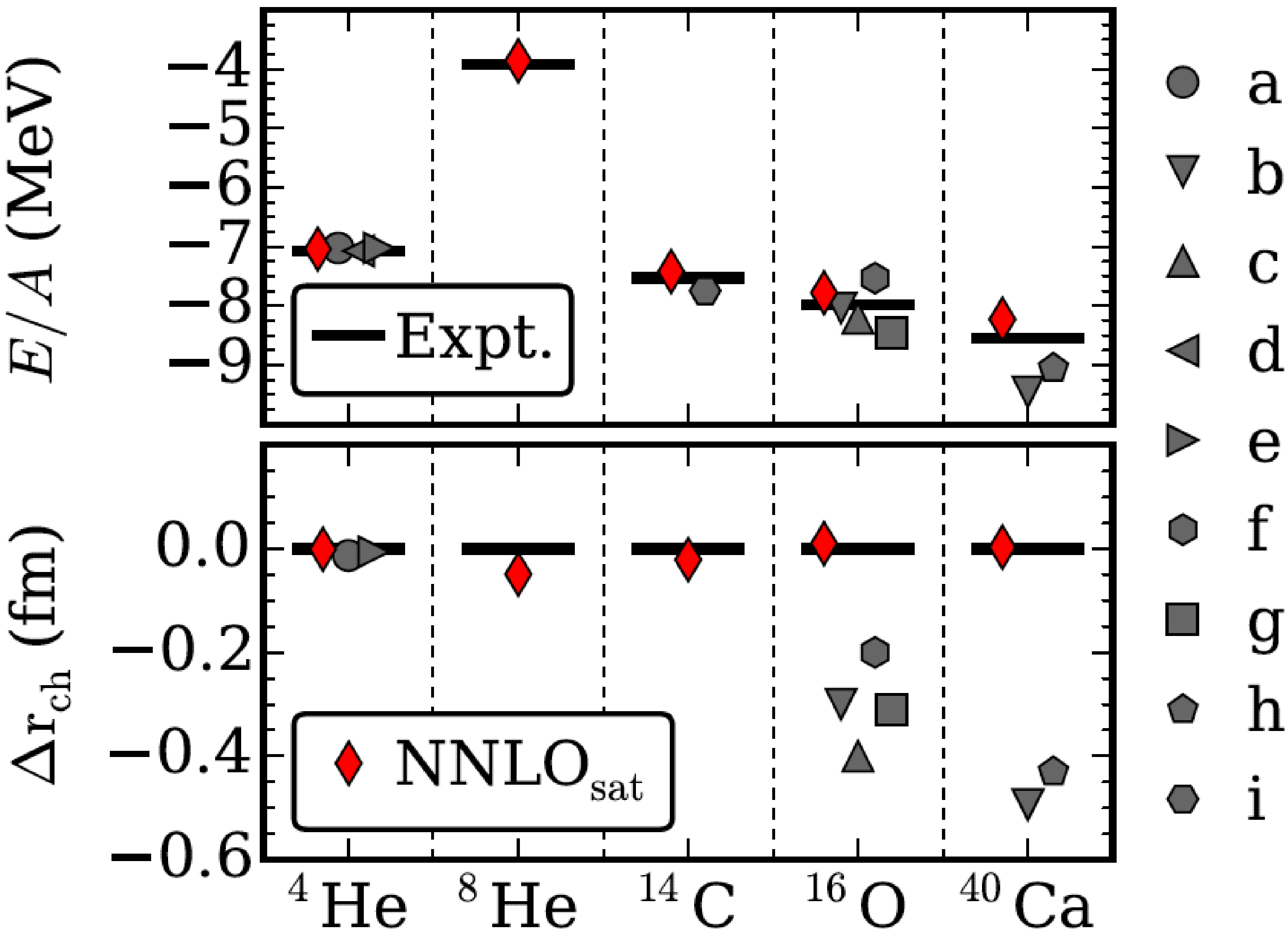
J. Piekarewicz e al, PRC 85, 041302(R) (2012)



P. -G. Reinhard et al, PRC 88, 034325 (2013)

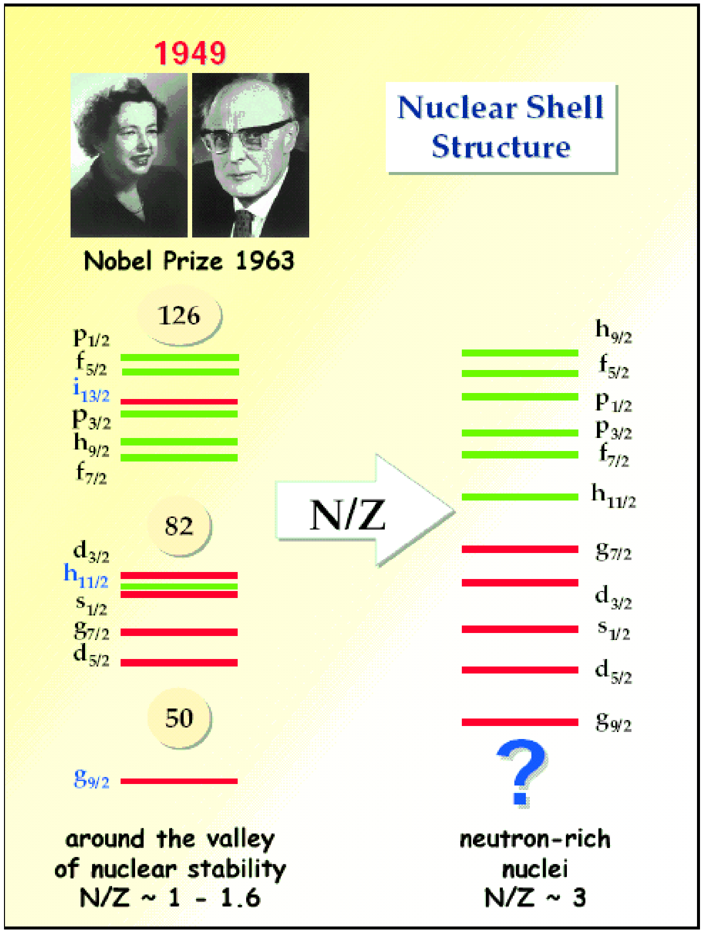
Accurate binding energies and radii from a chiral interaction

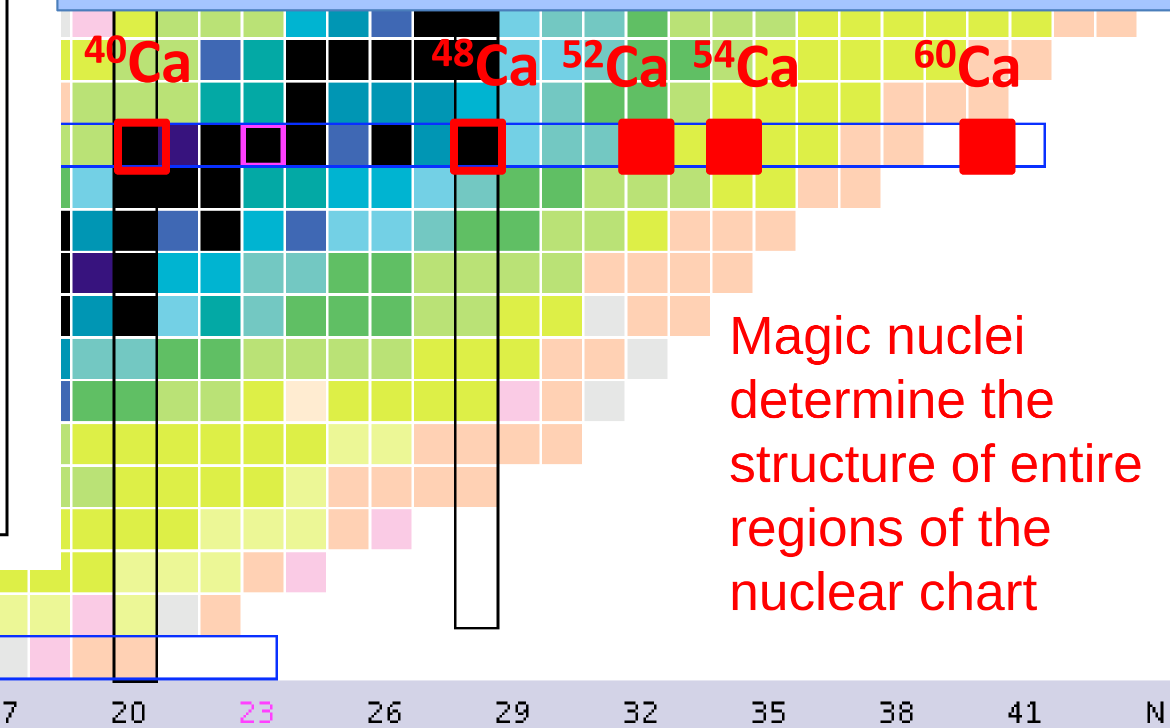
A. Ekström, G. Jansen, K. Wendt et al, arXiv:1502.04682 (2015)



Evolution of shell structure in neutron rich Calcium

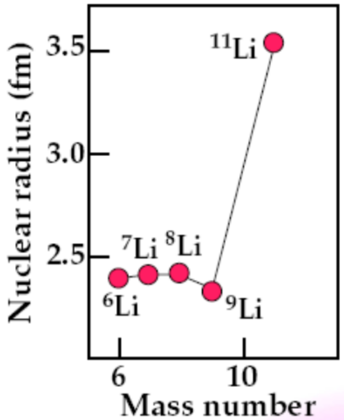
- How do shell closures and magic numbers evolve towards the dripline?
- What are the underlying mechanisms and how do we identify new shell structure?





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

Physics of nuclei at the edges of stability



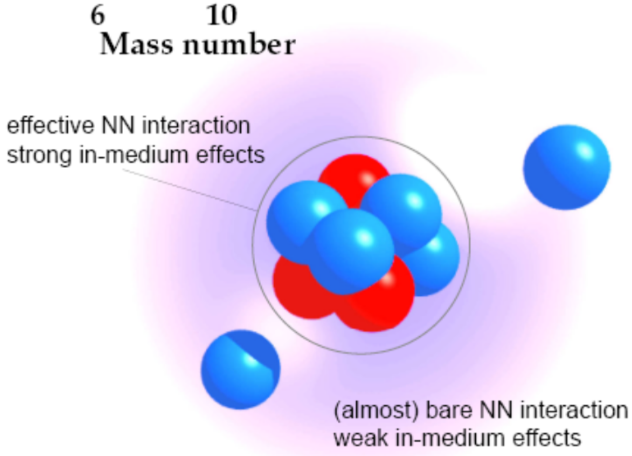
I. Tanihata et al.
Phys. Rev. Lett. 55, 2676 (1985)

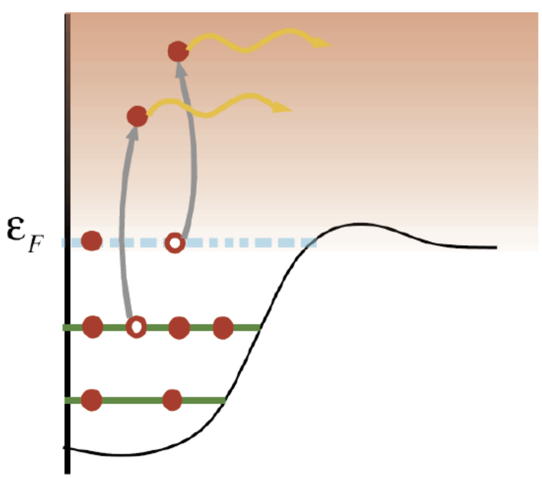
Interaction cross section measurements at Bevalac (790 MeV/u)

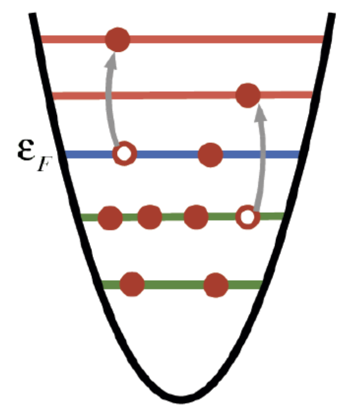
The Berggren completeness treats bound, resonant and scattering states on equal footing.

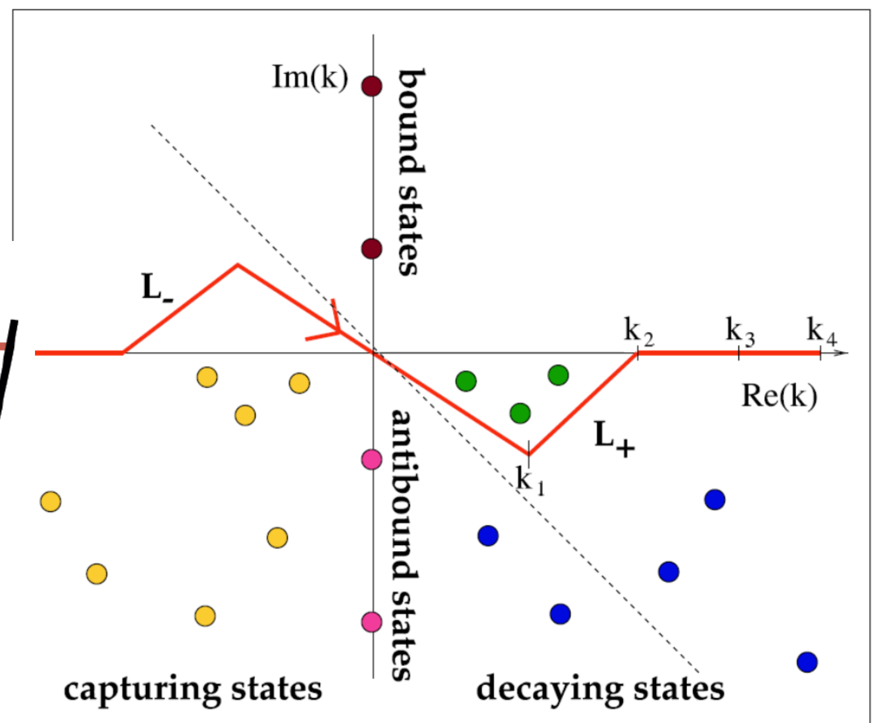
Has been successfully applied in the shell model in the complex energy plane to light nuclei. For a review see

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







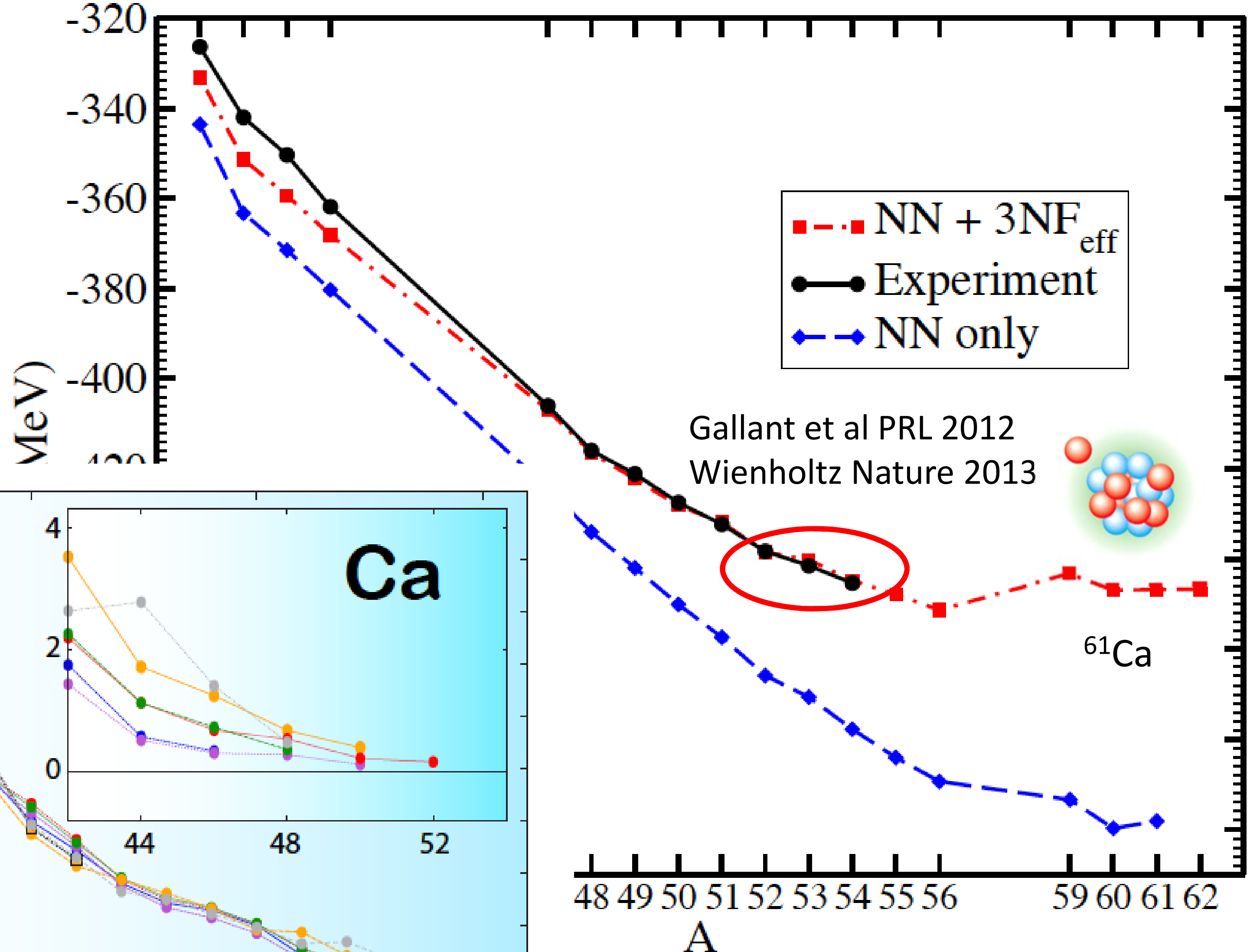


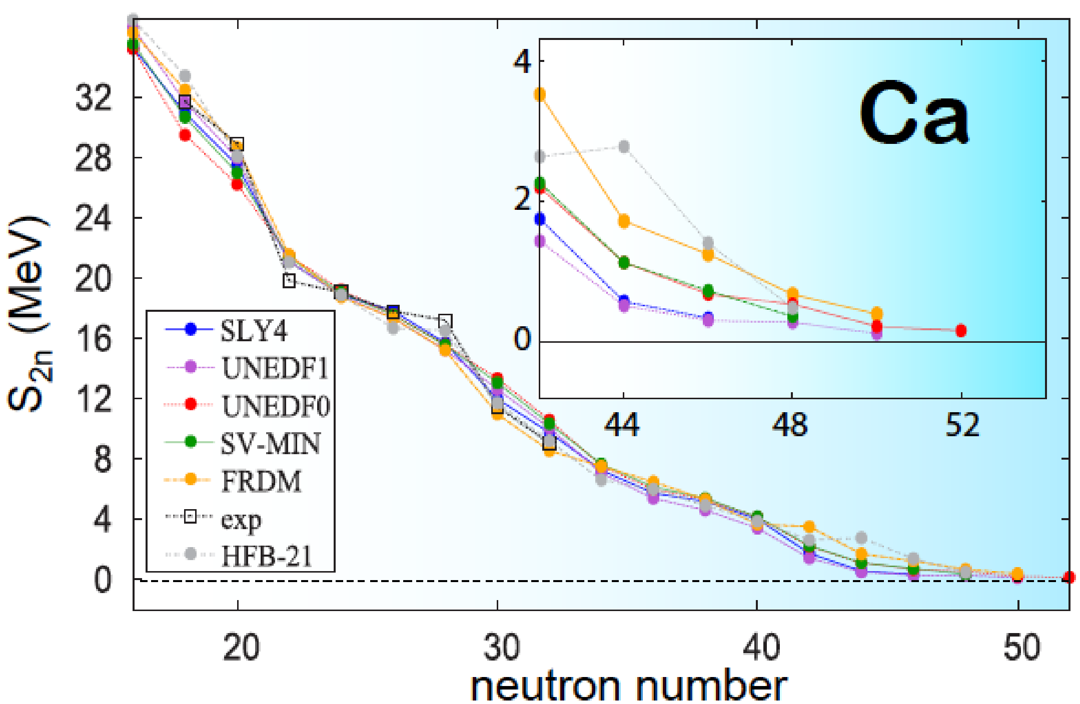
Neutron rich calcium isotopes

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

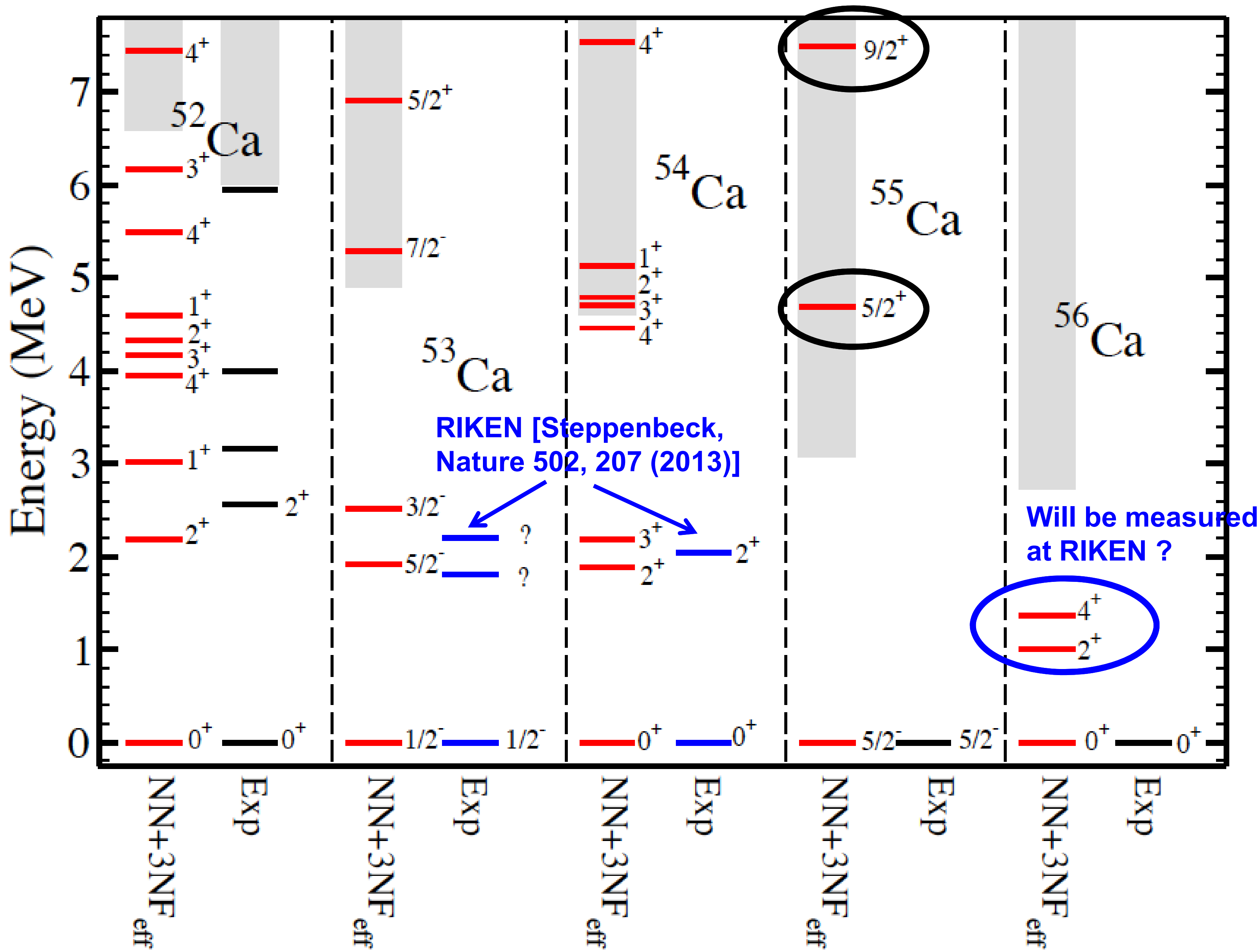
C Forssén et al
Phys. Scr. 014022 (2013)

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

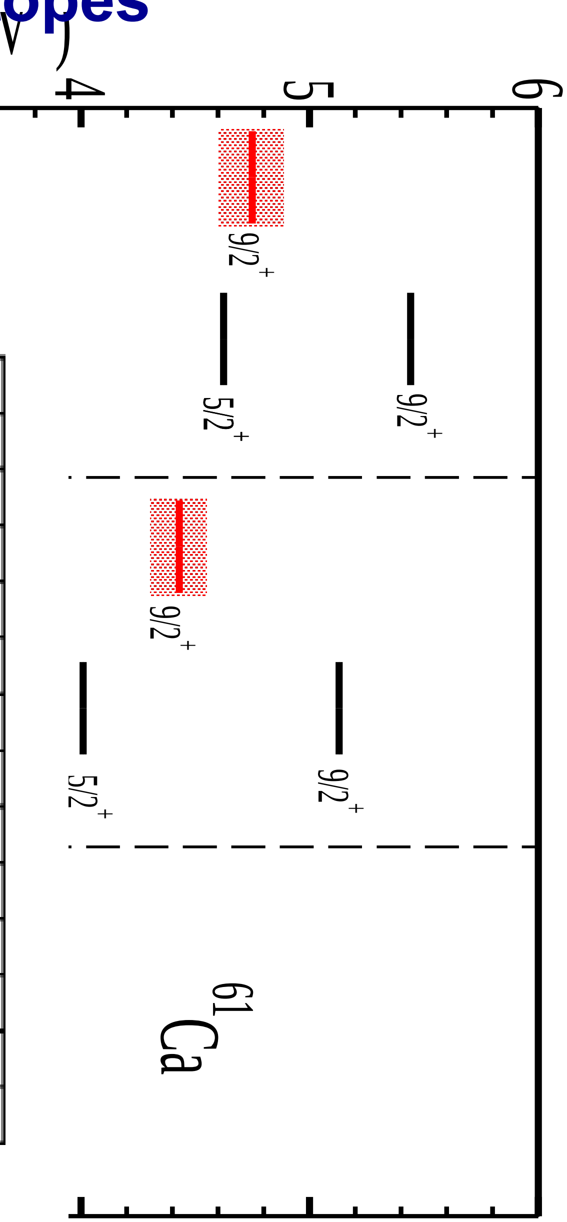




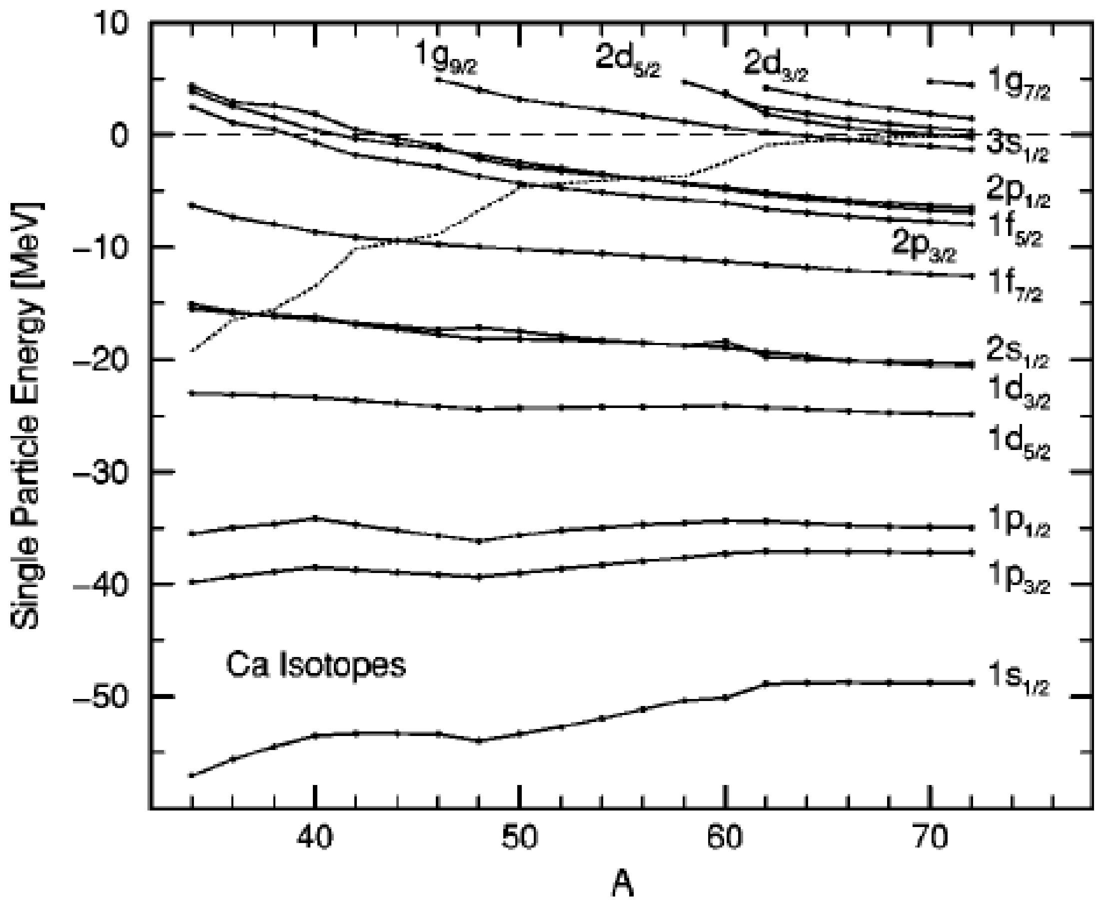
Spectra and shell evolution in Calcium isotopes



Effect of continuum on excited states in odd neutron rich Calcium isotopes



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



Elastic proton/neutron scattering on 40Ca

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

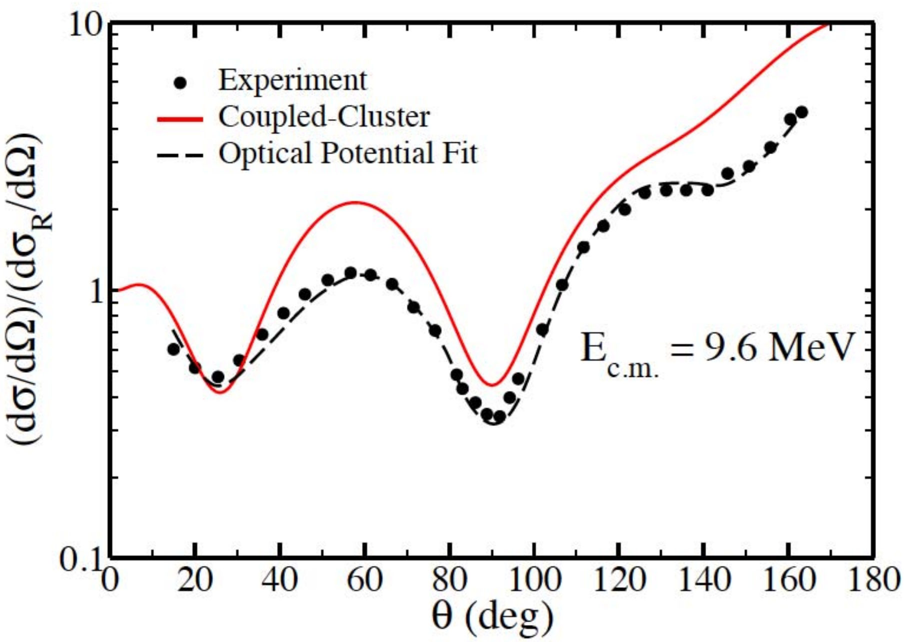
The one-nucleon overlap function:

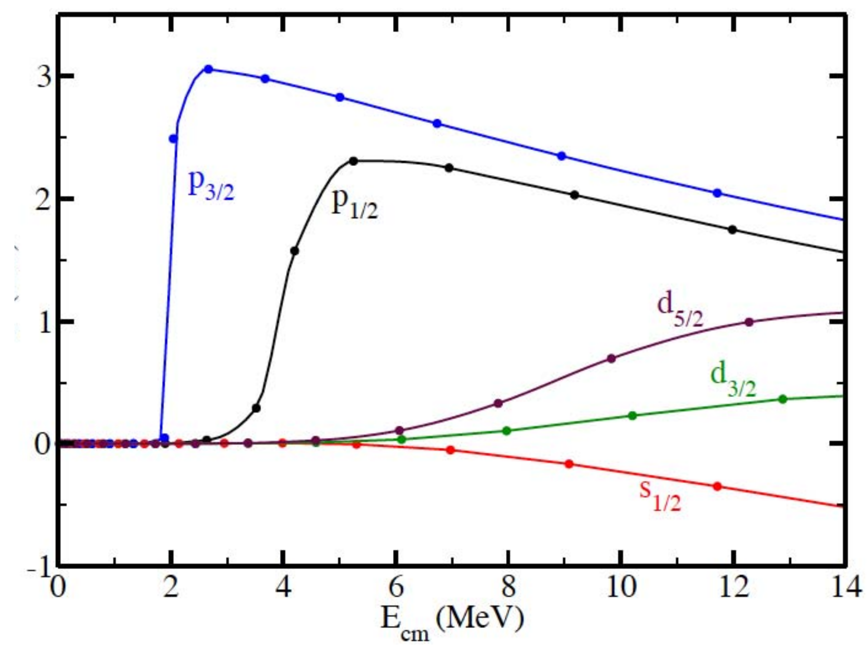
$$O_A^{A+1}(lj;r) = \sum_n \left\langle A+1 \left\| \tilde{a}^\dagger_{nlj} \right\| A \right\rangle \phi_{nlj}(r)$$

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

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

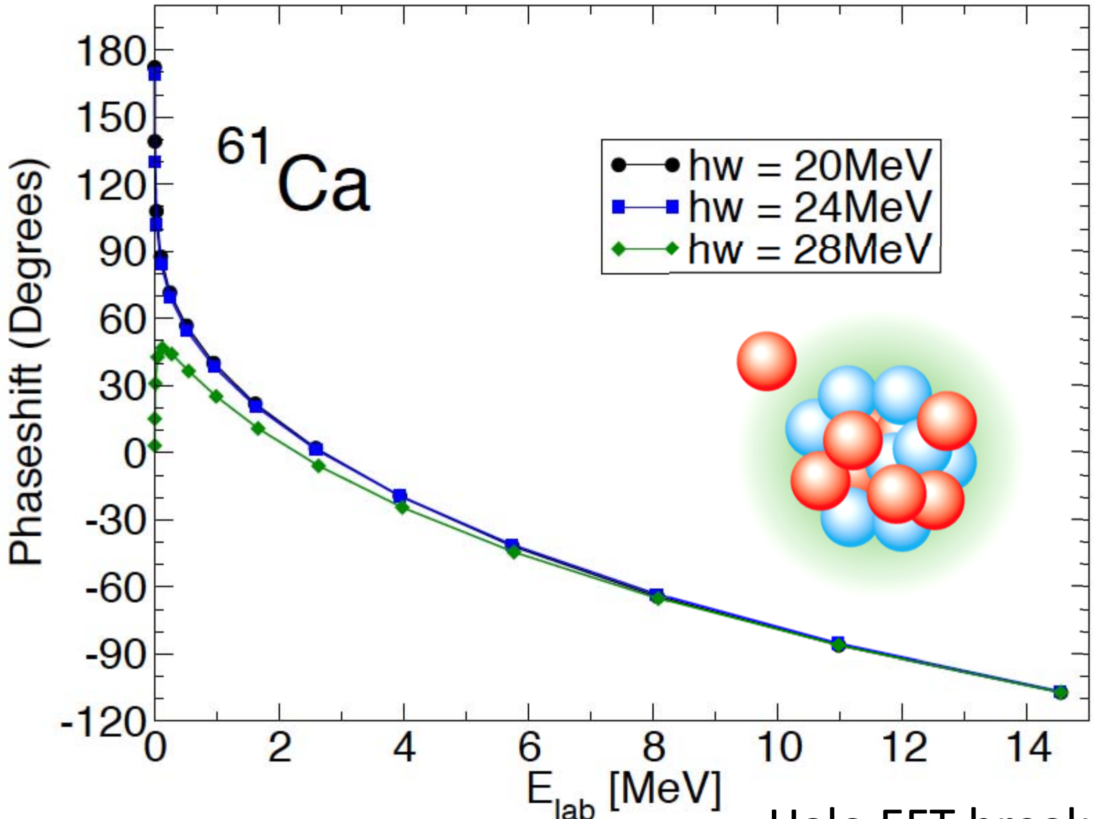
$$O_A^{A+1}(lj;kr) = C_{lj} \left[F_{\ell,\eta}(kr) - \tan\delta_l(k) G_{\ell,\eta}(kr) \right]$$





Efimov physics around neutron rich ^{60}Ca

G. Hagen, P. Hagen, H.-W. Hammer, and L. Platter, PRL 111, 132501 (2013)



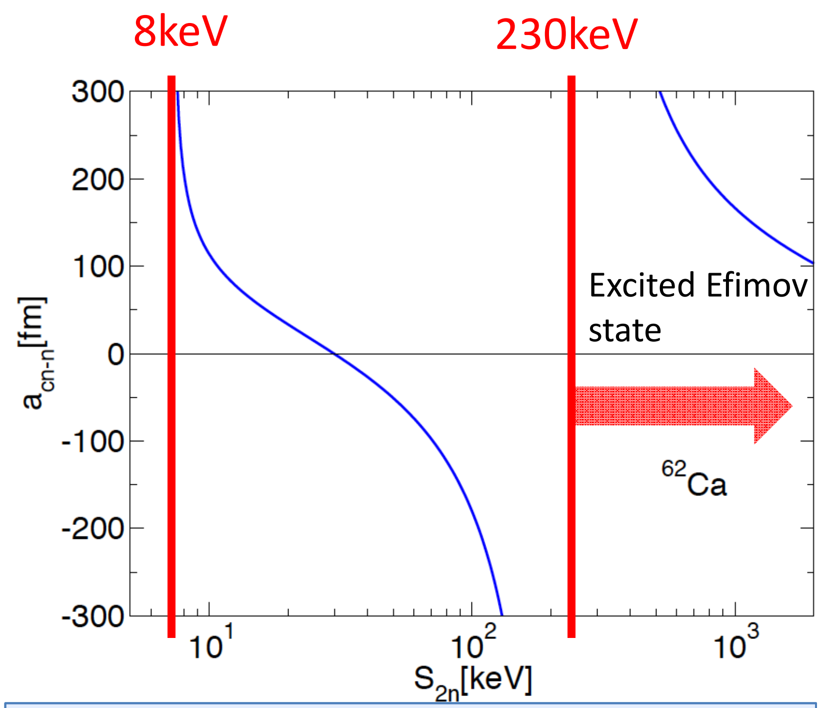
- Large S-wave scattering length in ^{61}Ca implies Halo phenomena
- Core-*n*-*n* are effective degrees of freedom
- Novel Approach: Merge halo-EFT and input from CC to study properties of ^{62}Ca

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

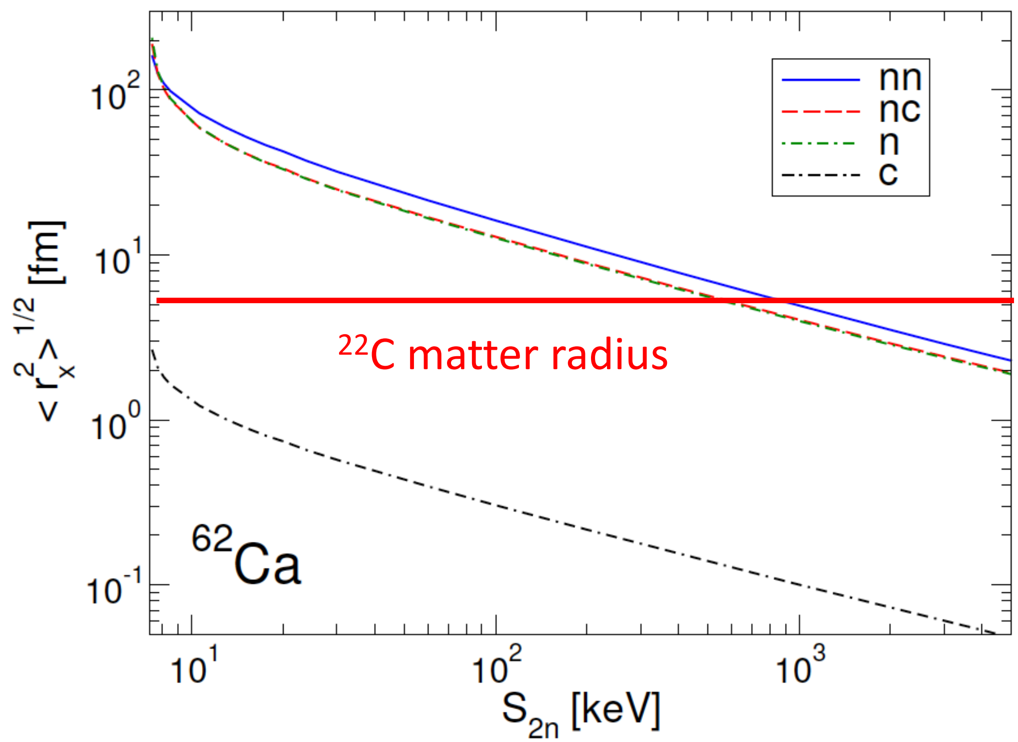
	^{53}Ca		^{55}Ca		^{61}Ca	
J^π	Re[E]	Γ	Re[E]	Γ	Re[E]	Γ
$5/2^+$	1.99	1.97	1.63	1.33	1.14	0.62
$9/2^+$	4.75	0.28	4.43	0.23	2.19	0.02

Efimov physics around neutron rich ^{60}Ca



- 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 indicates that it can be the largest and heaviest halo in the chart of nuclei so far.



Summary

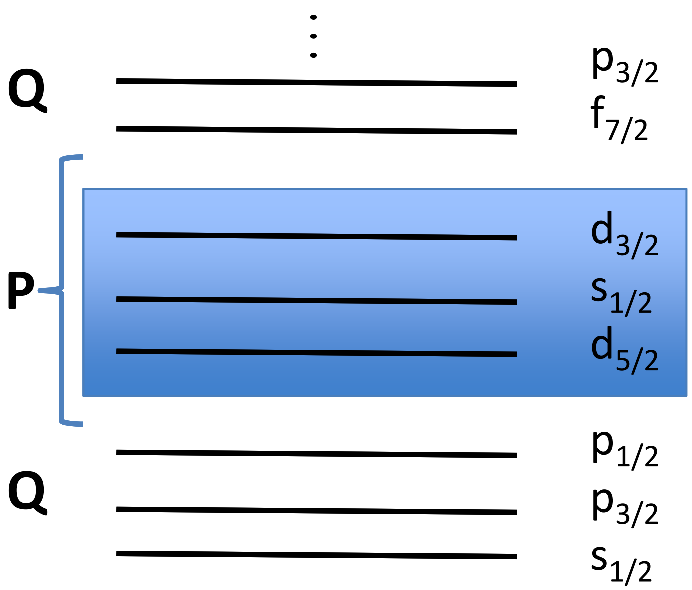
- Continuum coupling impacts level ordering and excitation energies of states in neutron rich odd calcium isotopes
- Computed elastic neutron scattering on ^{60}Ca and found ½$^{+}$ as ground state of ^{61}Ca
- Used halo EFT to study Efimov physics in ^{62}Ca

- Optimization of chiral forces with consistent two-body currents
- Origin of quenched Gamow-Teller strengths traced to two-body currents
- Revisited the anomalous life time of ^{14}C: depends on 3NFs, 2BC and 1^{+} state in ^{14}N
- Predictions for neutron radius and dipole polarizability in ^{48}Ca relevant for C-REX (Calcium Radius Experiment) at JLab.

Road to ββ decay in ^{76}Ge: Coupled-cluster effective interactions

G. R. Jansen, J. Engel, G. Hagen, P. Navratil, A. Signoracci, PRL **113**, 142502 (2014).

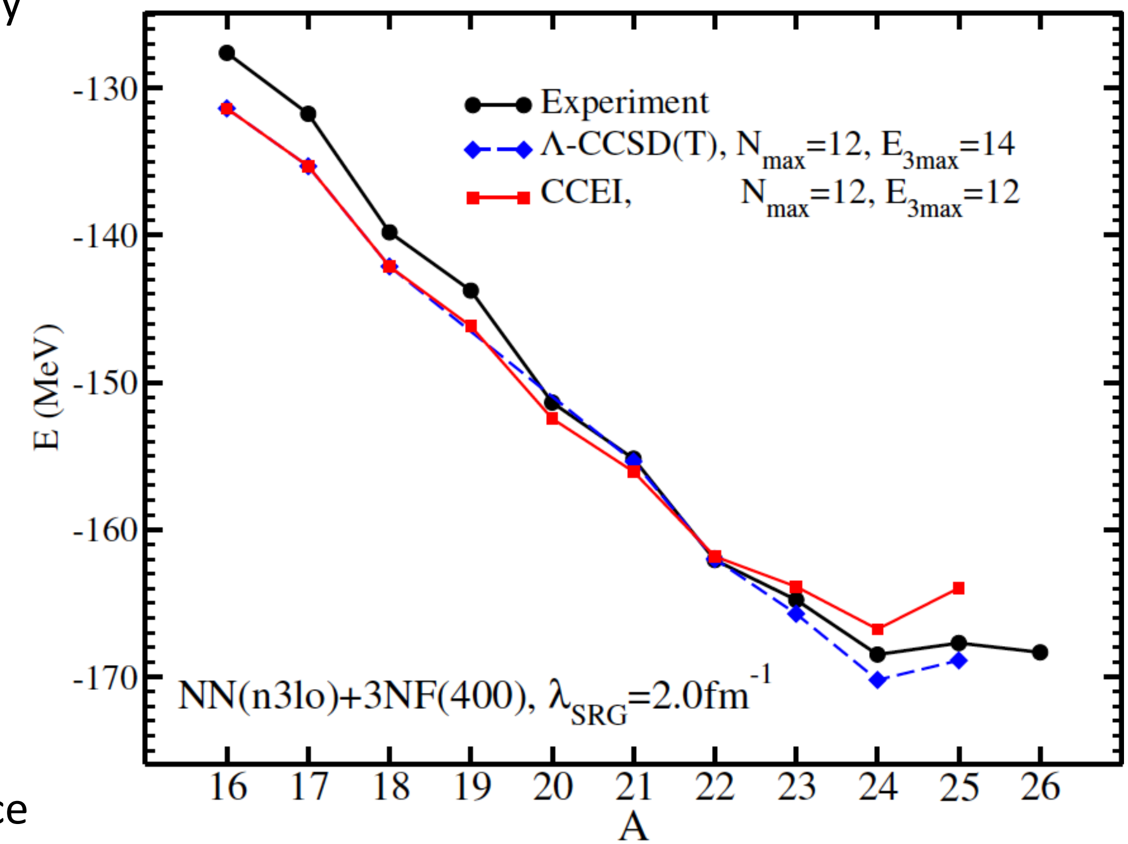
- Start from chiral NN(N3LO$_{EM}$) + 3NF(N2LO) interactions
- Solve for A+1 and A+2 using CC. Project A+1 and A+2 CC wave functions onto the *s*-*d* model space using Lee-Suzuki similarity transformation.



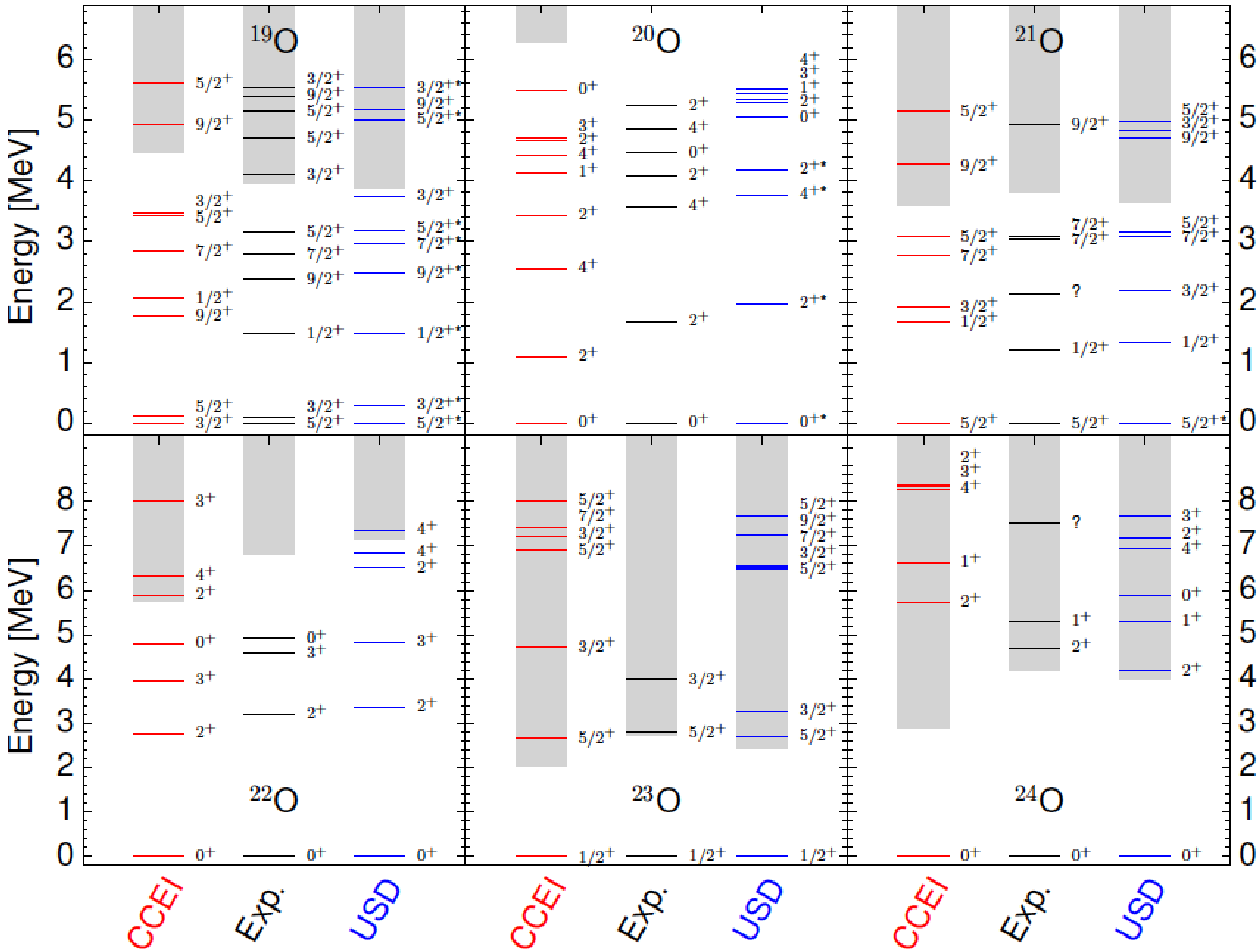
- Diagonalize the effective hamiltonian in the valence space

A. F. Lisetsky et al Phys. Rev. C 78, 044302

Comparison between coupled-cluster effective interaction (CCEI) and "exact" coupled-cluster calculation with inclusion of perturbative triples (Λ-CCSD(T)).



Coupled-cluster effective interactions for the shell model: Oxygen isotopes



Benchmarking different methods: Spectra in ^{22}O

In-medium SRG

S. Bogner et al, Phys. Rev. Lett. 113, 142501 (2014)

Coupled-Cluster Effective Interactions

G. R. Jansen et al,
Phys. Rev. Lett. 113, 142502 (2014)