Coupled-cluster theory for nuclei

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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. Practical solution to the center-of-mass problem

   [Hagen, TP, Dean, Phys. Rev. Lett. 103, 062503 (2009)]
4. Does ^{28}O exist?

   [Hagen, TP, Dean, Horth-Jensen, Velamur Asokan, Phys. Rev. C 80, 021306(R) (2009)]

Energy scales and relevant degrees of freedom

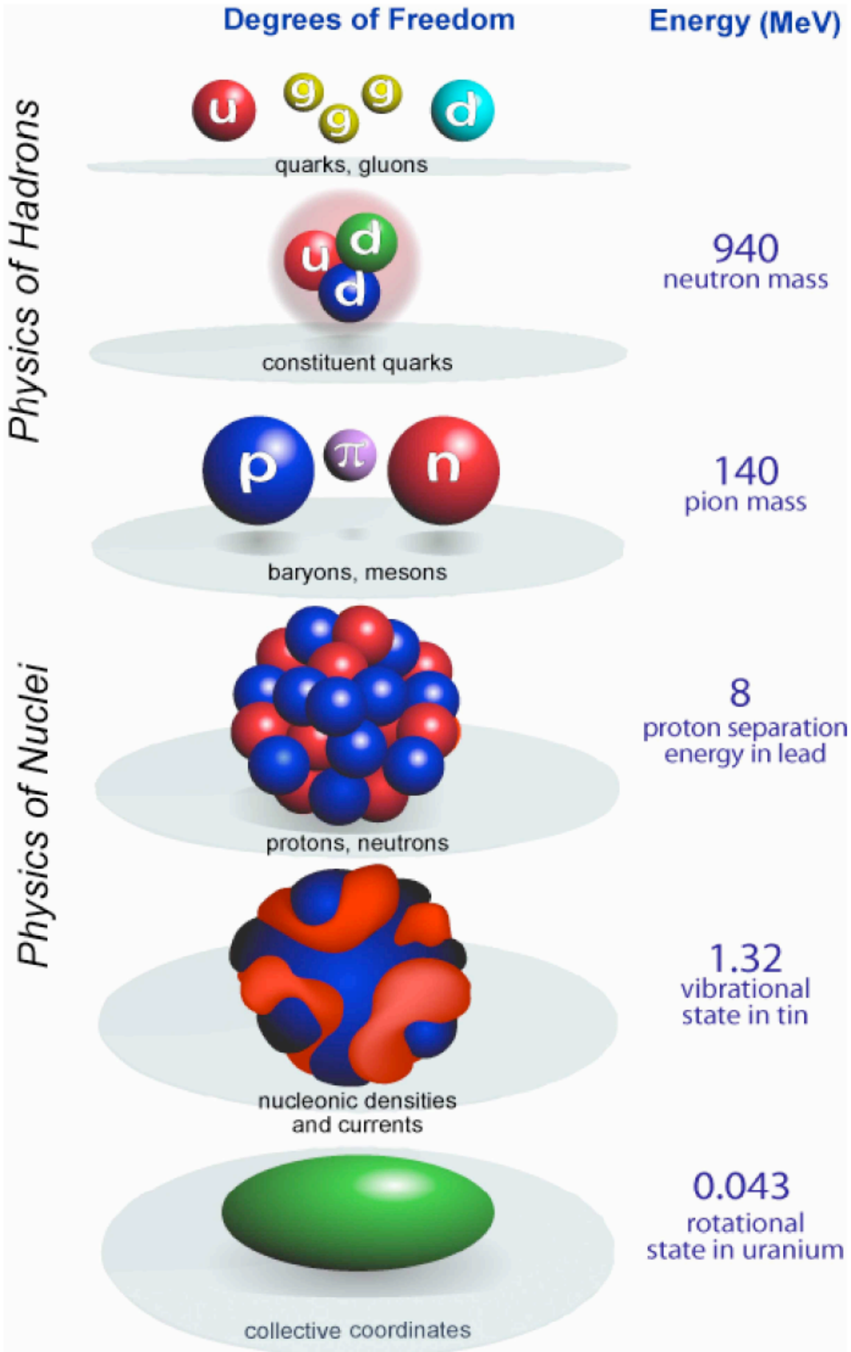
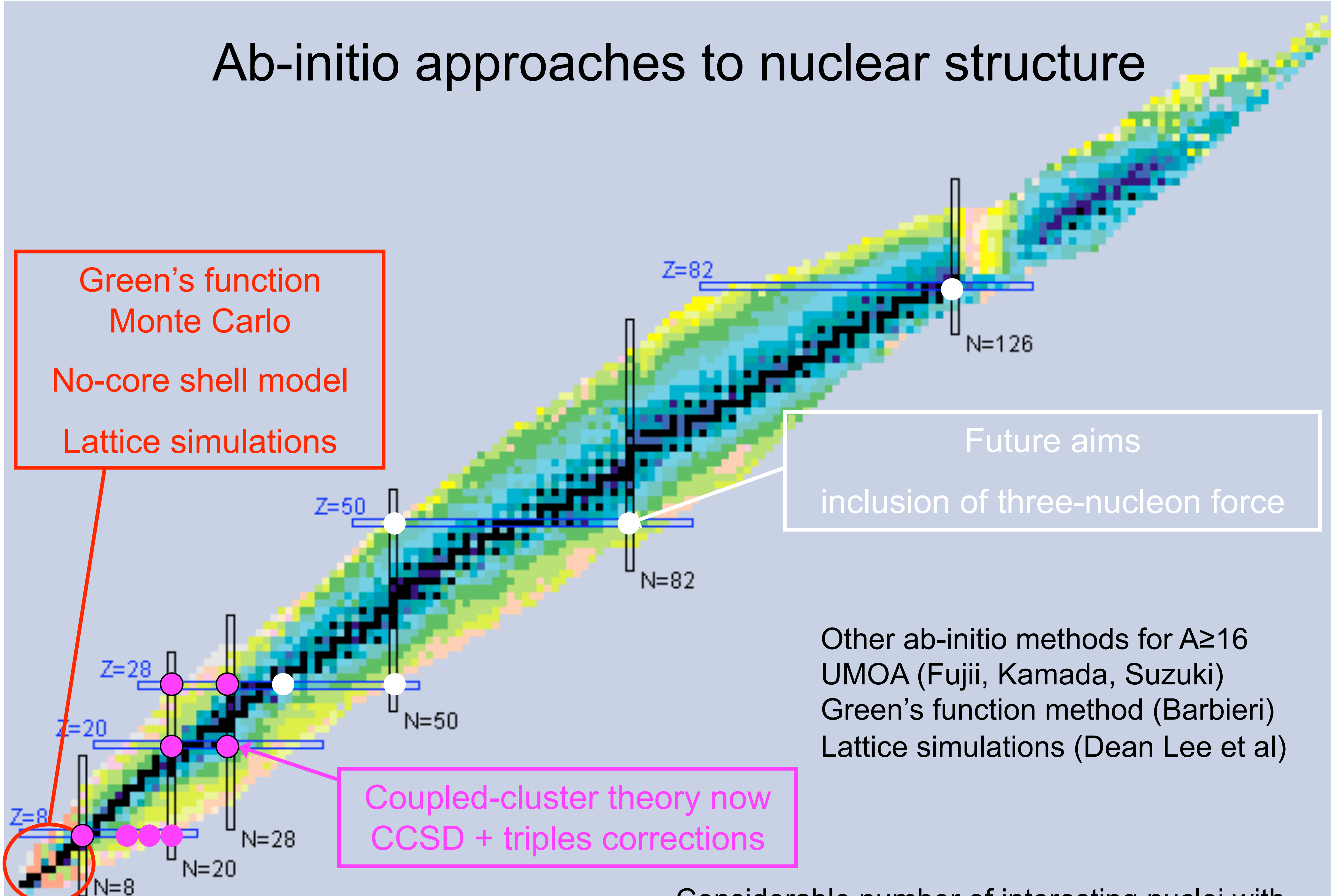


Fig.: SciDAC review (2007)

Ab-initio approaches to nuclear structure



Other ab-initio methods for A≥16
UMOA (Fujii, Kamada, Suzuki)
Green's function method (Barbieri)
Lattice simulations (Dean Lee et al)

Considerable number of interesting nuclei with closed subshells…

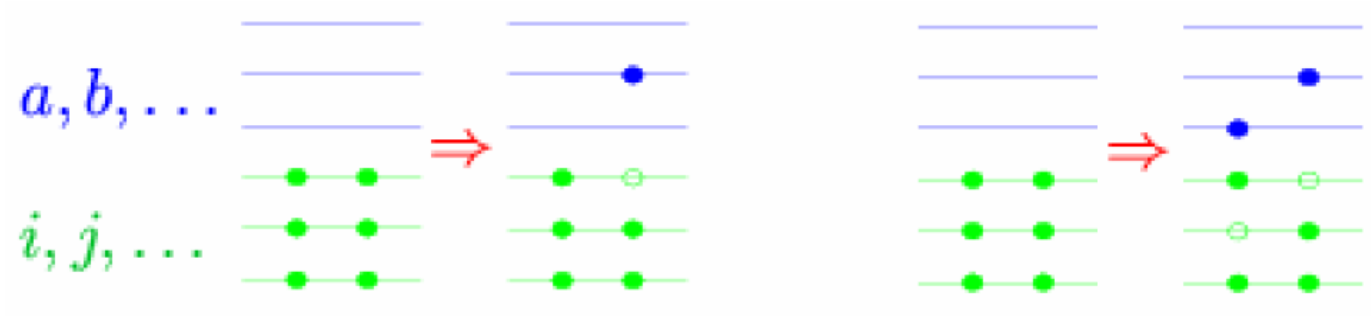
Coupled-cluster method (CCSD)

Ansatz:

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

- ☺ Scales gently (polynomial) with increasing problem size o^2u^4 .
- ☺ Truncation is the only approximation.
- ☺ Size extensive (error scales with A)

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



Coupled cluster equations

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

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

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

Peculiarities of coupled-cluster theory for nuclei

Interaction: One of the main questions / aims

1. A few high-precision potentials available
2. Renormalization scale / scale of external probe provides families of interactions
3. Model-space dependencies must be examined (no “standard” basis sets or model spaces)

Hamiltonian:

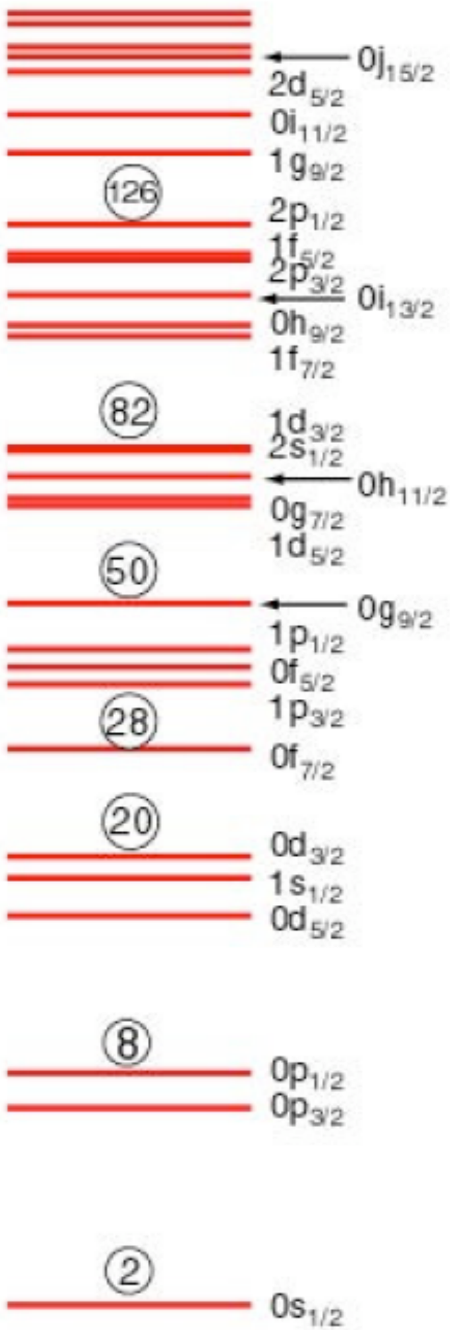
1. Nucleons are fundamental degrees of freedom (single-particle states carry orbital, spin, and isospin labels)
2. Hamiltonian is scalar under rotation
   - Cluster excitation operator is scalar, too
   - Number of j-shells ~ $A^{2/3}$ for nucleus with mass numbers A
   - **Much larger model spaces accessible (*m*-scheme: 8-10 shells; spherical scheme: 20 shells).**
   - **1 order of magnitude increase in number of single-particle states.**

$$\hat{T} = \sum_{j_a j_i} t_{j_i}^{j_a} \left(\hat{a}_{j_a}^\dagger \times \hat{a}_{j_i}\right)^{(0)}$$

$$+ \sum_{j_a, j_b, j_i, j_j} \sum_J t_{j_i j_j}^{j_a j_b}(J) \left(\left(\hat{a}_{j_a}^\dagger \times \hat{a}_{j_b}^\dagger\right)^{(J)} \times \left(\hat{a}_{j_j} \times \hat{a}_{j_i}\right)^{(J)}\right)^{(0)}$$

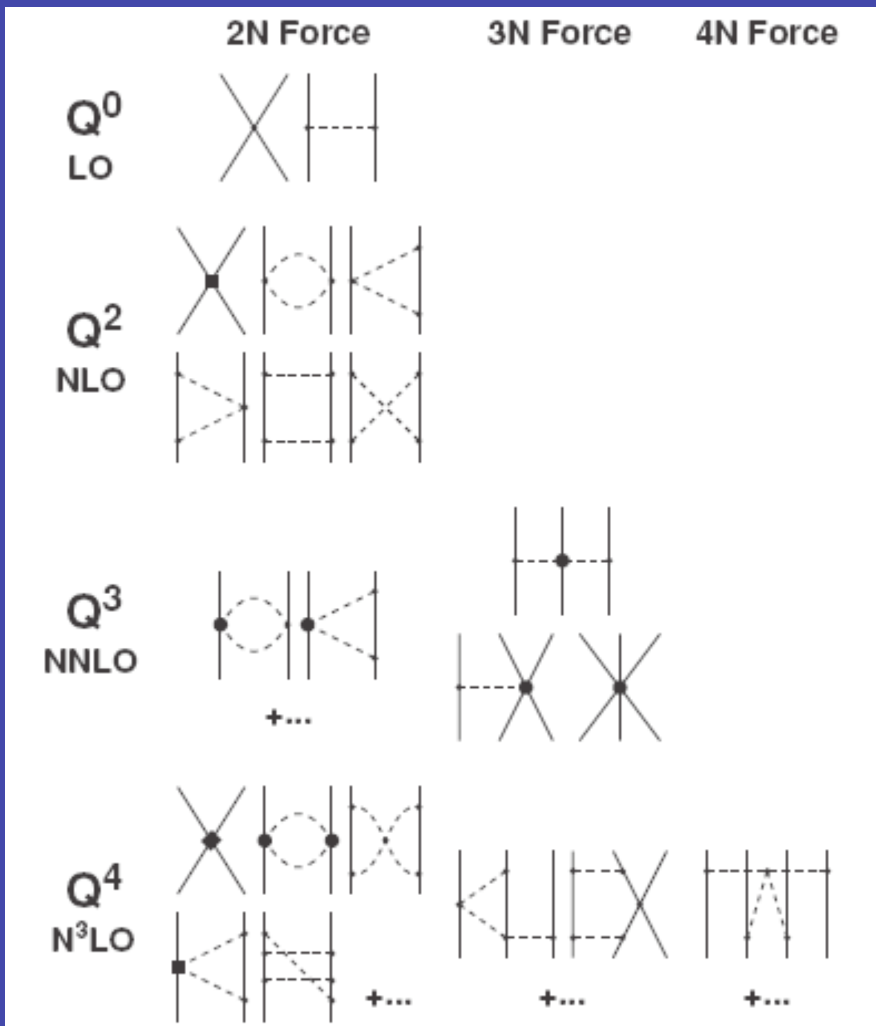
Nuclear shell model

1. Traditional shell model:
    - Quantum well + strong spin-orbit force
    - "Freeze" core nucleons and work with valence nucleons
2. "Ab-initio" methods:
    - Shell model provides basis for wave-function based methods
3. Harmonic oscillator basis allows to keep all symmetries within CI
    - Parameters: oscillator frequency, number of major oscillator shells
    - All nucleons active



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

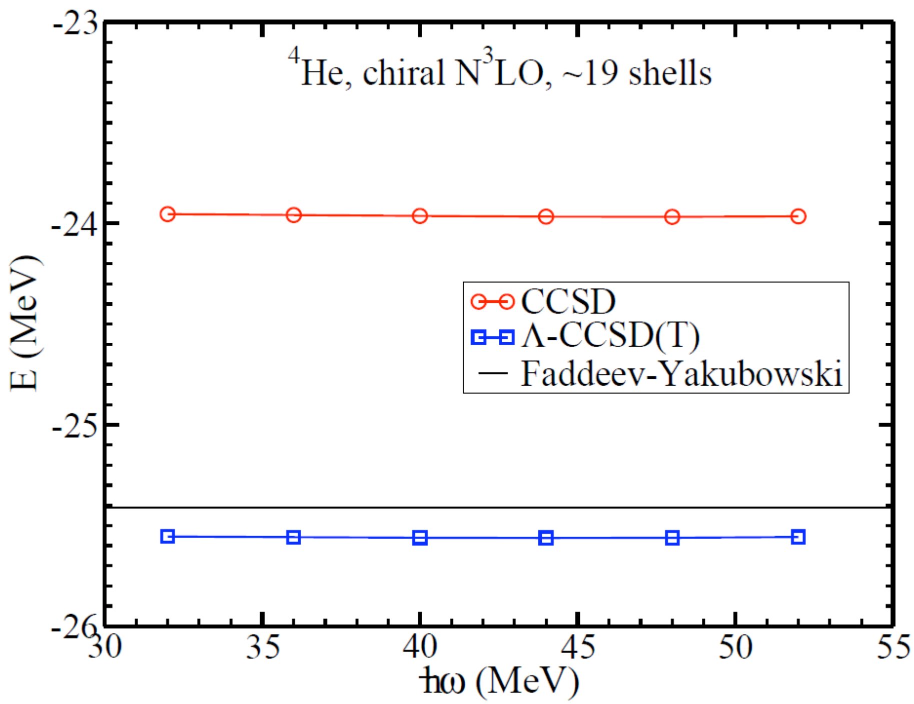
- A=3, 4: Faddeev-Yakubowski method
- A≤10: Hyperspherical Harmonics
- *p*-shell nuclei: NCSM, GFMC(AV18)
- ^{16,22,24,28}O, ^{40,48}Ca, ^{48}Ni: Coupled cluster, UMOA, Green's functions (NN so far)
- Lattice simulations
- Nuclear matter

Questions:

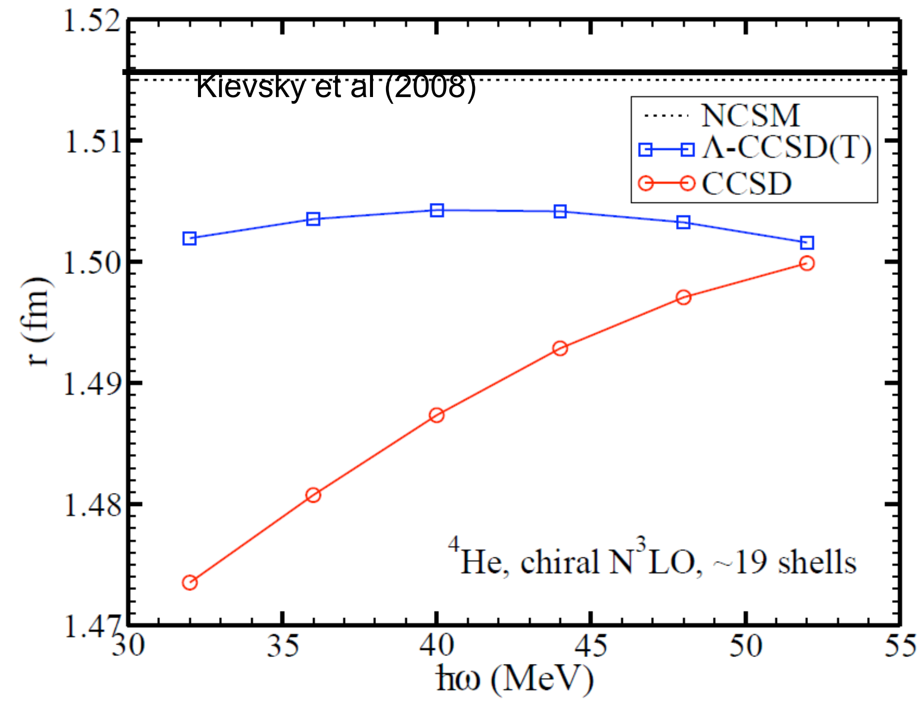
1. Can we compute nuclei from scratch?
2. Role/form of three-nucleon interaction
3. Saturation properties

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

Ground-state energy



Matter radius

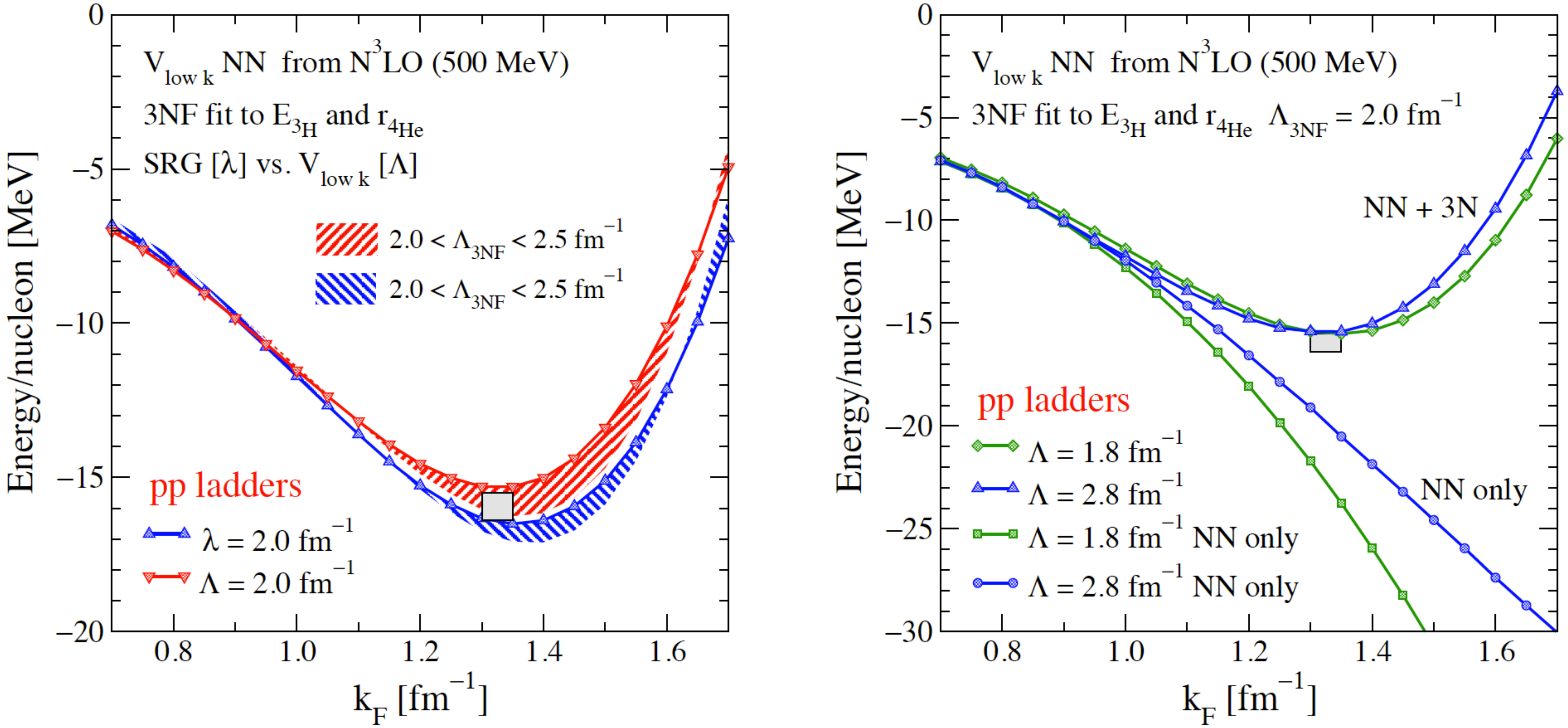


1. Results exhibit very weak dependence on the employed model space.
2. The coupled-cluster method, in its Λ-CCSD(T) approximation, overbinds by 150keV; radius too small by about 0.01fm.
3. Independence of model space of N major oscillator shells with frequency ω:

   $N\hbar\omega > \hbar^2\Lambda_\chi^2/m$ 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 ~ $(R\Lambda_\chi)^3$

Nuclear matter with low-momentum interactions



- Saturation of nuclear matter with low-momentum NN and NNN forces.
- Almost no cutoff dependence → physics almost complete
- Perturbative calculation already gives good results.

Bogner, Furnstahl, Schwenk & Nogga, arXiv:0903.3366

Ground-state energies of medium-mass nuclei

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

Nucleus	E/A	V/A	$\Delta E/A$
^{4}He	-5.99	-22.75	1.08
^{16}O	-6.72	-30.69	1.25
^{40}Ca	-7.72	-36.40	0.84
^{48}Ca	-7.40	-37.97	1.27
^{48}Ni	-6.02	-36.04	1.21

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

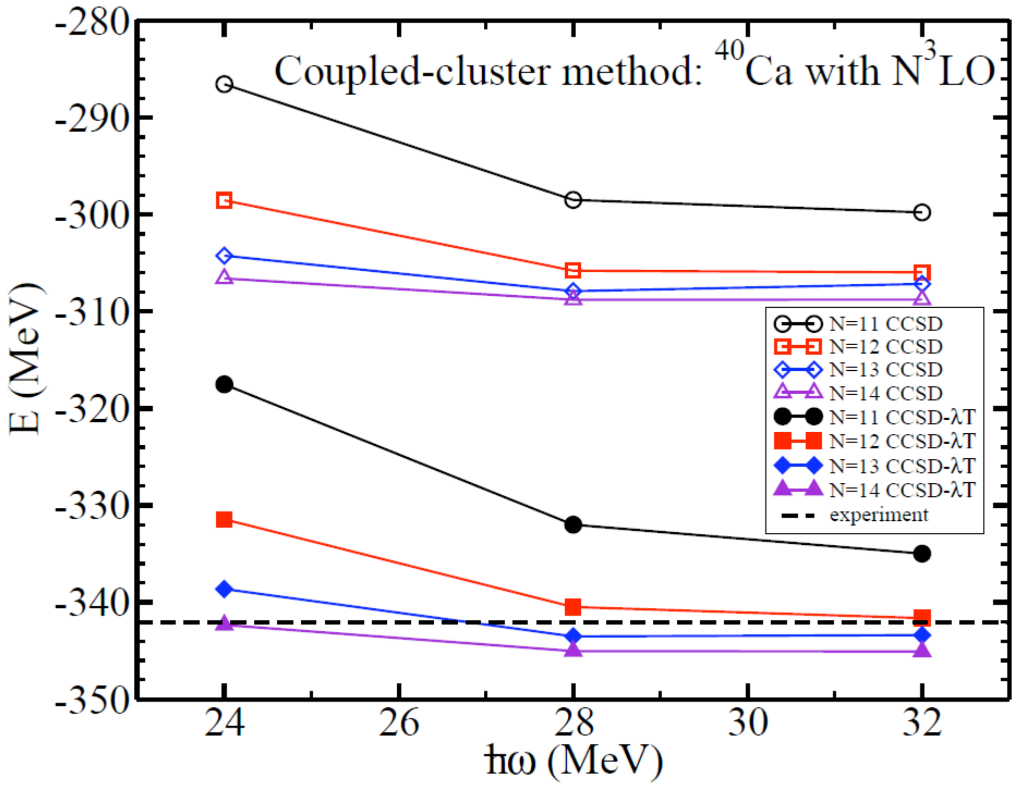
Main results

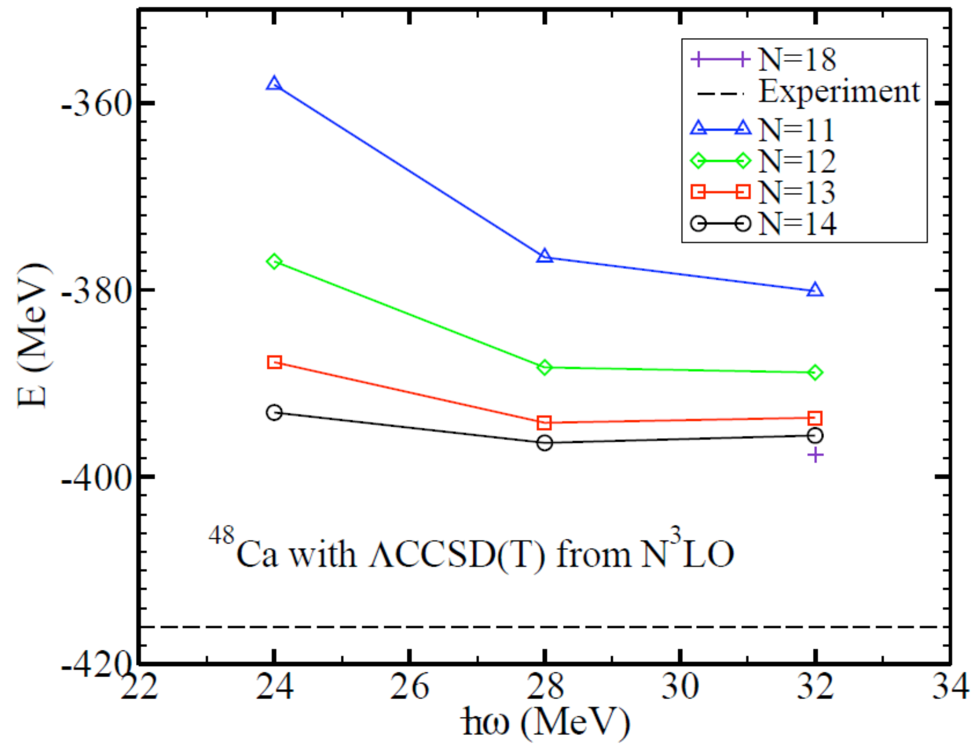
1. Well converged CCSD results with respect to size of model space (< 1% change in binding energy when going from 14 to 15 oscillator shells.
2. Three-nucleon force and triples corrections expected to yield ~1MeV additional binding?
3. Mirror nuclei ^{48}Ca and exotic ^{48}Ni differ by 1.38 MeV / A → close to mass-table predictions

How do corrections due to three-body clusters modify this picture?

Ground-state energies of medium-mass nuclei

CCSD results for chiral N³LO (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)]

Center-of-mass coordinate

The nuclear Hamiltonian is invariant under rotations and translations

Approach that preserves both symmetries:

☺ Jacobi coordinates

☹ Antisymmetrization very expensive → limited to A≤10 or so

[Faddeev Yakubowsky; Hyperspherical Harmonics; Manchester group's CCM].

Antisymmetry best dealt within second quantization:

☹ No single-particle basis available that consists of simultaneous eigenstates of the angular momentum operator and the momentum operator.

☺ Within a complete Nħω oscillator space, the wave function is guaranteed to factorize

$$\psi = \psi_{\rm cm}\psi_{\rm in}$$

Intrinsic wave function ψ_{in} invariant under translation

Center-of-mass wave function ψ_{cm} is Gaussian whose width is set by the oscillator length of the employed oscillator basis

The factorization is key. The form of ψ_{cm} is irrelevant.

Center-of-mass coordinate (cont'd)

Intrinsic nuclear Hamiltonian
$$\begin{aligned} H_{\rm in} &= T - T_{\rm cm} + V \;, \\ &= \sum_{1\le i<j\le A} \left(\frac{(\vec{p}_i - \vec{p}_j)^2}{2mA} + V(\vec{r}_i - \vec{r}_j) \right) \end{aligned}$$

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

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?

Q:How can one demonstrate the factorization of wave function ψ:

A: Find a suitable center-of-mass Hamiltonian H_{cm} whose eigenstate is ψ.

Our approach:

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

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

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*

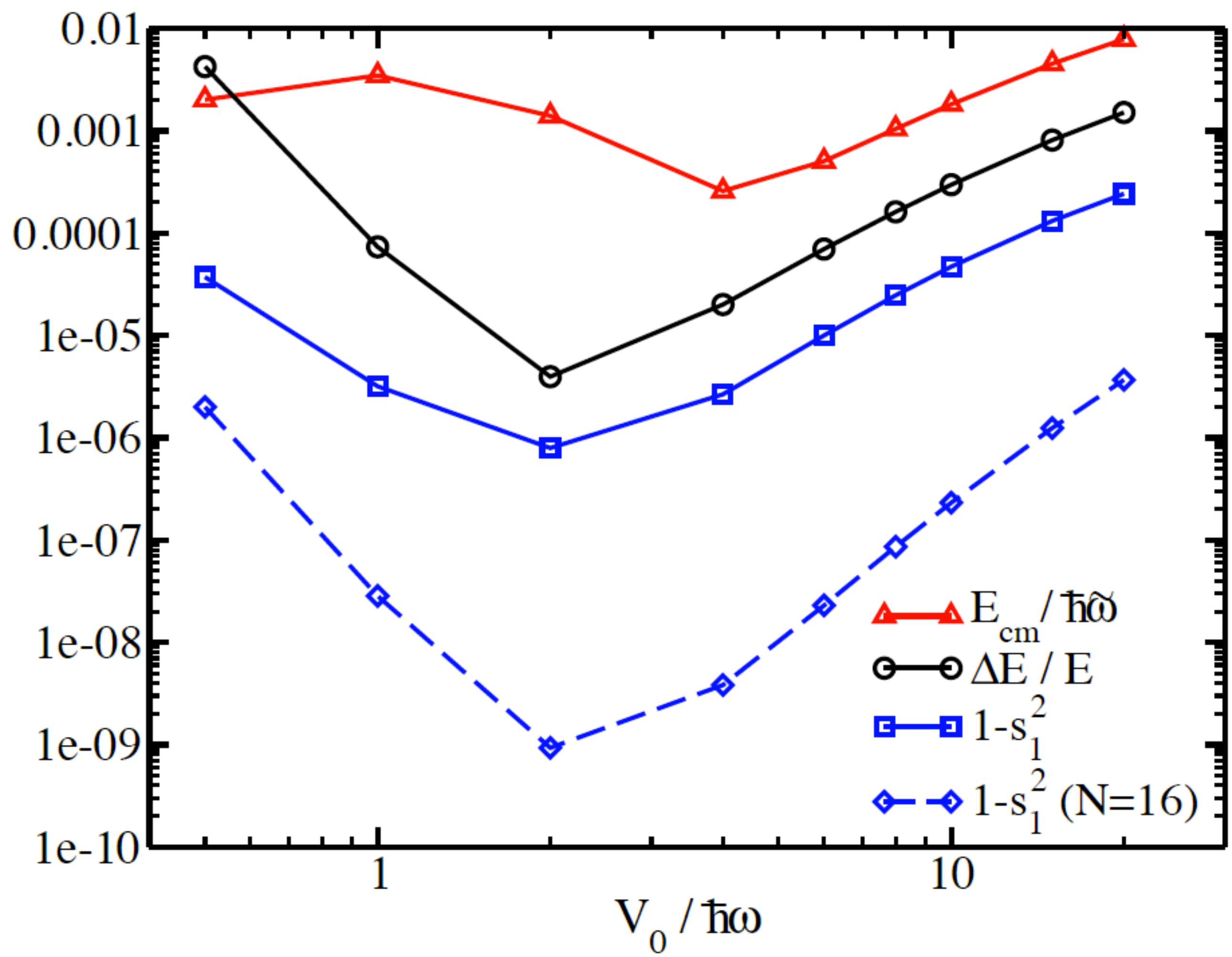
$$\Phi_m(x_1/l)\Phi_n(x_2/l)$$

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



Determination of ψ_{cm}

Assumption: ψ_{cm} is (approximately) a Gaussian for all model-space frequencies

- Gaussian center-of-mass wave function is the zero-energy ground state of

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

- Determine unknown frequency from from taking expectation value of identity

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

- Use

$$E_{\rm cm}(\tilde{\omega}) = 0$$

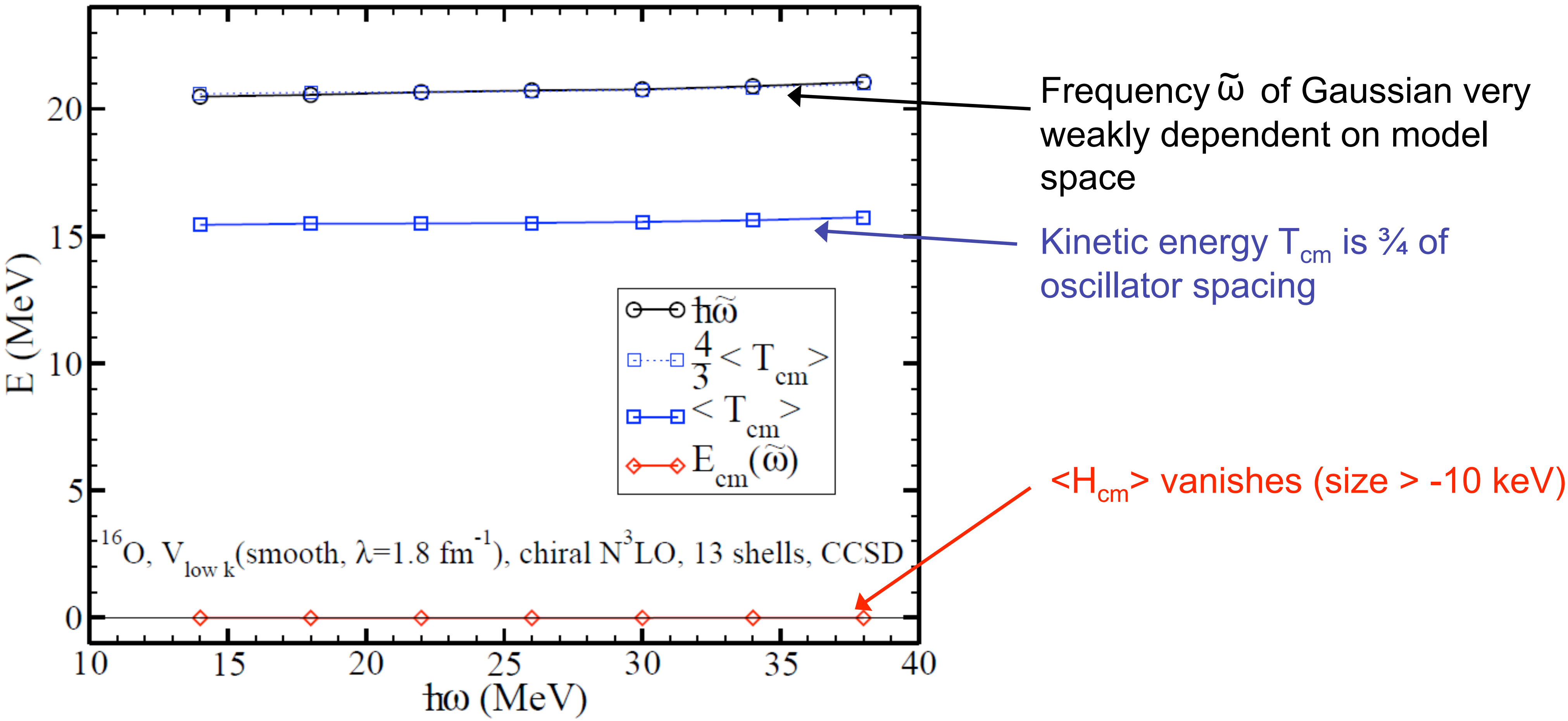
$$\langle T_{\rm cm}\rangle = \tfrac{3}{4}\hbar\tilde{\omega}$$

Two possible frequencies

$$\hbar\tilde{\omega} = \hbar\omega + \frac{2}{3}E_{\rm cm}(\omega) \pm \sqrt{\frac{4}{9}(E_{\rm cm}(\omega))^2 + \frac{4}{3}\hbar\omega E_{\rm cm}(\omega)}$$

Gaussian center-of-mass wave function

^{16}O with V_{lowk} (1.8 fm^{-1}, smooth) within CCSD



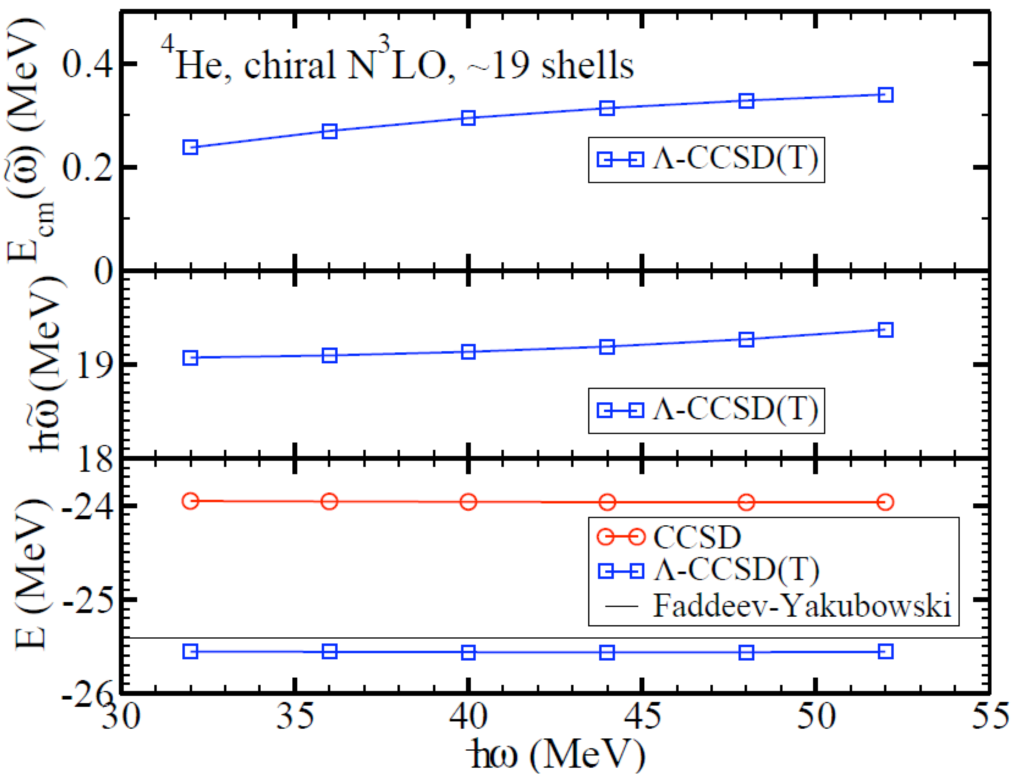
The intrinsic Hamiltonian does not reference the center-of-mass coordinate.

Yet, the resulting center-of-mass wave function is a Gaussian.

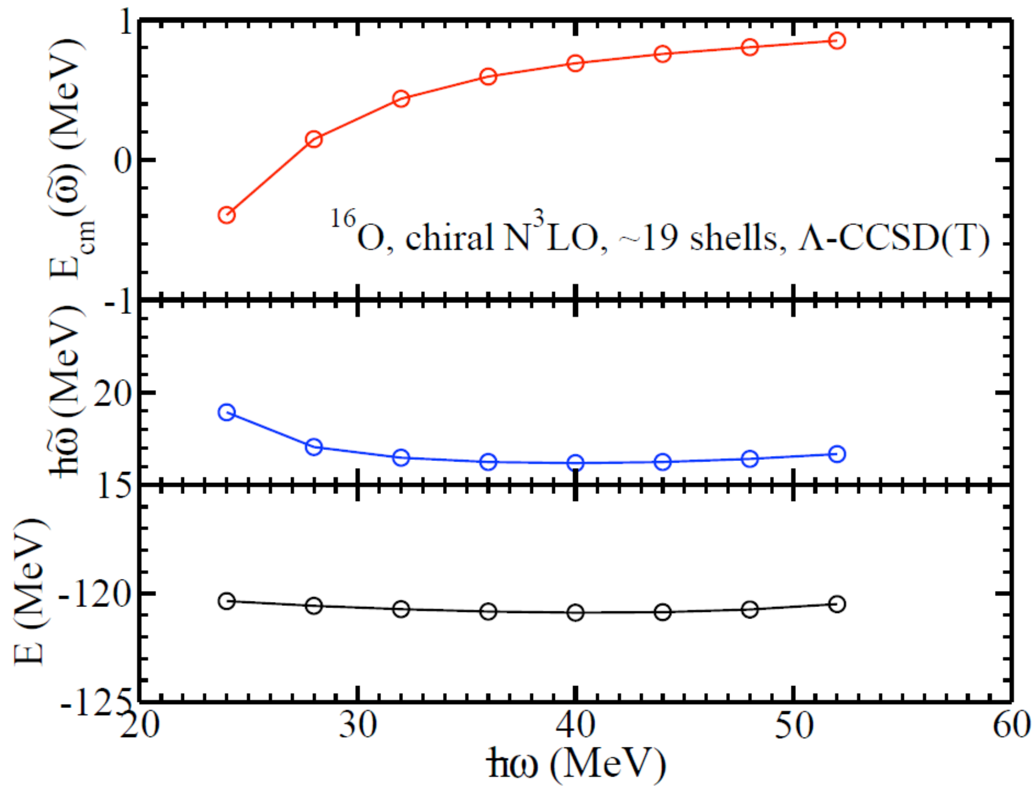
Approximate factorization also for “hard” interactions:

^{4}He, ^{16}O, and ^{48}Ca from Entem & Machleidt’s chiral N^{3}LO

^{4}He



^{16}O



Coupled-cluster wave function factorizes approximately.

Note: spurious states are separated by about 15 – 20 MeV >> E_{cm}.

No understanding of Gaussian CoM wave function (yet).

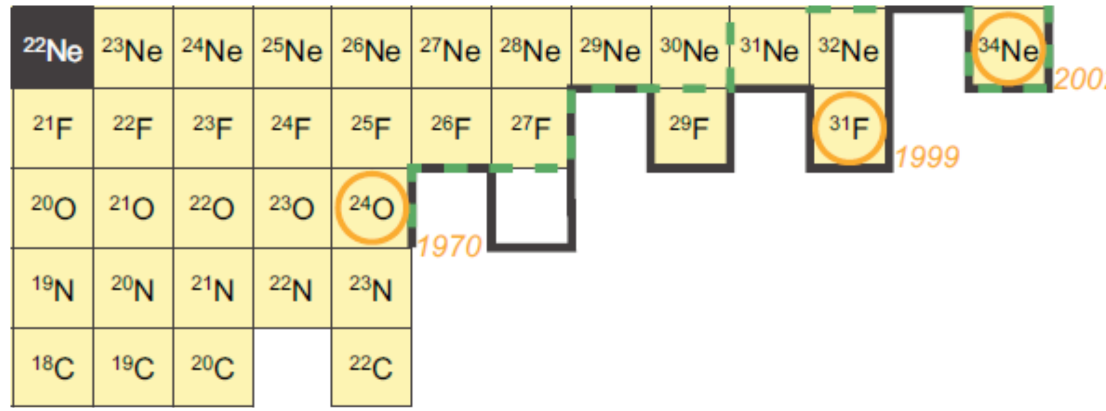
Nucleus	$\hbar\tilde{\omega}$
^{4}He	19.1 MeV
^{16}O	16.5 MeV
^{48}Ca	14.9 MeV

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

Neutron drip line in oxygen isotopes

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!?)



Theoretical situation

- USD interaction predicts stable ^{26,28}O (Brown)
- sf-pf shell calculation can reproduce data after adjusting TBME (Otsuka et al.)
- Shell model w/ continuum couplings employs two different interactions for oxygen isotopes near and far away from b-stability to reproduce data (Volya & Zelevinsky)
- Shell model with 3NF: ^{24}O is last bound isotope (Otsuka, Suzuki, Holt, Schwenk, Akaishi).

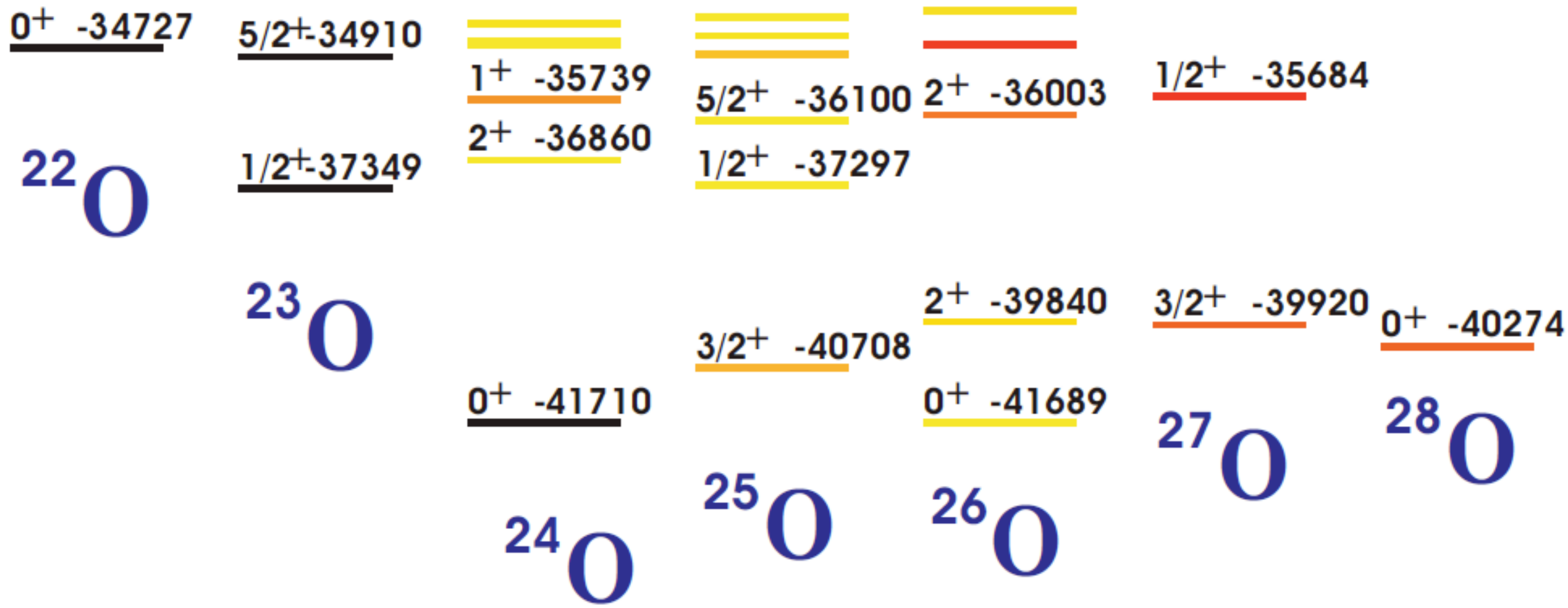
Most theoretical papers rule out a stable ^{28}O.

No approach flawless, i.e. no approach includes everything (continuum effects, 3NFs, no adjustments of interaction)

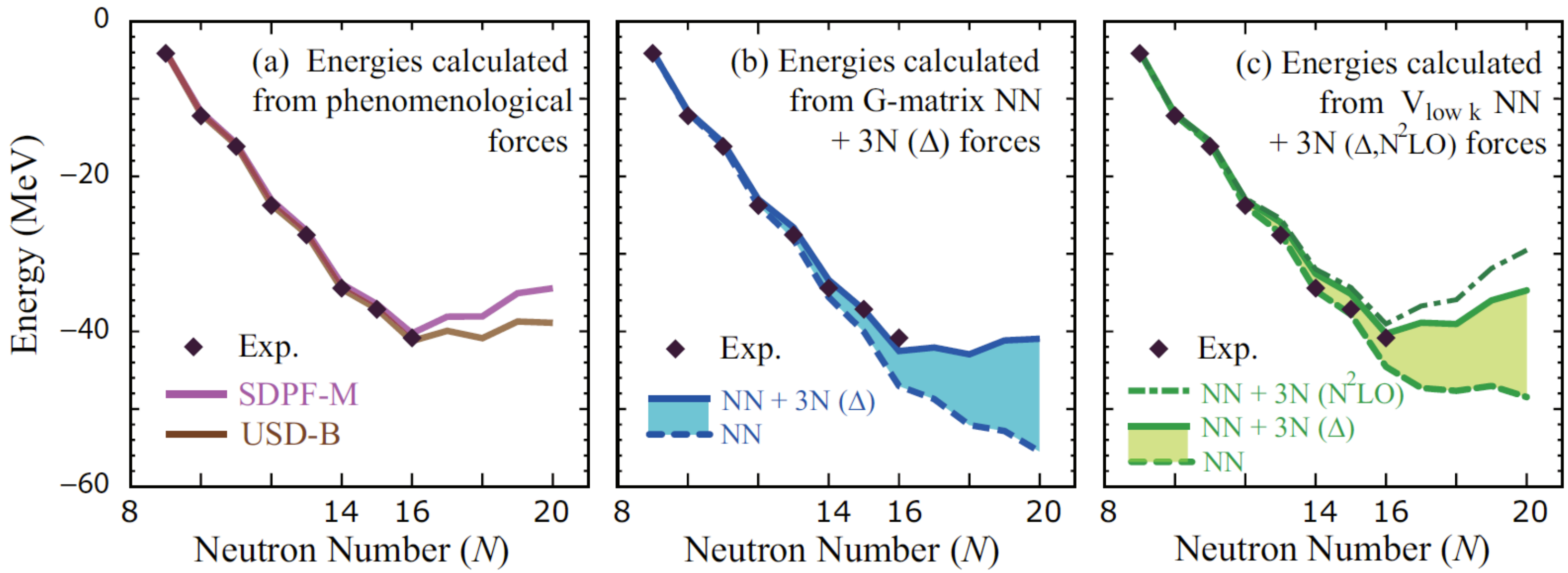
Theoretical difficulties: uncertainties in the effective interaction, quantify the resulting errors.

→ ab-initio calculations: coupled-cluster can address closed sub-shell nuclei ^{22,24,28}O with chiral interactions; study cutoff dependence

Examples of theoretical calculations

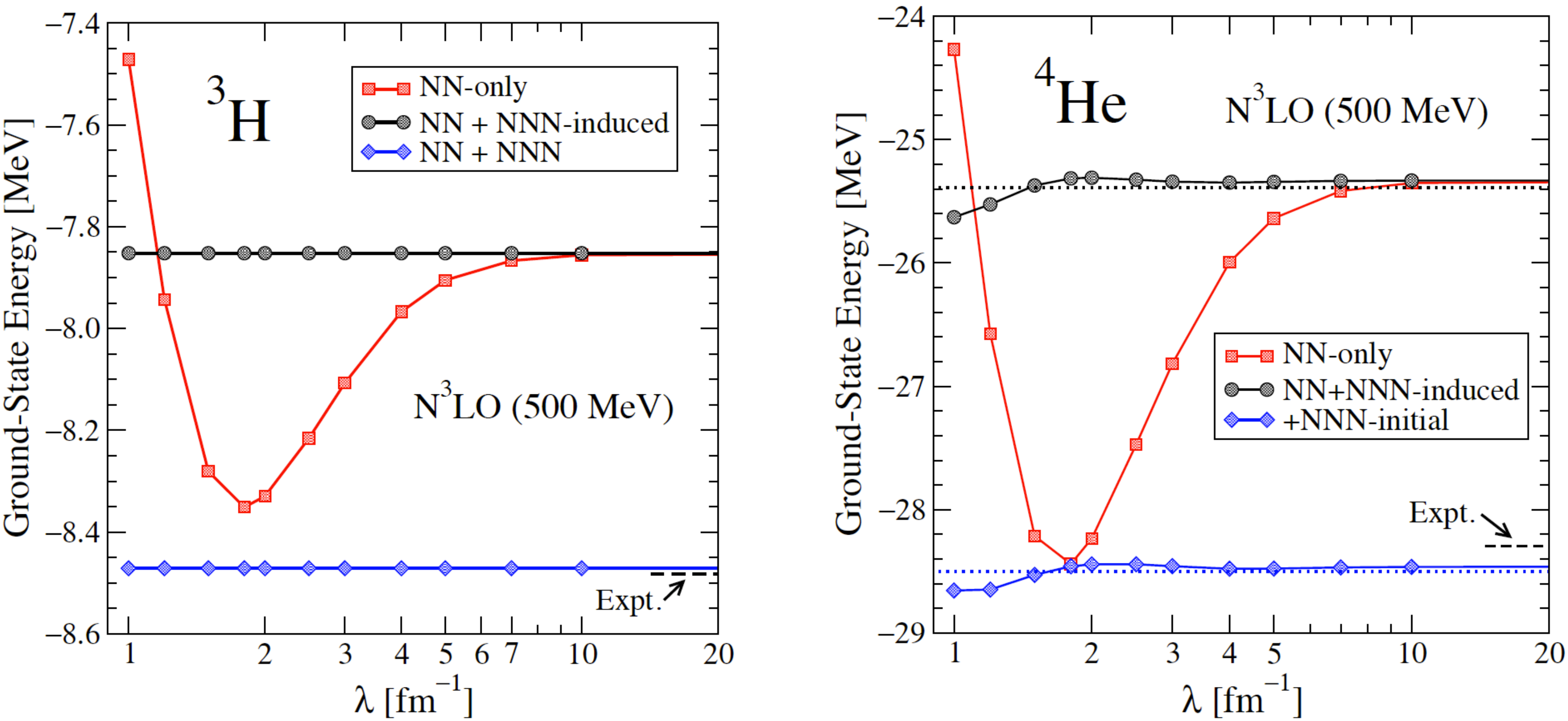


Volya & Zelevinsky, Phys. Rev. Lett. 94 (2005) 052501: Continuum + empirical interaction



Otsuka, Suzuki, Holt, Schwenk, Akaishi, arXiv:0908.2607: 3NF within small model space

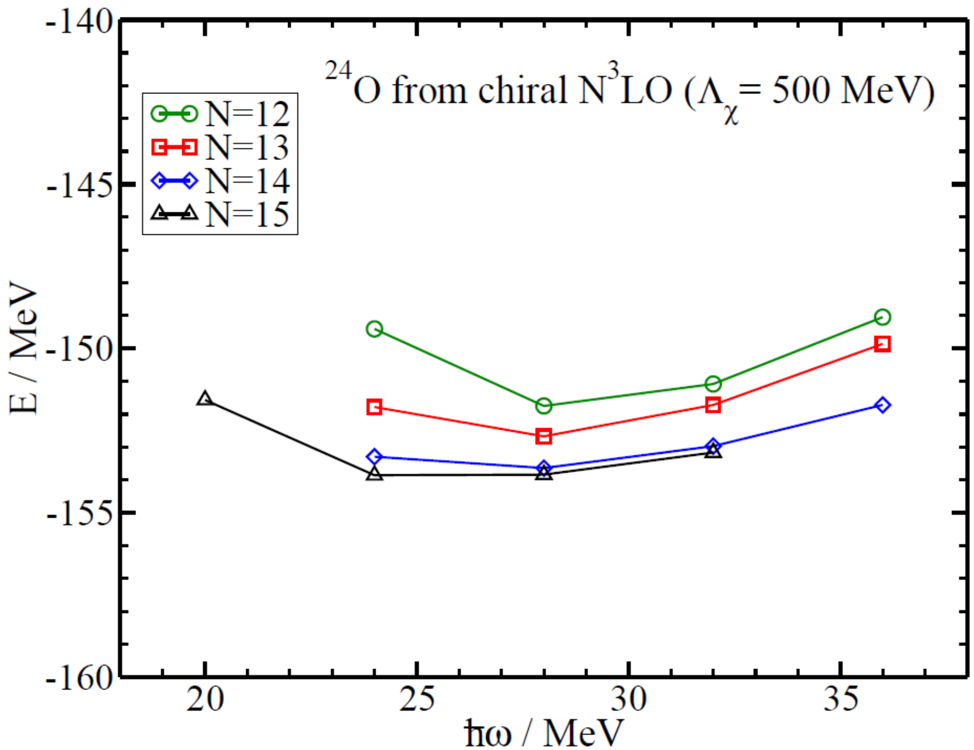
Solution of ^3H and ^4He with induced and initial 3NF

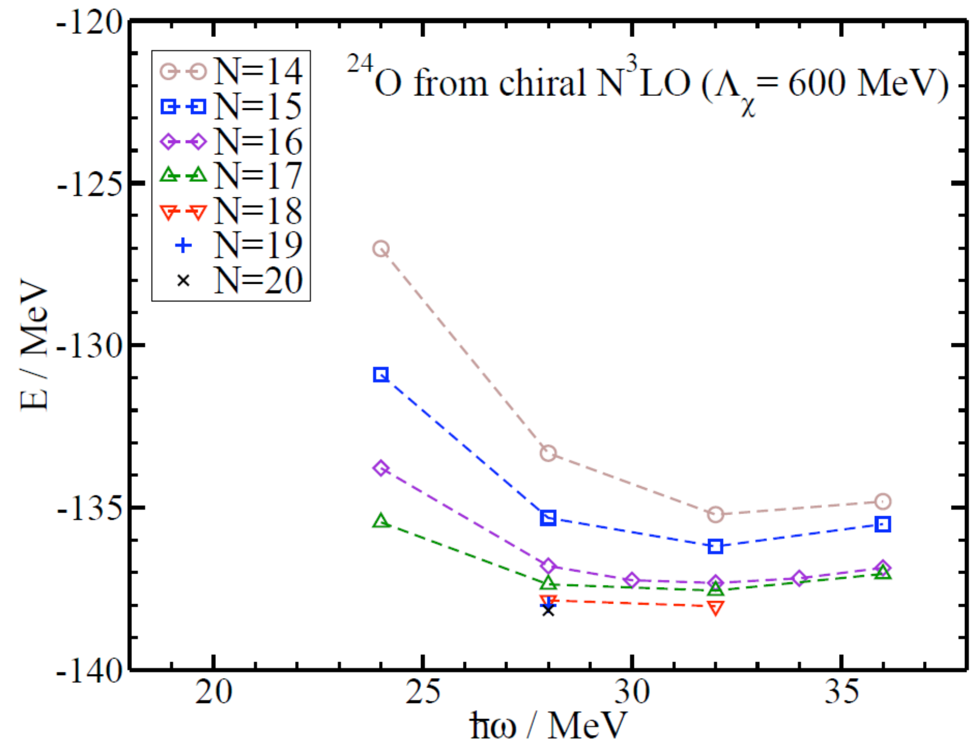


Jurgenson, Navratil & Furnstahl, Phys. Rev. Lett. 103, 082501 (2009)

Cutoff-dependence hints at missing physics, specifically short-ranged many-body forces.

Neutron-rich oxygen isotopes





Λ_χ=500 MeV potential converges in about 15 major oscillator shells

Λ_χ=600 MeV potential converges in about 20 shells

Summary of results

Energies	^{16}O	^{22}O	^{24}O	^{28}O
$(\Lambda_\chi = 500$ MeV$)$				
E_0	24.11	50.37	56.19	71.58
$\Delta E_{\rm CCSD}$	-144.77	-175.79	-190.39	-207.67
ΔE_3	-13.31	-19.22	-19.64	-19.85
E	-120.66	-144.64	-153.84	-155.94
$(\Lambda_\chi = 600$ MeV$)$				
E_0	22.08	46.33	52.94	68.57
$\Delta E_{\rm CCSD}$	-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	

← ~90% of correlation energy ($\Delta E_{\rm CCSD}$)

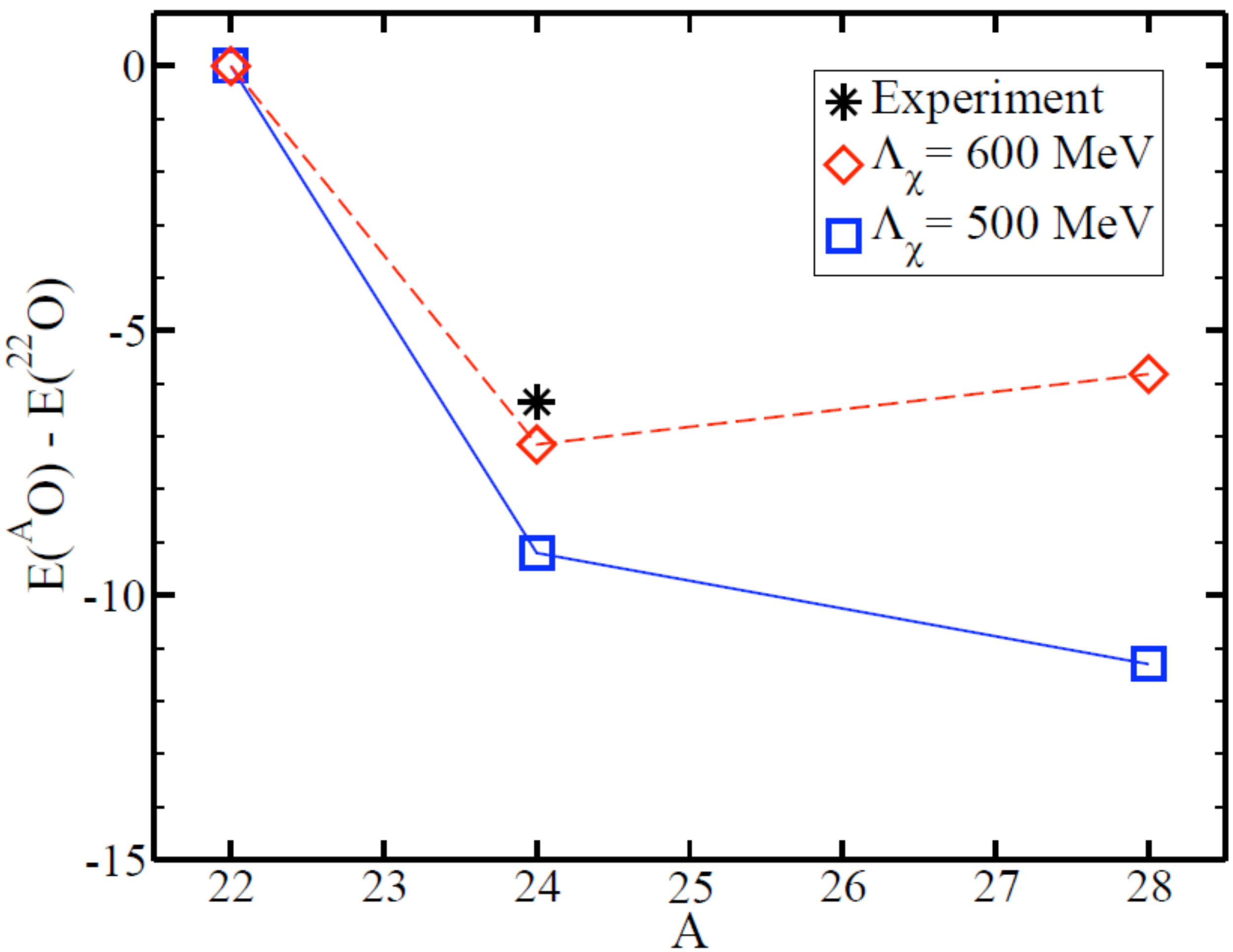
← ~10% of correlation energy (ΔE_3)

Estimate of theoretical uncertainties:

1. Finite model space ~2MeV
2. Truncation at triples clusters ~2MeV (educated guess)
3. Omission of three-nucleon forces (cutoff dependence) ~15MeV

[Hagen, TP, Dean, Horth-Jensen, Velamur Asokan, Phys. Rev. C 80, 021306(R) (2009)]

Is ^{28}O bound relative to ^{24}O?



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.

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

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

Neutron-rich oxygen isotopes:

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

Outlook

Towards heavier masses (Ni, Sn, Pb isotopes) & inclusion of 3NFs
Single-particle energies from ab-initio calculations
Drip-line nuclei (He, Li, O, Ca)
α-particle excitations (low-lying 0^+ states in doubly magic nuclei)