Ab initio nuclear structure calculations

Thomas Papenbrock

and OAK RIDGE NATIONAL LABORATORY

TECHNISCHE UNIVERSITÄT DARMSTADT

Coworkers: G. Hagen, D. J. Dean, M. Hjorth-Jensen, B. Velamur Asokan

Happy Birthday, Jochen!

EMMI workshop “Strongly coupled systems” GSI, November 15-17 2010

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Overview

1. Introduction
2. Medium-mass nuclei – saturation properties of NN interactions

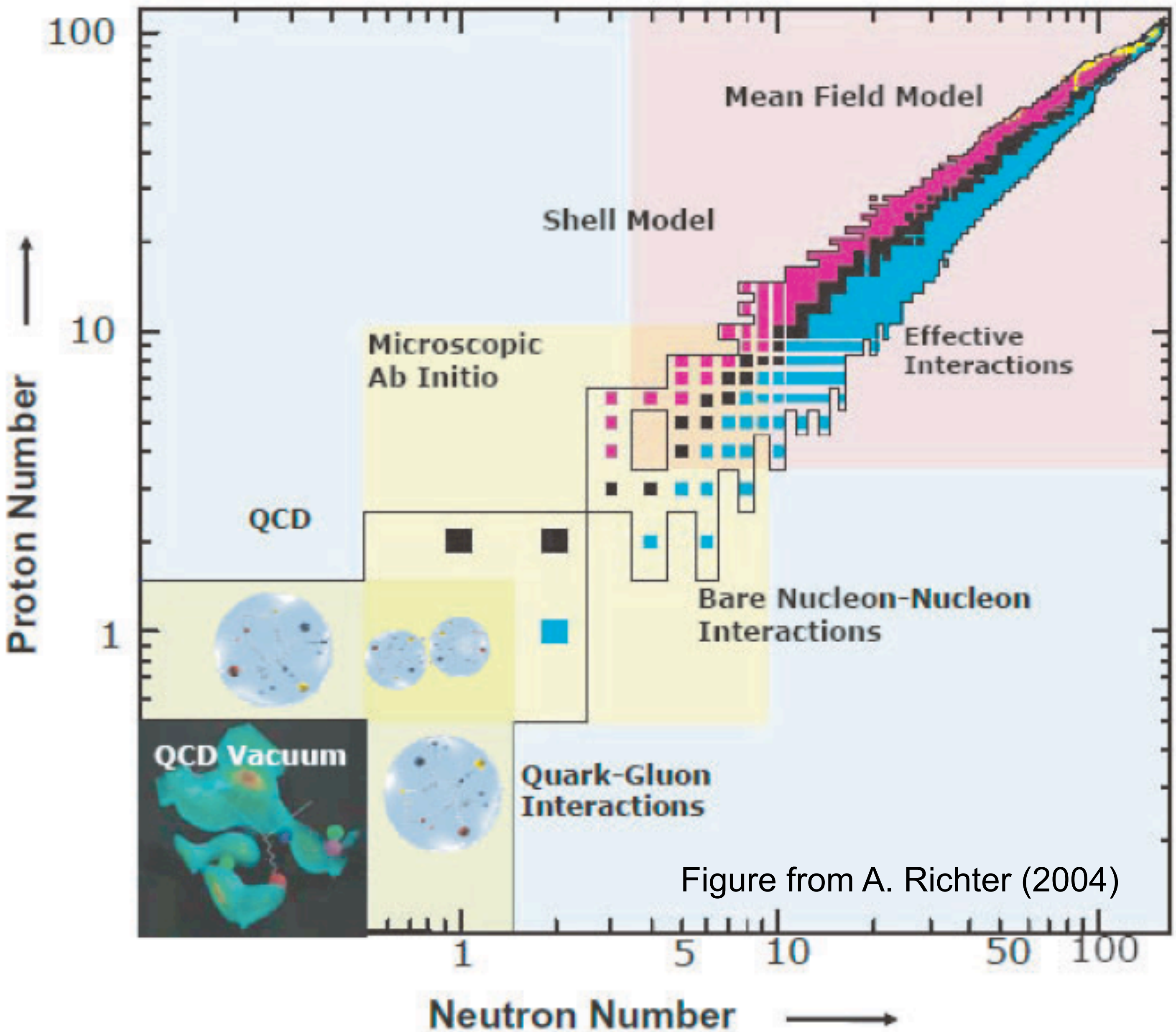
   [Hagen, TP, Dean, Hjorth-Jensen, Phys. Rev. Lett. 101, 092502 (2008)]
3. Proton-halo state in ^{17}F

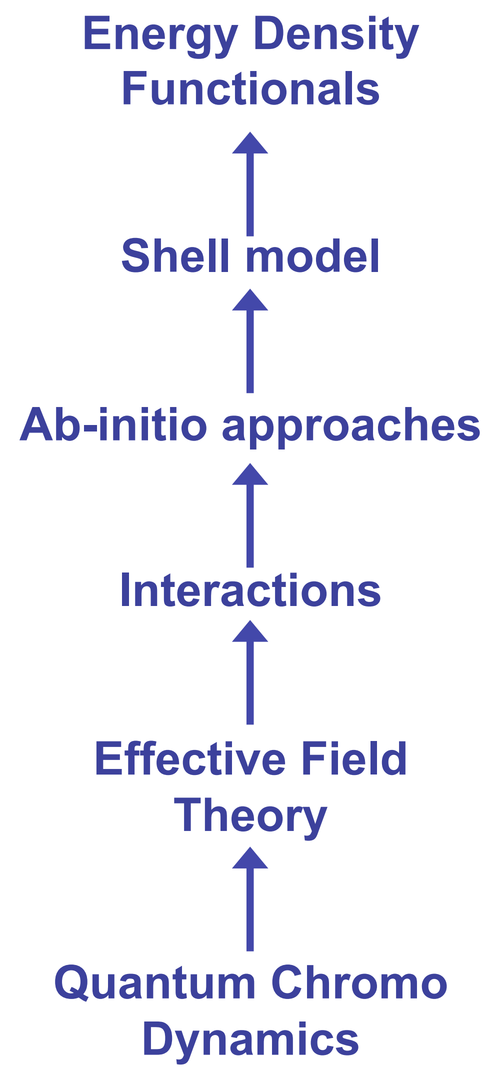
   [G. Hagen, TP, M. Hjorth-Jensen, Phys. Rev. Lett. 104, 182501 (2010]
4. Does ^{28}O exist?

   [Hagen, TP, Dean, Horth-Jensen, Velamur Asokan, Phys. Rev. C 80, 021306(R) (2009)]
5. Practical solution to the center-of-mass problem

   [Hagen, TP, Dean, Phys. Rev. Lett. 103, 062503 (2009)]

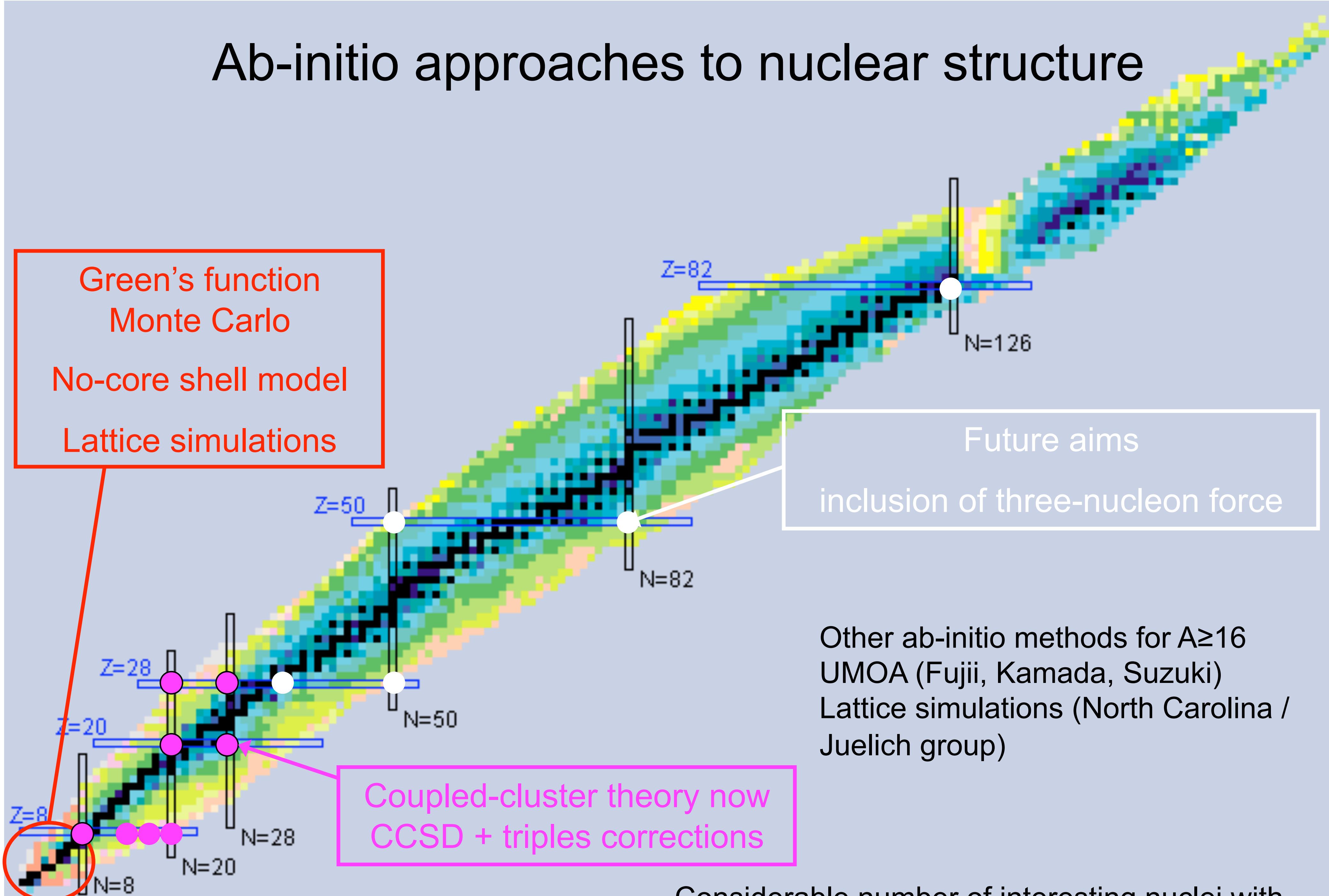
Model-independent description of atomic nuclei





Aim: Reliable predictions with error estimates.

Ab-initio approaches to nuclear structure



Other ab-initio methods for A≥16
UMOA (Fujii, Kamada, Suzuki)
Lattice simulations (North Carolina / Juelich group)

Considerable number of interesting nuclei with closed subshells…

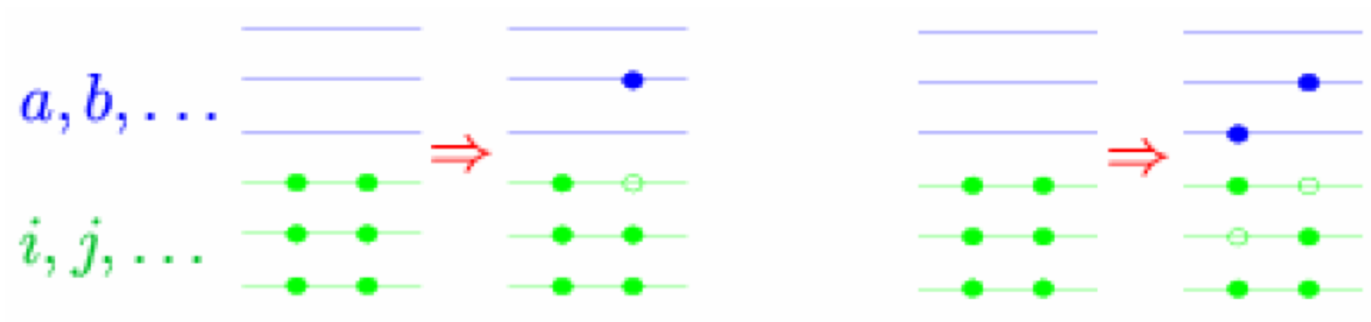
Coupled-cluster method (in CCSD approximation)

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)
- ☹ Limited to certain nuclei

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



Coupled cluster equations

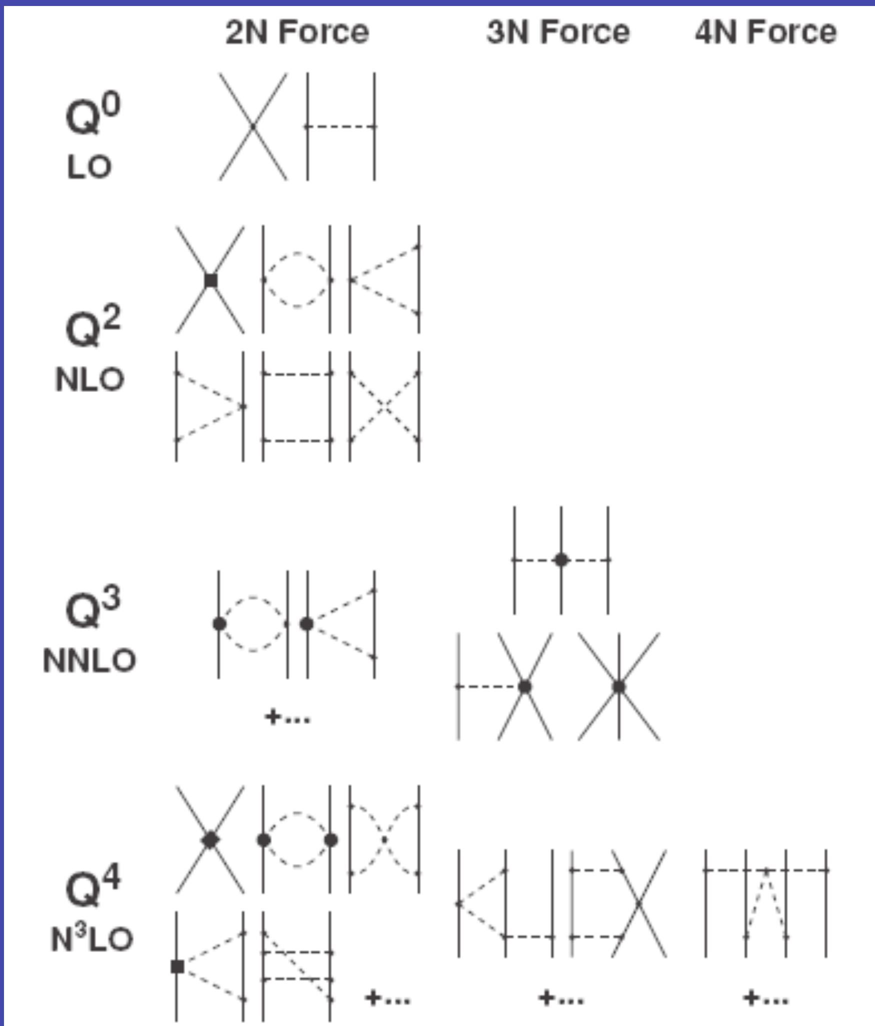
$$
\begin{aligned}
E &= \langle\Phi|\overline{H}|\Phi\rangle \\
0 &= \langle\Phi_i^a|\overline{H}|\Phi\rangle \\
0 &= \langle\Phi_{ij}^{ab}|\overline{H}|\Phi\rangle
\end{aligned}
$$

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

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

Nuclear potential from chiral effective field theory

Diagrams



van Kolck (1994); Epelbaum et al (2002); Machleidt & Entem (2005);

Ab-initio structure calculations with potentials from chiral EFT

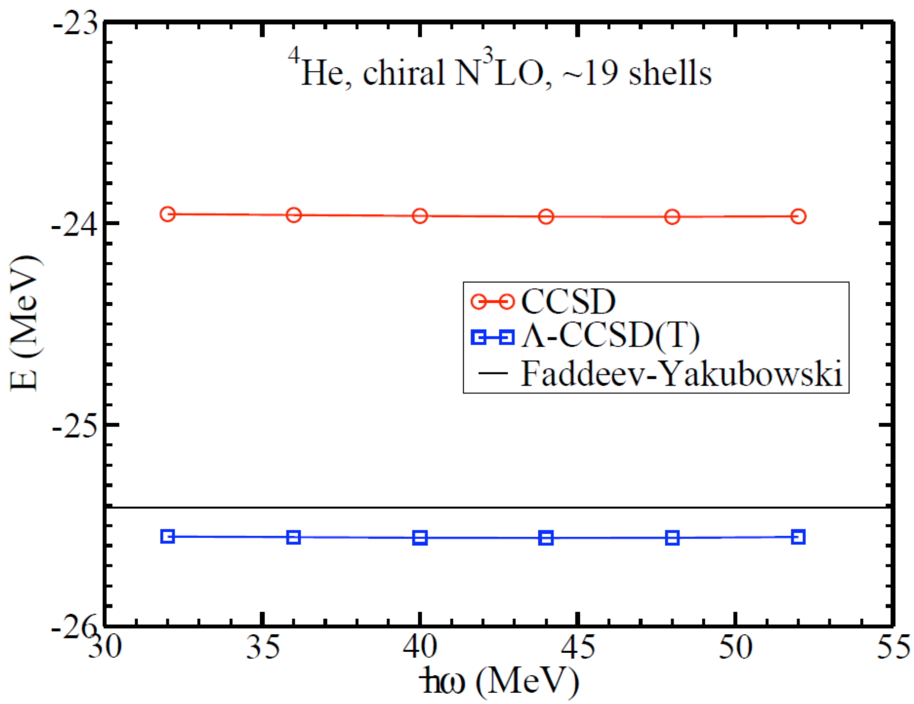
- A=3, 4: Faddeev-Yakubowski method
- A≤10: Hyperspherical Harmonics
- *p*-shell nuclei: NCSM, GFMC(AV18)
- ^{16,22,24,28}O, ^{40,48}Ca, ^{48}Ni: Coupled cluster, UMOA, Green's functions (NN so far)
- Lattice simulations
- Nuclear matter

Questions:

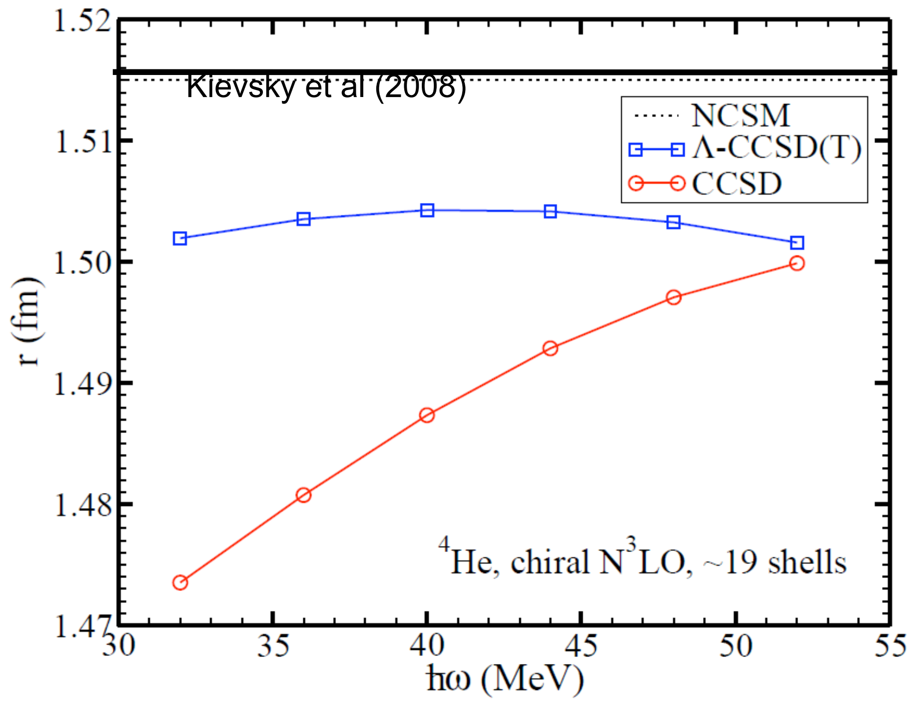
1. Can we compute nuclei from scratch?
2. Role/form of three-nucleon interaction
3. Saturation properties

Precision and accuracy: ^{4}He, chiral N^{3}LO [Entem & Machleidt]

Ground-state energy



Matter radius



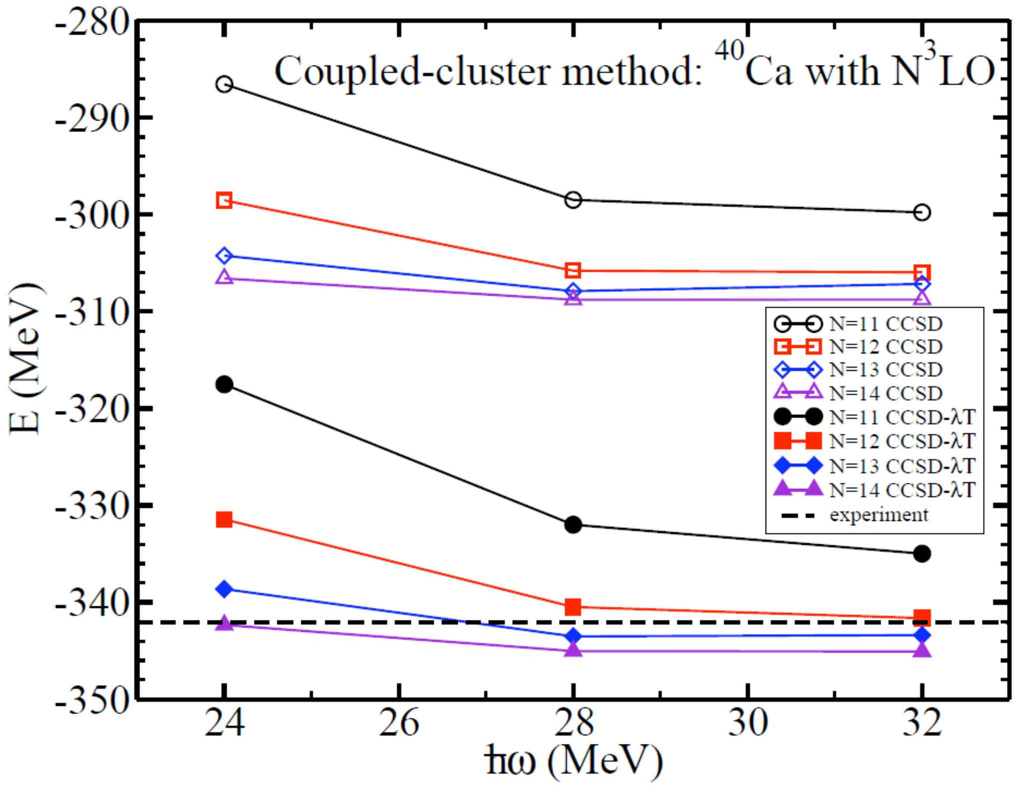
1. Results exhibit very weak dependence on the employed model space.
2. The coupled-cluster method, in its Λ-CCSD(T) approximation, overbinds by 150keV; radius too small by about 0.01fm.
3. Independence of model space of N major oscillator shells with frequency ω:

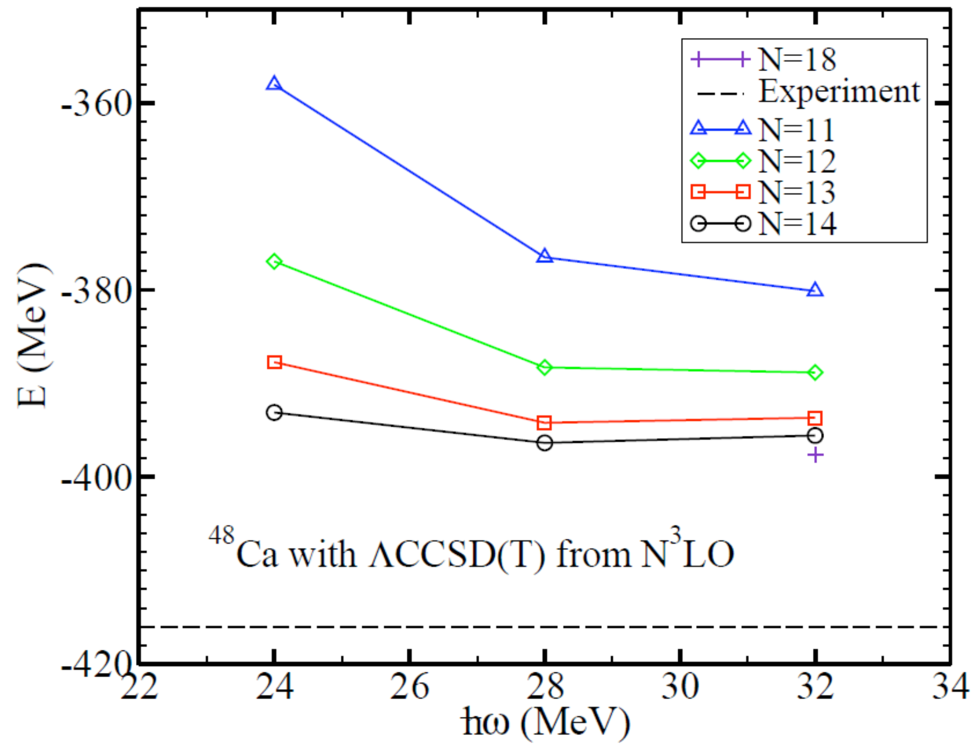
   $N\hbar\omega > \hbar^2\Lambda_\chi^2/m$ to resolve momentum cutoff Λ_χ

   $\hbar\omega < N\hbar^2/(mR^2)$ to resolve nucleus of radius R
4. Number of single-particle states ~ $(R\Lambda_\chi)^3$

Ground-state energies of medium-mass nuclei

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





Binding energy per nucleon

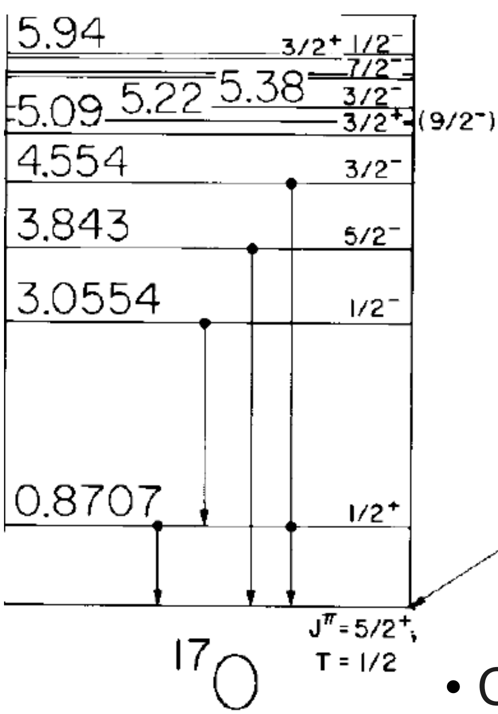
Nucleus	CCSD	Λ-CCSD(T)	Experiment
^{4}He	5.99	6.39	7.07
^{16}O	**6.72**	**7.56**	7.97
^{40}Ca	7.72	8.63	8.56
^{48}Ca	7.40	8.28	8.67

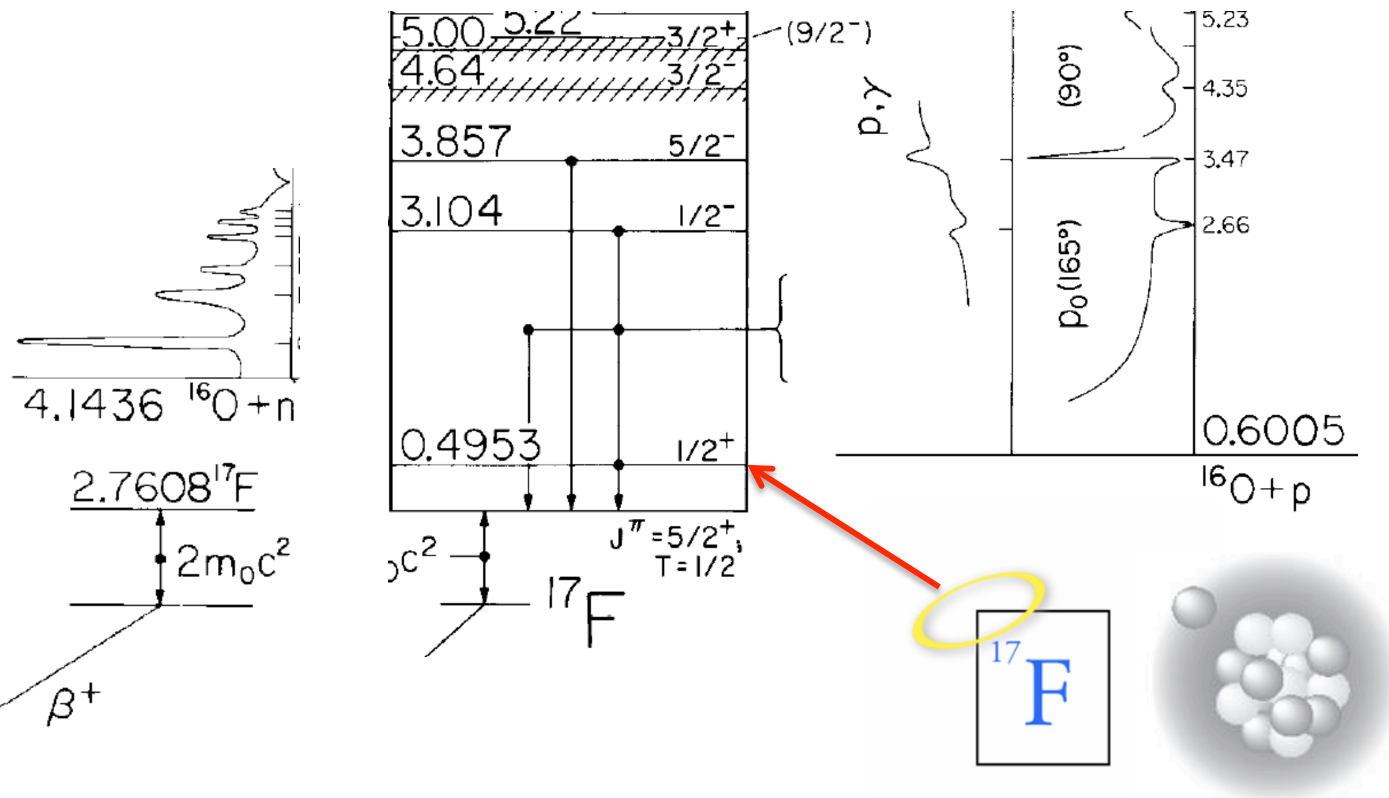
Compare ^{16}O to different approach Fujii et al., Phys. Rev. Lett. 103, 182501 (2009)

B/A=**6.62** MeV (2 body clusters)
B/A=**7.47** MeV (3 body clusters)

[Hagen, TP, Dean, Hjorth-Jensen, Phys. Rev. Lett. 101, 092502 (2008)]

Ab initio description of proton halo state in ^{17}F





- Continuum has to be treated properly
- Focus is on single-particle states
- Previous study: shell model in the continuum with^{16}O core

[K. Bennaceur, N. Michel, F. Nowacki, J. Okolowicz, M. Ploszajczak, Phys. Lett. B 488, 75 (2000)]

Bound states and resonances in ^{17}F and ^{17}O

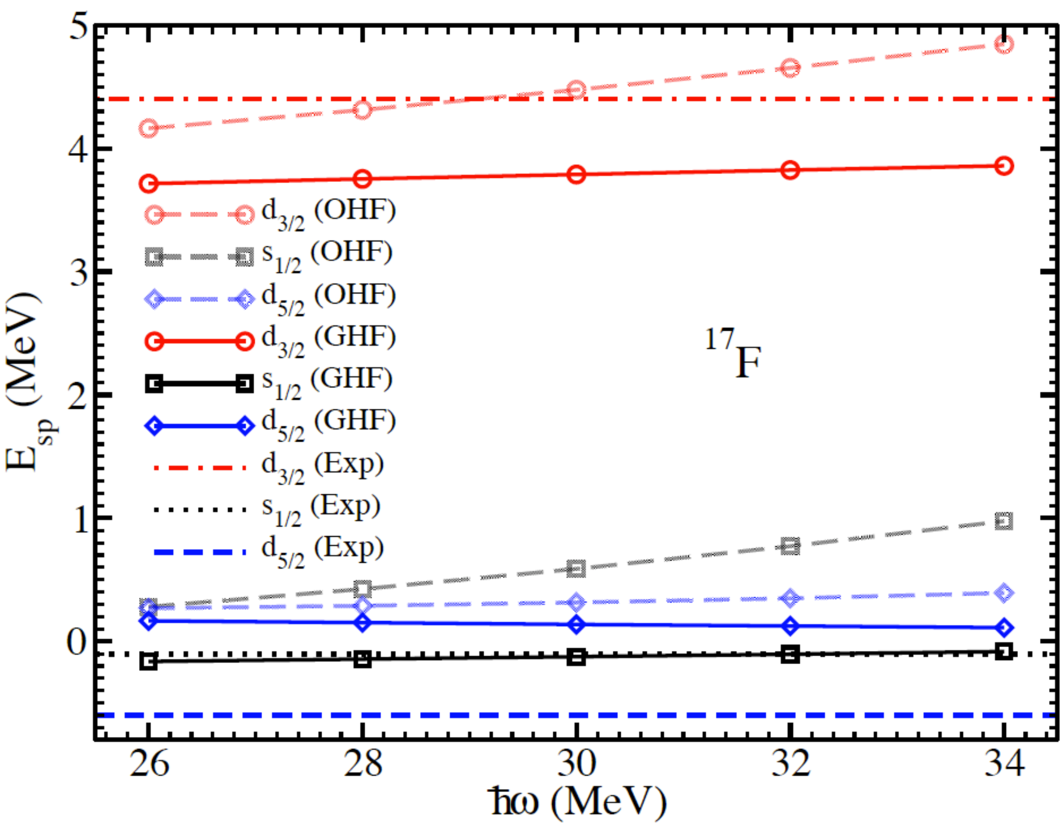
Single-particle basis consists of bound, resonance and scattering states

- Gamow basis for $s_{1/2}$ $d_{5/2}$ and $d_{3/2}$ single-particle states
- Harmonic oscillator states for other partial waves

Computation of single-particle states via "Equation-of-motion CCSD"

- Excitation operator acting on closed-shell reference
- Here: superposition of one-particle and 2p-1h excitations

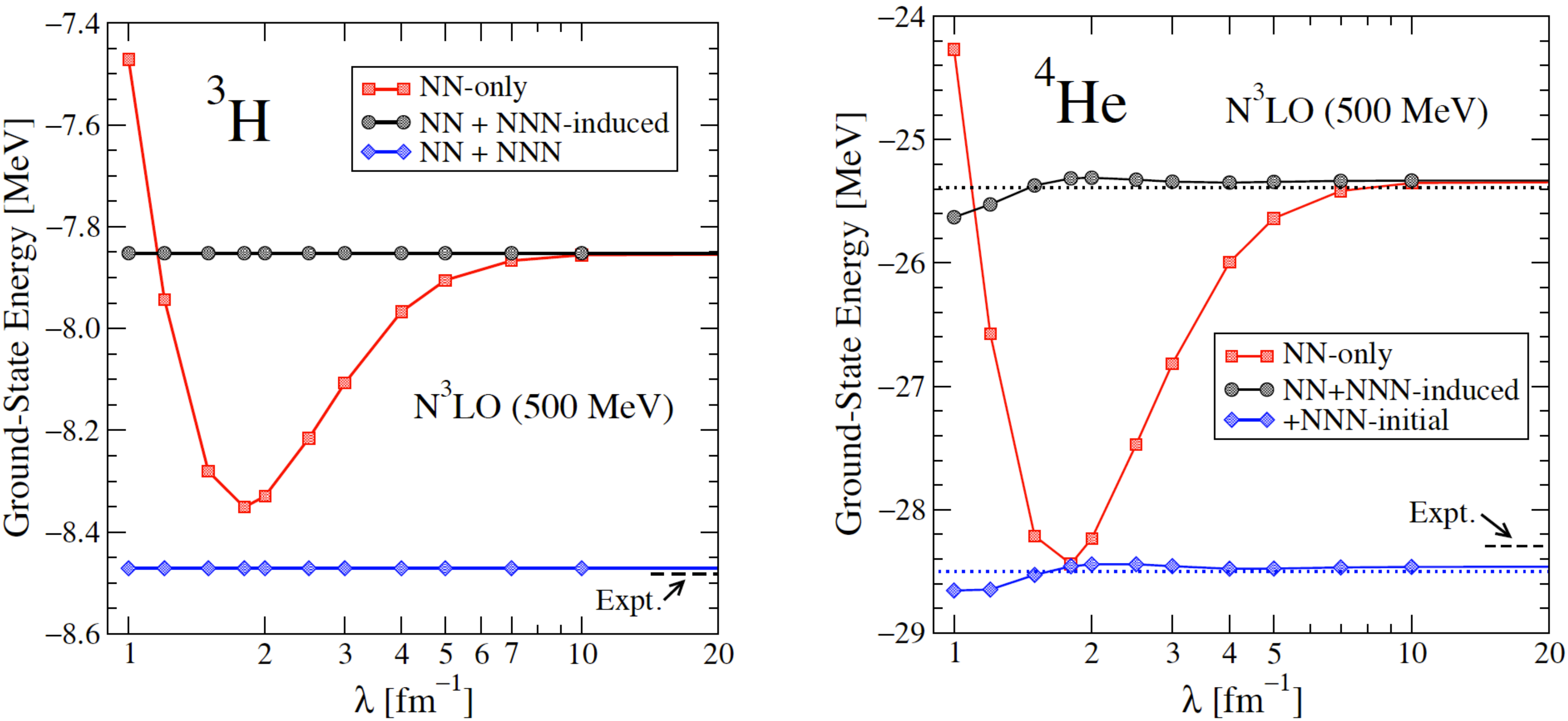
$$R_\mu = r^a a_a^\dagger + \frac{1}{2} r_j^{ab} a_a^\dagger a_b^\dagger a_j \qquad \left[\overline{H}, R_\mu\right] |\phi_0\rangle = \omega_\mu R_\mu |\phi_0\rangle$$



- Gamow basis weakly dependent on oscillator frequency
- $d_{5/2}$ not bound; spin-orbit splitting too small
- $s_{1/2}$ proton halo state close to experiment

[G. Hagen, TP, M. Hjorth-Jensen, Phys. Rev. Lett. 104, 182501 (2010)]

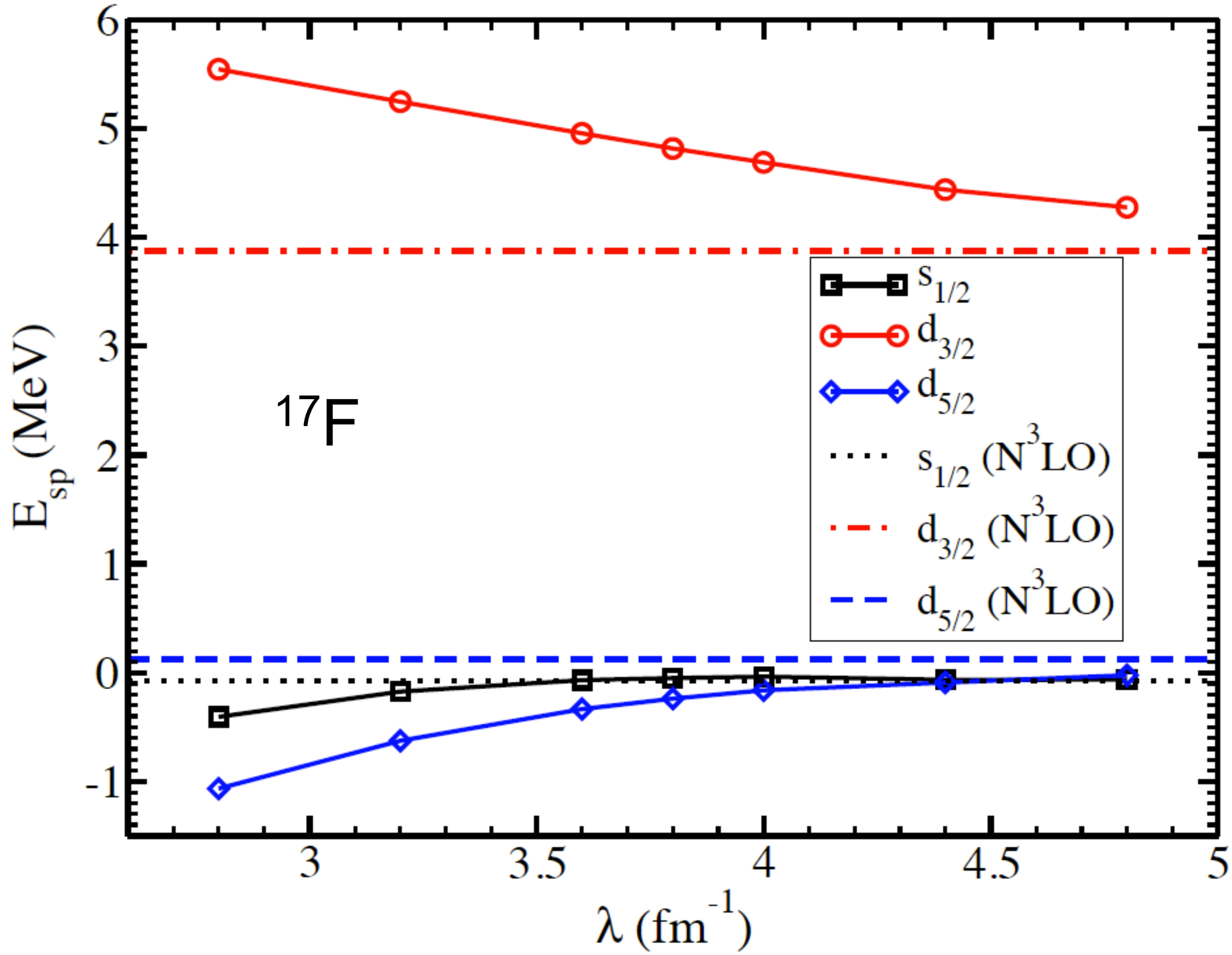
Insights from cutoff variation
^{3}H and ^{4}He with induced and initial 3NF



[Jurgenson, Navratil & Furnstahl, Phys. Rev. Lett. 103, 082501 (2009)]

Cutoff-dependence implies missing physics from short-ranged many-body forces.

Variation of cutoff probes omitted short-range forces



- Proton-halo state ($s_{1/2}$) very weakly sensitive to variation of cutoff
- Spin-orbit splitting increases with decreasing cutoff

[G. Hagen, TP, M. Hjorth-Jensen, Phys. Rev. Lett. 104, 182501 (2010)]

Results for single-particle energies and decay widths

	^{17}O			^{17}F		
	$1/2^+$	$5/2^+$	E_{so}	$1/2^+$	$5/2^+$	E_{so}
GHF	-2.8	-3.2	4.3	-0.082	0.11	3.7
Exp.	-3.272	-4.143	5.084	-0.105	-0.600	5.000

- Level ordering correctly reproduced in ^{17}O
- Spin-orbit splitting too small

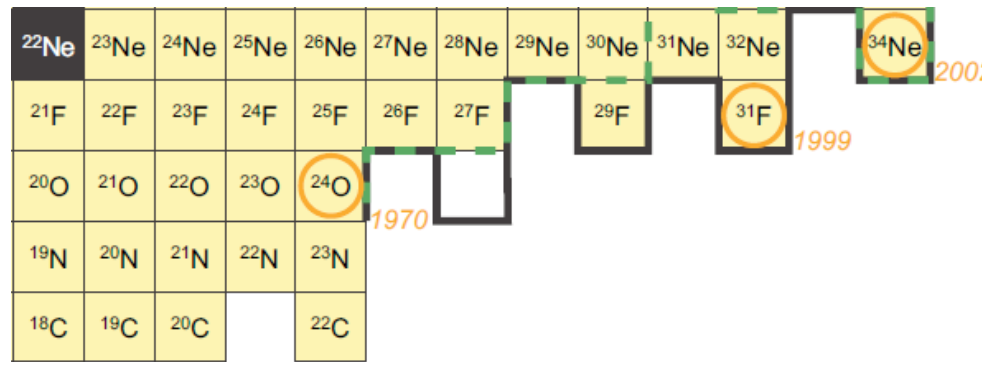
Life times of resonant states

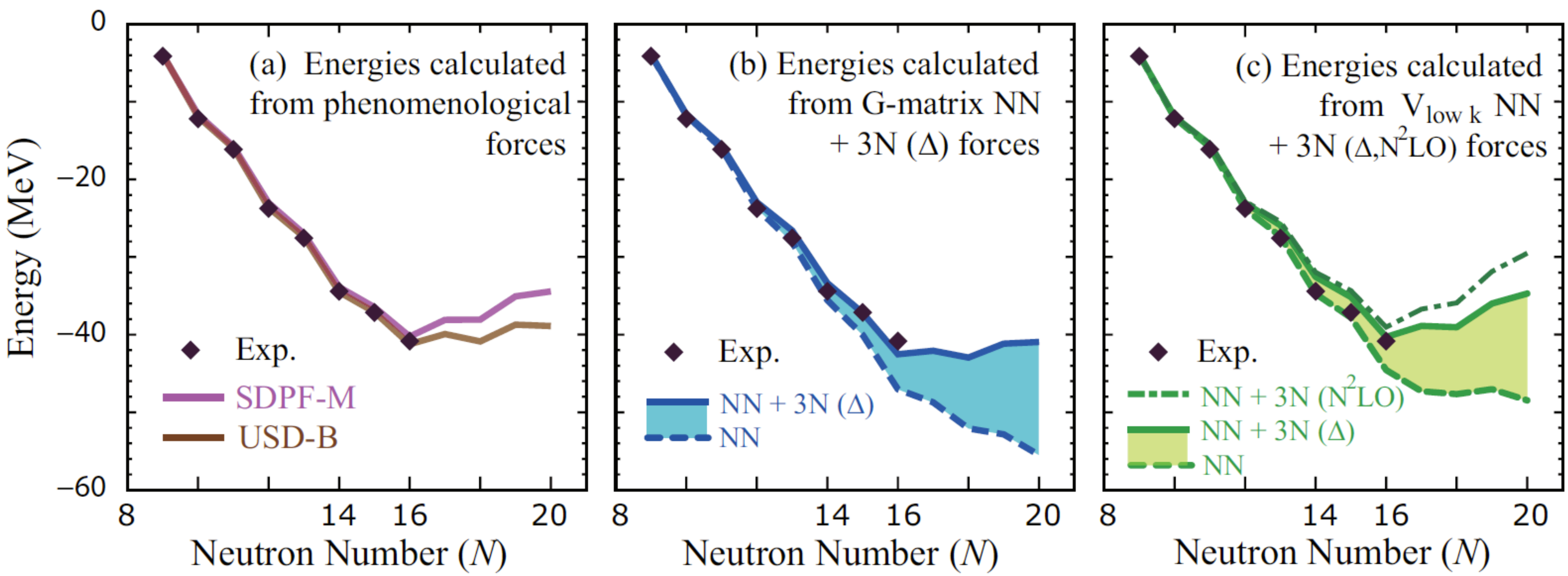
	^{17}O $3/2^+$		^{17}F $3/2^+$	
	E_{sp}	Γ	E_{sp}	Γ
This work	1.1	0.014	3.9	1.0
Experiment	0.942	0.096	4.399	1.530

Is ^{28}O a bound nucleus?

Experimental situation

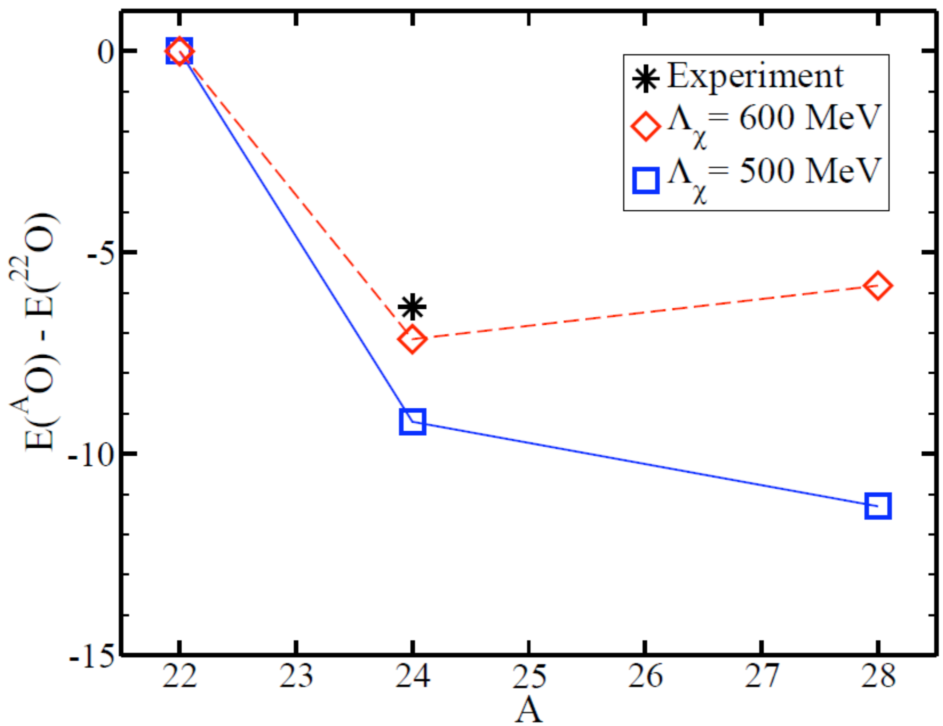
- “Last” stable oxygen isotope ^{24}O
- ^{25}O unstable (Hoffman et al 2008)
- $^{26,28}O$ not seen in experiments
- ^{31}F exists (adding on proton shifts drip line by 6 neutrons!?)





Shell model (sd shell) with monopole corrections from three-nucleon force predicts ^{24}O as last stable isotope of oxygen.[Otsuka, Suzuki, Holt, Schwenk, Akaishi, Phys. Rev. Lett. 105, 032501 (2010)]

Neutron-rich oxygen isotopes from chiral NN forces



• Chiral NN forces only: Too close to call. Theoretical uncertainties >> differences in binding energies.

• Chiral potentials by Entem & Machleidt's different from *G*-matrix-based interactions.

• Ab-initio theory cannot rule out a stable ^{28}O.

• Three-body forces largest potential contribution that decides this question.

[G. Hagen, TP, D. J. Dean, M. Hjorth-Jensen, B. Velamur Asokan, Phys. Rev. C 80, 021306(R) (2009)]

No theoretical approach flawless yet. (No approach includes everything (continuum effects, 3NFs, no adjustments of interaction). Stay tuned …

Practical solution of the center-of-mass problem

Intrinsic nuclear Hamiltonian

Obviously, H_{in} commutes with any Hamiltonian H_{cm} of the center-of-mass coordinate

Situation: The Hamiltonian depends on 3(A-1) coordinates, and is solved in a model space of 3A coordinates. What is the wave function in the center-of-mass coordinate?

Demonstration that ground-state wave function factorizes: $\psi = \psi_{\rm cm}\psi_{\rm in}$

Demonstrate that $\langle H_{cm} \rangle \approx 0$ for a suitable center-of-mass Hamiltonian with zero-energy ground state.

$$H_{\rm cm}(\tilde{\omega}) = T_{\rm cm} + \frac{1}{2}mA\tilde{\omega}^2 R_{\rm cm}^2 - \frac{3}{2}\hbar\tilde{\omega}$$

Frequency $\tilde{\omega}$ to be determined.

Toy problem

Two particles in one dimension
with intrinsic Hamiltonian

$$H = \frac{p^2}{2m} + V(x)$$
$$V(x) = -V_0 \exp\left(-(x/l)^2\right)$$

$$x = (x_1 - x_2)/\sqrt{2}$$
$$p = (p_1 - p_2)/\sqrt{2}$$

Single-particle basis of oscillator wave functions with *m,n=0,..,N*

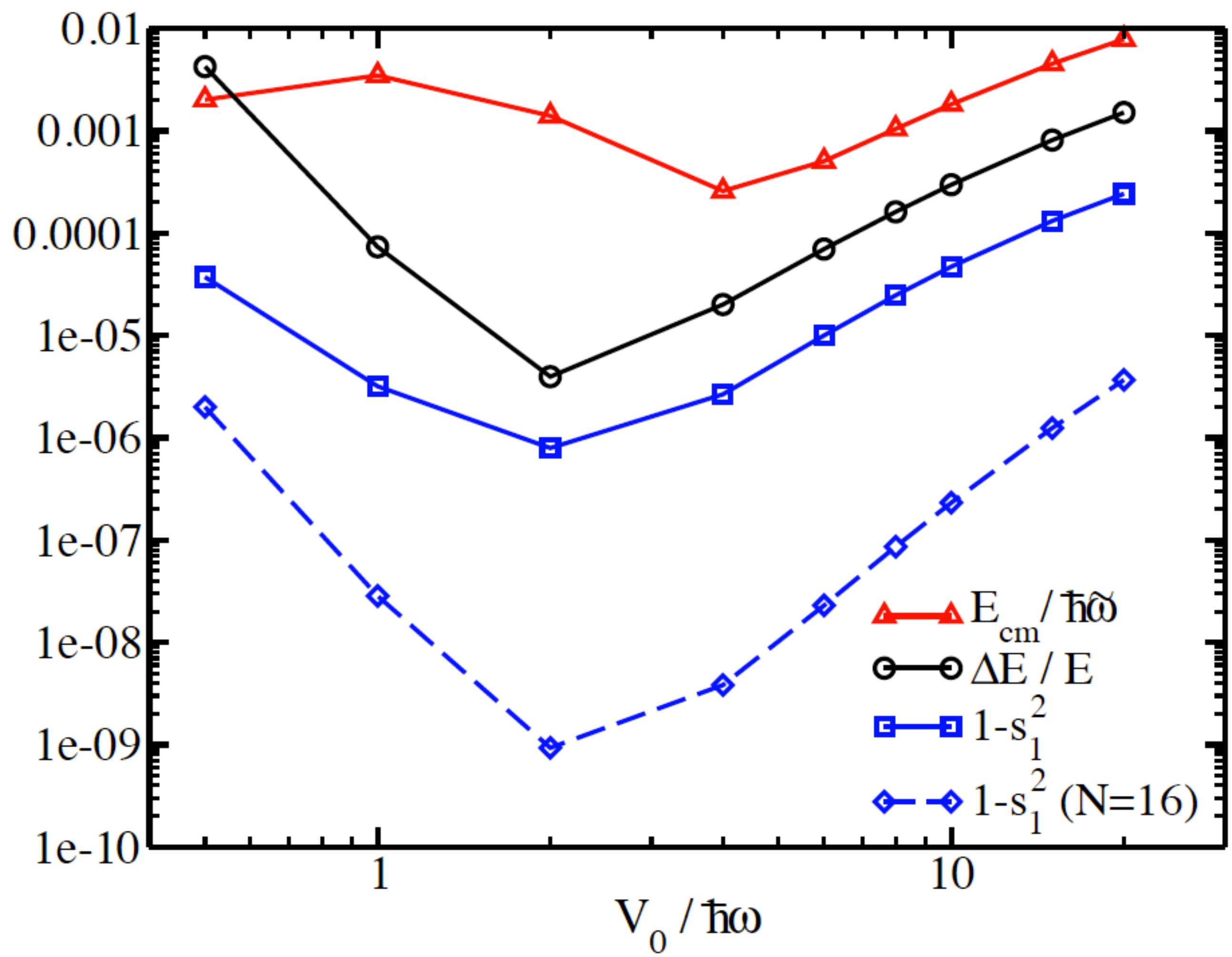
$$\Phi_m(x_1/l)\Phi_n(x_2/l)$$

Results:

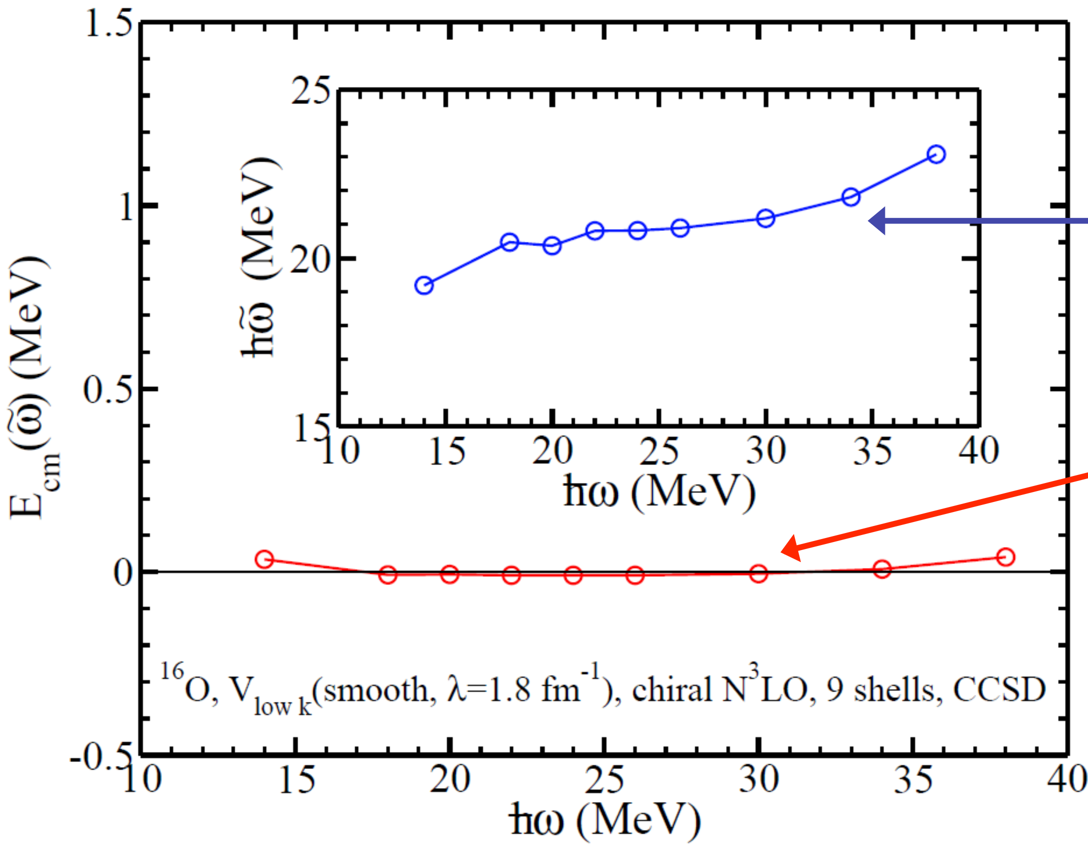
1. Ground-state is factored with $s_1 \approx 1$

$$\psi_A = \sum_j s_j \psi_{\rm cm}^{(j)} \psi_{\rm in}^{(j)}$$

2. CoM wave function is approximately a Gaussian



Coupled-cluster wave function factorizes to a very good approximation



Curve becomes practically constant in larger model spaces

E_{cm} is practically zero (size -0.01 MeV due to non-variational character of CCSD).

Note: spurious CoM excitations are of order 20 MeV << E_{cm}.

Coupled-cluster state is ground state of suitably chosen center-of-mass Hamiltonian.

Factorization between intrinsic and center-of-mass coordinate realized within high accuracy.

Note: Both graphs become flatter as the size of the model space is increased.

[Hagen, TP, Dean, Phys. Rev. Lett. 103, 062503 (2009)]

Summary

Saturation properties of medium-mass nuclei:

- "Bare" interactions from chiral effective field theory can be converged in large model spaces
- Chiral NN potentials miss ~0.4 MeV per nucleon in binding energy in medium-mass nuclei

A=17 nuclei:

- Equation-of-motion CCSD combined with a Gamow basis
- Accurate computation of proton-halo state in ^{17}F; halo weakly dependent on cutoff

Neutron-rich oxygen isotopes:

- Ab-initio theory with nucleon-nucleon forces only cannot rule out a stable ^{28}O
- Greatest uncertainty from omitted three-nucleon forces

Practical solution to the center-of-mass problem:

- Demonstration that coupled-cluster wave function factorizes into product of intrinsic and center-of-mass state
- Center-of-mass wave function is Gaussian
- Factorization very pure for "soft" interactions and approximate for "hard" interaction

Outlook

Inclusion of three-nucleon forces

Towards heavier masses (Ca, Ni, Sn, Pb isotopes)

α-particle excitations (low-lying 0^+ states in doubly magic nuclei)