Towards *ab initio* nuclear structure and reactions with coupled-cluster theory

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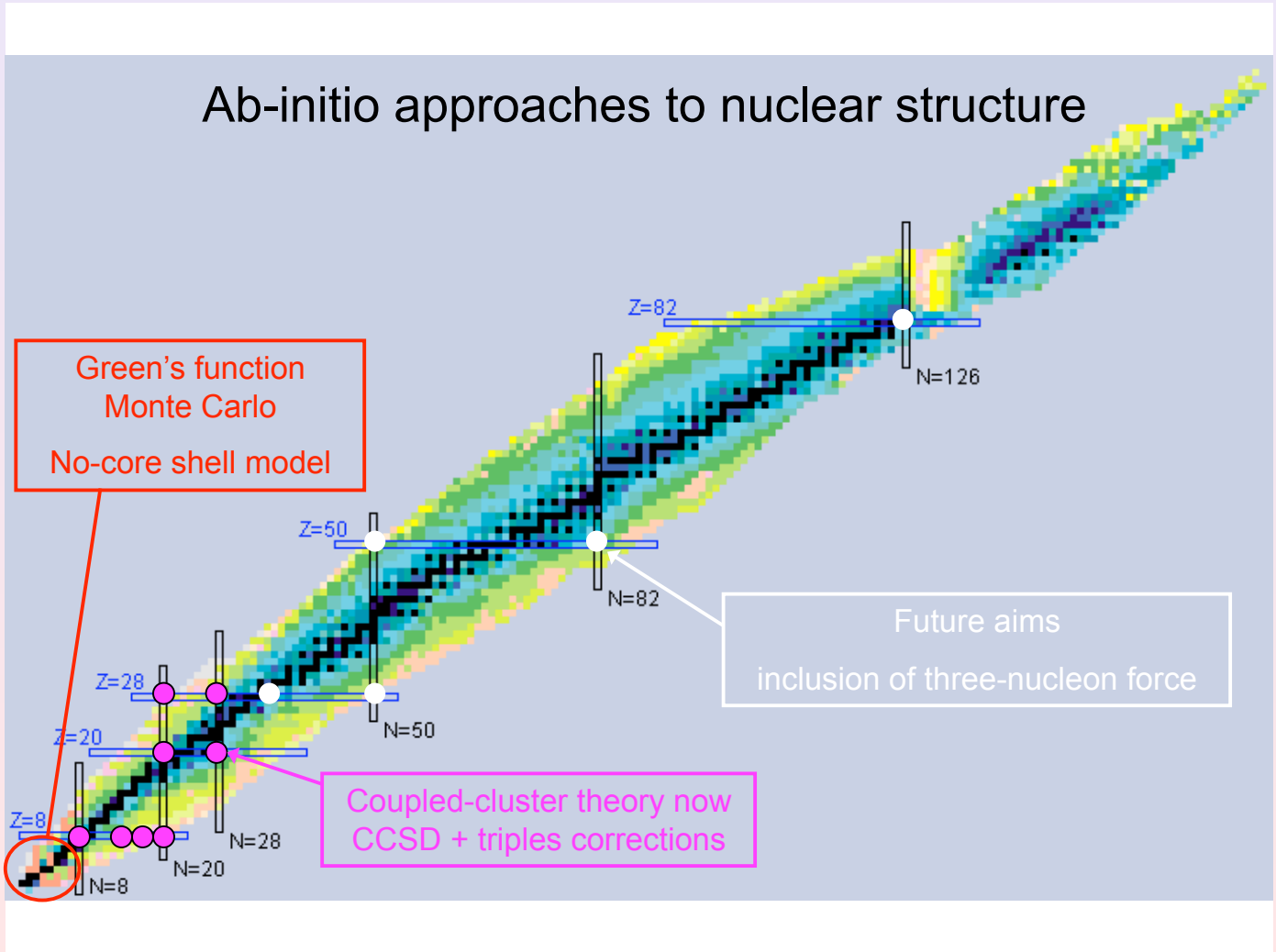
CEA Saclay,
Orme Des Merisiers, May 13

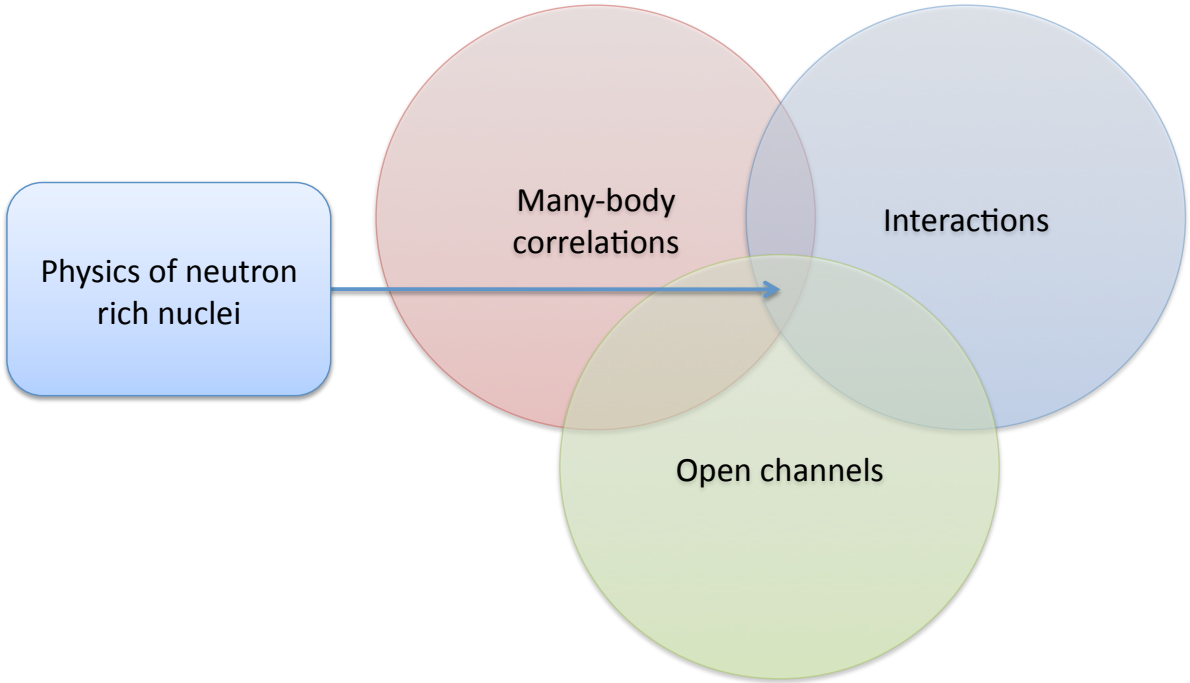
Outline

1. Coupled-Cluster approach to nuclear structure
   - Brief overview of Coupled-Cluster theory
   - Coupled-Cluster approach to medium mass nuclei. ^{16}O, ^{40,48}Ca with chiral interactions (NN-only)
2. Coupled-Cluster approach to loosely bound and unbound nuclear systems.
   - Microscopic description of resonances and halo states in ^{17}F and ^{17}O
   - Towards ab-initio reaction theory with coupled-cluster theory: Overlap functions and nucleon-nucleus scattering
3. Probing the dripline with Coupled-Cluster theory
   - Low-lying states in ^{18}O and ^{18}Ne with two-particle attached EOM-CCSD
   - Shell evolution in Oxygen and Calcium isotopes
4. Conclusion

Ab-initio approaches to light and medium mass nuclei



Physics of neutron rich nuclei: A challenge for theory



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)

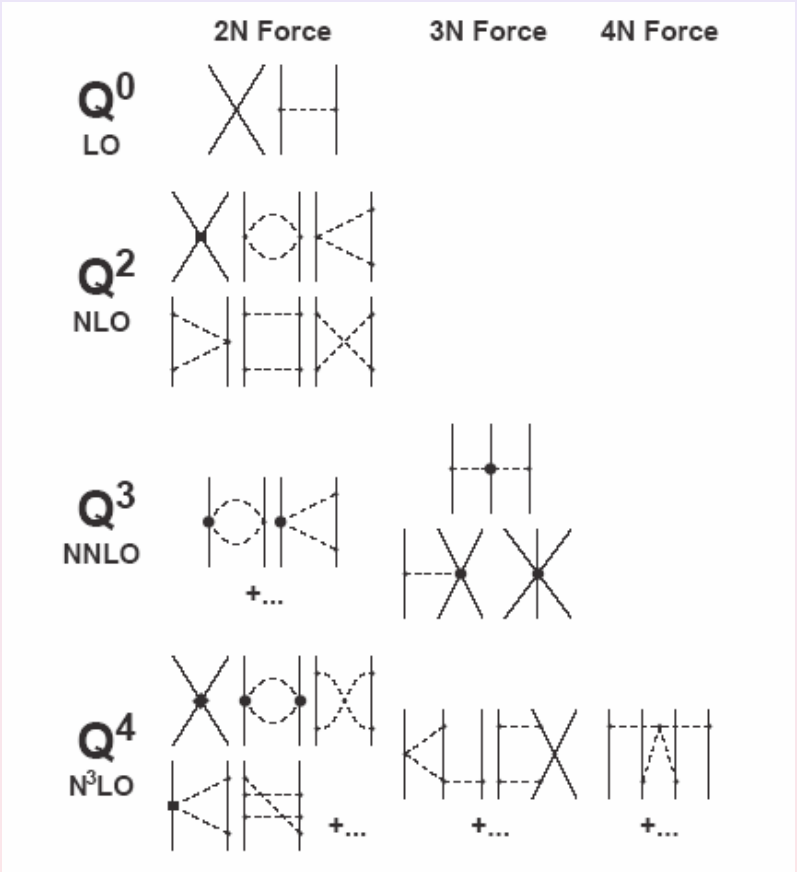
Lagrangian
→ infinite sum of Feynman diagrams.

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 Theory

Exponential Ansatz for Ψ

$$|\Psi\rangle = e^{\hat{T}}|\Phi_0\rangle, \quad \hat{T} = \hat{T}_1 + \hat{T}_2 + \ldots + \hat{T}_A$$

$$\hat{T}_1 = \sum_{i,a} t_i^a \hat{a}_a^\dagger \hat{a}_i, \; \hat{T}_2 = \frac{1}{2} \sum_{i<j,a<b} t_{ij}^{ab} \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i.$$

Coupled-Cluster Equations

$$\Delta E = \langle \Phi_0 | \left(H_N exp(T) \right)_C | \Phi_0 \rangle$$

$$0 = \langle \Phi_p | \left(H_N exp(T) \right)_C | \Phi_0 \rangle$$

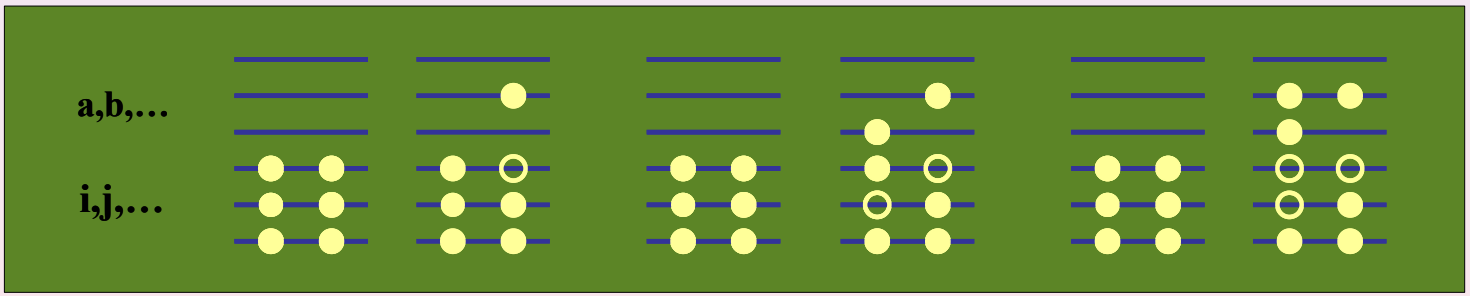
$$\bar{H} = \left(H_N exp(T) \right)_C$$

1. Coupled-Cluster Theory is fully microscopic .
2. Coupled-Cluster is size extensive. No unlinked diagrams enters, and error scales linearly with number of particles.
3. Low computational cost (CCSD scales as $n_o^2 n_u^4$).
4. Capable of systematic improvements.
5. Amenable to parallel computing.

Coupled-Cluster in pictures

$$\left|\Psi\right\rangle = e^{T^{(A)}}\left|\Phi\right\rangle, \quad T^{(A)} = \sum_{k=1}^{m_A} T_k$$

$$T_1 = \sum_{\substack{i \\ a}} t_i^a \left|\Phi_{\ i}^{\ a}\right\rangle, \quad T_2 = \sum_{\substack{i>j \\ a>b}} t_{ij}^{ab} \left|\Phi_{\ ij}^{\ ab}\right\rangle, \quad T_3 = \sum_{\substack{i>j>k \\ a>b>c}} t_{ijk}^{abc} \left|\Phi_{\ ijk}^{\ abc}\right\rangle$$



Equation-of-Motion CC for open-shell nuclei

Equation-of-Motion Coupled-Cluster theory

The idea of Equation-of-Motion Coupled-Cluster theory is to calculate ground- and excited states of system B by acting with a excitation operator Ω_k on the ground state of system A

$$|\psi_k^B\rangle = \Omega_k |\psi_0^A\rangle, \;\; |\psi_0^A\rangle = \exp(T)|\phi_0^A\rangle$$

Define the excitation operators $\Omega_k = R_k^{(A\pm1)}$

$$\begin{aligned} R_k^{(A+1)} &= r^a a_a^\dagger + \frac{1}{2} r_j^{ab} a_a^\dagger a_b^\dagger a_j + \ldots, \\ R_k^{(A-1)} &= r_i a_i + \frac{1}{2} r_{ij}^b a_b^\dagger a_i a_j + \ldots, \end{aligned}$$

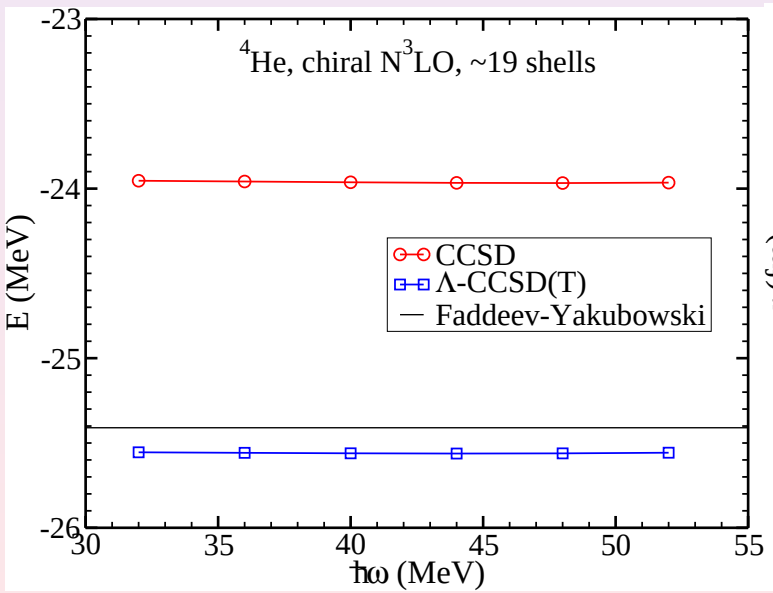
Particle-Attached/Removed EOM-CC equations

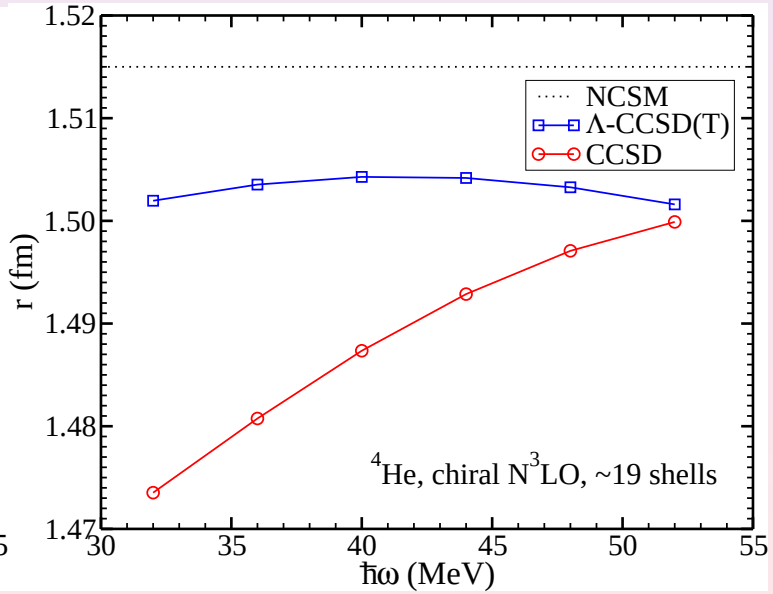
$$\left[\overline{H}, R_k^{(A\pm1)}\right] |\phi_0\rangle = \left(\overline{H} R_k^{(A\pm1)}\right)_C |\phi_0\rangle = \omega_k R_k^{(A\pm1)} |\phi_0\rangle,$$

Precision and accuracy: ^{4}He and chiral N^{3}LO (500 Mev)

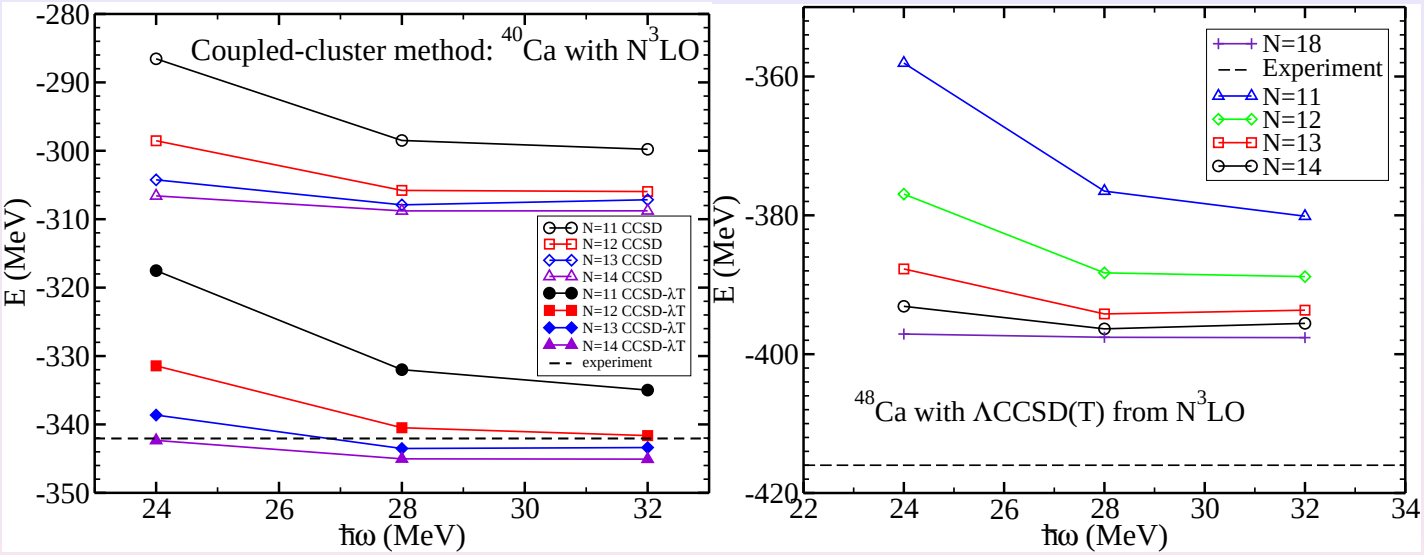
- Results exhibit practically no dependence on the employed model space.
- The Coupled-Cluster method in its Λ-CCSD(T) approximation overbinds by 150 keV, radius too small by about 0.01fm.

G. Hagen, T. Papenbrock, D. J. Dean, M. Hjorth-Jensen, Phys. Rev. C 82, 034330 (2010).





Saturation of N^{3}LO (NN only) in medium mass nuclei



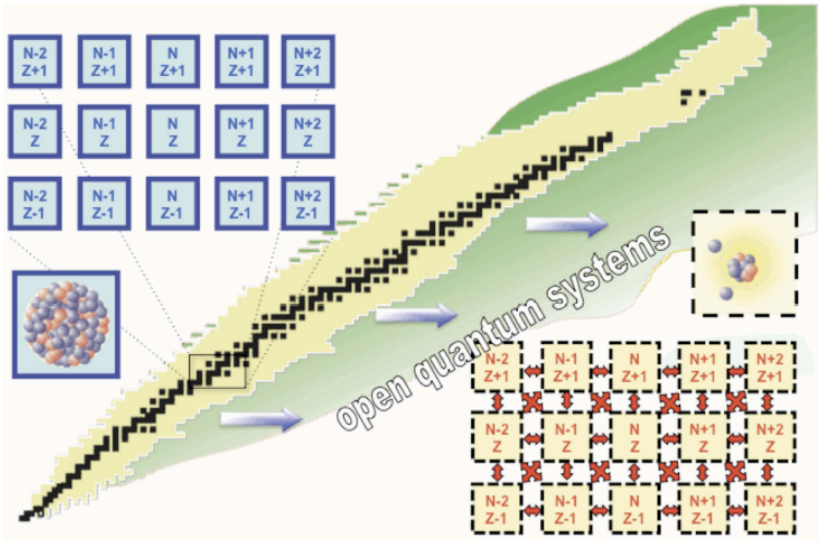
G. Hagen, T. Papenbrock, D. J. Dean, M. Hjorth-Jensen, Phys. Rev. Lett. 101, 092502 (2008).

G. Hagen, T. Papenbrock, D. J. Dean, M. Hjorth-Jensen, Phys. Rev. C 82, 034330 (2010).

- $\sim$ 400keV/A missing for ^{16}O and ^{48}Ca.
- Interesting isospin behavior of 3NF in Calcium isotopes.

	CCSD		ΛCCSD(T)	
Nucleus	E/A	$\Delta E/A$	E/A	$\Delta E/A$
^{16}O	-6.72	1.25	-7.56	0.41
^{40}Ca	-7.72	0.84	-8.63	-0.08
^{48}Ca	-7.40	1.27	-8.26	0.40

Role of continuum in structure of nuclei



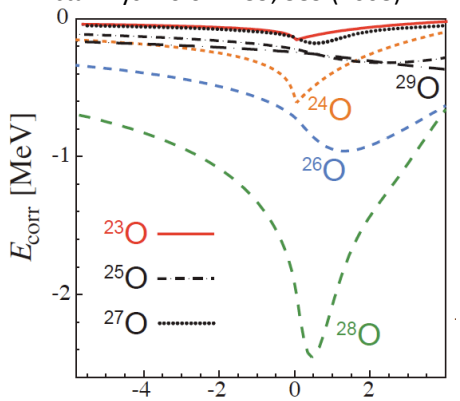
S. Quaglioni and P. Navratil,
Phys. Rev. Lett. 101, 092501 (2008)

		^{10}Be	^{11}Be($\frac{1}{2}^-$)		^{11}Be($\frac{1}{2}^+$)	
	$N_{\max}$	$E_{g.s.}$	E	E_{th}	E	E_{th}
NCSM [13, 14]	8/9	-57.06	-56.95	0.11	-54.26	2.80
NCSM [13, 14],[a]	6/7	-57.17	-57.51	-0.34	-54.39	2.78
NCSM/RGM[a]			-57.59	-0.42	-57.85	-0.68
Expt.		-64.98	-65.16	-0.18	-65.48	-0.50

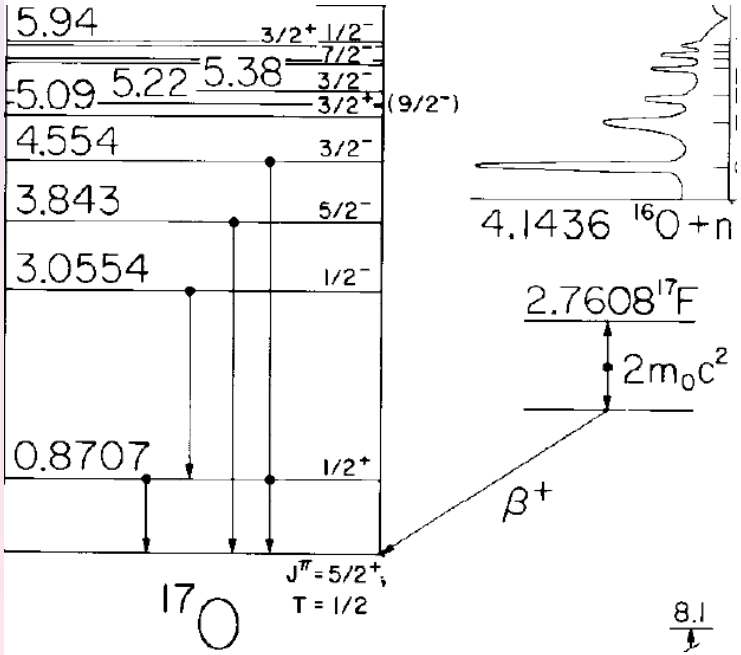
[a]present calculation

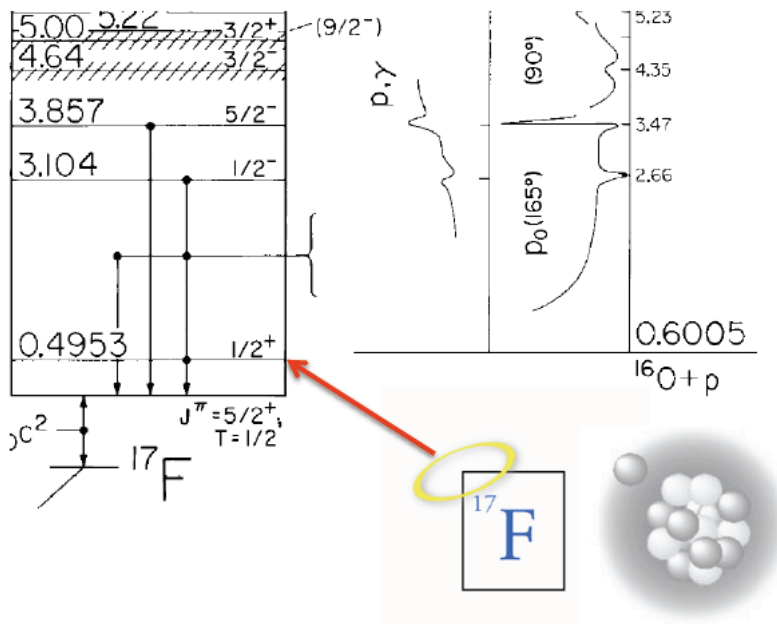
TABLE II: Calculated energies (in MeV) of the ^{10}Be g.s. and of the lowest negative- and positive-parity states in ^{11}Be, obtained using the CD-Bonn NN potential [15] at $\hbar\Omega = 13$ MeV. The NCSM/RGM results were obtained using $n+^{10}$Be configurations with $N_{\max} = 6$ g.s., 2^+_1, 2^+_2, and 1^+_1 states of ^{10}Be.

J. Okolowicz, M. Ploszajczak, Yan-an Luo
Acta Phys. Polon B 39, 389 (2008).

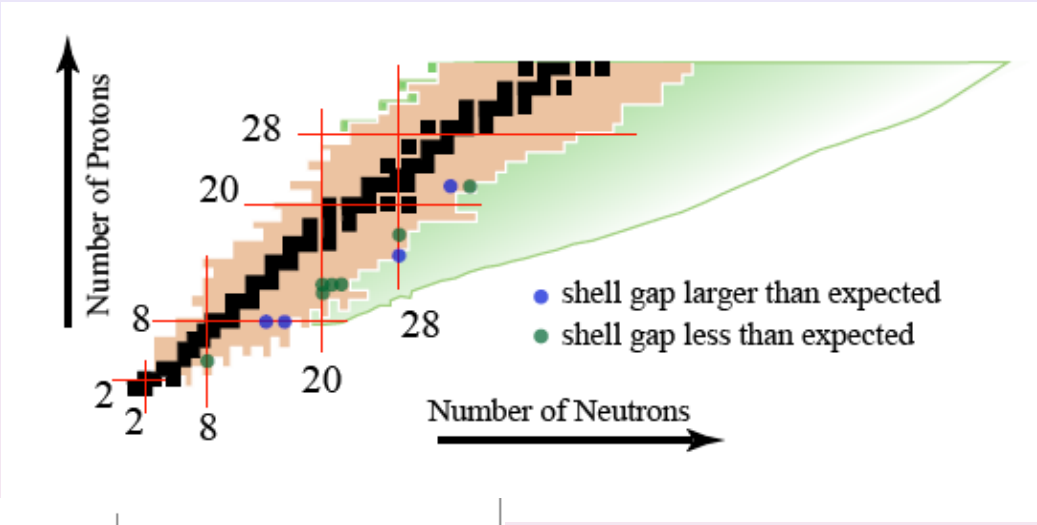


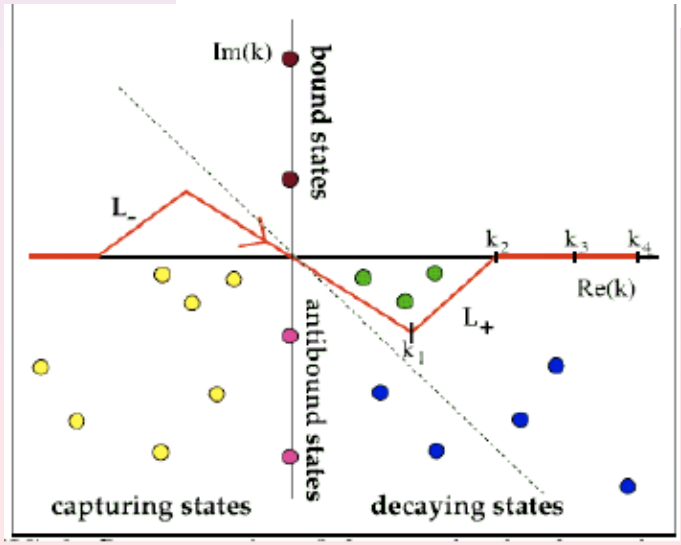
Weakly bound and unbound states in ^{17}F an ambitious testing ground for ab-initio theory

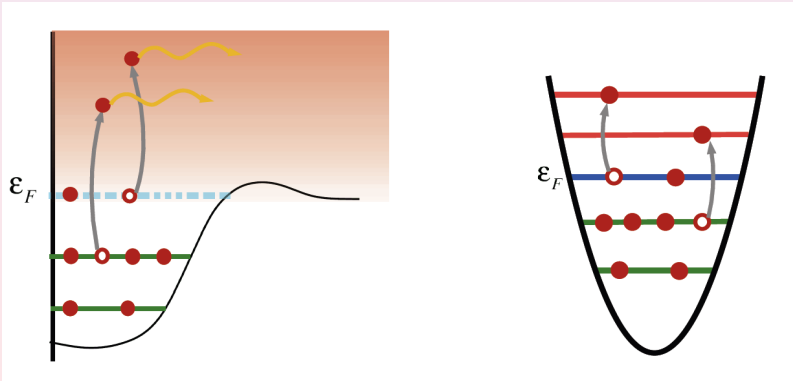




Coupled-Cluster approach to open quantum systems



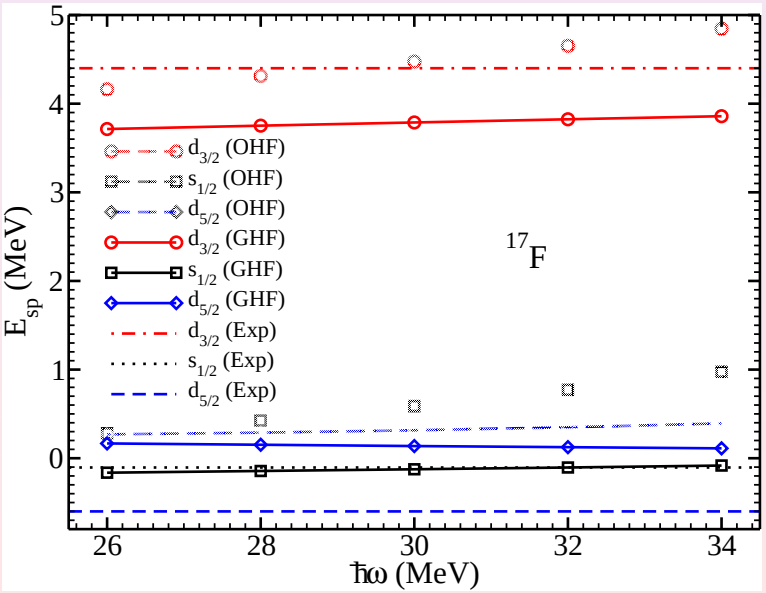




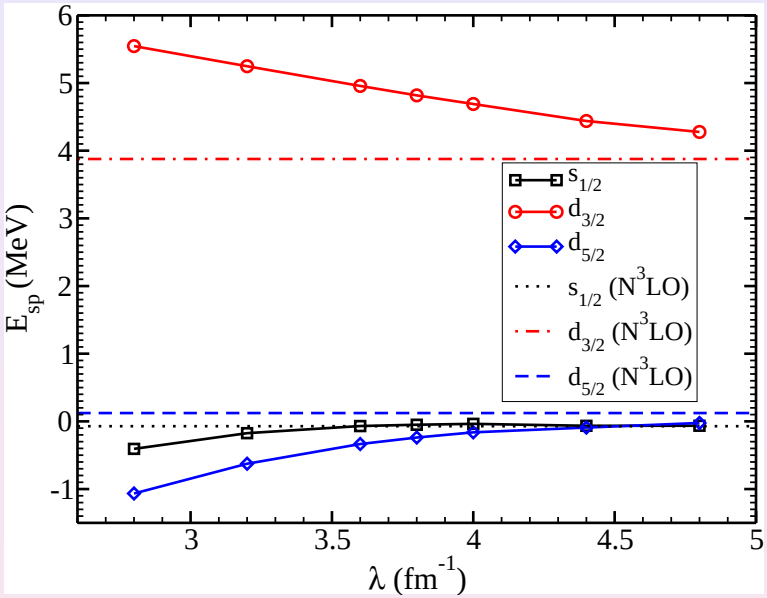
Low-lying states in ^{17}F and the role of continuum

- 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).



Cutoff dependence on Low-lying states in ^{17}F



- Cuttoff dependence on the low-lying states in ^{17}F.
- Spin-orbit splitting increases between the $d_{5/2}$-$d_{3/2}$ orbitals with decreasing cutoff λ.
- $s_{1/2}$ state show very weak dependence on the cutoff.
- The $1/2^+$ state is a *halo* state which extends far beyond the range of the interaction. Renormalizing the interaction by integrating out high momentum modes does not alter the long range physics.

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

Spectroscopic factors with coupled-cluster theory

Overlap functions for one-nucleon removal.

$$O^A_{A-1}(lj;r) \equiv \langle A-1||\tilde{a}_{lj}(r)||A\rangle = (-)^{j-m}\frac{\langle A-1 M_{A-1}|a_{ljm}(r)|AM_A\rangle}{(J_A M_A j-m \mid J_{A-1}M_{A-1})}$$

The spectroscopic factor is defined as the norm the overlap function:

$$S^A_{A-1}(lj) = \sum_n |\langle A-1||\tilde{a}_{nlj}||A\rangle|^2 = \sum_n \frac{|\langle A-1|a_{nljm}|A\rangle|^2}{(J_A M_A j-m \mid J_{A-1}M_{A-1})^2}$$

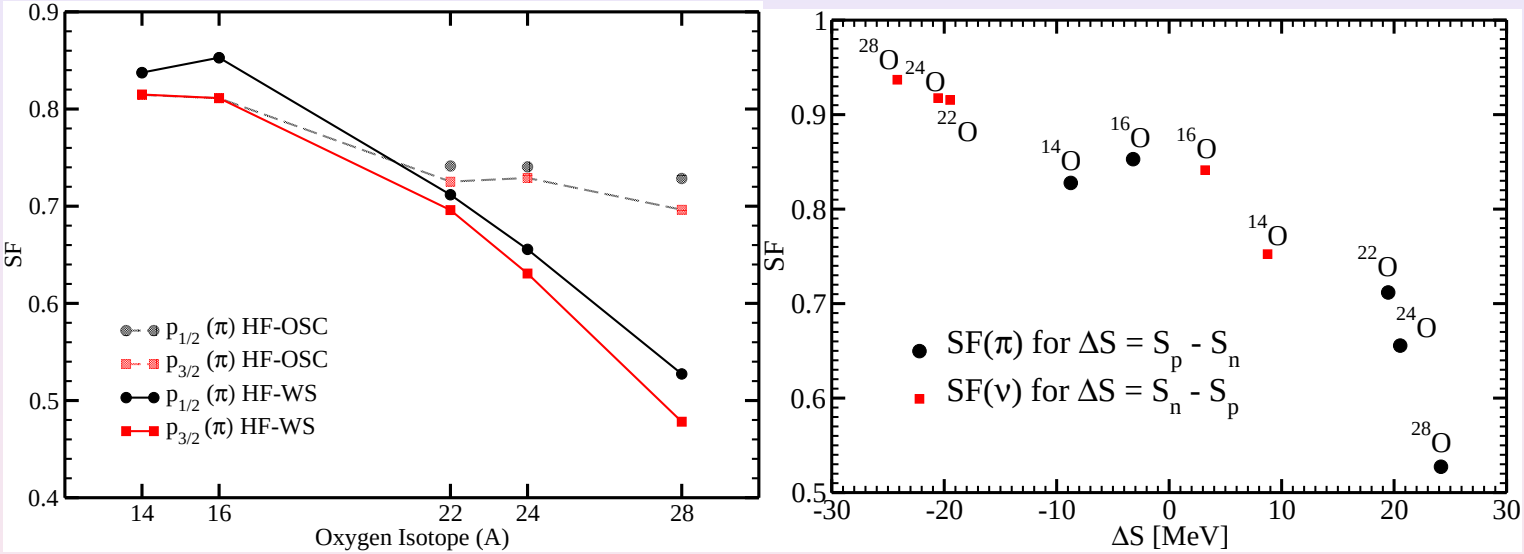
Spectroscopic factors in coupled-cluster formalism

$$S^A_{A-1}(lj) = \sum_n \frac{\langle\phi_0|L^A_0 \overline{a^\dagger_{nljm}} R^{A-1}_\mu|\phi_0\rangle \langle\phi_0|L^{A-1}_\mu \overline{a_{nljm}} R^A_0|\phi_0\rangle}{(J_A M_A j-m \mid J_{A-1}M_{A-1})^2}$$

First application to SFs in ^{16}O:

Ø. Jensen, G. Hagen, T. Papenbrock, D. J. Dean, J. S. Vaagen, Phys. Rev. C 82, 014310 (2010).

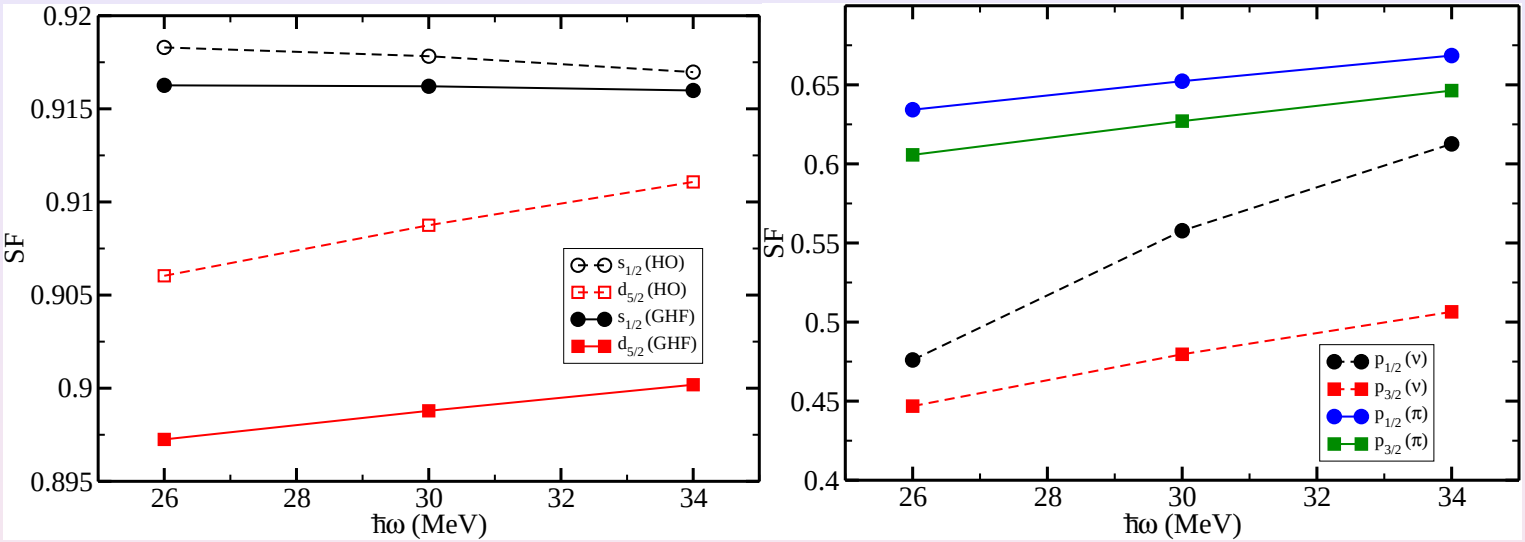
Quenching of SFs in the oxygen isotopes



Spectroscopic factor for proton removal from Oxygen isotopes

- We find a significant quenching of the spectroscopic factors due to coupling to the scattering continuum in the neutron rich oxygen isotopes.
- **Ø. Jensen, GH, Hjorth-Jensen, Brown, Gade submitted to PRL, arXiv:1104.1552 (2011)**

How closed shell is ^{24}O ?



Spectroscopic factor for nucleon removal from ^{24}O

- We find a large spectroscopic factor for $s_{1/2}$ and $d_{5/2}$ neutron removal in ^{24}O. This is consistent with experiment and indicates shell closure in ^{24}O.
- Removal of deeper lying states in ^{24}O show a considerable $\hbar\omega$ dependence pointing to stronger fragmentation and larger role of correlations.
- **Ø. Jensen, G. Hagen and M. Hjorth-Jensen, Phys. Rev. C(R) 83, 021305 (2011)**
  R. Kanungo et al, Phys. Rev. Lett. 102, 152501 (2009).

Overlap functions and nucleon-nucleus elastic scattering

Elastic scattering, or capture of a nucleon on a target nucleus with mass A is given by the overlap function

$$O_A^{A+1}(lj;r) = \left\langle A \left\| \tilde{a}_{lj}(r) \right\| A+1 \right\rangle .$$

The overlap function is given in the coupled-cluster formalism

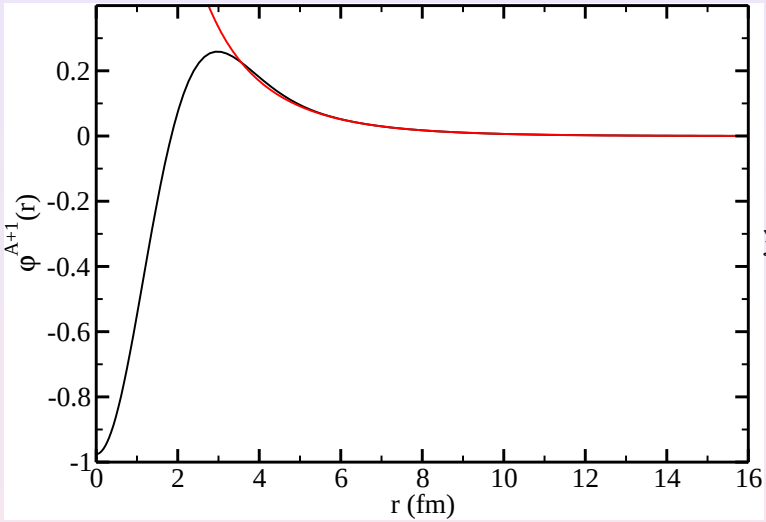
$$O_A^{A+1}(lj;r) = \sum_n \left\langle L_0^A(J_A) || \overline{\tilde{a}_{nlj}} || R_\mu^{A+1}(J_{A+1}) \right\rangle \phi_{nlj}(r)$$

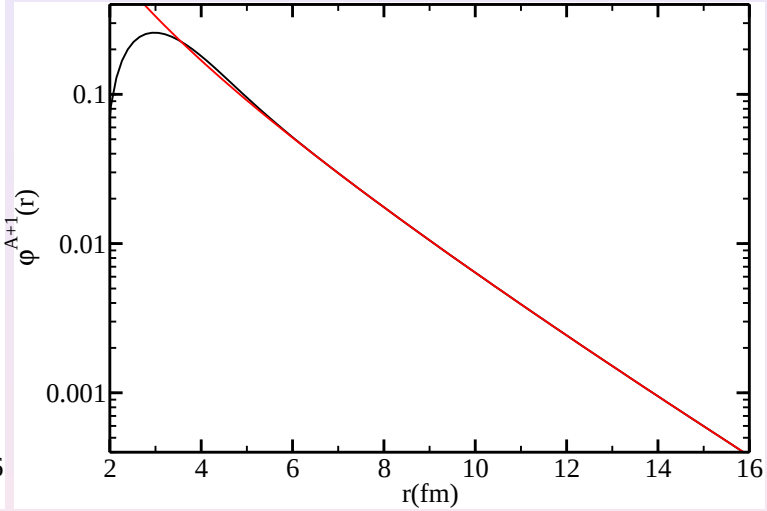
Outside the range of the interaction the overlap function is proportional to a single-particle wave function.

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

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

Asymptotic normalization coeffcients

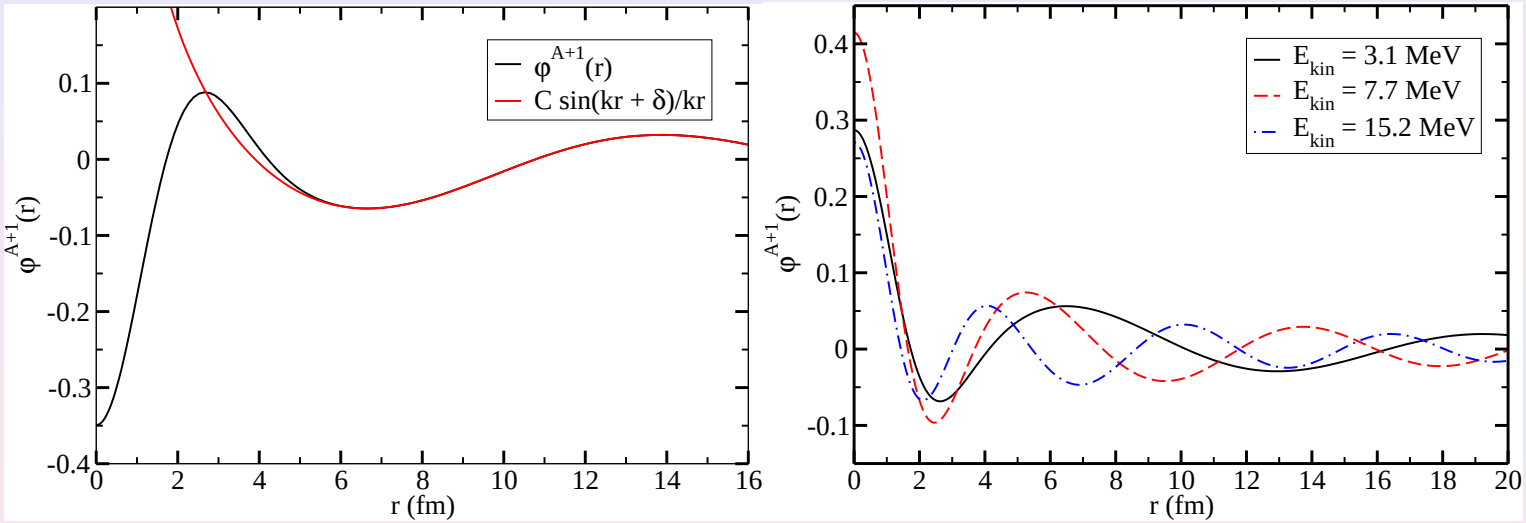




Overlap function for a bound $A+1$ nucleus

- 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.

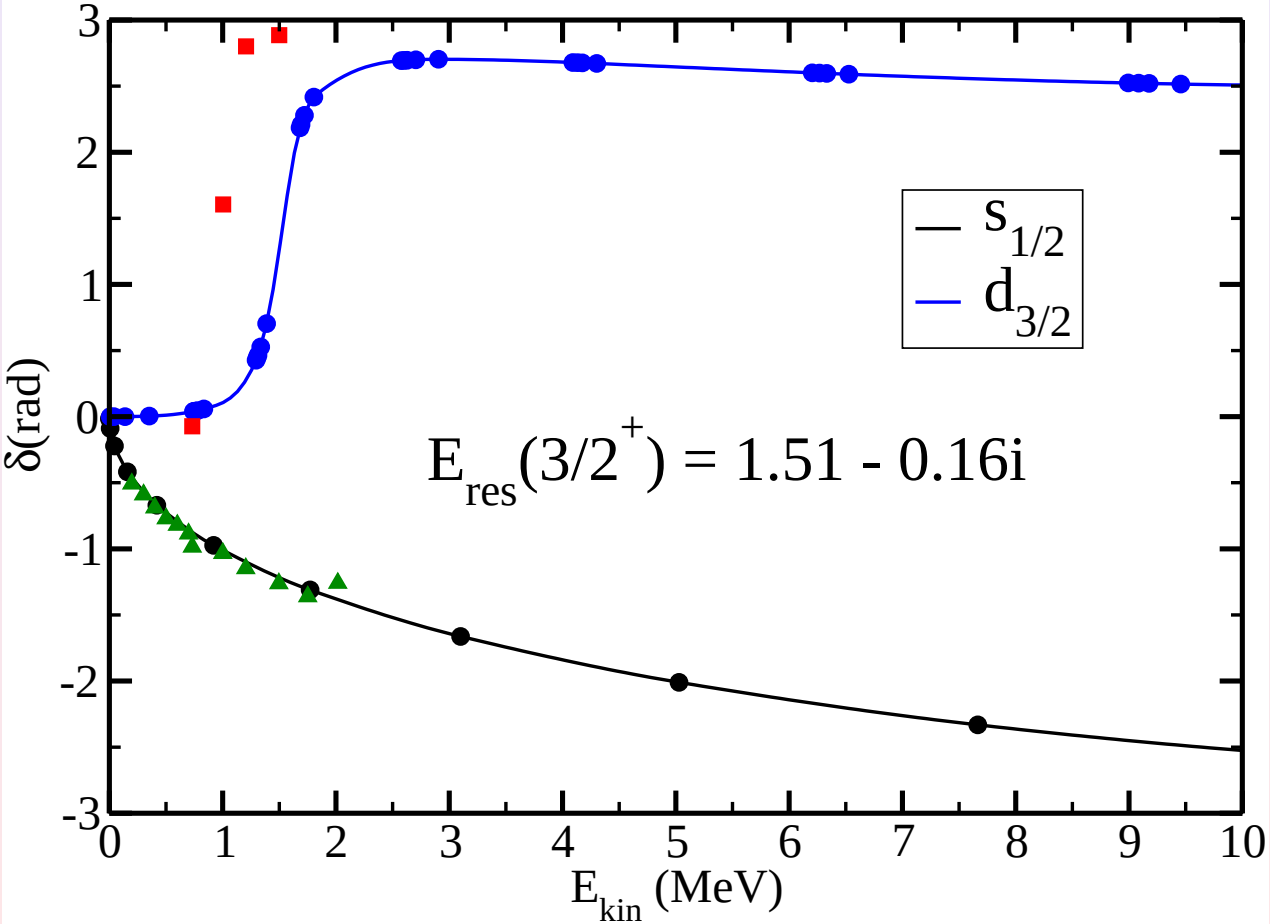
Overlap functions for $A+1$ scattering states



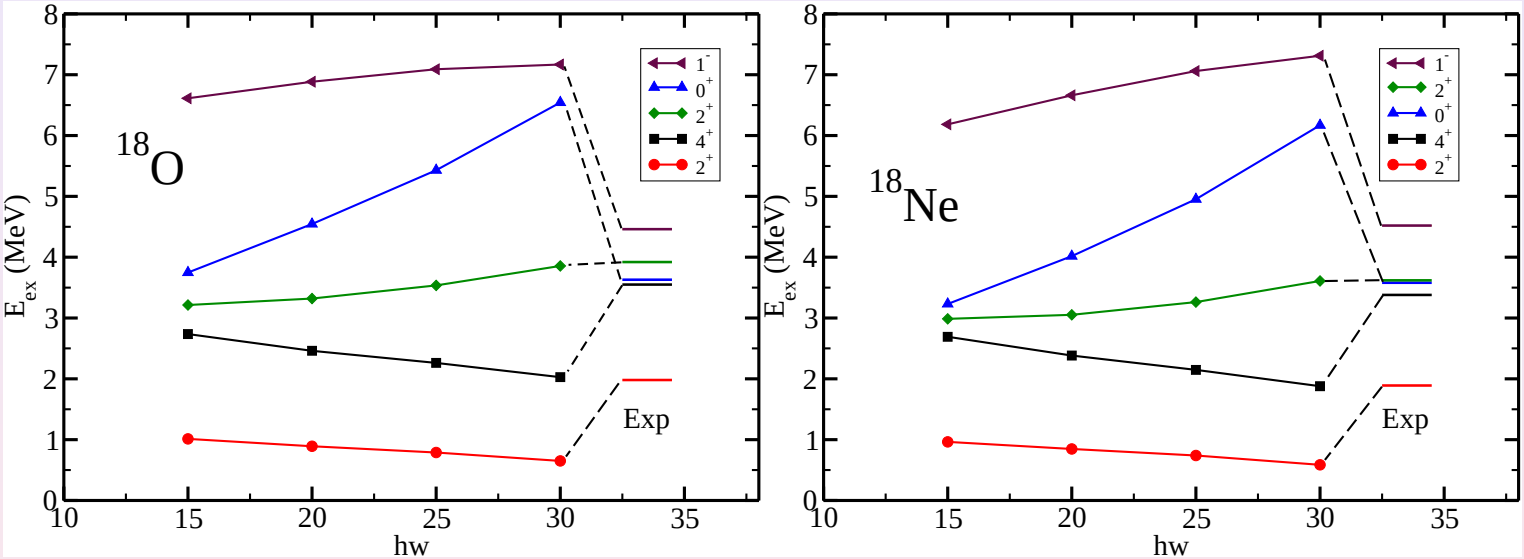
Overlap functions

- One neutron overlap functions for a $J^\pi = 1/2^+$ scattering state with energy 4.075267MeV in ^{17}O with the ground state of ^{16}O. The red line gives the asymptotic form of the radial overlap.

$s_{1/2}$ and $d_{3/2}$ phase shifts for elastic neutron scattering on ^{16}O (Preliminary)



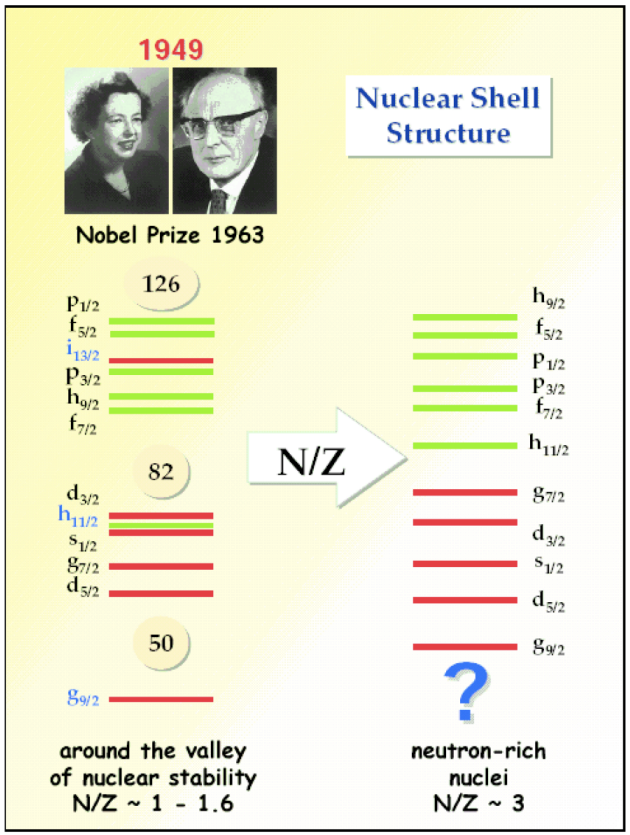
Going beyond closed-shell nuclei. Low-lying states in ^{18}O and ^{18}Ne (Preliminary)



- SRG evolved interaction with $\lambda = 2.0\mathrm{fm}^{-1}$.
- Model space consists of 8 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 and ^{18}Ne.

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

Shell evolution towards the drip line



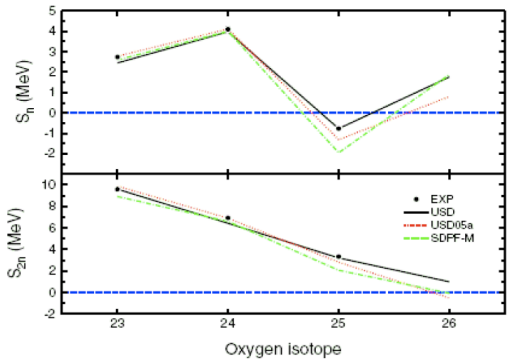


FIG. 4 (color online). The experimental [25,26] (data points) and theoretical [13–15] (lines) one- and two-neutron separation energies for the $N = 15$–18 oxygen isotopes. The experimental error is shown if it is larger than the symbol size.

25O neutron separation energy: -820 keV
the width was measured to be 90(30) keV
giving a lifetime of t ~ 7x10-21 sec

C. Hoffman PRL 100 (2008) 152502

Effective single-particle energies in correlated many-nucleon systems

Effective single-particle energies (ESPEs)

- How can we define single-nucleon shell structure in a system that is strongly correlated; i.e. how are ESPEs related to (correlated) observable?
- ESPEs are the eigen solutions of the *centroid* matrix :

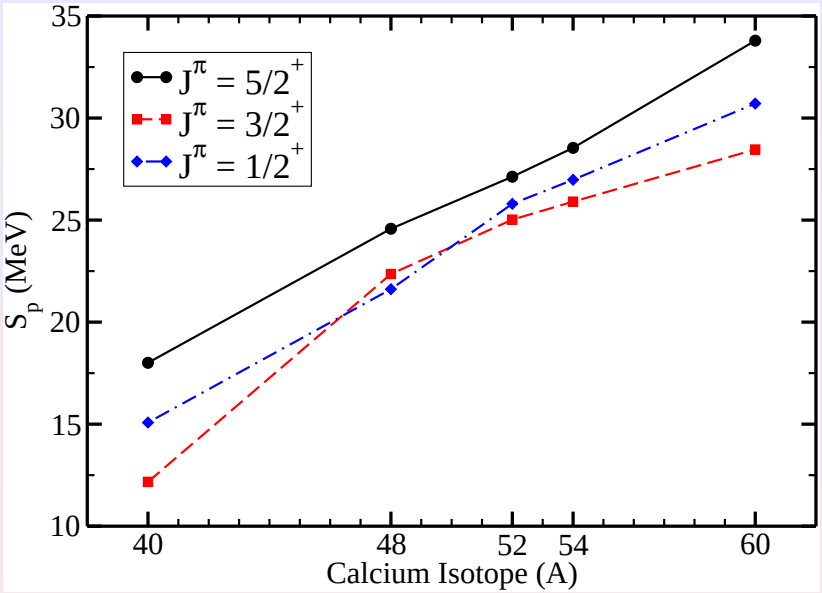
$$h_{pq}^{\text{cent}} \equiv \sum_{\mu \in \mathcal{H}_{A+1}} \bar{S}_{\mu}^{+pq} E_{\mu}^{+} + \sum_{\mu \in \mathcal{H}_{A-1}} S_{\mu}^{-pq} E_{\mu}^{-} \quad .$$

- The *centroid* matrix can be written in terms of the correlated density matrix

$$h_{pq}^{\text{cent}} = T_{pq} + \sum_{rs} \bar{V}_{prqs}^{\text{2N}} \rho_{sr}^{[1]}$$

- **T. Duguet, J. Sadoudi, V. Somà, G. Hagen, and C. Barbieri, In preparation (2011)**

Low-lying states in neutron rich Potassium isotopes



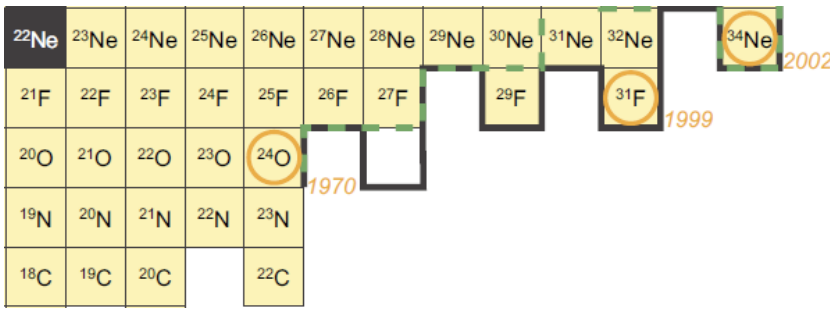
- Proton separation energies $S_p = -E_\mu^- = E_\mu^{A-1} - E_0^A$ in ^{40,48,52,54,60}Ca.
- Low lying states in Potassium isotopes calculated using PA/PR-EOMCCSD with "bare" chiral interactions.
- Model space consists of 15 major harmonic oscillator shells with fixed oscillator frequency $\hbar\omega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

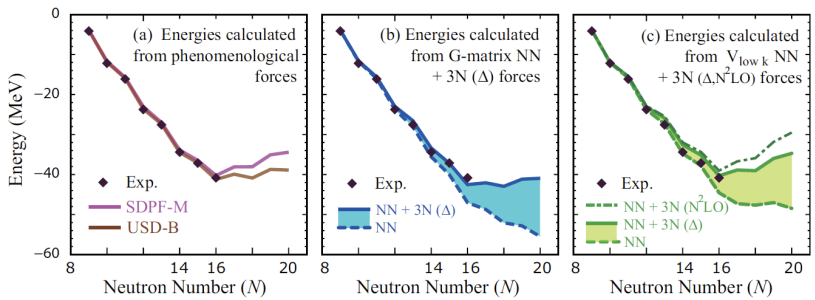
	^{39}K		^{47}K	
J^π	E_{CC} (MeV)	E_{Exp} (MeV)	E_{CC} (MeV)	E_{Exp} (MeV)
$3/2^+$	0.00	0.00	0.00	0.00
$1/2^+$	2.90	2.52	-0.75	-0.36
$5/2^+$	5.84	4.51	2.22	3.00

Shell evolution and the dripline in Oxygen isotopes

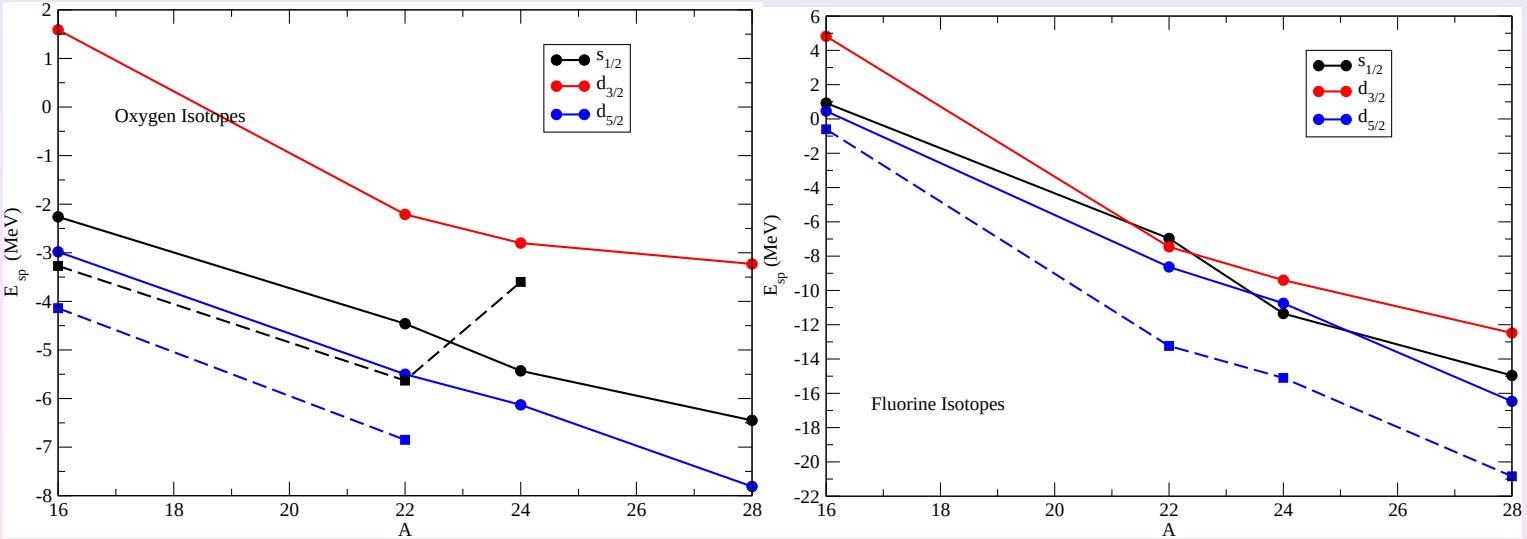
- Evidence of new magic numbers in oxygen isotopes $N = 14$ and $N = 16$.
- All shell model calculation in the $s - d$ shell with realistic NN interactions predicts dripline beyond ^{28}O.
- Results from Otsuka et al. with inclusion of 3NF predicts ^{28}O unstable.
- Adding one more proton binds 6 more neutrons in fluorine isotopes.
- Can Ab-initio theory throw light on this ?

T. Otsuka et al, Phys. Rev. Lett. 105, 032501 (2010)



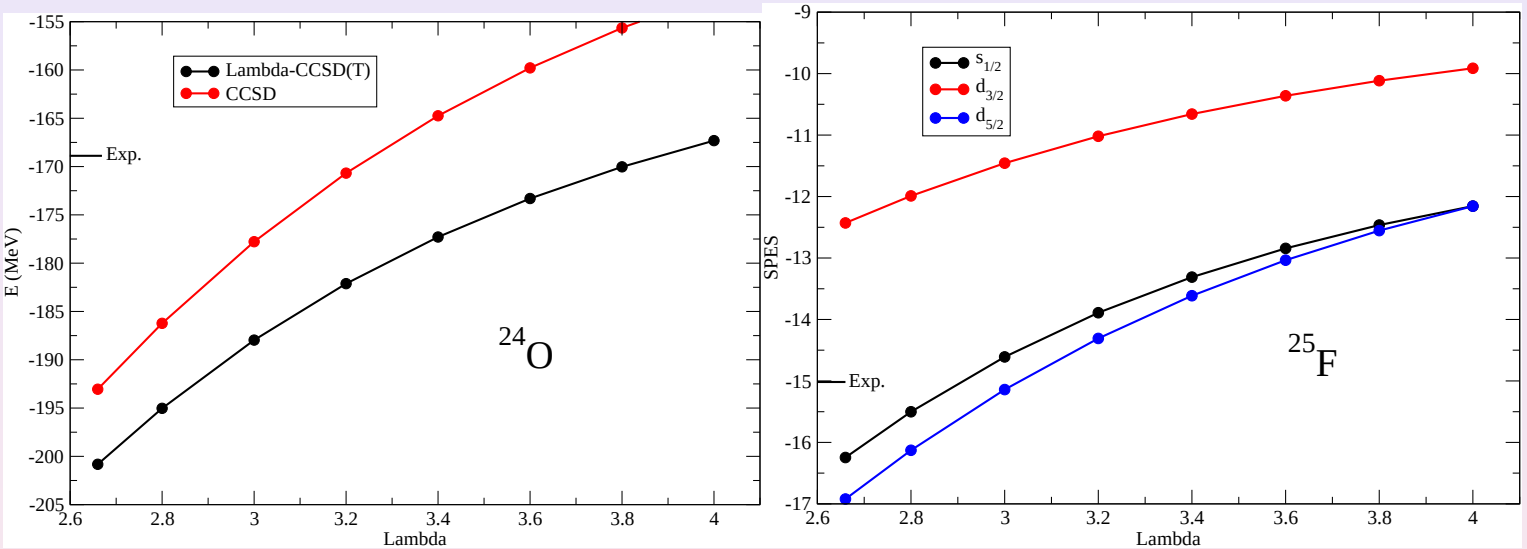


Shell evolution and separation energies in oxygen isotopes



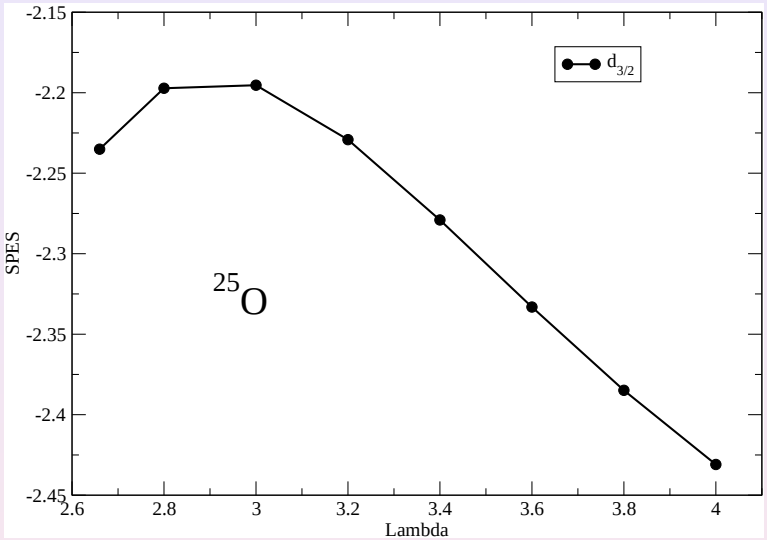
- Low lying states in oxygen and fluorine isotopes calculated using PA/PR-EOMCCSD with "bare" chiral interactions.
- Model space consists of 15 major harmonic oscillator shells with fixed oscillator frequency $\hbar\omega = 32$MeV.
- ^{25}O is stable with respect to neutron emission. Interesting inversion of ground state in ^{25}F.
- What is the role of continuum and three-body forces ?

Cutoff dependence in ^{24}O and ^{25}F



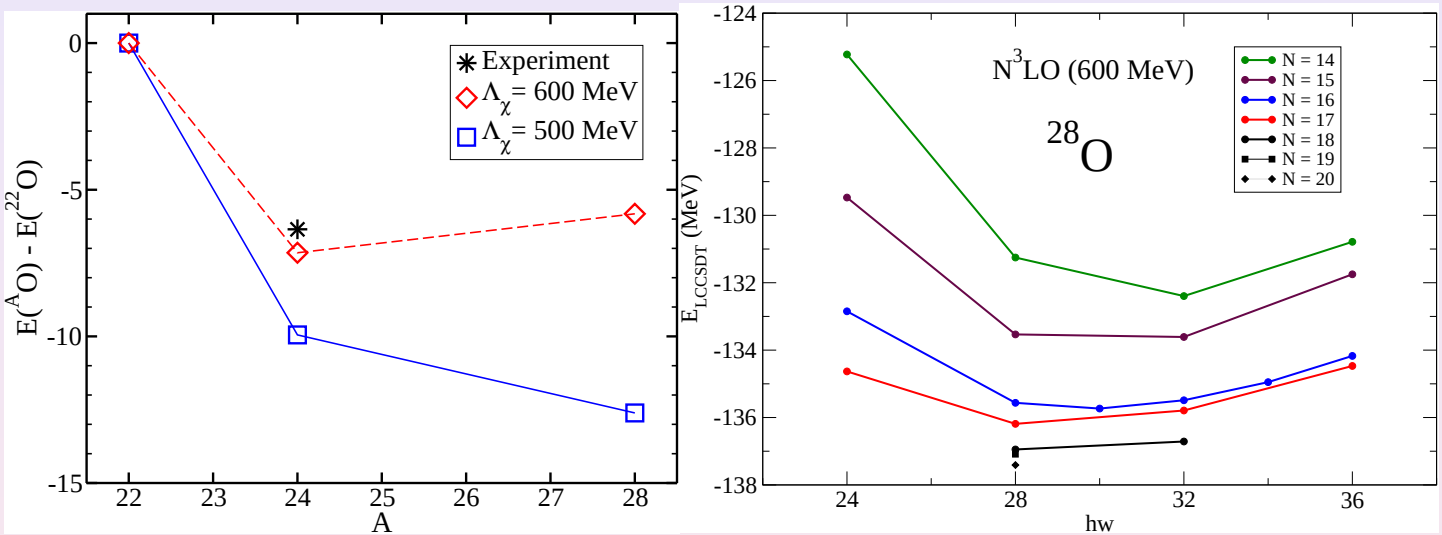
- Variation of the cutoff as a tool to probe the effects of missing many-body forces.
- No unique cutoff that will reproduce data in ^{24}O and ^{25}F simultaneously.
- Three-nucleon forces are needed. Continuum coupling might bring additional binding in the low-lying states in ^{25}F.

Cutoff dependence in ^{25}O



- Cuttoff dependence on the $3/2^+$ state in ^{25}O.
- Calculations done in 15 major oscillator shells with fixed oscillator frequency $\hbar\omega = 32$MeV.
- There are no two-body forces within the family of phase-equivalent low-momentum interactions derived from N^{3}LO that will make ^{25}O unstable.
- Three-nucleon forces are needed to match theory with experiment in ^{25}O!

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



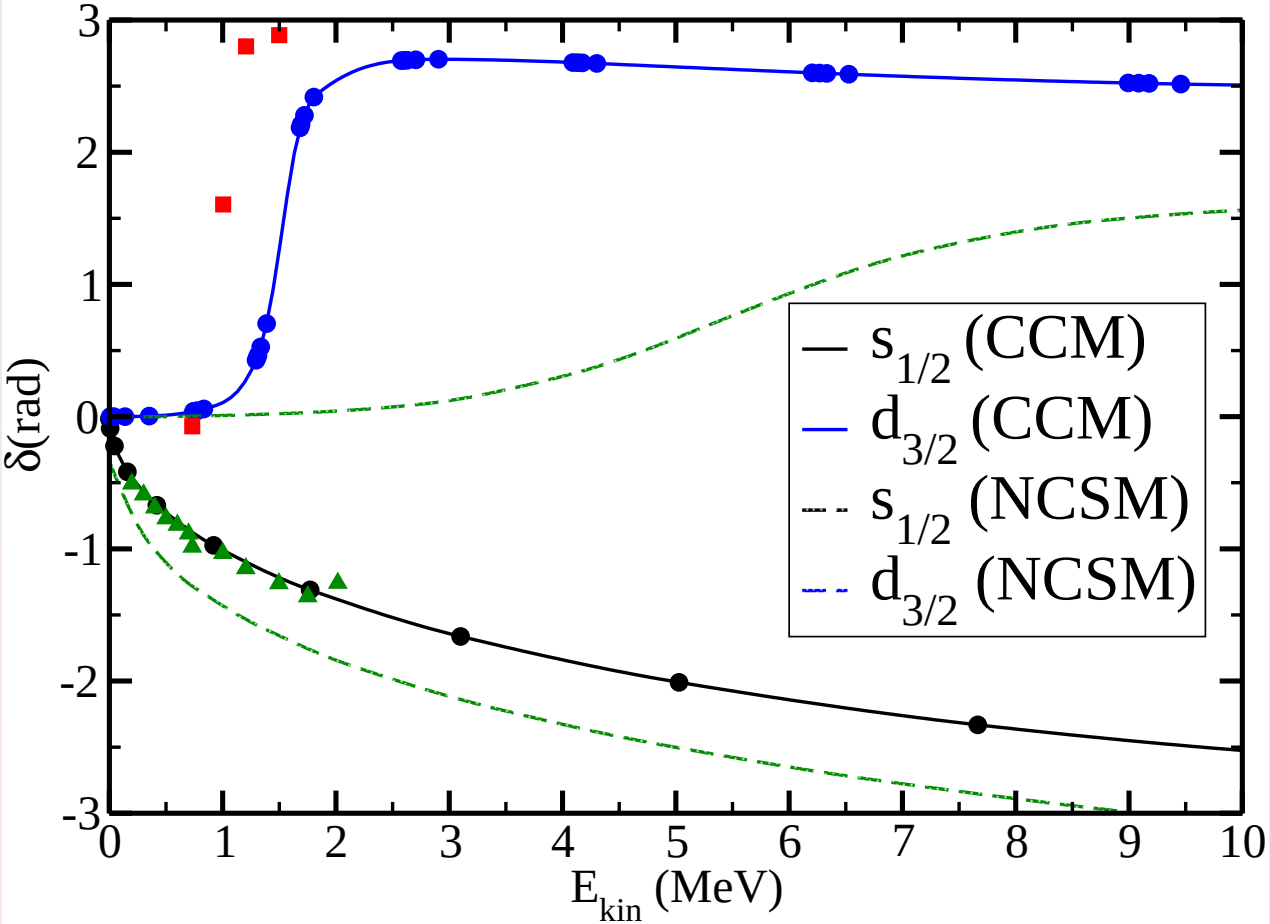
G. Hagen, T. Papenbrock, D. J. Dean, M. Hjorth-Jensen, B. Velamur Asokan, Phys. Rev. C 80, 021306 (2009).

- No sign of dramatic increase in binding energies of oxygen isotopes.
- Ab-initio Coupled-Cluster calculations can not 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.

Conclusion

- Coupled-Cluster approach to medium mass and driplines with "bare" chiral interactions. $\sim$ 400keV/A missing for ^{16}O and ^{48}Ca.
- PA-EOM Coupled-Cluster method has been succesfully applied to the description of weakly bound and unbound states in ^{17}O and ^{17}F.
- Coupling to the continuum plays a significant role on states close to the particle emission threshold.
- Ab-initio coupled-cluster computation of one-nucleon overlap functions allows for a simple and intuitive description of nuclear reactions.
- Presented the first successful calculation of scattering phaseshifts with coupled-cluster theory, the results for ^{17}O are very promising!
- Study of evolution of proton and neutron single-particle energies in Oxygen and Calcium isotopes.
- Energy spacing between excited states in ^{39,47}K and the level inversion in ^{47}K are well reproduced.
- Coupled-cluster calculations of oxygen isotopes cannot rule out a stable ^{28}O.

$s_{1/2}$ and $d_{3/2}$ phase shifts for elastic neutron scattering on ^{16}O (Preliminary)



Overlap functions for $A+1$ scattering states: Accuracy

ϵ_μ^{A+1} (MeV)	$\lvert r^a\rvert^2$	$\lvert r_i^{ab}\rvert^2$	δ_0
0.00025	0.99999	0.00000	-0.01664
0.00716	0.99999	0.00000	-0.08917
0.04465	0.99997	0.00003	-0.22240
0.15869	0.99985	0.00015	-0.41719
0.41917	0.99951	0.00049	-0.67063
0.91951	0.99873	0.00127	-0.97373
1.77221	0.99719	0.00281	-1.31085
3.10046	0.99443	0.00557	-1.66256
5.02790	0.98938	0.01061	-2.00957
7.66533	0.97913	0.02087	-2.33112
11.0793	0.95347	0.04652	-2.58973
15.2047	0.86866	0.13133	-2.69405
19.4601	0.52493	0.47506	-2.32111
22.2231	0.27238	0.72762	-0.76552

$A+1$ scattering states from *ab initio* coupled cluster theory

The lowest lying $J^\pi = 1/2^+$ single-particle energies with corresponding squared sum of the 1p and 2p1h amplitudes and computed phases shifts

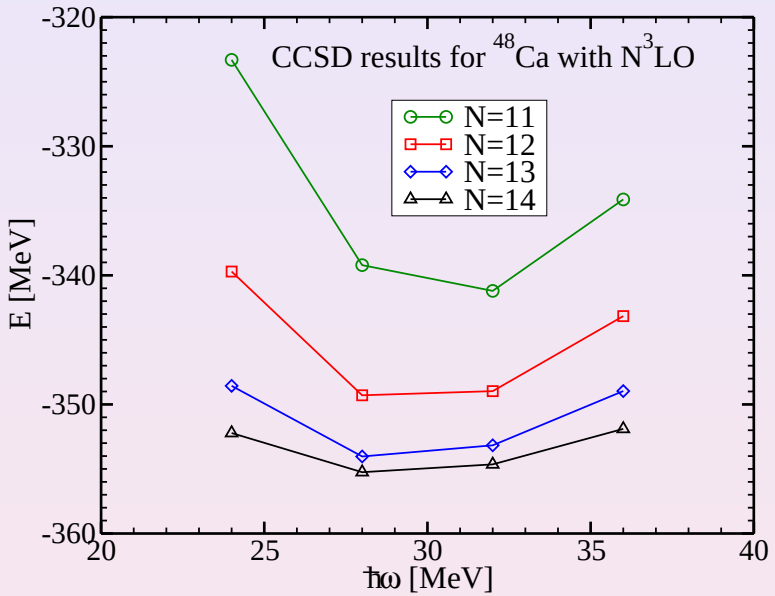
Coupled-Cluster versus DMC for quantum dots.

ω	R	E_0	CCSD	CCSD(T)	Λ-CCSD(T)	DMC
0.28	14	63.2557	62.0634	61.9265	61.9466	
	16	63.3032	62.0646	61.9214	61.9423	
	18	63.3369	62.0656	61.9181	61.9395	
	20	63.3621	62.0664	61.9156	61.9375	61.922(2)
0.5	14	95.4164	93.9921	93.8700	93.8833	
	16	95.4676	93.9904	93.8632	93.8771	
	18	95.5043	93.9895	93.8588	93.8730	
	20	95.5320	93.9891	93.8558	93.8702	93.867(3)
1.0	14	157.6437	155.9740	155.8795	155.8863	
	16	157.7002	155.9669	155.8687	155.8758	
	18	157.7413	155.9627	155.8618	155.8690	
	20	157.7725	155.9601	155.8571	155.8646	155.868(6)

Table: Coupled-Cluster versus DMC for 20 electrons confined in a two-dimensional quantum dot. M. Pedersen Lohne, G. Hagen, M. Hjorth-Jensen, S. Kvaal, F. Pederiva, arXiv:1009.4833.

CCSD results for Chiral N^{3}LO (NN only)

- Mirror nuclei ^{48}Ca and ^{48}Ni differ by 1.38 MeV/A $\rightarrow$ close to mass table predictions.
- 3NF and triples expected to yield $\sim$ 1MeV/A ?
- Radii and and densities stronger model space dependence.
- **G. Hagen et. al, Phys. Rev. Lett. 101, 092502 (2008).**



Nucleus	E/A	V/A	Q	$\Delta E/A$	$< r^2 >_{ch}^{1/2}$	$< r^2 >_{ch}^{1/2}$ (Exp)
^{4}He	-5.99	-22.75	0.90	1.08		1.673(1)
^{16}O	-6.72	-30.69	1.08	1.25	2.72(5)	2.737(8)
^{40}Ca	-7.72	-36.40	1.18	0.84	3.25(9)	3.4764
^{48}Ca	-7.40	-37.97	1.21	1.27	3.24(9)	3.4738
^{48}Ni	-6.02	-36.04	1.20	1.21	3.52(15)	?

Coupled-Cluster method and the Center of Mass

Center of mass issues

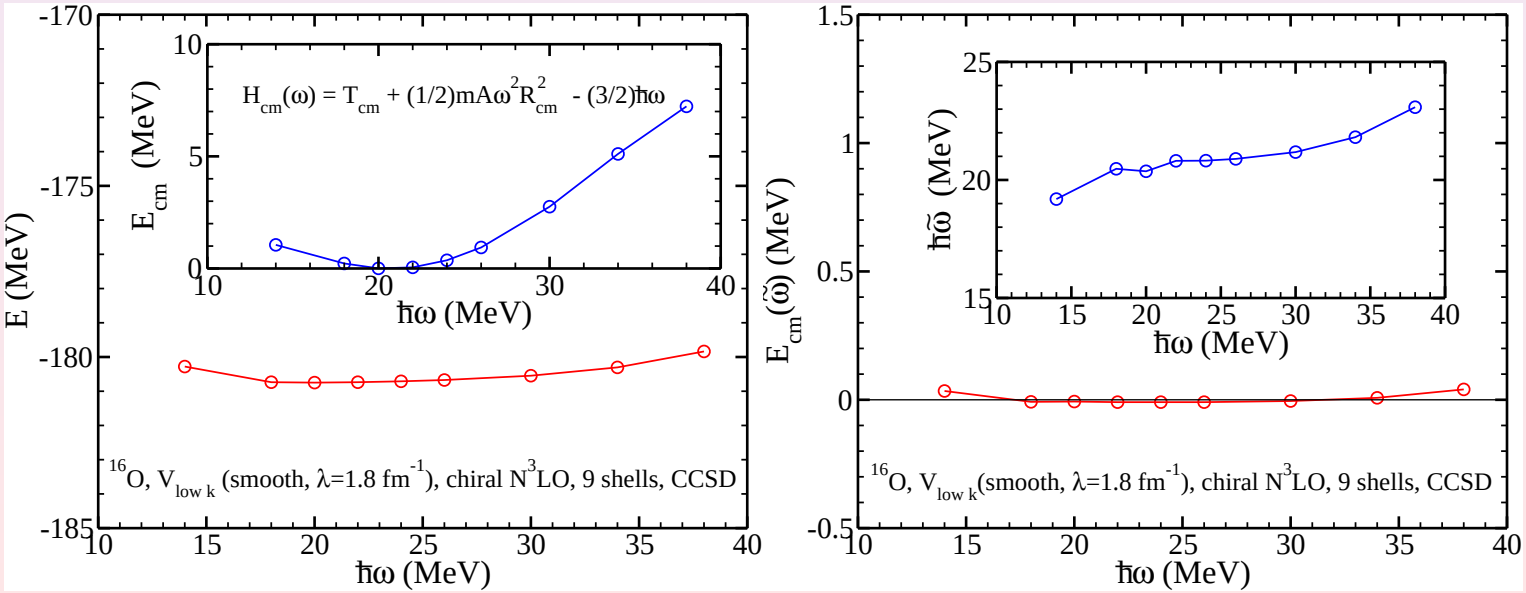
1. Is factorization of CoM wave function and intrinsic wave function possible in finite spaces other than the $N\hbar\Omega$ space of the No-Core shell-model approach ?
2. Is the expectation value of $H_{cm}(\omega) = T_{cm} + \frac{1}{2}mA\omega^2 R_{cm}^2 - \frac{3}{2}\hbar\omega$ a meassure of the quality of the calculated intrinsic energy ?

^{16}O with $V_{\mathrm{low-k}}$ (1.8/fm, smooth) within CCSD

- Center of mass energy $E_{cm}(\omega) = \langle H_{cm} \rangle$ does vanish at $\hbar\omega \sim 20$MeV, and we have $\psi_{int}\psi_{cm}$.
- Take expectation value of the generalized CoM Hamiltonian $H_{cm}(\tilde{\omega}) = T_{cm} + \frac{1}{2}mA\tilde{\omega}^2 R_{cm}^2 - \frac{3}{2}\hbar\tilde{\omega}$.
- CC wave function factorizes and the CoM wave function is a Gaussian with almost constant width $\hbar\tilde{\omega} \sim 20MeV$

G. Hagen,T. Papenbrock, D. J. Dean, Phys. Rev. Lett. 103, 062503 (2009).

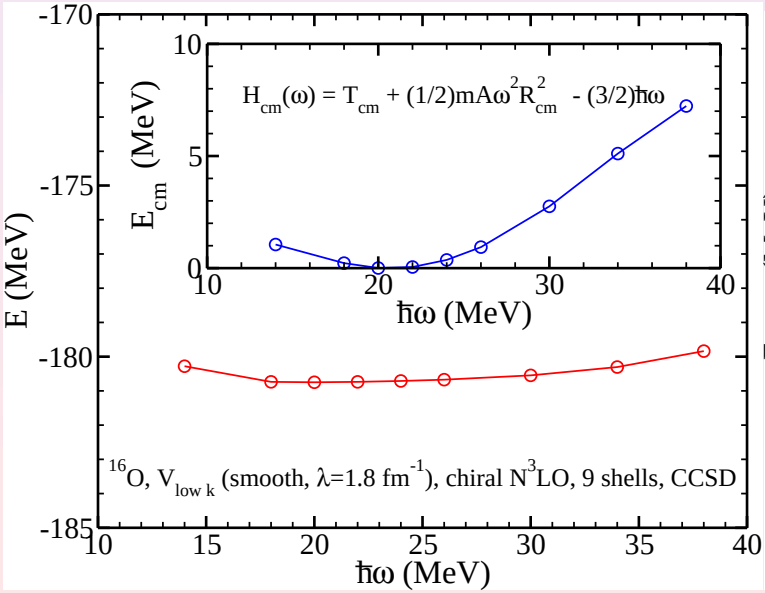
G. Hagen, T. Papenbrock, D. J. Dean, M. Hjorth-Jensen, Phys. Rev. C 82, 034330 (2010).

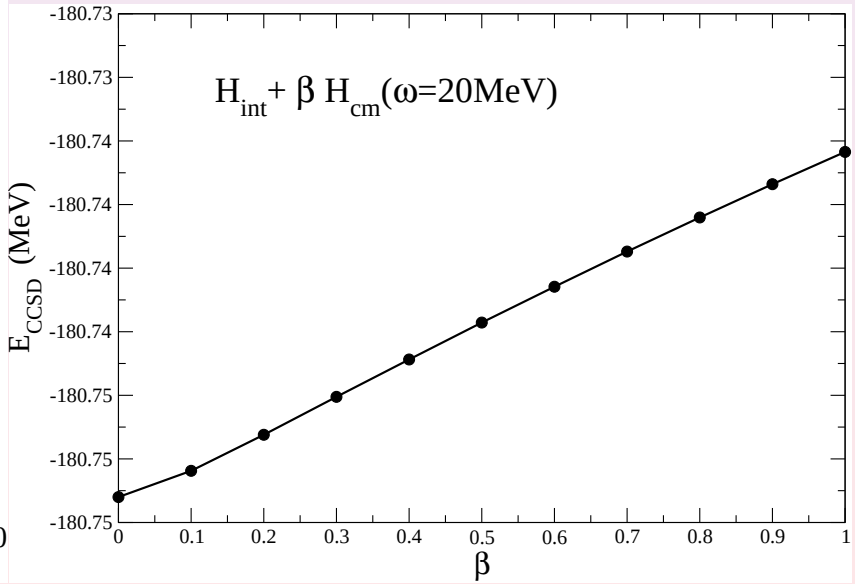


^{16}O with $V_{\mathrm{low-k}}$ (1.8/fm, smooth) within CCSD

- Center of mass energy $E_{cm}(\omega) = \langle H_{cm} \rangle$ does vanish at $\hbar\omega \sim 20$MeV.
- At this model-space the CC wave function factorizes: $\psi_{int}\psi_{cm}$.
- Approximate constancy of energy suggests that it factorizes approximately for many frequencies.
- What is ψ_{cm} ?

G. Hagen,T. Papenbrock, D. J. Dean, Phys. Rev. Lett. 103, 062503 (2009).



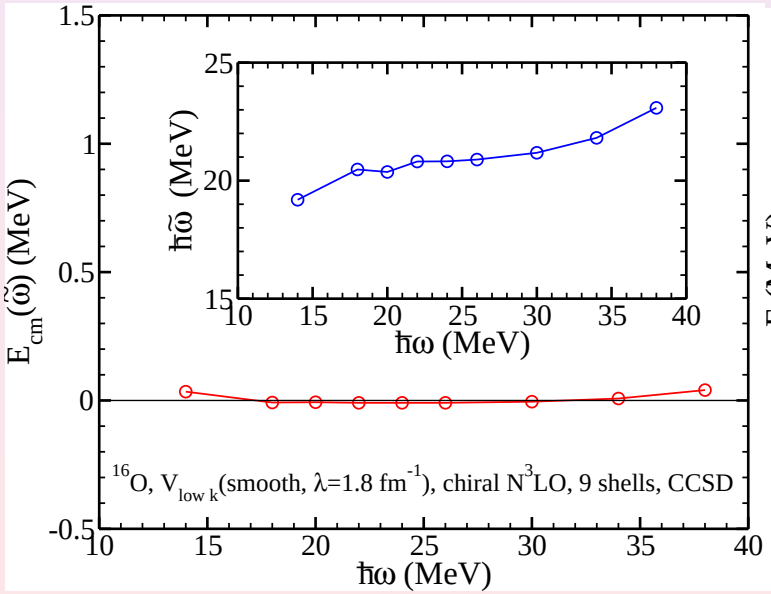


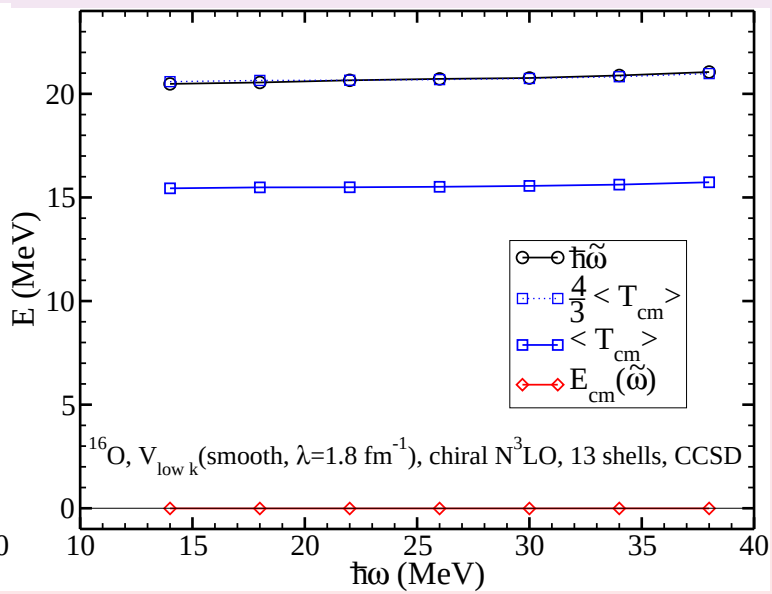
If CC wave function factorizes what is ψ_{cm} ?

- Assumption: CoM wave function is always a gaussian (approximately).
- Take expectation value of the generalized CoM Hamiltonian $H_{cm}(\tilde{\omega}) = T_{cm} + \frac{1}{2} m A \tilde{\omega}^2 R_{cm}^2 - \frac{3}{2}\hbar\tilde{\omega}$.
- Use $E_{cm}(\tilde{\omega}) = 0$ and $\langle T_{cm} \rangle = \frac{3}{4}\hbar\tilde{\omega}$.
- Determine unknown frequency from taking the expectation value of the identity
  $H_{cm}(\omega) + \frac{3}{2}\hbar\omega - T_{cm} = \frac{\omega^2}{\tilde{\omega}^2}\left(H_{cm}(\tilde{\omega}) + \frac{3}{2}\hbar\tilde{\omega} - T_{cm}\right)$
- Gives quadratic equation for unknown frequency:
  $\hbar\tilde{\omega} = \hbar\omega + \frac{2}{3}E_{cm}(\omega) \pm \sqrt{\frac{4}{9}(E_{cm})^2 + \frac{4}{3}\hbar\omega E_{cm}(\omega)}$

Coupled-Cluster wave function factorizes: $\psi_{int}\psi_{cm}$

- CC wave function factorizes and the CoM wave function is a Gaussian with almost constant width $\hbar\tilde{\omega} \sim 20MeV$ for all different $\hbar\omega$ values of the basis !
- Expectation value of T_{cm} is 3/4 of oscillator spacing $\hbar\tilde{\omega}$.
- Why is the CoM wave function a Gaussian ?
- Why does the CoM wave function come at a constant $\hbar\omega$ independent of basis ?

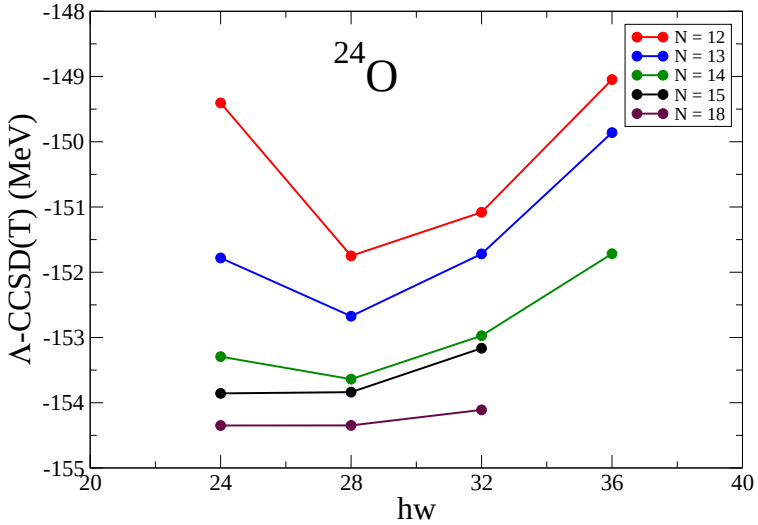


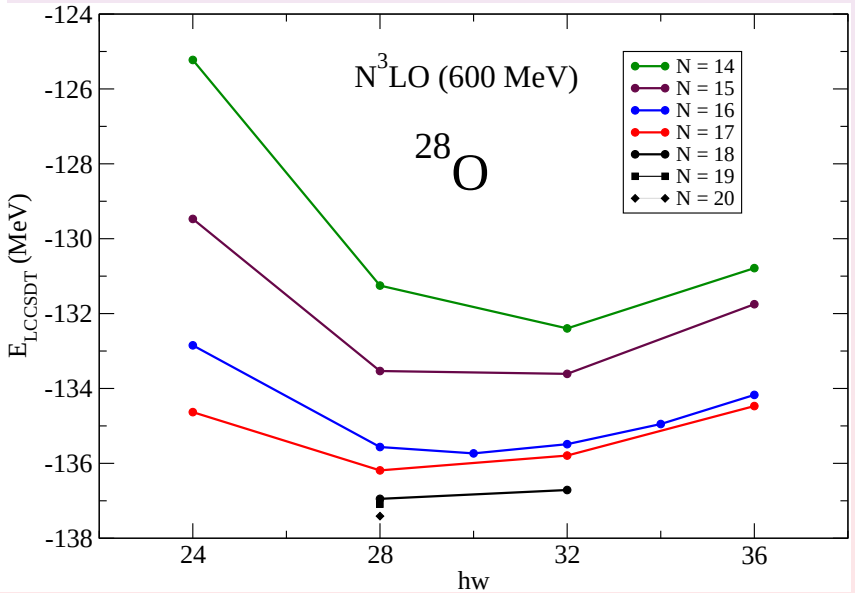


Convergence of ^{24}O and ^{28}O with chiral interactions

- Λ-CCSD(T) ground state calculations of ^{24}O and ^{28}O using chiral interactions with cutoffs 500 and 600 MeV respectively.
- Convergence is slower for the 600 MeV cutoff interaction, and need N $\sim$ 20 major shells to reach convergence for ^{28}O.

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





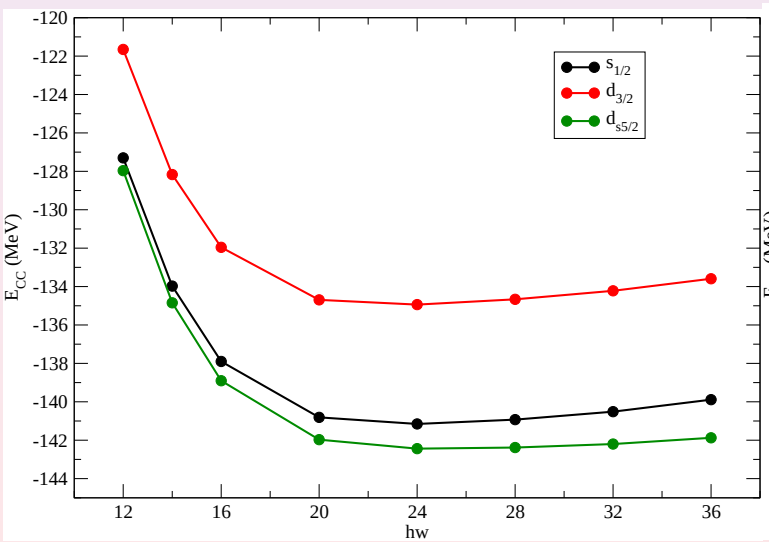
Cutoff dependence and summary of results for Oxygen isotopes

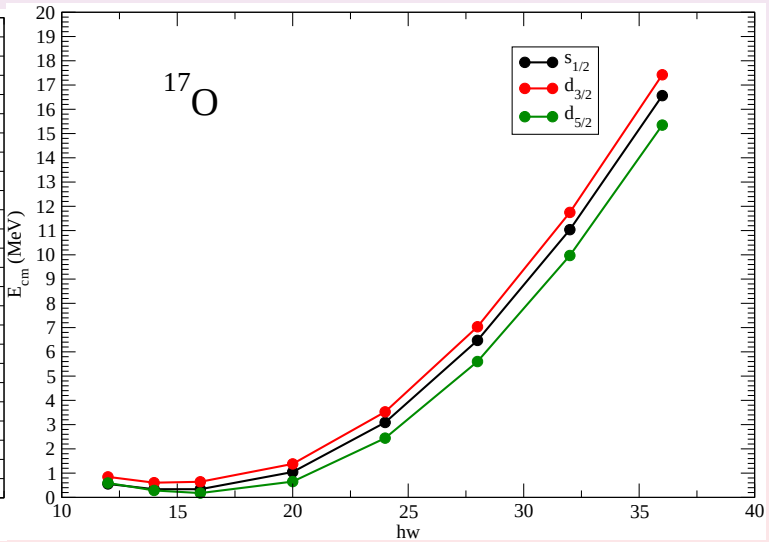
Energies	^{16}O	^{22}O	^{24}O	^{28}O
($\Lambda_\chi = 500$ MeV)				
E_0	25.946	46.52	50.74	63.85
ΔE_{CCSD}	-133.53	-171.31	-185.17	-200.63
ΔE_3	-13.31	-19.61	-19.91	-20.23
E	-120.89	-144.40	-154.34	-157.01
($\Lambda_\chi = 600$ MeV)				
E_0	22.08	46.33	52.94	68.57
ΔE_{CCSD}	-119.04	-156.51	-168.49	-182.42
ΔE_3	-14.95	-20.71	-22.49	-22.86
E	-111.91	-130.89	-138.04	-136.71
Experiment	-127.62	-162.03	-168.38	

	^{16}O	^{22}O	^{24}O	^{28}O
$\langle r^2 \rangle^{1/2}$	2.296	2.405	2.658	2.825
Expt.	2.54(2)	2.88(6)	3.19(13)	

Low-lying states in ^{17}O with V_{srg} (2.8/fm) and the center of mass

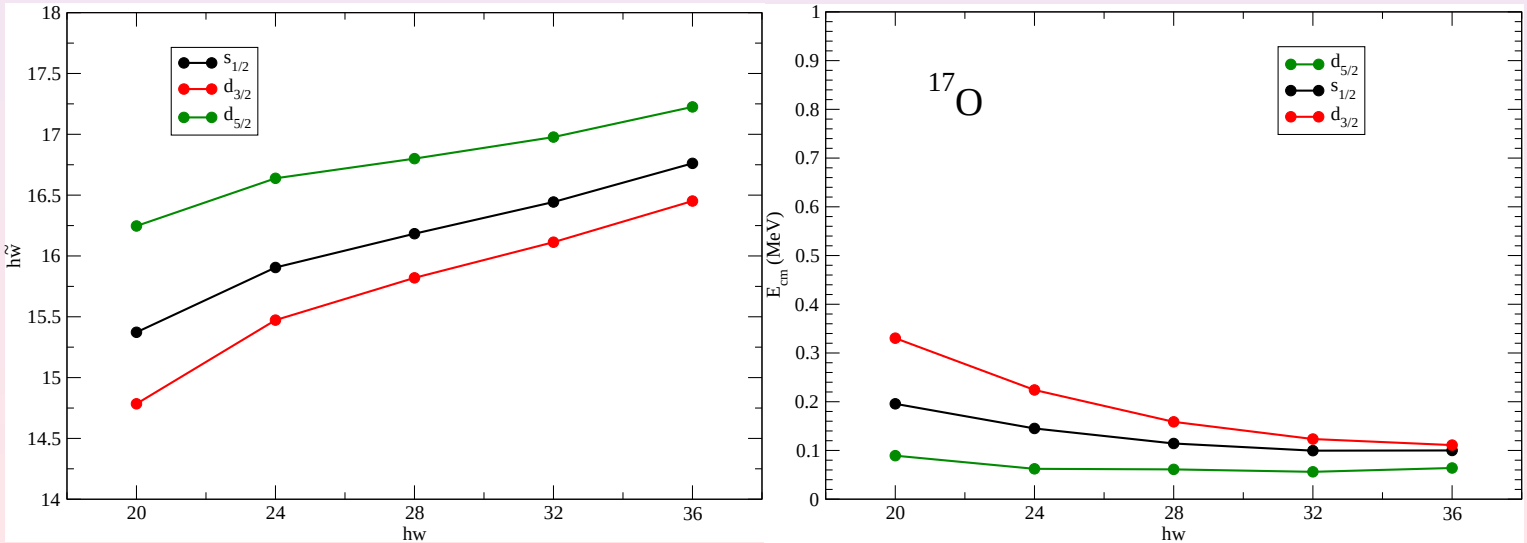
- Low-lying $1/2^+, 3/2^+ and 5/2^+$ states in ^{17}O calculated using PA-EOM-CCSD in 13 major oscillator shells.
- The expectation value of $H_{cm}(\omega) = T_{cm} + \frac{1}{2} mA\omega^2 R_{cm}^2 - \frac{3}{2}\hbar\omega$ meassures to what degree the CoM is a Gaussian with oscillator frequency ω.



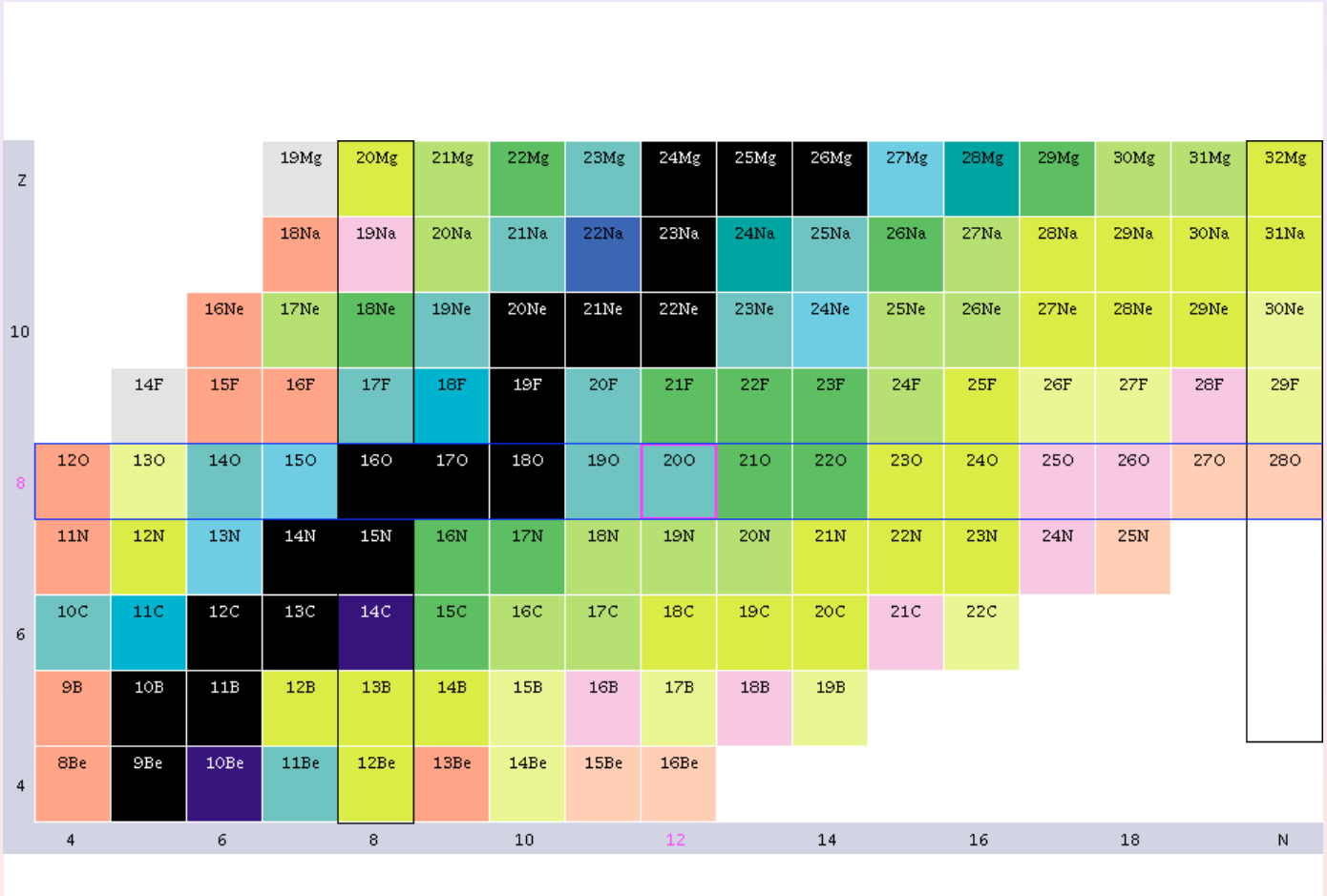


Coupled-Cluster wave function factorizes: $\psi_{int}\psi_{cm}$

- Assumption: CoM wave function is always a gaussian (approximately).
- Take expectation value of the generalized CoM Hamiltonian $H_{cm}(\tilde{\omega}) = T_{cm} + \frac{1}{2}mA\tilde{\omega}^2 R_{cm}^2 - \frac{3}{2}\hbar\tilde{\omega}$.
- CC wave function factorizes and the CoM wave function is a Gaussian with almost constant width $\hbar\tilde{\omega} \sim 16MeV$ for all different $\hbar\omega$ values of the basis.

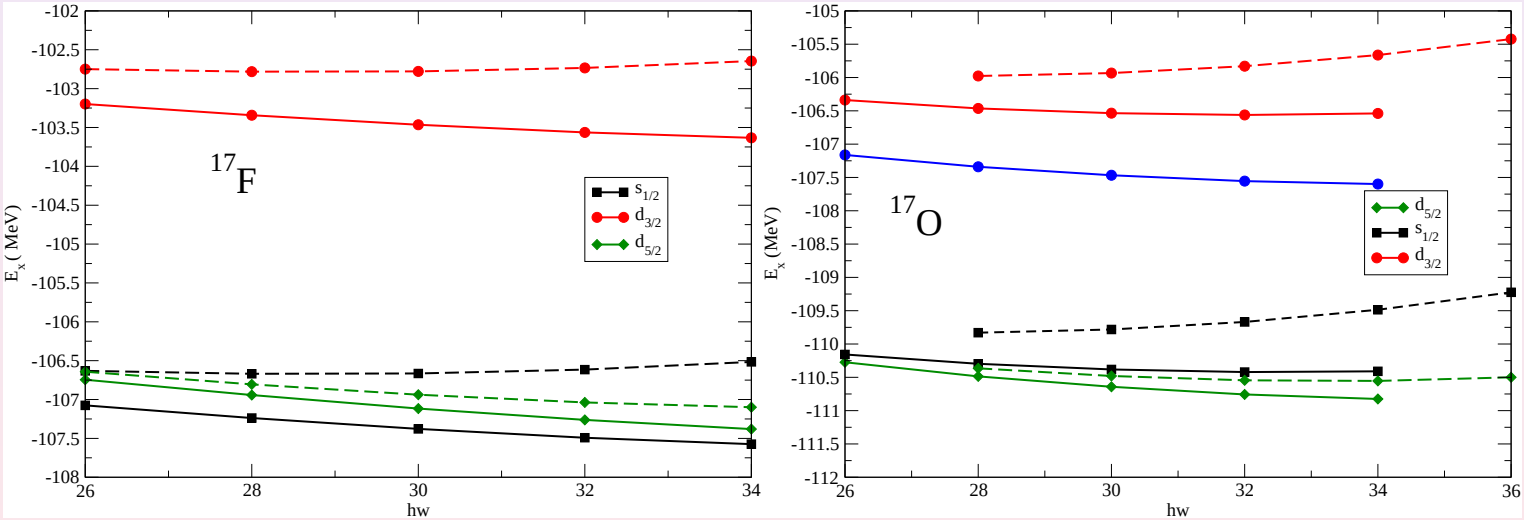


Most nuclei are open-shell. How to access these nuclei with coupled-cluster method?



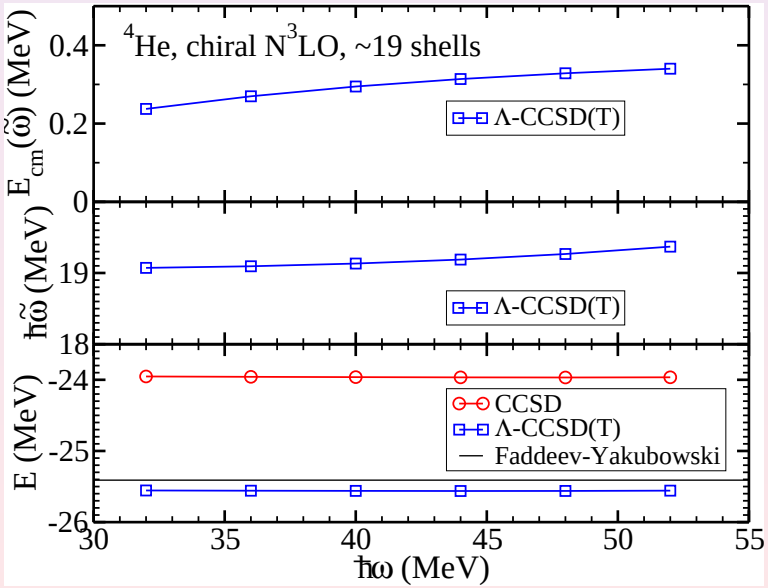
Low-lying states in ^{17}O and ^{17}F

- Low-lying states in ^{17}F and ^{17}O using a Gamow-Hartree-Fock basis and a Oscillator-Hartree-Fock basis.



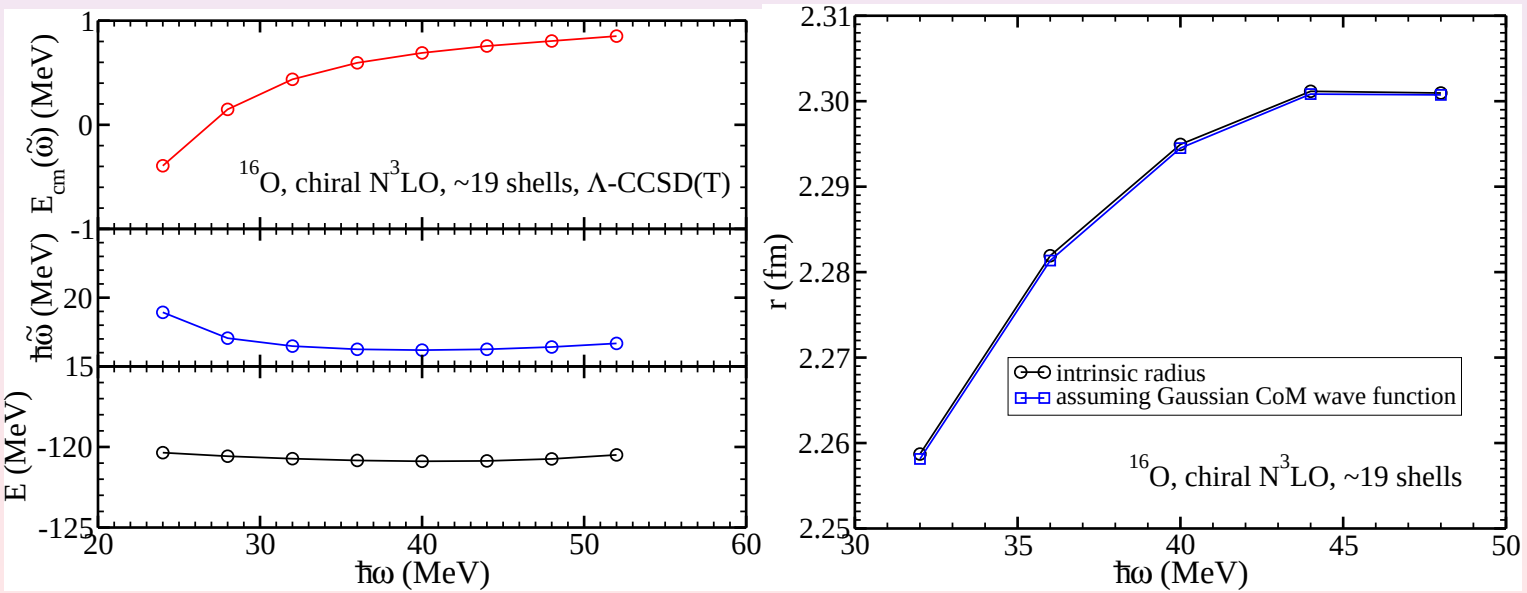
Approximate factorization also for "hard" interactions

- Ground state of ^{4}He using HF basis and N = 18 for the bare N^{3}LO (500 MeV) chiral interaction.
- CC wave function factorizes (approximately) and the CoM wave function is a Gaussian with almost constant width $\sim$ 19.1 MeV, for all different $\hbar\omega$ values of the basis.

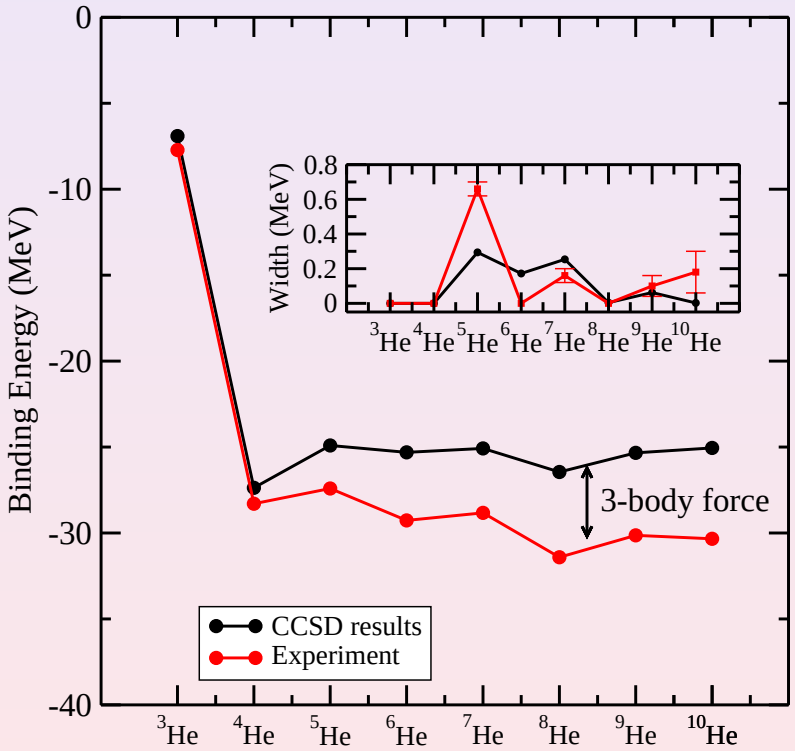


Approximate factorization also for "hard" interactions

- Ground state of ^{16}O, using HF basis and N = 18 for the bare N^{3}LO (500 MeV) chiral interaction, factorizes approximately within Λ−CCSD(T).
- RMS radii, $\langle \frac{1}{A}\sum_{i=1}^{A} r_i^2 - R_{cm}^2 \rangle^{1/2}$, using intrinsic radius operator and subtracting $\langle R_{cm}^2 \rangle \sim \frac{62.2071}{A\hbar\omega}$, assuming a Gaussian for the center of mass agrees.
- Small negative values for $E_{cm}(\tilde{\omega})$ coming from cluster truncation and non-varitional character of CCM.



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