Coupled-cluster theory for medium-mass nuclei

Tentative solution of the center-of-mass problem

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Effective field theories and the many-body problem

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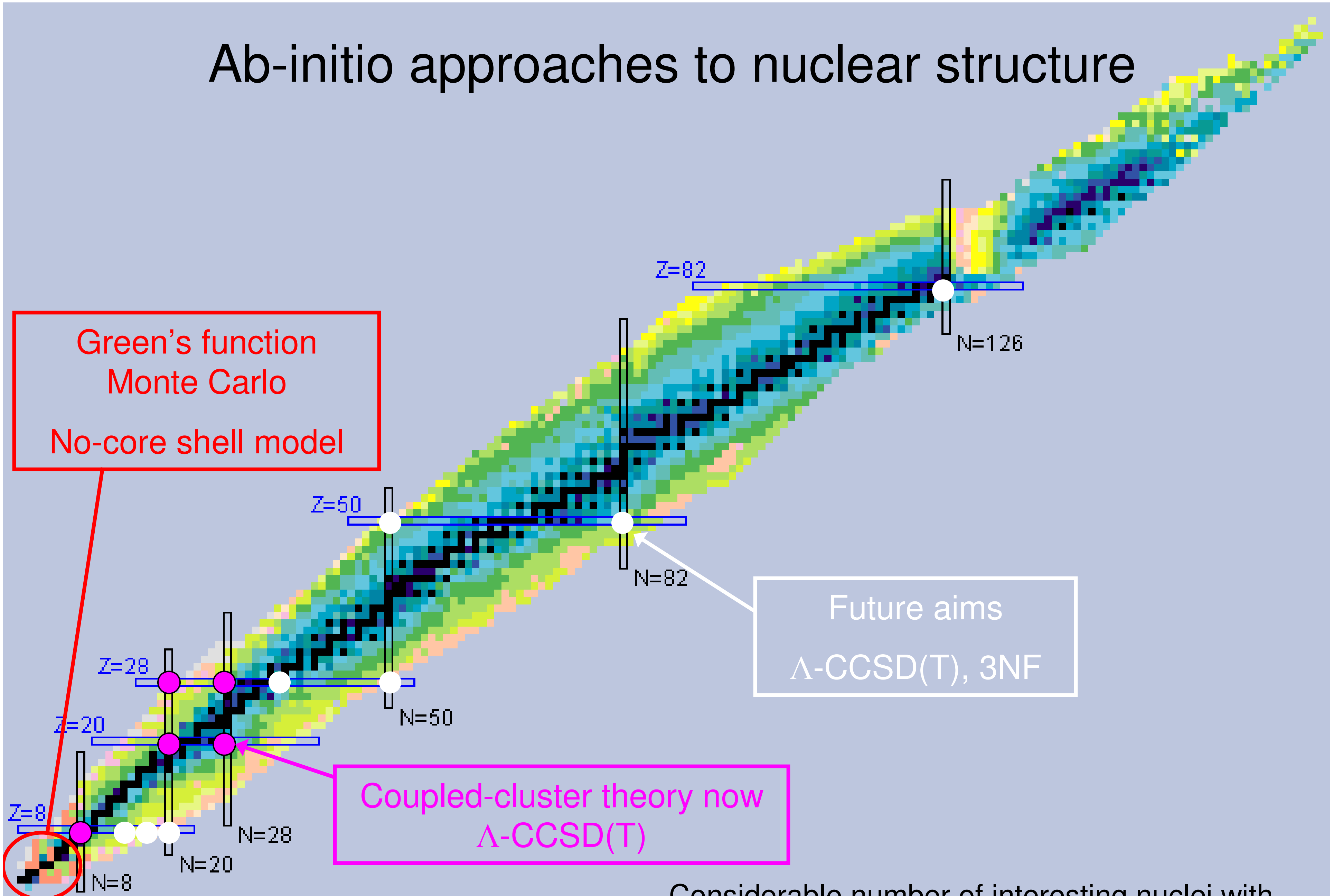
Overview

1. Introduction
2. Solution to the center-of-mass problem
3. Does ^{28}O exist?

Ab-initio approaches to nuclear structure



Considerable number of interesting nuclei with closed subshells…

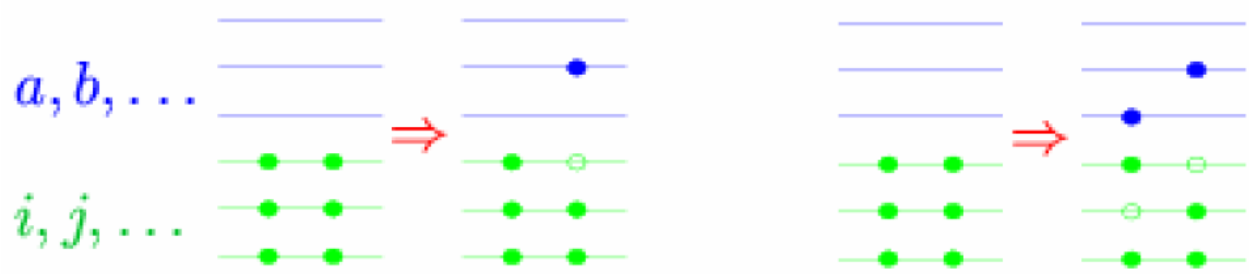
Coupled-cluster theory (CCSD)

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)

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



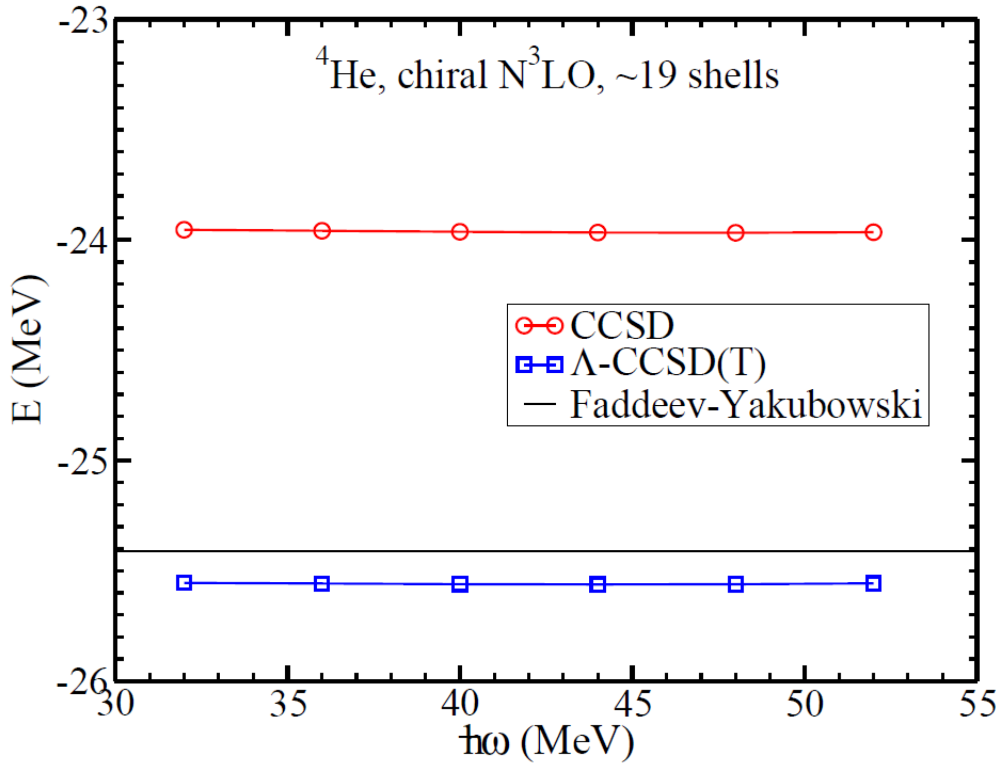
Coupled cluster equations

$$
\begin{aligned}
E &= \langle\Phi|\overline{H}|\Phi\rangle \\
0 &= \langle\Phi_i^a|\overline{H}|\Phi\rangle \\
0 &= \langle\Phi_{ij}^{ab}|\overline{H}|\Phi\rangle \\
\overline{H} &\equiv e^{-T}He^{T} = \left(He^{T}\right)_c = \left(H + HT_1 + HT_2 + \frac{1}{2}HT_1^2 + \ldots\right)_c
\end{aligned}
$$

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

Test of accuracy: ^{4}He from a chiral N^{3}LO [Entem & Machleidt]

Please note: The full potential is iterated within coupled-cluster



1. Results exhibit practically no dependence on the employed model space.
2. The coupled-cluster method, in its Λ-CCSD(T) approximation, overbinds by 150keV.
3. Independence of model space of N major oscillator shells with frequency ω:

   $N\hbar\omega > \hbar^2\lambda^2/m$ to resolve momentum cutoff λ

   $\hbar\omega < N\hbar^2/(mR^2)$ to resolve nucleus of radius R

Center-of-mass coordinate

The nuclear Hamiltonian is invariant under rotations and translations

Approach that preserves both symmetries:

☺ Jacobi coordinates

☹ Antisymmetrization scales as A! → limited to A<8 or so.

Antisymmetrization 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 $N\hbar\omega$ oscillator space, the wave function is guaranteed to factorize

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

Intrinsic wave function $\psi_{\rm in}$ invariant under translation

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

Please note: The factorization is key. The form of $\psi_{\rm cm}$ is irrelevant. It only needs to be the ground state of a suitably chosen center-of-mass Hamiltonian.

Center-of-mass coordinate (cont'd)

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

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

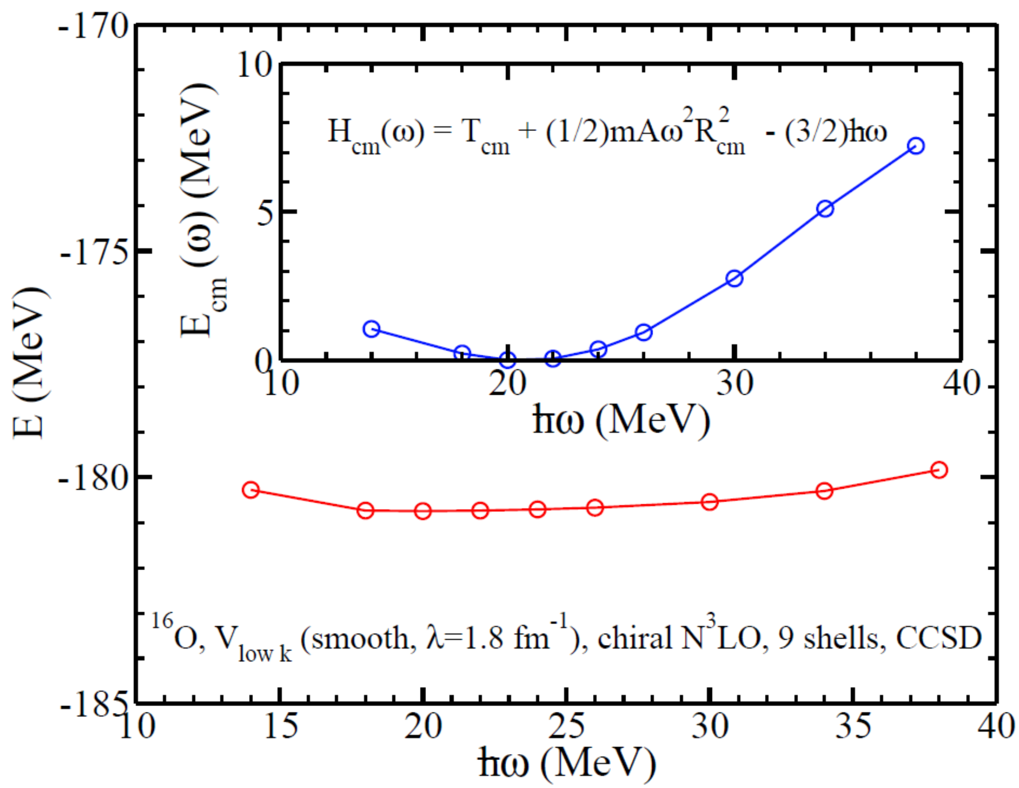
Please note:

1. To demonstrate the factorization, one (only) needs to find a suitable center-of-mass Hamiltonian whose ground state is ψ_{cm}.
2. NCSM employs harmonic oscillator Hamiltonian for H_{cm}
3. Of course:

Factorization can be guaranteed analytically in an $N\hbar\omega$ oscillator space.

Not working in such a space does not imply absence of factorization.

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



1. Hartree-Fock basis used. Not an $N\hbar\omega$ space
2. Ground-state energy varies little with frequency of oscillator basis.
3. Ground-state energy obviously independent of center-of-mass energy.
4. Center-of-mass energy generally nonzero → coupled-cluster wave function not eigenstate of $H_{cm}(\omega)$. [Beware of misconception: this does not imply that the wave function does not factorize.]

However:

1. Center-of-mass energy $E_{cm}(\omega) \equiv \langle H_{cm}(\omega)\rangle$ does vanish at $\hbar\omega \approx 20$MeV
2. **At $\hbar\omega \approx 20$MeV, the coupled-cluster wave function factorizes**
3. Approximate constancy of energy suggests approximate factorization for range of frequencies.
4. What is ψ_{cm}?

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

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

- Determine unknown frequency from from taking expectation value of identity

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

- Use

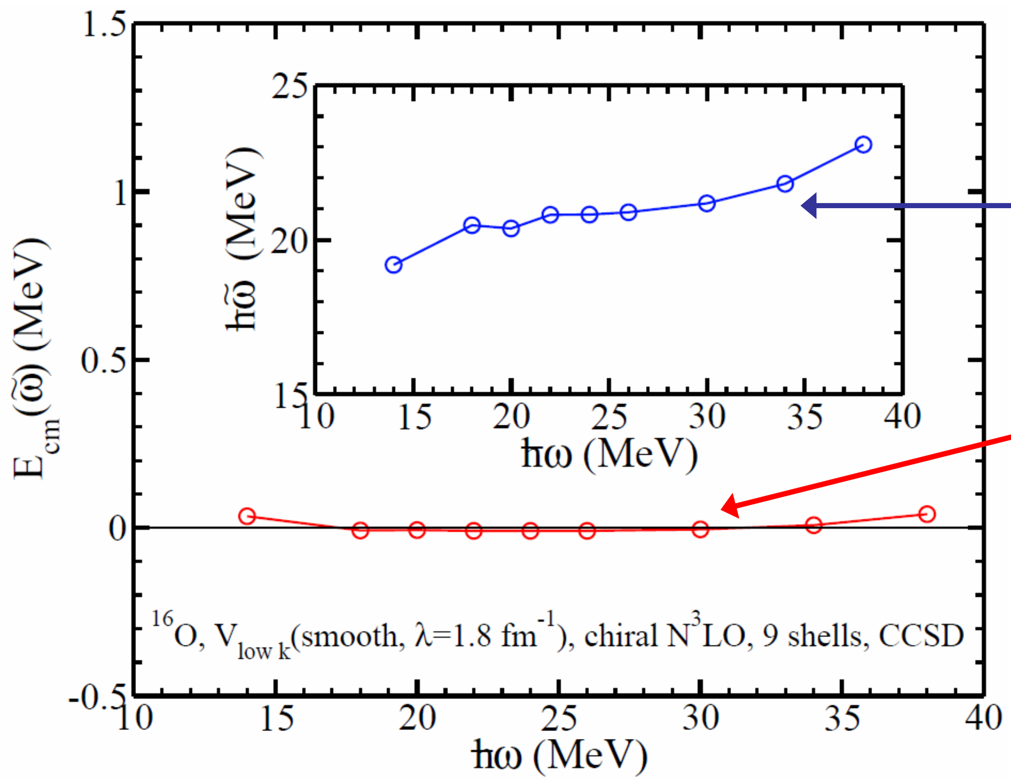
$$E_{\text{cm}}(\tilde{\omega}) = 0$$

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

Two possible solutions

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

Coupled-cluster wave function factorizes to a very good approximation!



Curve becomes practically constant in larger model spaces

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

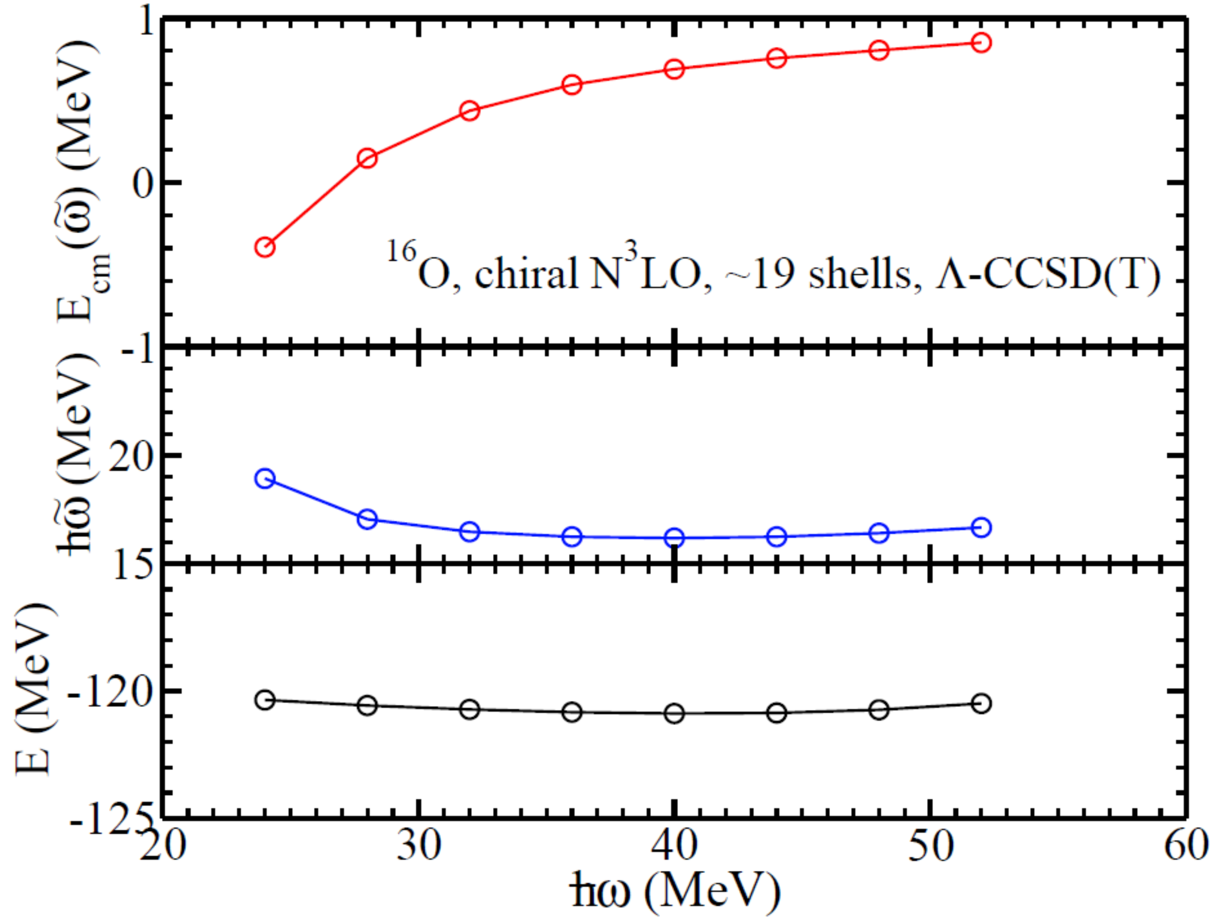
Note: spurious CoM excitations are of order 20 MeV >> E_{cm}.

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.

Factorization also for harder interactions: ^{16}O from Entem & Machleidt's chiral N^{3}LO



H_{cm} expectation value ~ 1 MeV

→ Spurious admixture ≲ 6% squared overlap.

Frequency of CoM Hamiltonian

(scale of spurious excitations)

Ground-state energy

Coupled-cluster wave function factorizes approximately.

Note: spurious states are separated by about 16MeV >> E_{cm}.

No solid understanding of Gaussian CoM wave function (yet).

Intermission

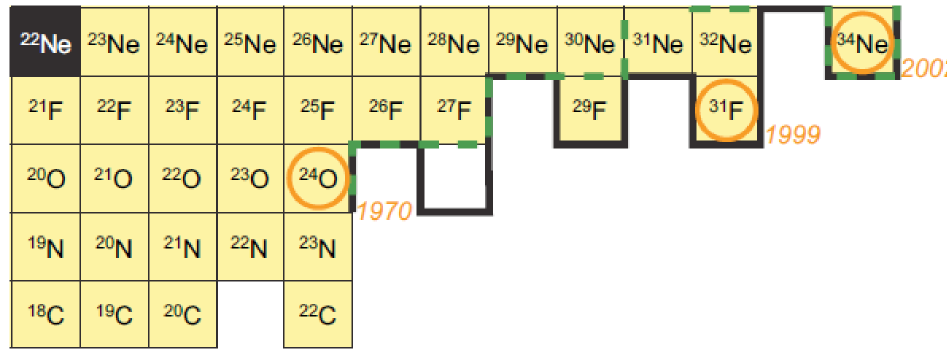
1. Numerical evidence for factorization of coupled-cluster wave function as product of intrinsic and CoM wave function.
2. CoM wave function is approximate Gaussian whose frequency is not identical to the underlying oscillator basis
3. Simple procedure yields frequency of Gaussian CoM wave function
4. Results can be checked (and utilized?) by NCSM

Arguments you might have heard (?)	**More precise (and correct) statement**
Only an $N\hbar\omega$ space can provide a separation of intrinsic and center-of-mass coordinates	In an $N\hbar\omega$ space, the separation of intrinsic and center-of-mass coordinates is guaranteed
A nonzero expectation value of H_{cm} indicates center-of-mass problems	State in question is not an eigenstate of this particular center-of-mass Hamiltonian. Does not address question of factorization.
Method X breaks translational invariance	Everyone does (since wave function not eigenstate of total momentum). The question is whether method X can factorize into intrinsic and CoM state

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

• sf-pf shell calculation can reproduce data only after adjusting TBME (Otsuka et al.)

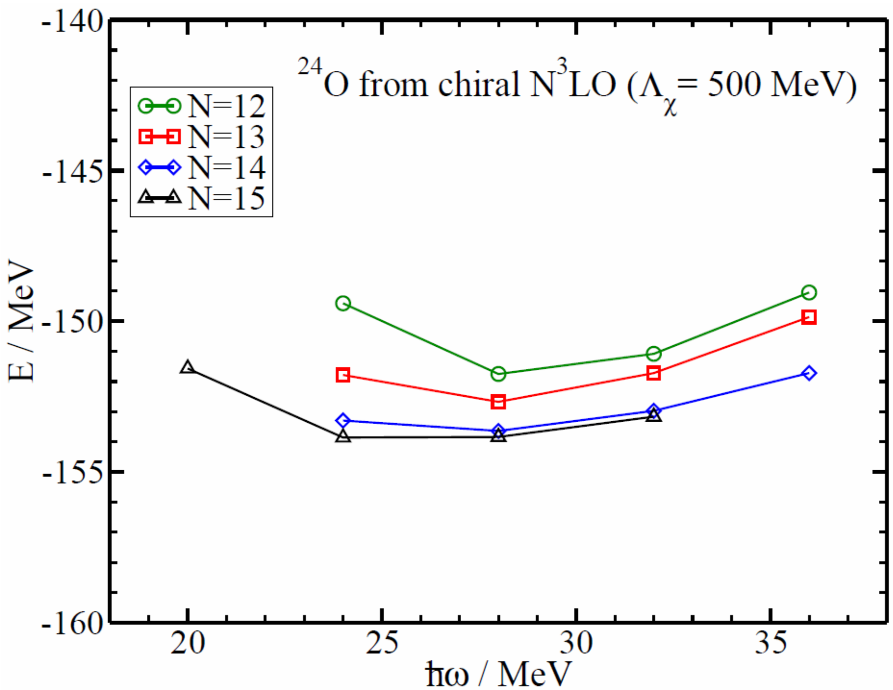
• Shell-model w/ continuum couplings employs two different interactions for oxygen isotopes near and far away from b-stability to reproduce data (Volya & Zelevinsky)

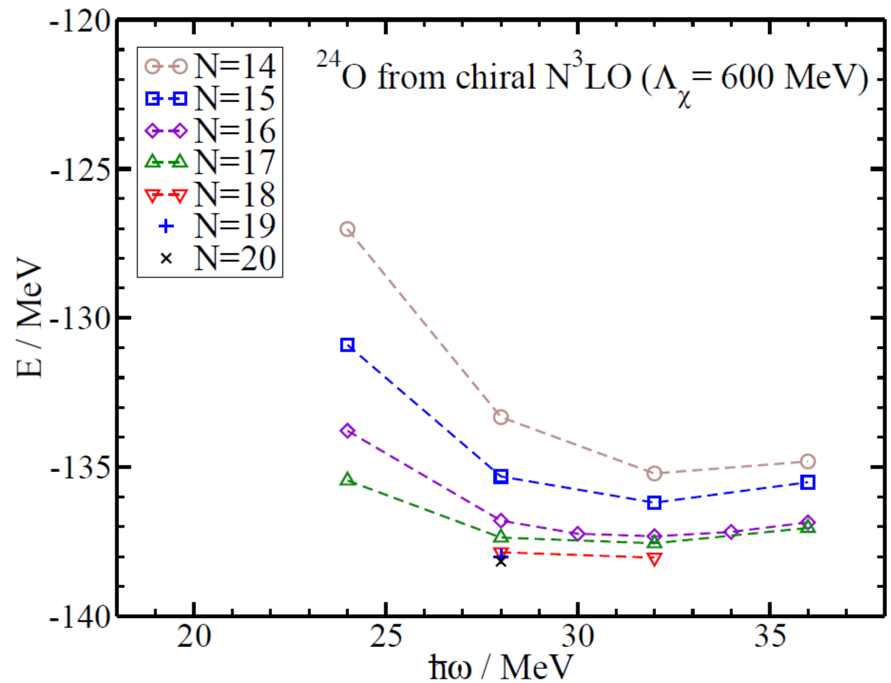
It seems that most theoretical papers rule out a stable ^{28}O

Theory has obvious difficulty due to uncertainties in the effective interaction, and the difficulty to 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

Neutron-rich oxygen isotopes





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

Λ=600 MeV potential converges in about 20 shells

Summary of preliminary results

Energies	^{16}O	^{22}O	^{24}O	^{28}O
$(\Lambda_\chi = 500 \text{ MeV})$				
E_0	24.11	50.37	56.19	71.58
ΔE_{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
$(\Lambda_\chi = 600 \text{ MeV})$				
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	

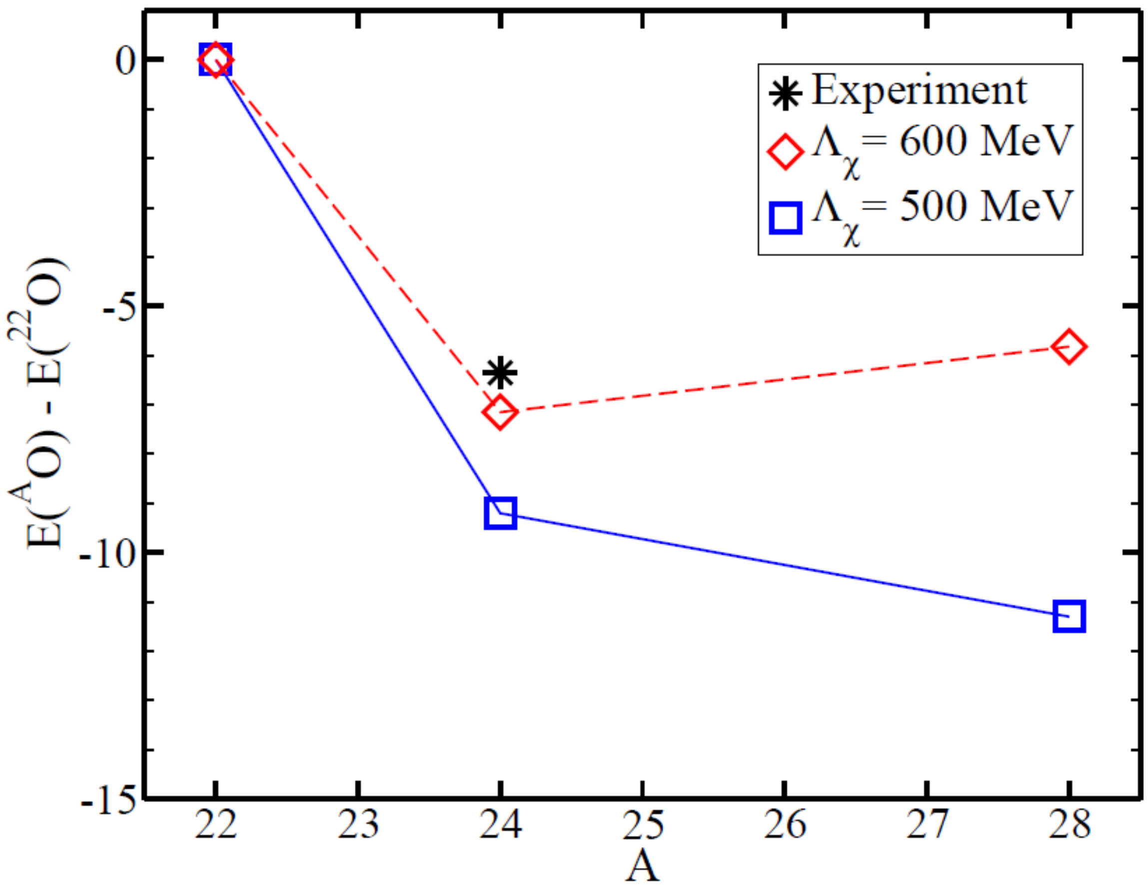
← ~90% of correlation energy

← ~10% of correlation energy

Estimate of theoretical uncertainties:

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

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



Too close to call. Theoretical uncertainties >> differences in binding energies.

Entem & Machleidt’s chiral potentials 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 and outlook

Medium-mass nuclei:

- Demonstration that coupled-cluster wave function factorizes into product of intrinsic and center-of-mass state.

Neutron-rich oxygen isotopes:

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