Towards nuclear reactions with coupled-cluster theory

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Outline

1. Coupled-Cluster approach to loosely bound and unbound nuclear systems.
   - Resonances and halo states in ^{17}F and ^{17}O
2. Coupled-cluster approach to nuclear reactions
   - Spectroscopic factors: A tool to study correlations
   - Overlap functions and elastic scattering: n+^{16}O
   - Neutron skins and densities from CCM. Is ^{23}O consistent with a halo picture?
   - Extracting ANC's from one-body densities: The radiative capture reaction $^{15}\mathrm{N}(\mathrm{p},\gamma)^{16}\mathrm{O}$.
3. Coupled-cluster approach to open-shell nuclei
   - Towards open-shell nuclei with CCM: ^{18}O
   - Towards the drip line in the Potassium isotopes
4. Conclusion

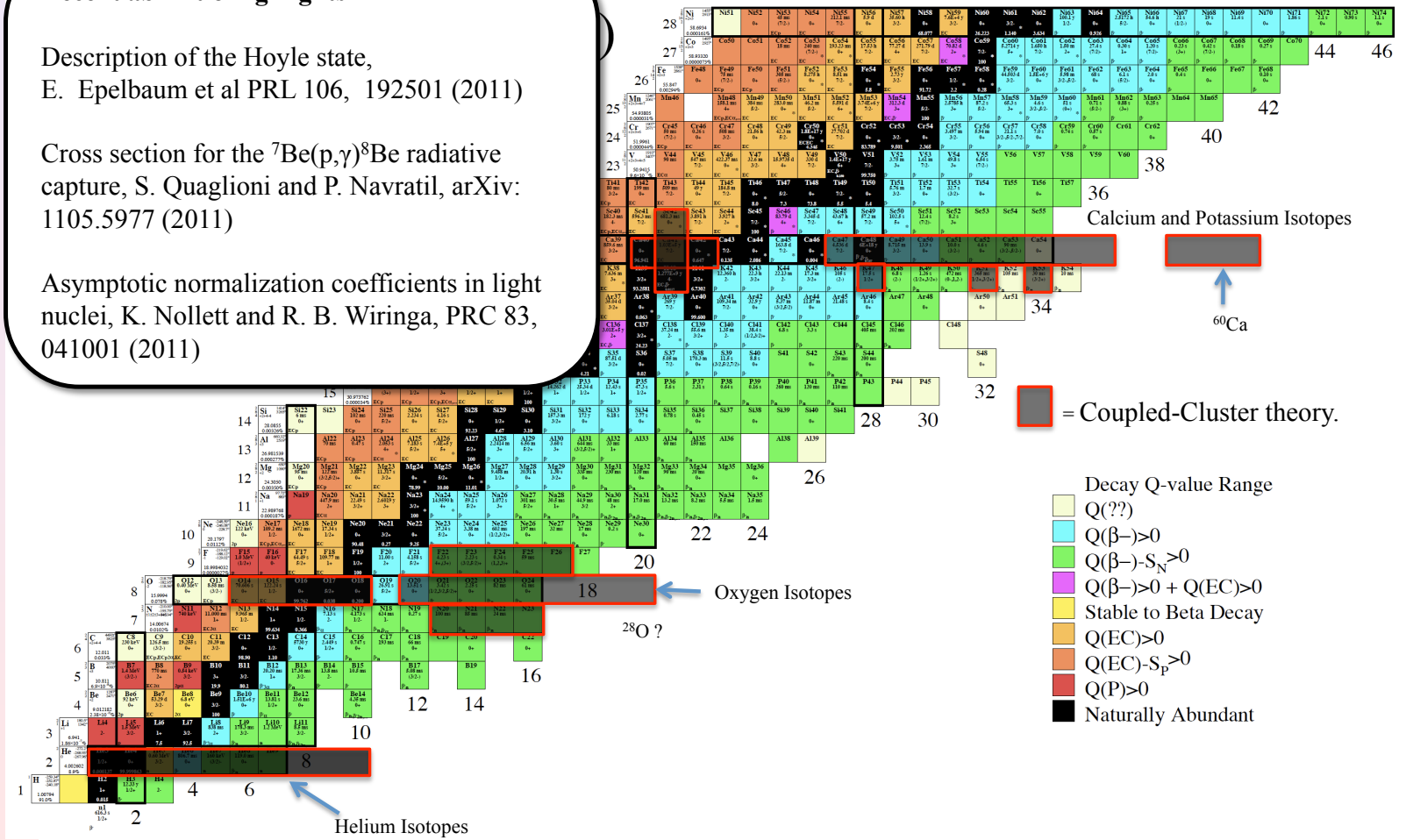
Ab-initio approaches to light and medium mass nuclei

Recent ab-initio highlights

Description of the Hoyle state,
E. Epelbaum et al PRL 106, 192501 (2011)

Cross section for the ^{7}Be(p,γ)^{8}Be radiative capture, S. Quaglioni and P. Navratil, arXiv: 1105.5977 (2011)

Asymptotic normalization coefficients in light nuclei, K. Nollett and R. B. Wiringa, PRC 83, 041001 (2011)



N-N force from Chiral perturbation theory

"If you want more accuracy, you have to use more theory (more orders)"

Effective Lagrangian → obeys QCD symmetries (spin, isospin, chiral symmetry breaking)

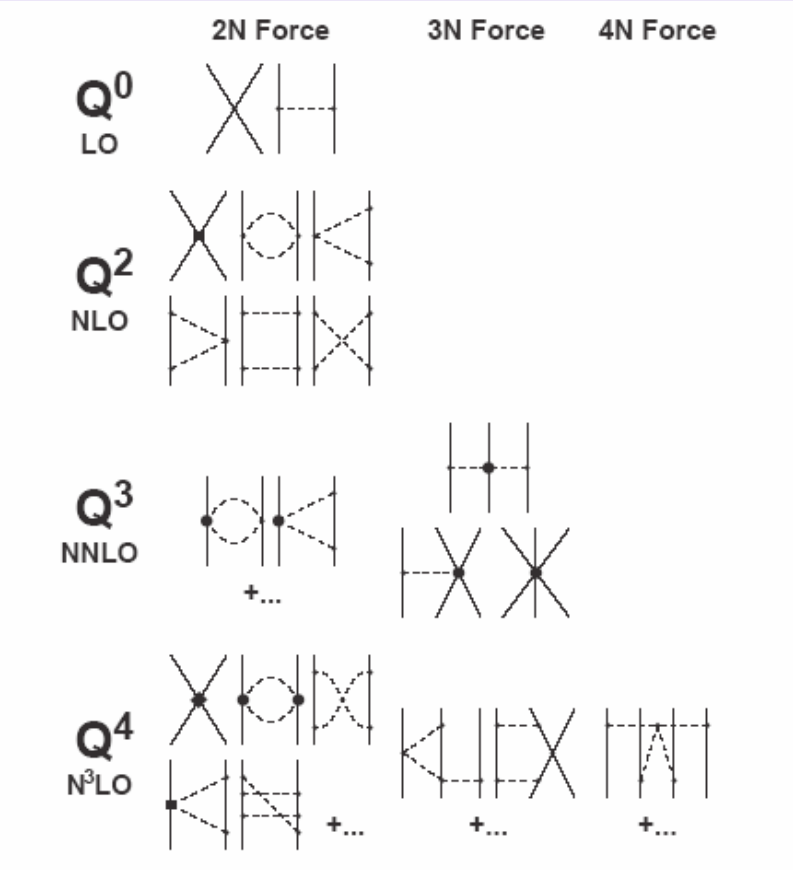
Lagrangian
→ infinite sum of Feynman diagrams.

Expand in $O(Q/\Lambda_{QCD})$

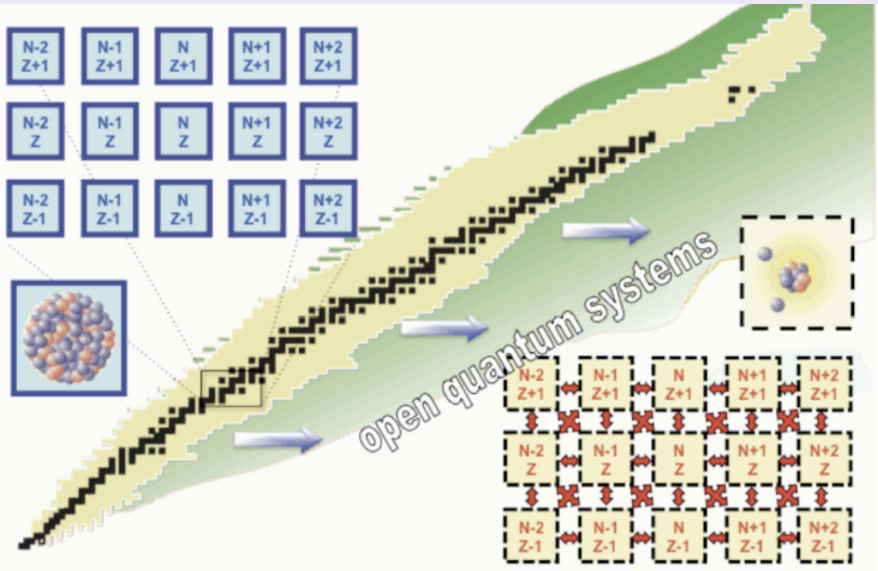
Weinberg, Ordonez, Ray, van Kolck

NN amplitude uniquely determined by two classes of contributions: contact terms and pion exchange diagrams.

24 paramters (rather than 40 from meson theory) to describe 2400 data points with

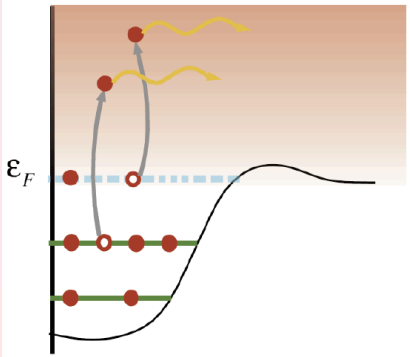


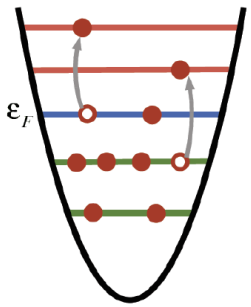
Coupled-Cluster approach to open quantum systems

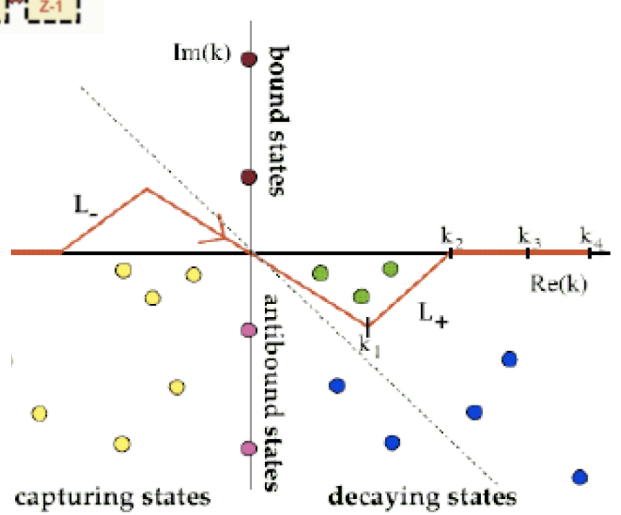


The Berggren completeness treats bound, resonant and scattering states on equal footing.

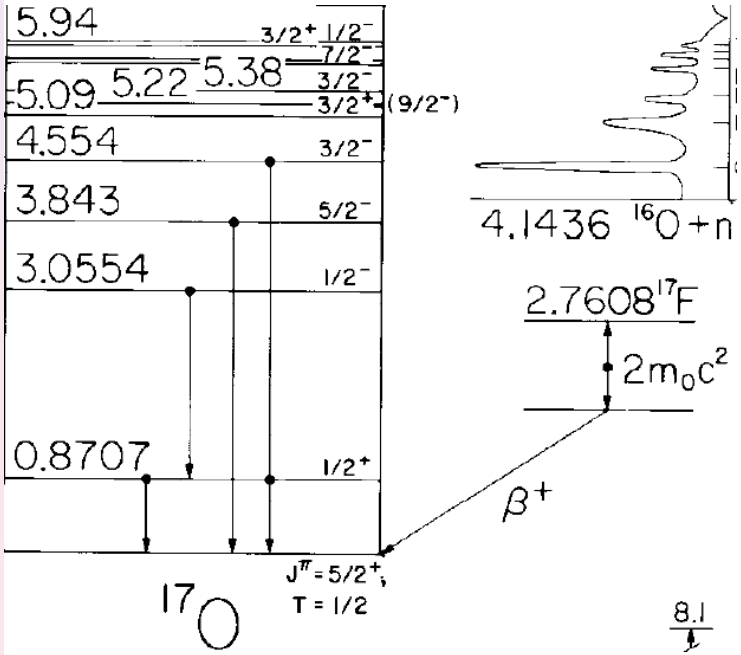
Has been successfully applied in the shell model in the complex energy plane to light nuclei. For a review see N. Michel et al J. Phys. G 36, 013101 (2009).

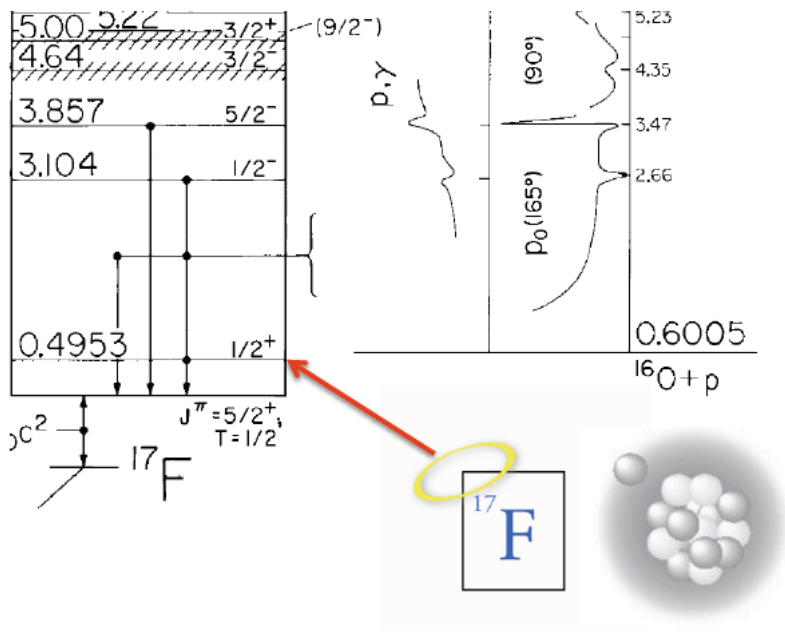






Weakly bound and unbound states in ^{17}F an ambitious testing ground for ab-initio theory

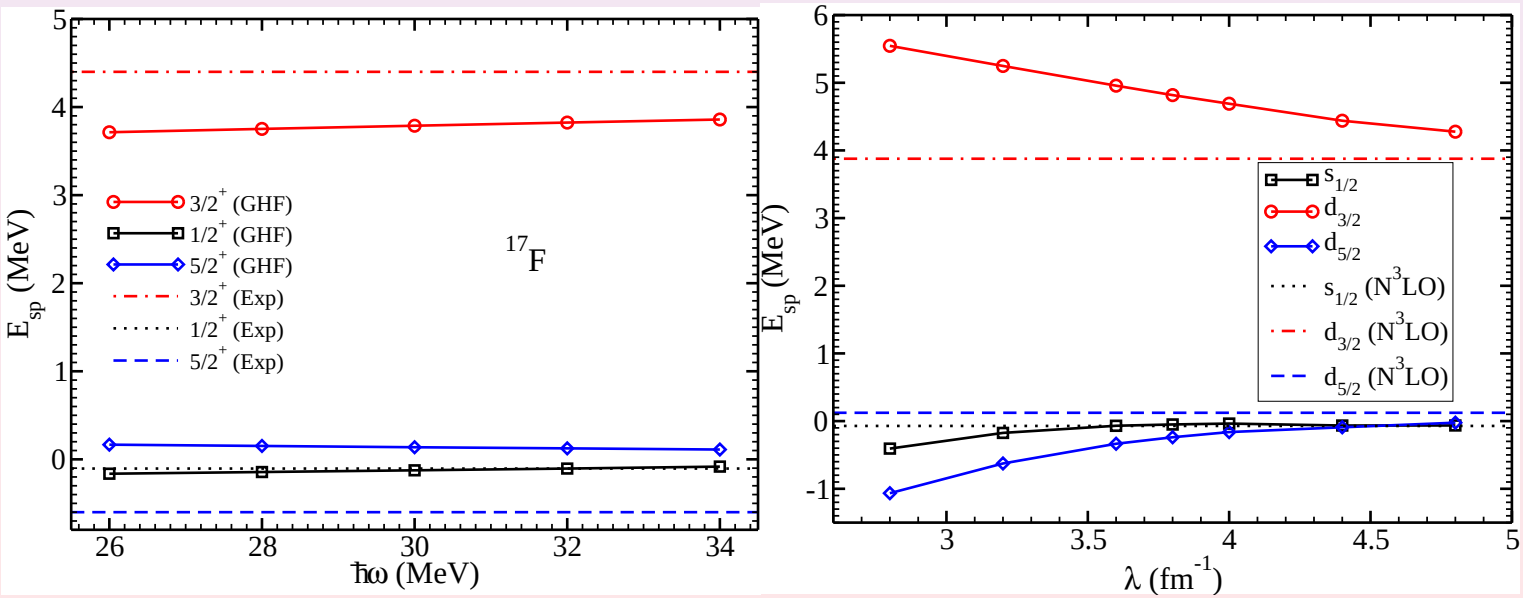




Low-lying states in ^{17}F and the role of continuum

- Low-lying single-particle states in ^{17}F using a Gamow-Hartree-Fock basis (GHF) and a Oscillator-Hartree-Fock (OHF) basis.
- Very weak dependence on the oscillator frequency $\hbar\omega$ for calculations done in a GHF basis.
- Significant effect of continuum coupling on the $1/2^+$ and $3/2^+$ states in ^{17}F.

G. Hagen, T. Papenbrock, M. Hjorth-Jensen, Phys. Rev. Lett. 104, 182501 (2010).



Summary of results for ^{17}O and ^{17}F

- Our calculations for the $1/2^+$ states in ^{17}F and ^{17}O agree remarkably well with experiment.
- Spin-orbit splitting between $d_{5/2}$-$d_{3/2}$ orbitals too compressed without three-nucleon forces.
- Our calculations of the widhts of the $3/2^+$ resonant states compare reasonably well with experiment.

	^{17}O			^{17}F		
	$(1/2)^+_1$	$(5/2)^+_1$	$E_{s.o.}$	$(1/2)^+_1$	$(5/2)^+_1$	$E_{s.o.}$
OHF	-1.888	-2.955	4.891	0.976	0.393	4.453
GHF	-2.811	-3.226	4.286	-0.082	0.112	3.747
Exp.	-3.272	-4.143	5.084	-0.105	-0.600	5.000

	^{17}O $(3/2)^+_1$		^{17}F $(3/2)^+_1$	
	Re[E_{sp}]	Γ	Re[E_{sp}]	Γ
PA-EOMCCSD	1.059	0.014	3.859	0.971
Experiment	0.942	0.096	4.399	1.530

Overlap functions and spectroscopic factors

Microscopic definition of Spectroscopic Factors (SF)

- Elastic scattering, capture and transfer of a nucleon on/to a target nucleus with mass A is given by the overlap function

$$O_A^{A+1}(lj;r) = \langle A \,\|\, \tilde{a}_{lj}(r) \,\|\, A+1 \rangle = \sum_n \langle A \,\|\, \tilde{a}_{nlj} \,\|\, A+1 \rangle \, \phi_{nlj}(r).$$

- The norm of the overlap functions defines the spectroscopic factor:

$$SF = \int_0^\infty dr r^2 \, |O_A^{A+1}(lj;r)|^2.$$

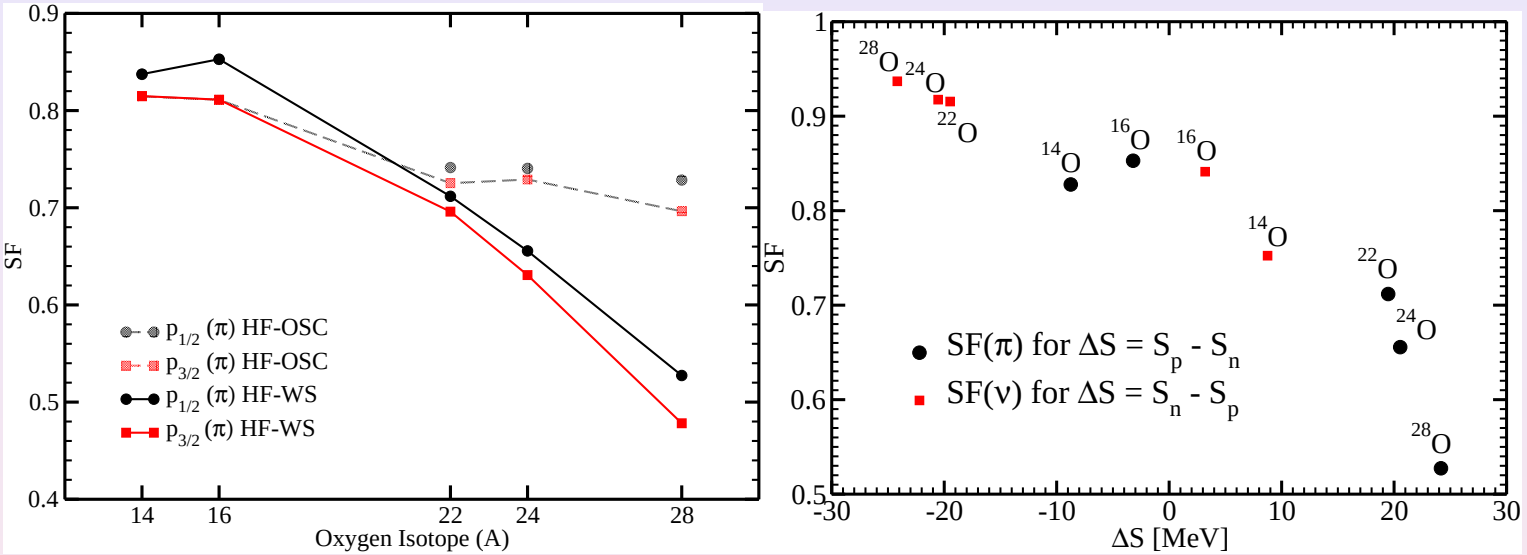
Asymptotic properties of the one-nucleon overlap function

Outside the range of the interaction the overlap function is proportional to a single-particle wave function.

$$O_A^{A+1}(lj;r) = C \frac{e^{-\kappa r}}{\kappa r} \qquad \text{(Bound states)}$$

$$O_A^{A+1}(lj;r) = A\,(j_l(kr) - \tan\delta_l n_l(kr)) \qquad \text{(Scattering states)}$$

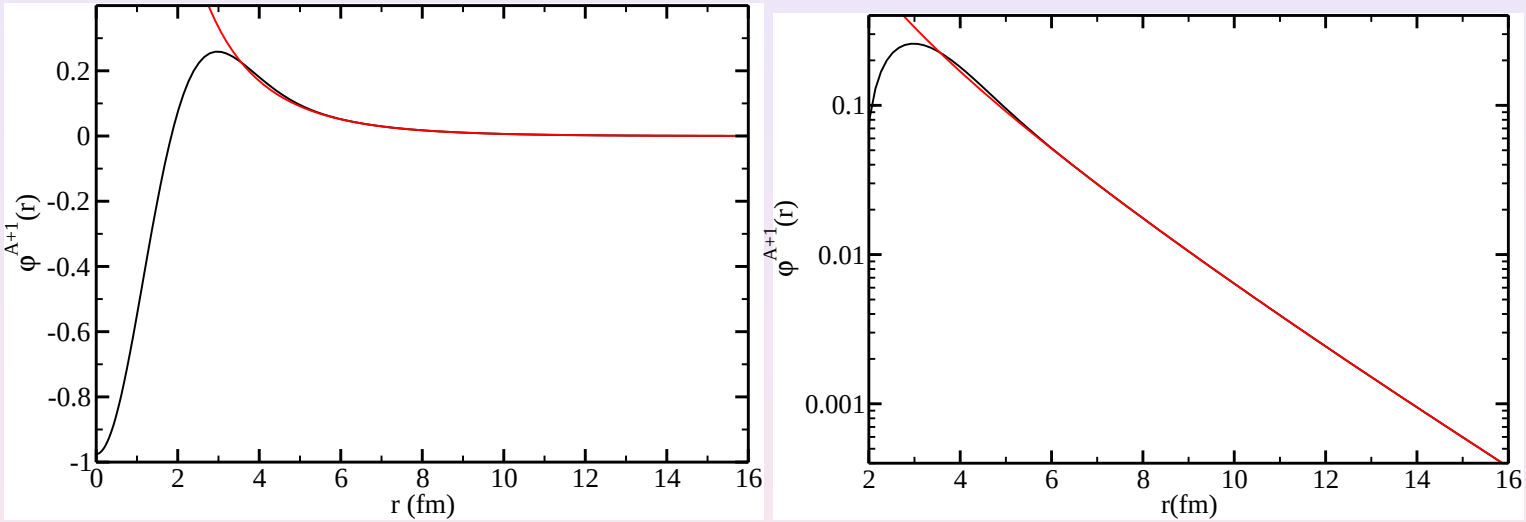
Quenching of SFs for proton removal in oxygen isotopes



Spectroscopic factor for proton removal from Oxygen isotopes

- SF is a useful tool to study the role correlations toward the dripline.
- We find a significant quenching of the SFs due to enhanced correlations coming from coupling to the scattering continuum.
- **Ø. Jensen, G. Hagen and M. Hjorth-Jensen, Phys. Rev. C(R) 83, 021305 (2011)**
  Ø. Jensen, G. Hagen, Hjorth-Jensen, Brown, Gade, in press Phys. Rev. Lett. 107, 032501 (2011).
  Threshold effects in SFs see N. Michel et al Phys. Rev. C(R) 75, 031301 (2007)

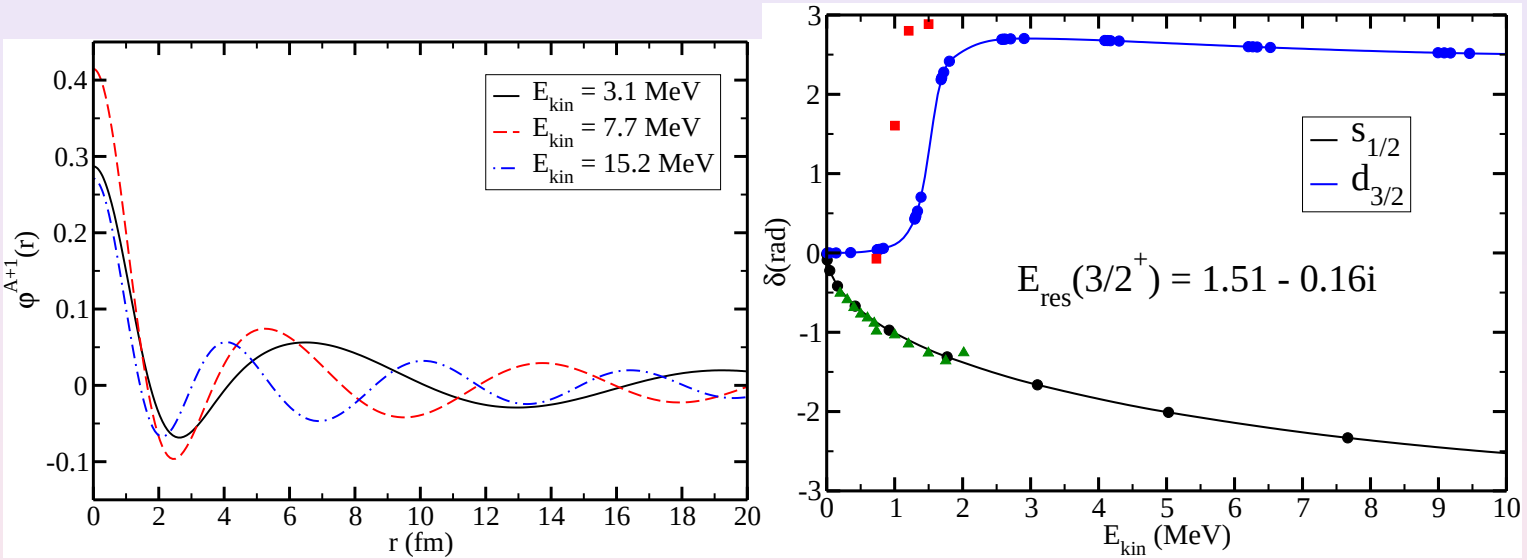
Overlap functions for bound states



Overlap function for a bound $A+1$ nucleus

- We use an SRG evolved interaction with cutoff $2.66\mathrm{fm}^{-1}$. The CCSD ground state energy for ^{16}O in $N = 11$ major shells is -140.52 MeV.
- One neutron overlap functions for the bound $J^\pi = 1/2^+$ state in ^{17}O with the ground state of ^{16}O. For ^{17}O we get $E_{sp}(1/2^+)$ = -3.83 MeV.

Elastic scattering of neutrons on ^{16}O with CCM (Preliminary)



Overlap functions provides a simple and intuitive picture of reactions

- **Left figure:** One neutron overlap functions for various $J^\pi = 1/2^+$ scattering states in ^{17}O using SRG evolved interaction with cutoff $\lambda = 2.66\mathrm{fm}^{-1}$
- **Right figure:** By matching the known asymptotic form of the overlap functions to scattering solutions we can extract low-energy elastic scattering phase shifts.

Intrinsic densities from microscopic CCM

Computing intrinsic densities

- The one-body density matrix for the A and $A-1$ nuclei are computed in the coupled-cluster formalism

$$\rho^A_{pq} = \langle \Phi_0 | L^A_0 \overline{a^\dagger_p a_q} R^A_0 | \Phi_0 \rangle, \;\; \rho^{A-1}_{pq} = \langle \Phi_0 | L^{A-1}_0 \overline{a^\dagger_p a_q} R^{A-1}_0 | \Phi_0 \rangle,$$

  and the local laboratory density is $\rho(r) = \sum_{pq} \rho_{pq} \phi_p(r) \phi_q(r)$

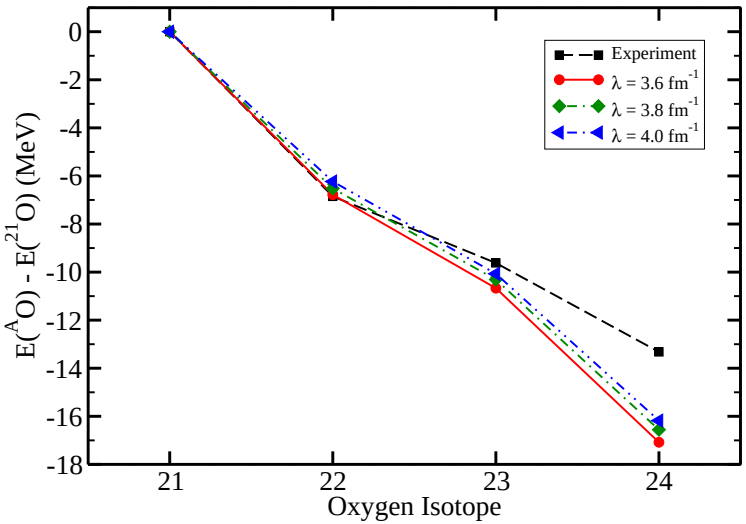
- CC wave function factorizes and the CoM wave function is a Gaussian with fixed width (G. Hagen *et al* Phys. Rev. Lett. **103**, 062503 (2009))

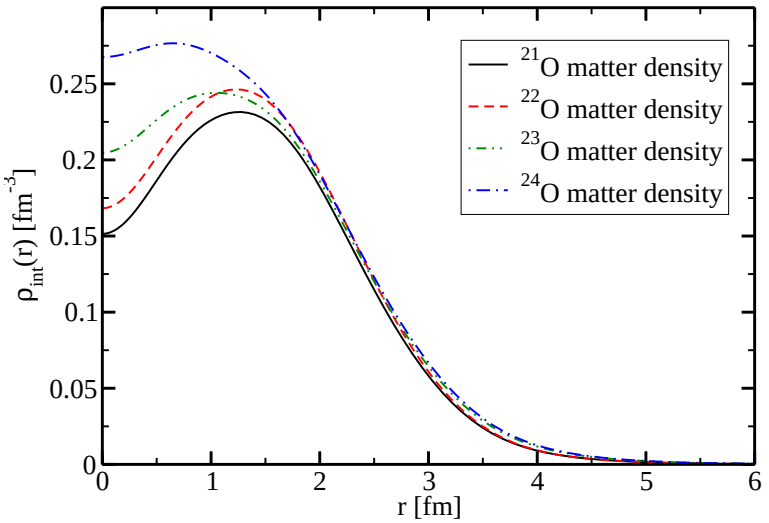
$$\Psi(r_1, \ldots, r_A) = \Gamma(R) \Psi_{int}(x)$$

- We can get the internal density σ by a deconvolution of the local laboratory density ρ (B. G. Giraud, Phys. Rev. C 77, 014311 (2008))

$$A^{-1} \rho(r) = A^{-1} \int dR \, [\Gamma(R)]^2 \, \sigma\left(\frac{A}{A-1}(r-R)\right)$$

Matter and charge radii in the ^{21,22,23,24}O isotopes





- Binding energies of ^{21,22,23,24}O with respect to the ground state of ^{21}O.
- Point matter and charge radii for computed from intrinsic densities
- We used the SRG evolved N^{3}LO nucleon-nucleon interaction with cutoffs $\lambda = 3.6, 3.8, 4.0\mathrm{fm}^{-1}$.
- Calculations converged with respect to the model-space.

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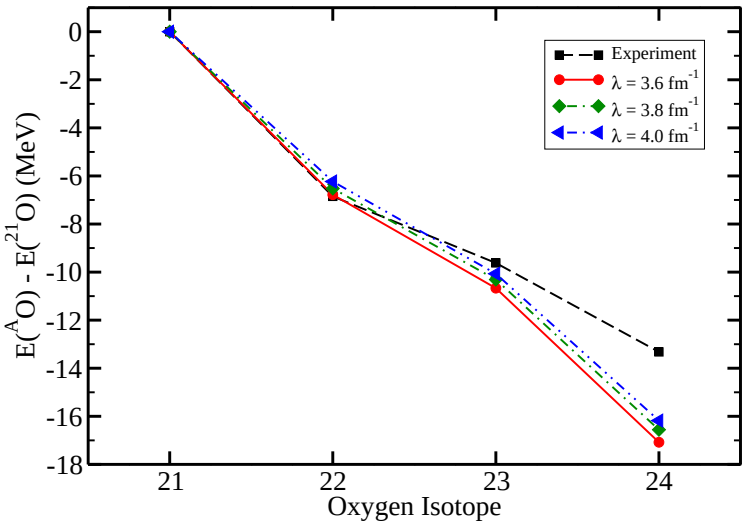

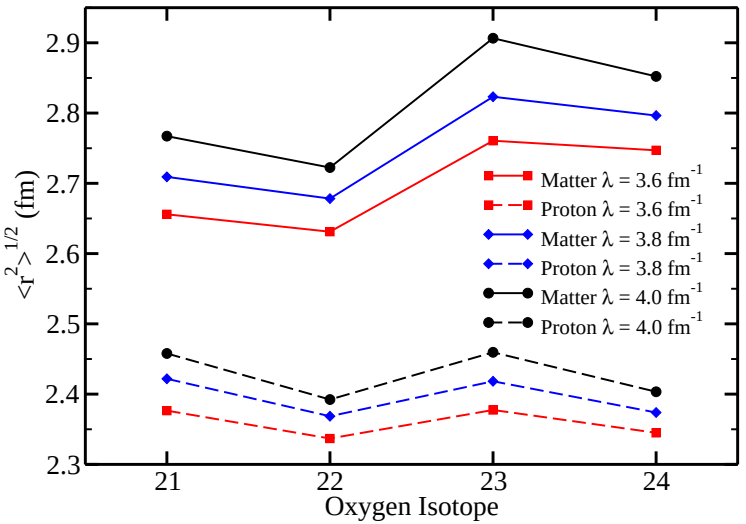

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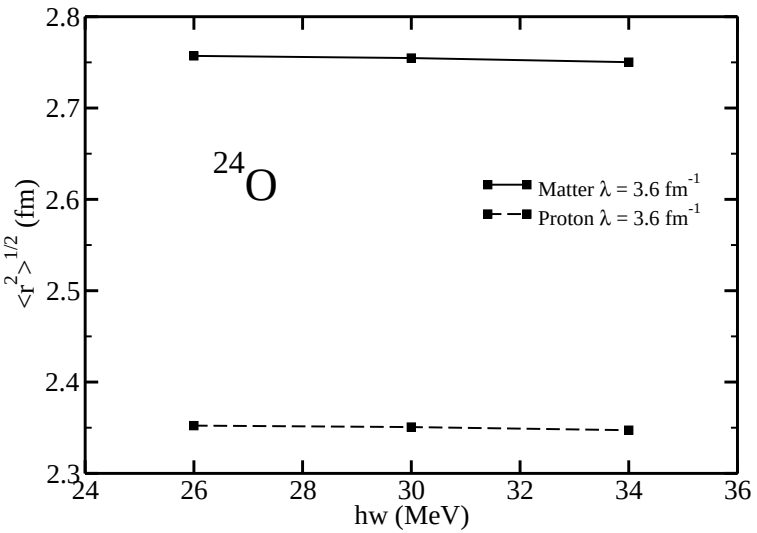

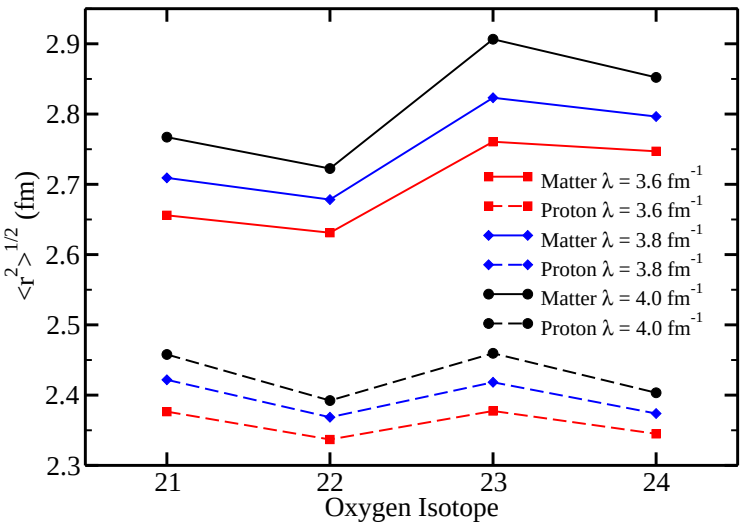

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ANC's from one-body densities?

Physics Letters B 314 (1993) 255–259
North-Holland

PHYSICS LETTERS B

On the relationship between single-particle overlap functions, natural orbitals and the one-body density matrix for many-fermion systems

D. Van Neck [1], M. Waroquier [2]
Institute for Nuclear Theory, University of Washington, Seattle, WA 98195, USA and Institute for Nuclear Physics, Proeftuinstraat 86, B-9000 Gent, Belgium

and

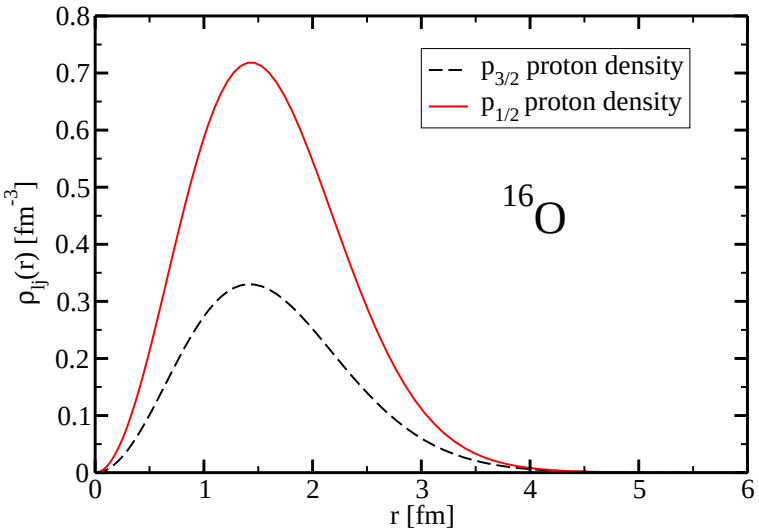
K. Heyde
Institute for Theoretical Physics, Proeftuinstraat 86, B-9000 Gent, Belgium

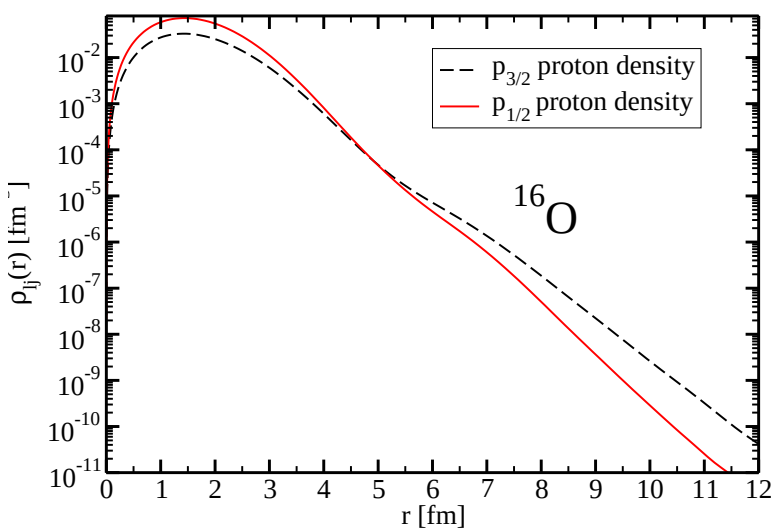
5. Conclusion

We have shown that, in principle, the overlap functions, spectroscopic factors and separation energies of the bound eigenstates of the $(A-1)$-particle system can be constructed by means of the exact OBDM of the groundstate of the A-particle system.

It is rather surprising that the latter quantity contains much of the dynamics in the $(A-1)$ system. The practical applicability is severely limited, however, by the need of a reliable calculation of the full OBDM (diagonal as well as off-diagonal elements) in coordinate space, at large radial distances. This

^{16}O proton density with NN from SRG $\lambda = 2.66\mathrm{fm}^{-1}$

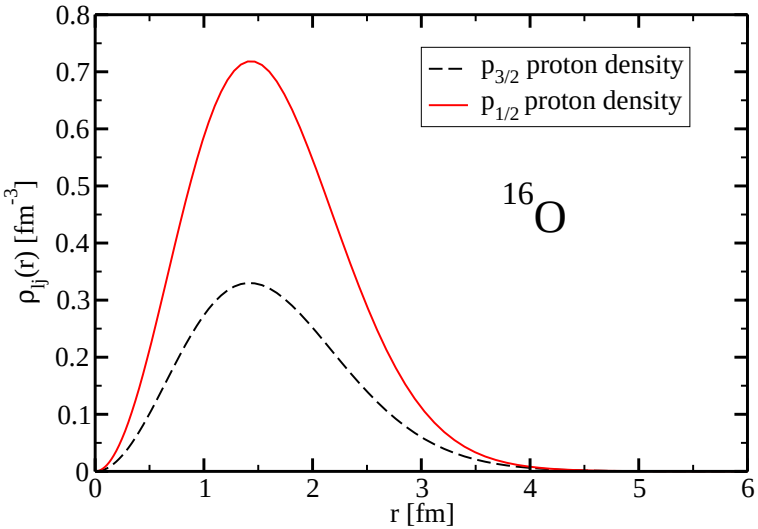


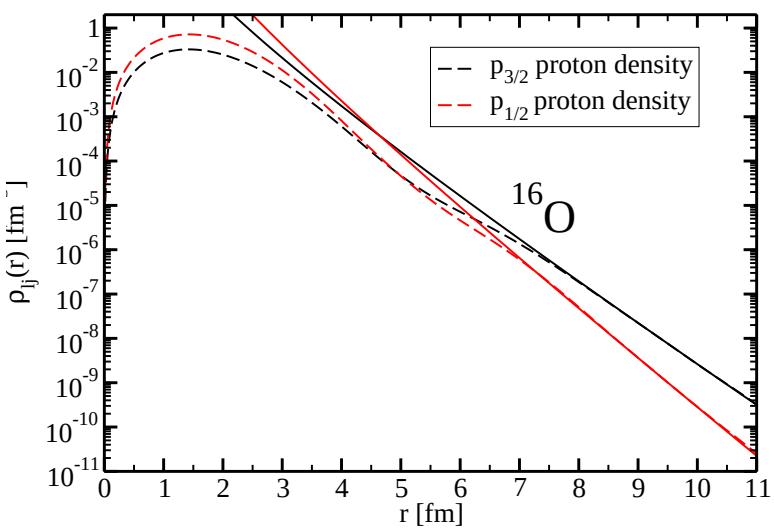


The density matrix can be written in terms overlap functions between nucleus A and its $A-1$ neighbour

$$\rho^A_{lj}(r) = \sum_\mu \langle A|a_{lj}(r)|A-1\rangle_{\mu\,\mu}\langle A-1|a^\dagger_{lj}(r)|A\rangle, \quad \rho^A_{lj}(r) \to |C_{lj}|^2 \frac{e^{-2\kappa_0 r}}{r^2}$$

ANC for the radiative capture $^{15}N(p,\gamma)^{16}O$ reaction



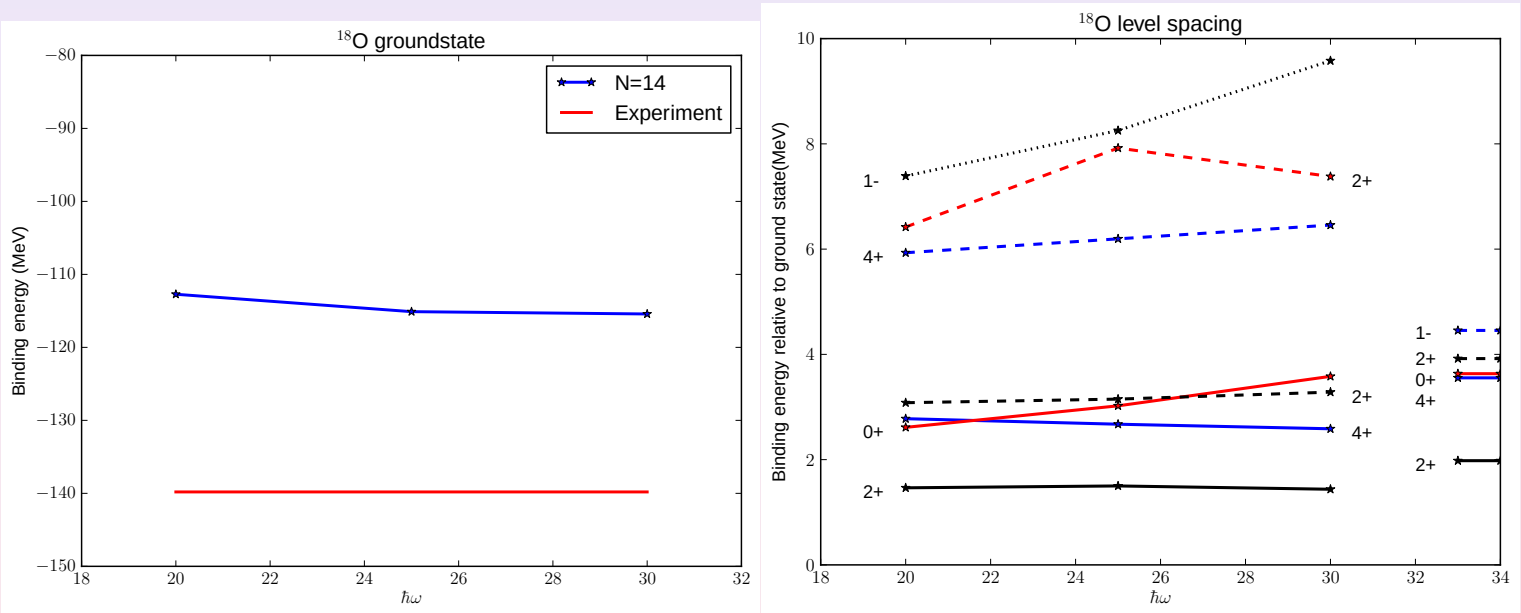


Proton separation energies in ^{16}O and ANC for $\langle {}^{15}Np|{}^{16}O\rangle$.

J^π	$E_{CC}(MeV)$	$E_{\rm exp}$ (MeV)	$\lvert C\rvert^2_{CC}$ (fm^{-1})	$\lvert C\rvert^2_{\rm exp}$ (fm^{-1})
$1/2^-$	17.99	12.13	621.66	529 ($\pm$9)
$3/2^-$	26.60	18.45	4301.17	?

Experiment: P. J. LeBlanc et al., Phys. Rev. C **82**, 055804 (2010).

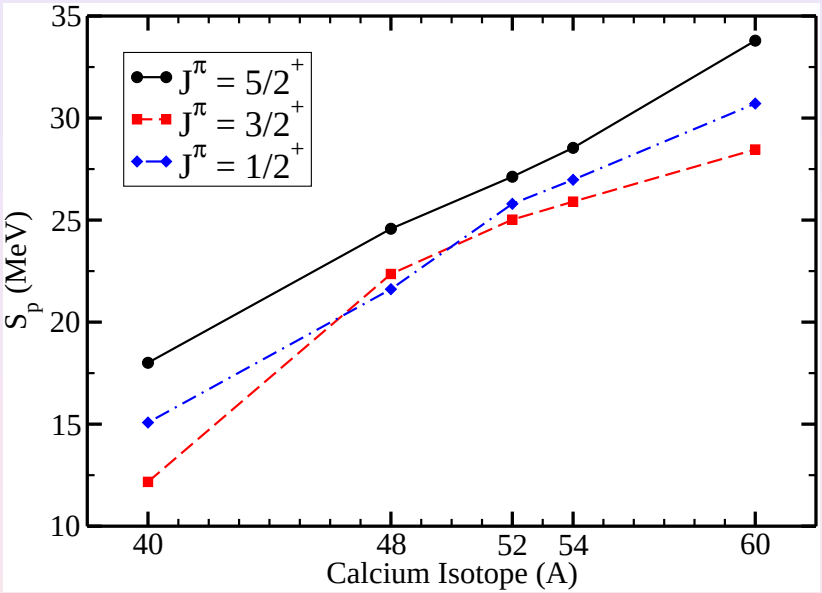
Going beyond closed-shell nuclei. Low-lying states in ^{18}O (Preliminary)



- Model space consists of 15 major oscillator shells.
- Two-particle attached equation-of-motion coupled-cluster works very well for low-lying states in open-shell nuclei like ^{18}O.

G. Jansen, M. Hjorth-Jensen, G. Hagen, T. Papenbrock, Phys. Rev. C 83, 054306 (2011).

Low-lying states in neutron rich Potassium isotopes



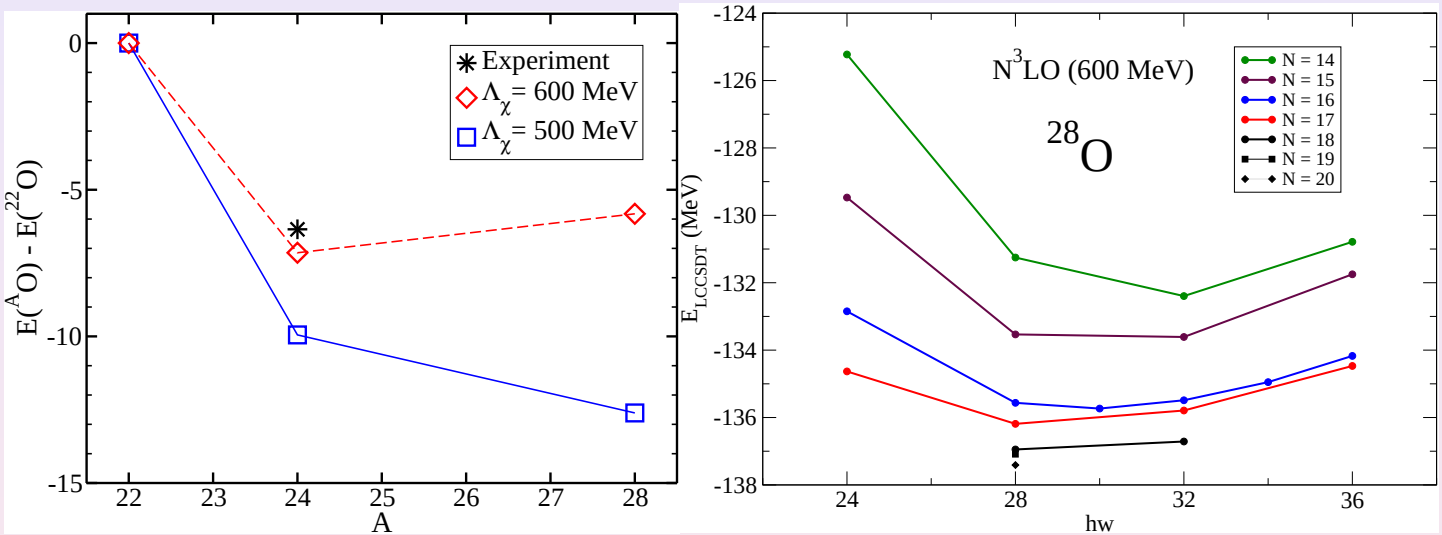
- Proton separation energies $S_p = -E_\mu^- = E_\mu^{A-1} - E_0^A$ in ^{40,48,52,54,60}Ca.
- Low lying states in Potassium isotopes calculated using PA/PR-EOMCCSD with "bare" chiral interactions.
- Model space consists of 15 major harmonic oscillator shells with fixed oscillator frequency $\hbar\omega = 30$MeV.

	^{39}K		^{47}K	
J^π	E_{CC} (MeV)	E_{Exp} (MeV)	E_{CC} (MeV)	E_{Exp} (MeV)
$3/2^+$	0.00	0.00	0.00	0.00
$1/2^+$	2.90	2.52	-0.75	-0.36
$5/2^+$	5.84	4.51	2.22	3.00

Conclusion

- Coupled-Cluster method has been succesfully applied to the description of weakly bound and unbound states in ^{17}O and ^{17}F.
- Microscopic calculations of spectroscopic factors for proton removal showed significant quenching in the neutron rich oxygen isotopes.
- Presented the first successful calculation of scattering phaseshifts with coupled-cluster theory, the results for ^{17}O are promising.
- Performed coupled-cluster calculations of intrinsic densities, charge and matter radii for ^{21,22,23,24}O.
- Extration of ANCs from one-body density matrices
- Extended coupled-cluster to nuclei with ± 2 nucleons outside a closed shell. Presented fully converged calculations for low-lying states in ^{18}O.
- Energy spacing between excited states in ^{39,47}K and the level inversion in ^{47}K are well reproduced.

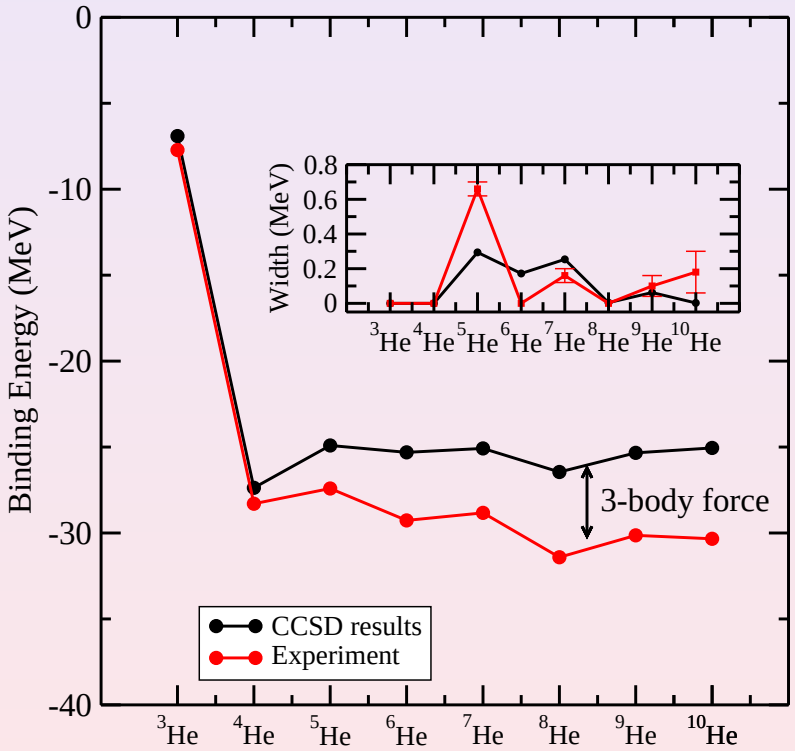
Can theory support the existence of ^{28}O ?



G. Hagen, T. Papenbrock, D. J. Dean, M. Hjorth-Jensen, B. Velamur Asokan, Phys. Rev. C 80, 021306 (2009).

- No sign of dramatic increase in binding energies of oxygen isotopes.
- Can ab-initio Coupled-Cluster calculations rule out the existence of ^{28}O ?
- Cutoff variation indicates that three-nucleon forces will play a crucial role in the determination of the neutron dripline.

CCSD results for Helium chain using $V_{\mathrm{low}-k}$



- $V_{\mathrm{low}-k}$ from N3LO with $\Lambda = 1.9\mathrm{fm}^{-1}$.
- G. Hagen et al., Phys. Lett. B 656, 169 (2007). arXiv:nucl-th/0610072.

- First *ab-initio* calculation of decay widths of a whole isotopic chain.
- CCM unique method for dripline nuclei.
- $\sim$ 1000 active orbitals
- Underbinding hints at missing 3NF