Coupled-cluster theory for medium-mass nuclei

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Overview

1. Coupled-cluster theory
2. Benchmark calculations
   [Hagen, Dean, Hjorth-Jensen, TP, Schwenk, arxiv:0707.1516 → Phys. Rev. C]
3. Correct scaling with system size – size (extensivity) matters
   [Dean, Hagen, Hjorth-Jensen, TP, Schwenk, arxiv:0709.0449]
4. Three-nucleon forces
   [Hagen, TP, Dean, Schwenk, Nogga, Wloch, Piecuch, Phys. Rev. C 76 (2007) 034302]
5. Weakly bound and unstable nuclei – ab initio calculation of life times
   [Hagen, Dean, Hjorth-Jensen, TP, nucl-th/0610072 → Phys. Lett. B]

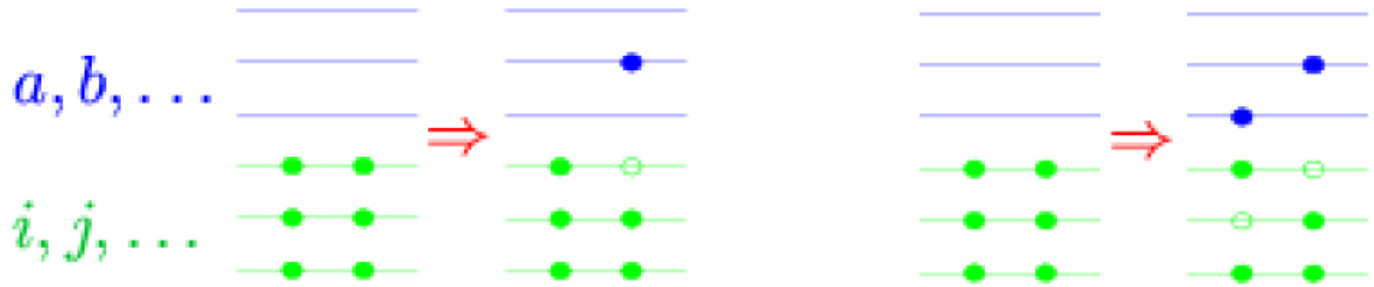
Coupled-cluster theory (CCSD)

Ansatz:

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

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

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



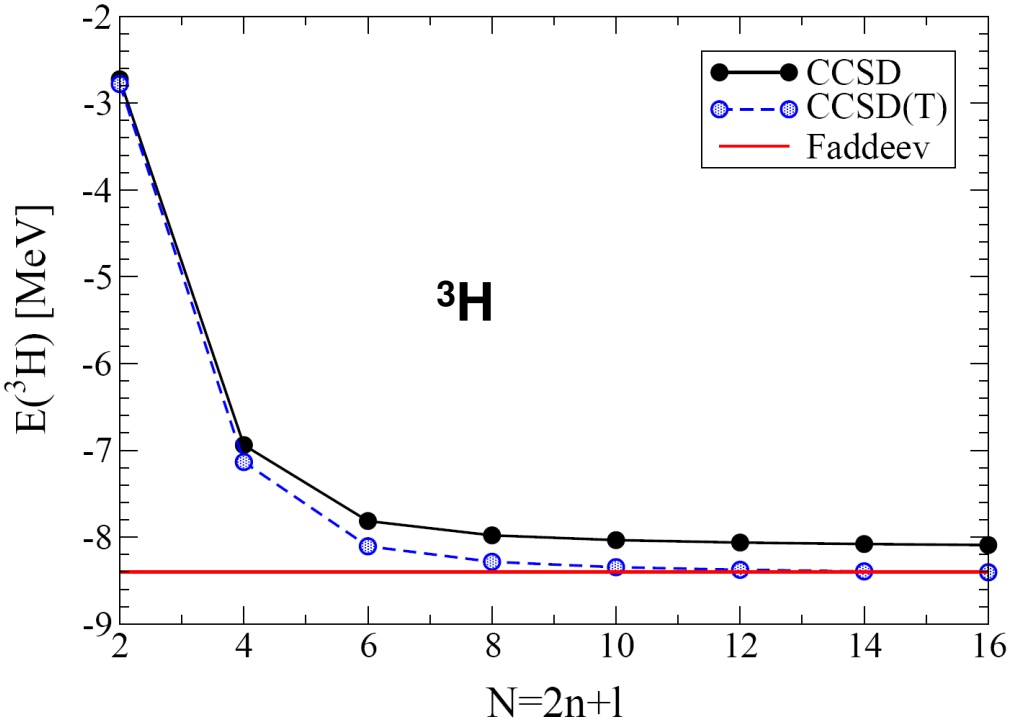
Coupled cluster equations

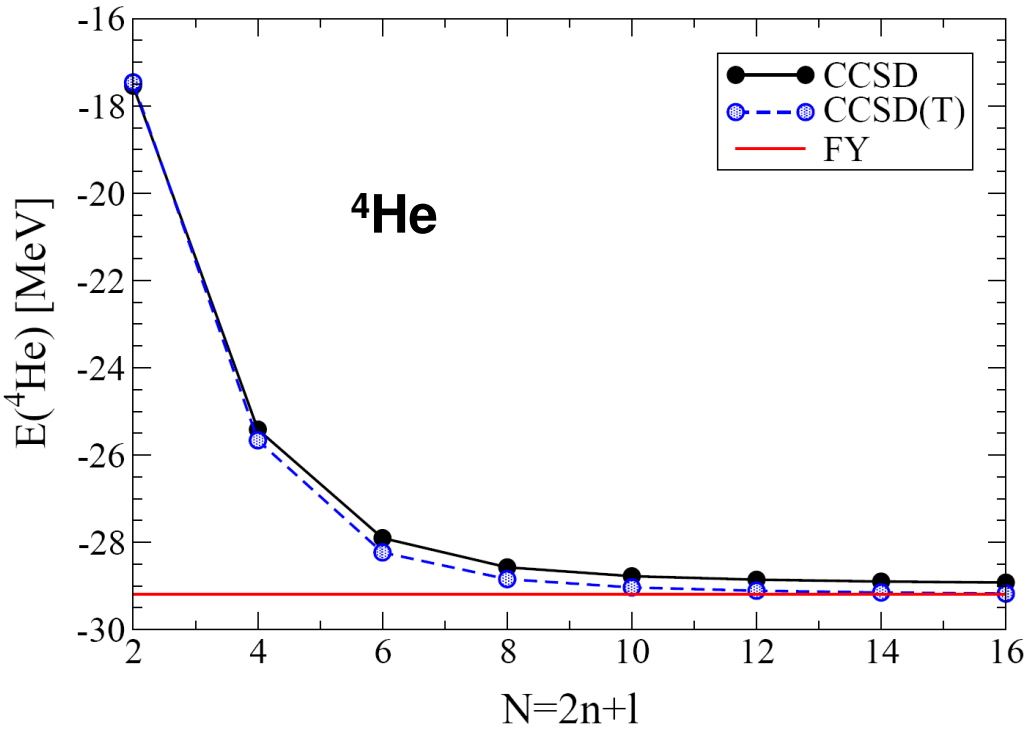
$$
\begin{aligned}
E &= \langle\Phi|\overline{H}|\Phi\rangle \\
0 &= \langle\Phi_i^a|\overline{H}|\Phi\rangle \\
0 &= \langle\Phi_{ij}^{ab}|\overline{H}|\Phi\rangle
\end{aligned}
$$

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

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

Coupled-cluster theory meets benchmarks for ^{3}H and ^{4}He



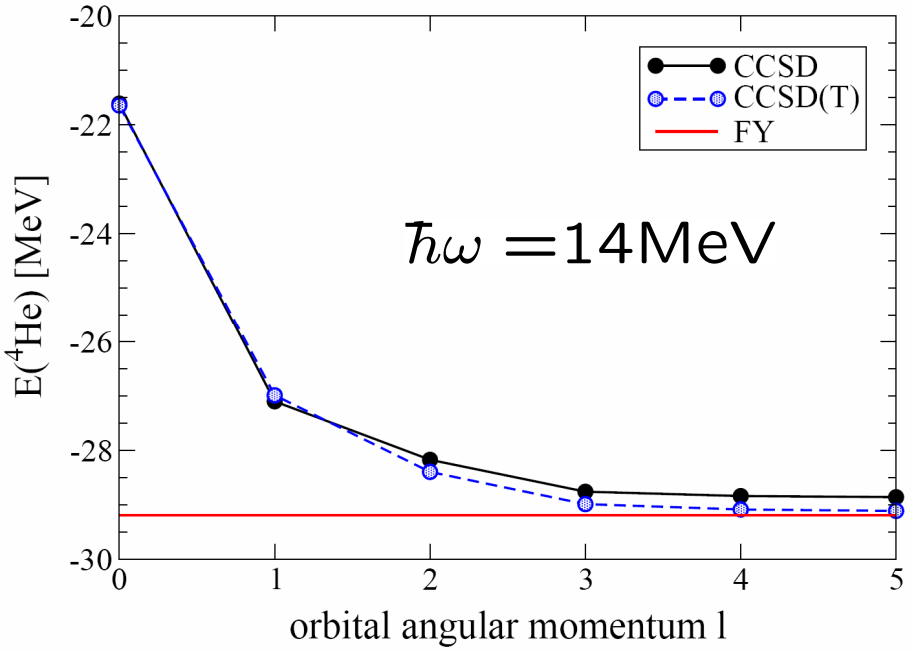


Interaction: $V_{low\text{-}k}$ with Λ=1.9 fm^{-1} from Argonne V18

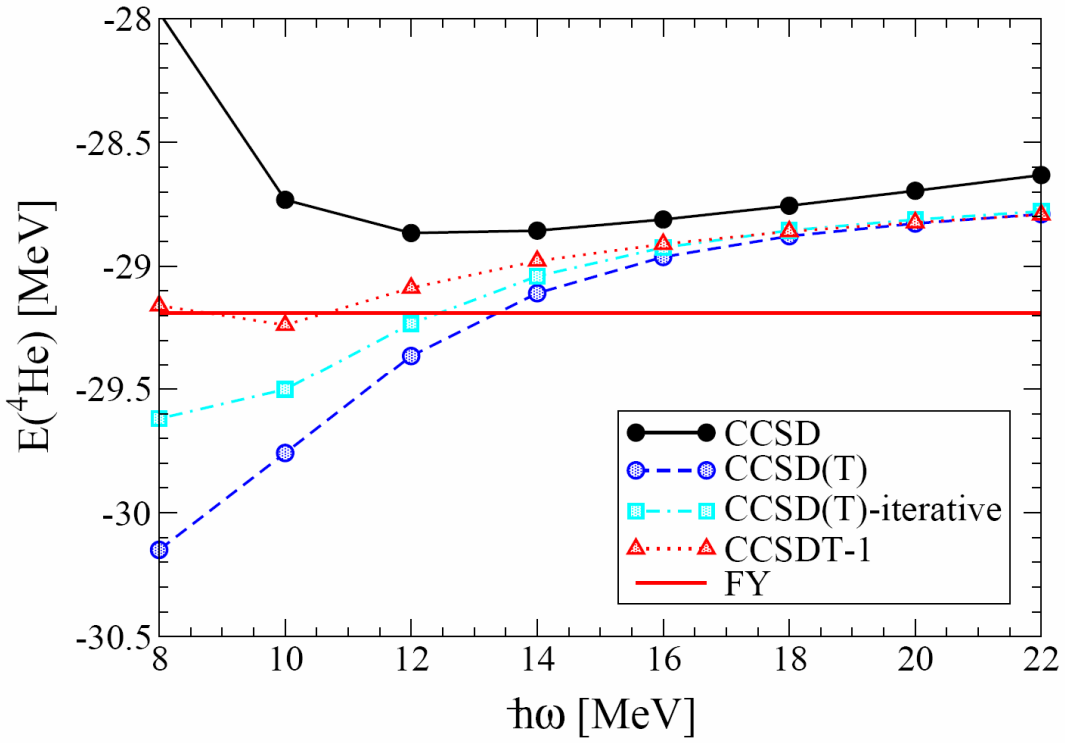
Exact results: Faddeev and Faddeev-Yakubowsky calculations

Main result: benchmarks are met.

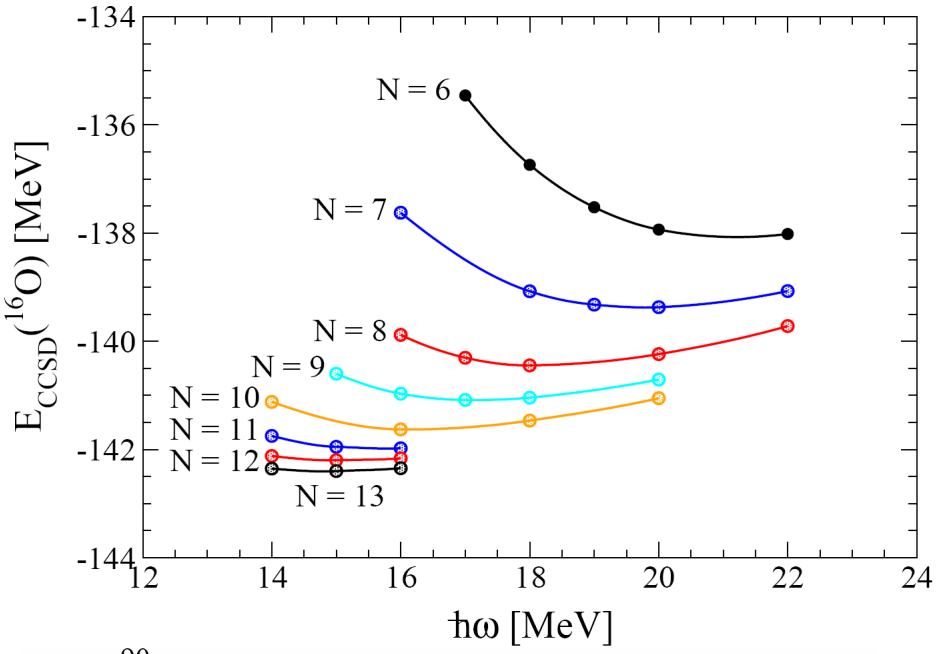
Convergence and hw-dependence for ^{4}He

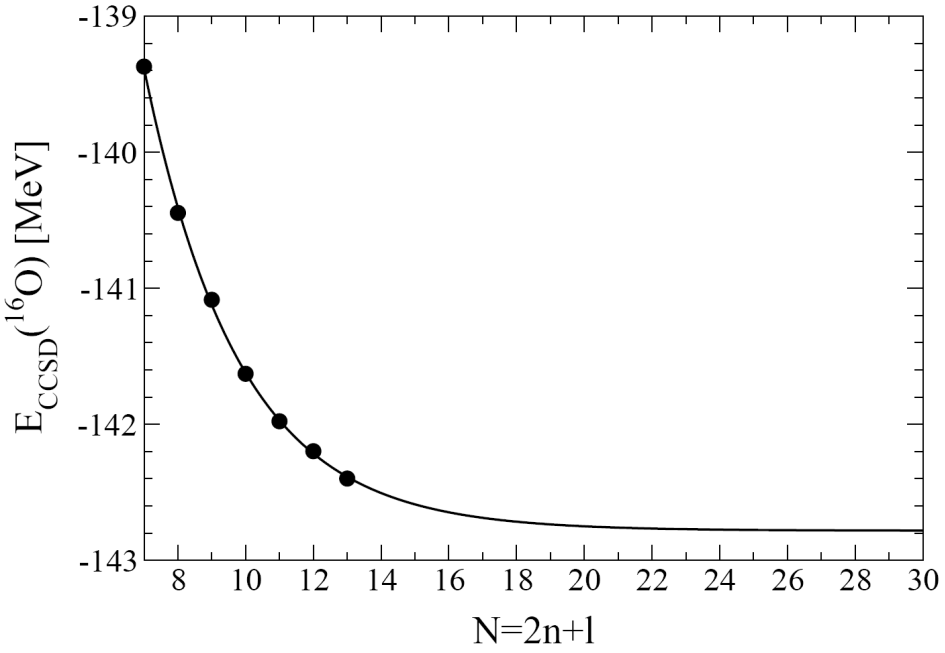


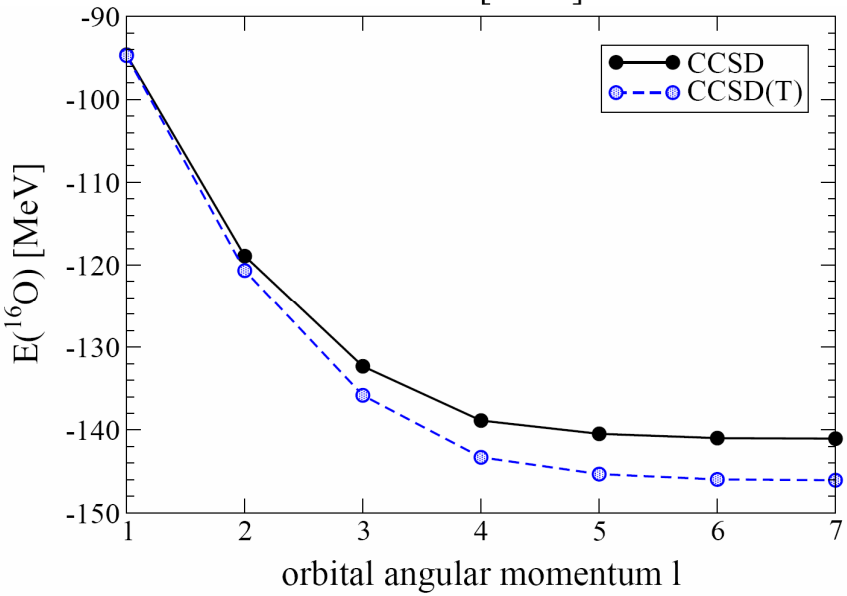
Perturbative and non-iterative triples correction diverge at small hw. Self-consistent corrections perform better.



^{16}O with $V_{low\text{-}k}$





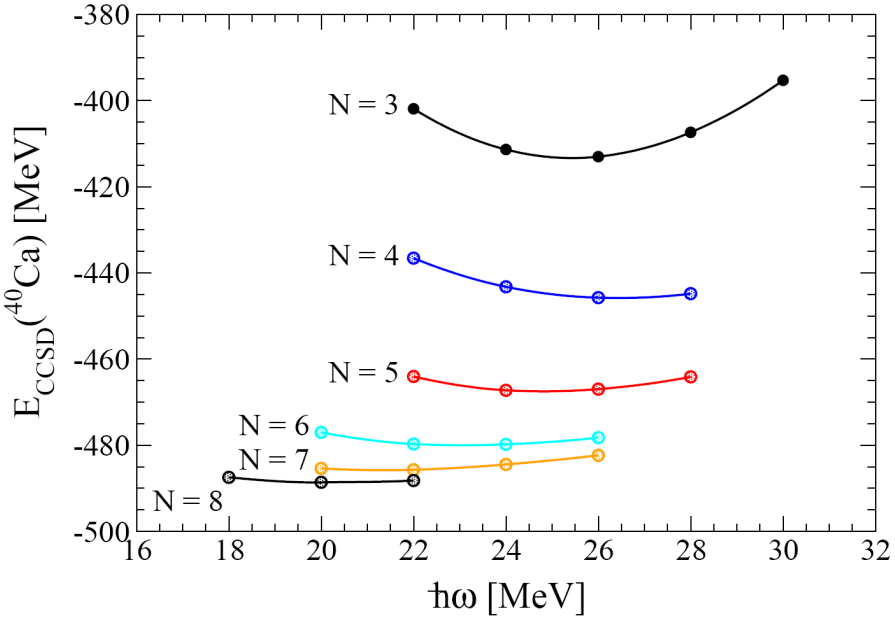


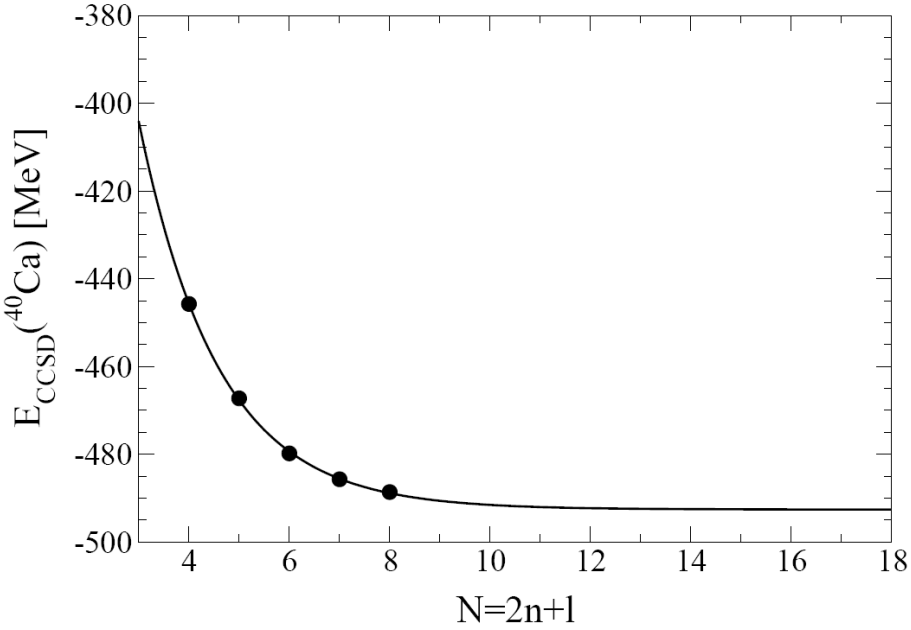
Interaction: $V_{low\text{-}k}$ with Λ=1.9 fm^{-1} from Argonne V18 (no three-body forces)

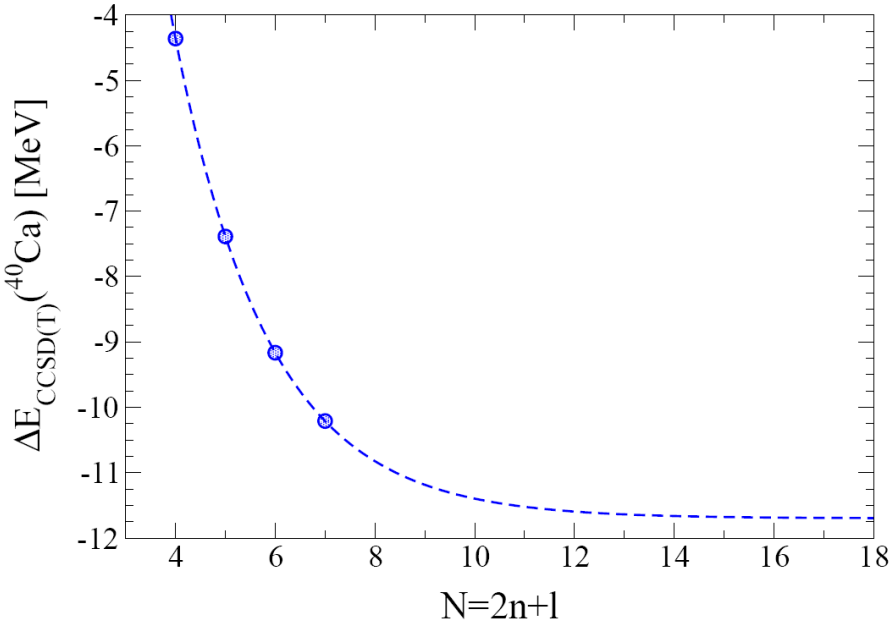
Model space: about 1000 single-particle orbitals

Main result: accuracy estimate about 1%

Coupled-cluster results for ^{40}Ca with $V_{low\text{-}k}$







Accuracy estimate: 1% level.

	^{4}He	^{16}O	^{40}Ca
E_0	-11.8	-60.2	-347.5
ΔE_{CCSD}	-17.1	-82.6	-143.7
$\Delta E_{\mathrm{CCSD(T)}}$	-0.3	-5.4	-11.7
$E_{\mathrm{CCSD(T)}}$	-29.2	-148.2	-502.9
exact (FY)	-29.19(5)		

^{40}Ca in particle-hole truncated no-core shell model

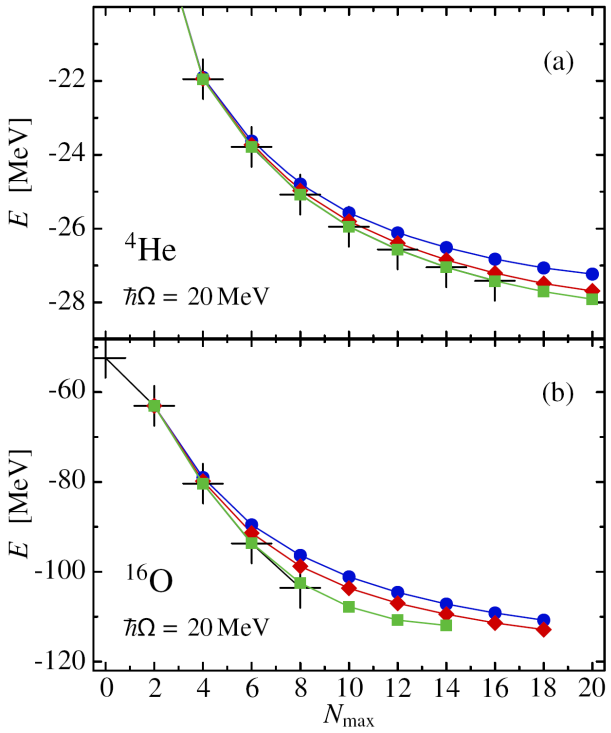


FIG. 3 (color online). Convergence of the ground-state energy for ^{4}He (a) and ^{16}O (b) versus N_{max} obtained using V_{UCOM}. Shown are three data sets corresponding to model spaces with up to $2p2h$ (●), $3p3h$ (◆), and $4p4h$ states (■), respectively. Black crosses (+) indicate the results of full NCSM calculations. Lines to guide the eye.

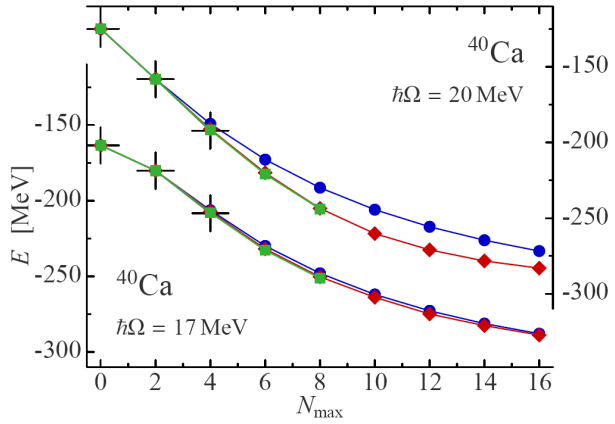


FIG. 4: (color online) Convergence of the ground-state energy of ^{40}Ca as function of model-space size N_{max} for $\hbar\Omega$ = 17 MeV (lower curves, left-hand axis) and 20 MeV (upper curves, right-hand axis) using the V_{UCOM} interaction. Symbols as described in Fig. 3.

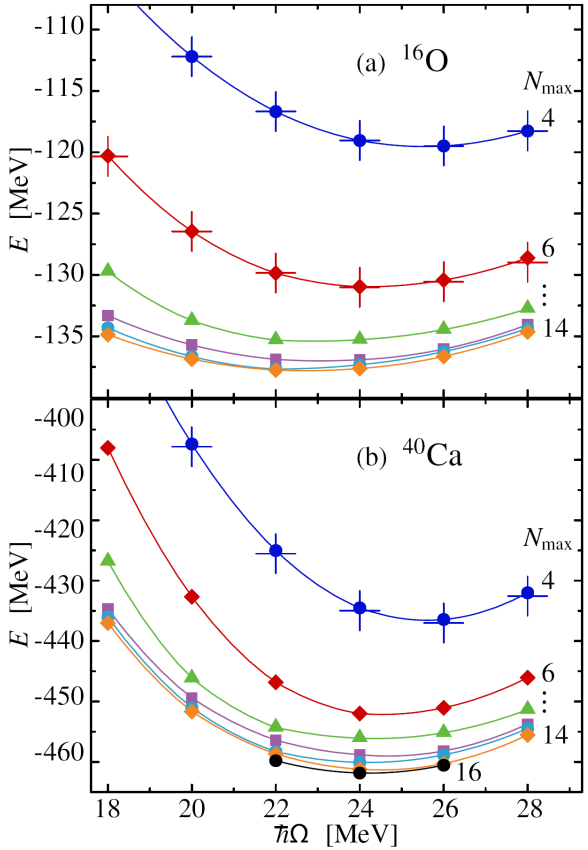


FIG. 5 (color online). Ground-state energy of ^{16}O (a) and ^{40}Ca (b) as function of the harmonic-oscillator frequency $\hbar\Omega$ for different model-space sizes up to N_{max} = 16 obtained with the $V_{low\,k}$ interaction. For ^{16}O up to $4p4h$ configurations are included, for ^{40}Ca up to $3p3h$. Crosses indicate the results of full NCSM calculations.

[Roth and Navratil, Phys. Rev. Lett. 99 (2007) 092501]

Convergence with respect to particle-hole truncation?

Which result is more accurate?

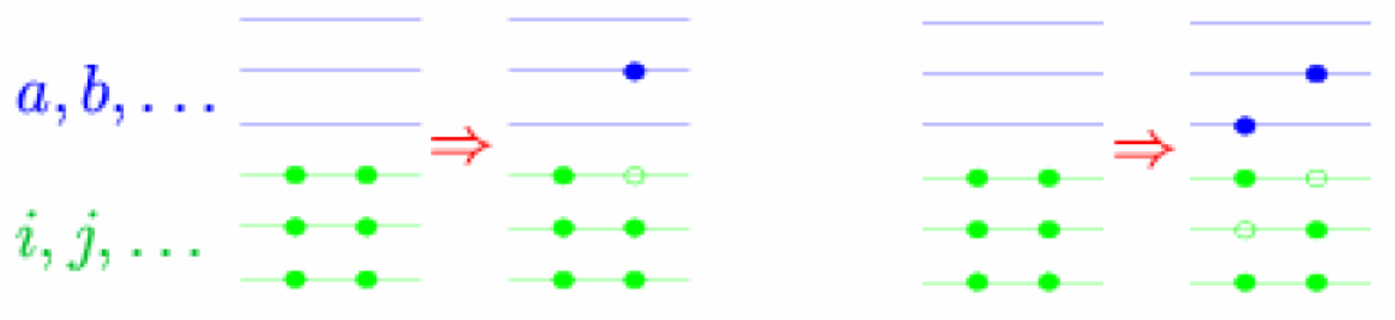
1. The case has no merit. (Neither approach agrees with the experimental value.)

	^{16}O	^{40}Ca
CCSD(T)	-148.2	-502.9
NCSM (4p4h/3p3h)	-137.8	-461.8

2. Both approaches rest on approximations. Let's understand their quality!

Truncated NCSM	**Coupled-cluster approach**
Model space restricted to np-nh excitations	Similarity transform with 2p-2h clusters
3p3h truncation level; 4p4h excitations only in small model space	CCSD + triples correction at large model space
Truncation not size consistent	Size extensive

Particle-hole truncation



Truncated No-Core Shell Model: Diagonalization of Hamiltonian matrix in Hilbert space of 0p-0h, 1p-1h, … 3p-3h excited states

Relationship between shell model and CC amplitudes

$$B_1 = T_1$$

$$B_2 = T_2 + \frac{1}{2}T_1^2$$

$$B_3 = T_3 + T_2T_1 + \frac{1}{6}T_1^3$$

$$B_4 = T_4 + T_3T_1 + \frac{1}{2}T_2^2 + \frac{1}{2}T_2T_1^2 + \frac{1}{24}T_1^4$$

$\cdots$

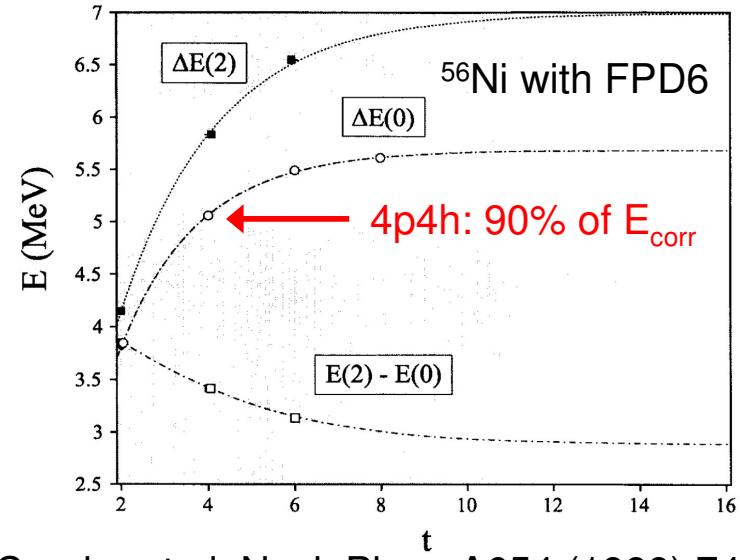
CCSD

CR-CCSD(T)

"Disconnected quadruples"

"Connected quadruples"

Quality of particle-hole truncation



[Caurier et al, Nucl. Phys. A654 (1999) 747c]

Figure 4. Gain in correlation energy for $J = 0, 2$ and excitation energy for $J=2$ in ^{56}Ni as a function of truncation level t (see text). Diamonds, crosses and squares are exact results. Continuous lines are exponential approximants.

ΔG	−2	−1	0	1	2
S_0	0.022	0.332	0.825	0.917	0.949
CCSD	−3.218	−2.048	−1.509	−1.202	−1.002
CR-CC(2,3)	−4.355	−2.437	−1.686	−1.298	−1.060
CR-CC(2,4)	−4.253	−2.415	−1.679	−1.295	−1.059
CISD	−2.148	−1.652	−1.327	−1.104	−0.943
CISDT	−2.706	−1.946	−1.488	−1.199	−1.004
CISDTQ	−4.013	−2.548	−1.758	−1.334	−1.079
Full CI	−10.198	−3.868	−1.909	−1.370	−1.091

[Horoi et al, Phys. Rev. Lett. 98, 112501 (2007)]

3p-3h truncation usually not very accurate

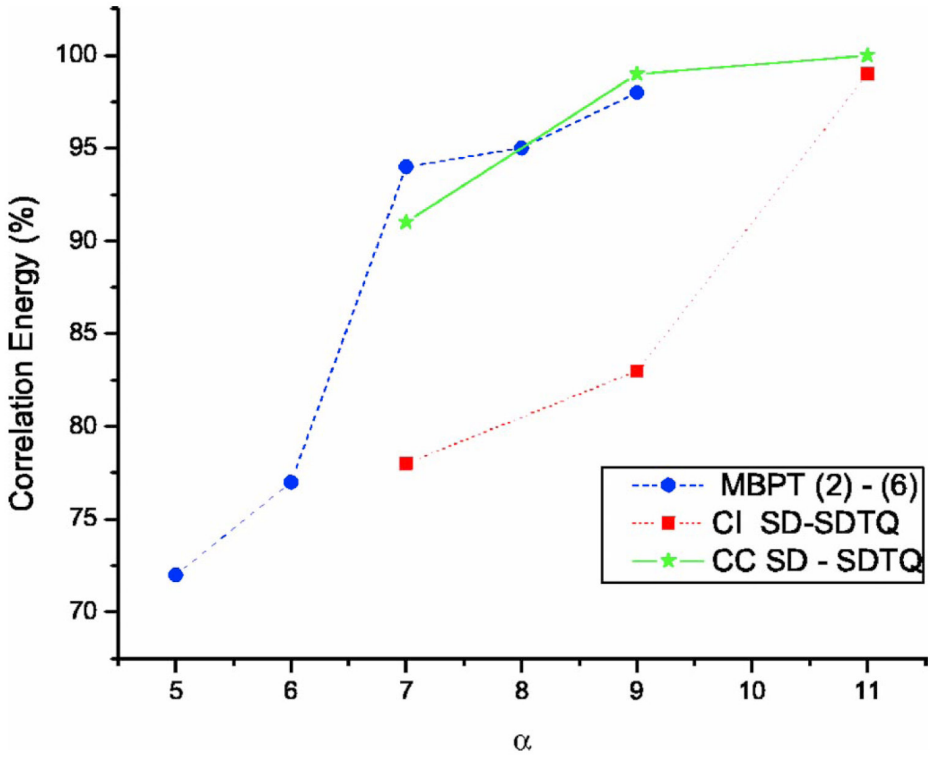


FIG. 3. (Color online) Performance of theories for the correlation energy in small molecules. Graphed is the percentage of the full correlation energy achieved by the CI, CC, and MBPT theories, as a function of the level of approximation. To facilitate comparisons, the ordinate gives the size-scaling parameter of the approximation $\alpha = \alpha_n + \alpha_N + \alpha_{it}$ in the computational cost function $n^{\alpha_n} N^{\alpha_N} N_{it}^{\alpha_{it}}$. Shown are MBPT (solid circles), approximations (2)–(6); CI (solid squares), approximations SD-SDTQ; and CC (stars), approximations SD-SDTQ. The correlation energy is defined with respect to the Hartree-Fock energy for the given basis set, and the full correlation energies are obtained from the FCI calculations quoted in Table I.

[Bartlett and Musial, Rev. Mod. Phys. 79 (2007) 291]


THE WORD
Size Extensivity

Size extensivity – consistent scaling with size

The binding energy of a nucleus is an extensive quantity: $BE \propto A$

Goldstone's linked cluster theorem (1955): Formal diagrammatic proof of Brueckner's conjecture that perturbation theory is size consistent. Only linked diagrams contribute to the energy of a (closed shell) nucleus.

→ Unlinked diagrams do not scale with mass number ***A***, and the sum of all unlinked diagrams is zero.

Theories that maintain a consistent scaling with size ("size-extensive"):

☺ Many-body perturbation theory

☺ "Exact" methods like matrix diagonalization within a full model space

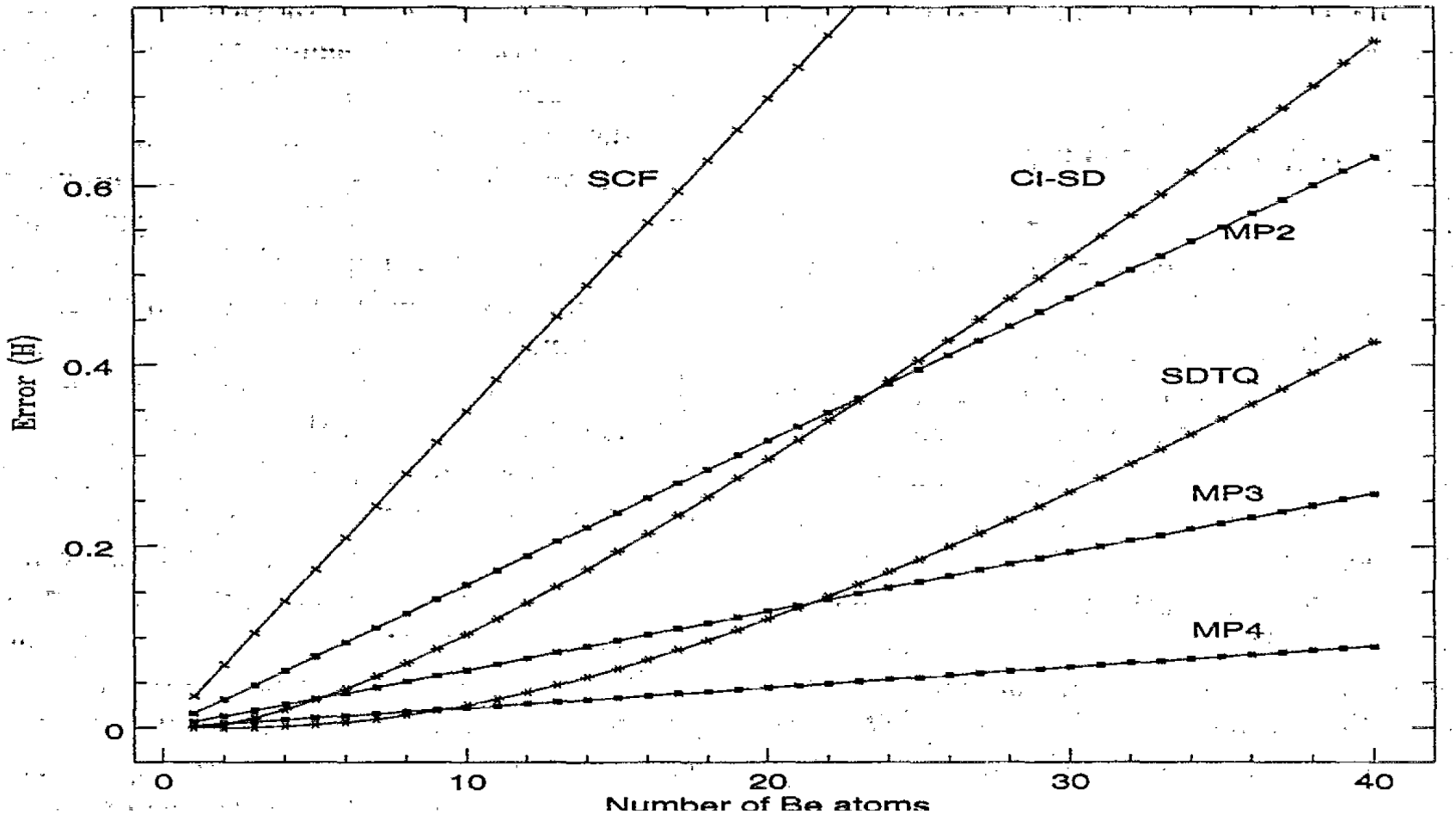
☺ Coupled-cluster theory (CCSD, CCSDT, …)

Theoretical approaches that are not size extensive:

☹ Diagonalization in a space of np-nh exitations (n < A). (CISD, CISDT…)

Size (extensivity) matters!

Only size extensive theories produce a result and an error that scale as ***A***.

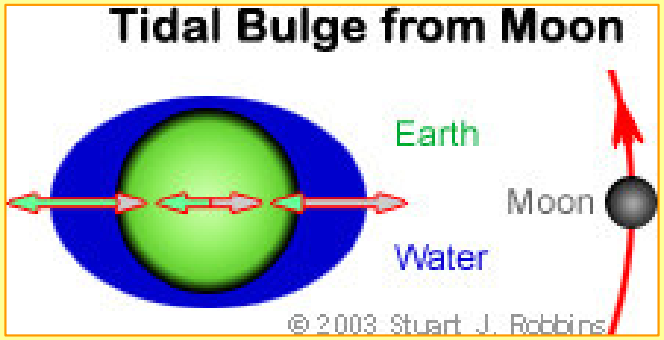


[Duch and Diercksen, J. Chem. Phys. 101 (1994) 3018]

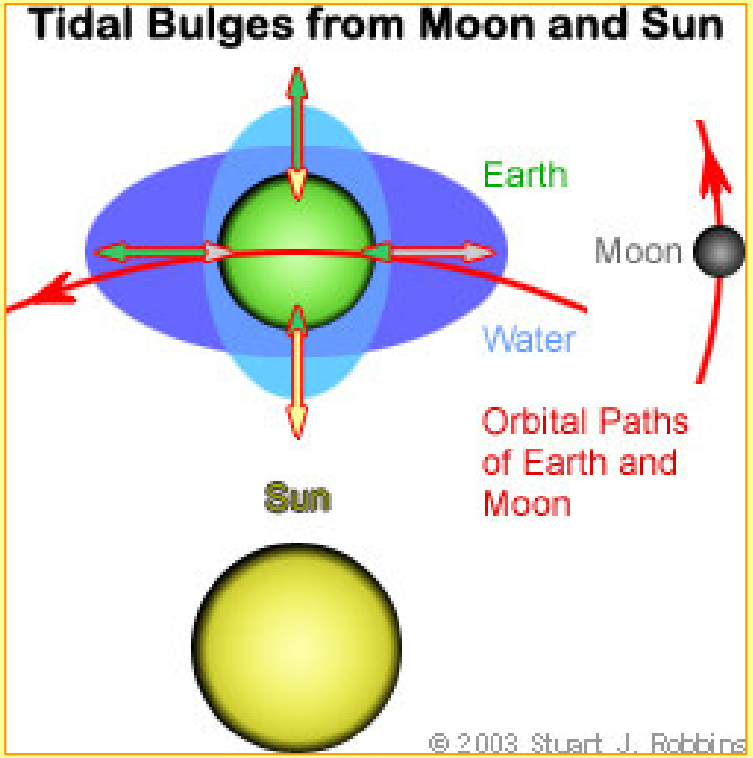
Three-nucleon forces: Why?

- Nucleons are not point particles (i.e. not elementary).
- We neglected some internal degrees of freedom (e.g. Δ-resonance, “polarization effects”, …), and unconstrained high-momentum modes.

Example from celestial mechanics:
Earth-Moon system: point masses and modified two-body interaction



Other tidal effects cannot be included in the two-body interaction! Three-body force unavoidable for point masses.



Renormalization group transformation: Removal of “stiff” degrees of freedom at expense of additional forces.

A theorem for three-body Hamiltonians

Polyzou and Glöckle, Few Body Systems 9, 97 (1990)

Different two-body Hamiltonians can be made to fit two-body and three-body data by including a 3NF into one of the Hamiltonians.

Theorem. *Let*

$$H_{ij} = H_i + H_j + V_{ij} \qquad \text{and} \qquad \bar{H}_{ij} = H_i + H_j + \bar{V}_{ij} \tag{1.1}$$

be two-body Hamiltonians with the same binding energies and scattering matrices for each pair of particles i and j. Assume that the two-body Hamiltonians are asymptotically complete and that the unitary transformations relating these two-body Hamiltonians, which necessarily exist, have bounded Cayley transforms. Then there exists a three-body interaction, W, such that the two three-body Hamiltonians

$$H = H_1 + H_2 + H_3 + V_{12} + V_{23} + V_{31} \tag{1.2}$$

and

$$\bar{H}' = \bar{H} + W \tag{1.3}$$

with

$$\bar{H} = H_1 + H_2 + H_3 + \bar{V}_{12} + \bar{V}_{23} + \bar{V}_{31} \tag{1.4}$$

have the same binding energies and scattering matrix.

Corollary. *Under the assumptions of the theorem, if $V_{(123)}$ is a three-body interaction then there exists another three-body interaction $\bar{V}_{(123)}$ such that*

$$H = H_1 + H_2 + H_3 + V_{12} + V_{23} + V_{31} + V_{(123)}$$

and

$$\bar{H} = H_1 + H_2 + H_3 + \bar{V}_{12} + \bar{V}_{23} + \bar{V}_{31} + \bar{V}_{(123)}$$

have the same binding energies and scattering matrix.

Implications:

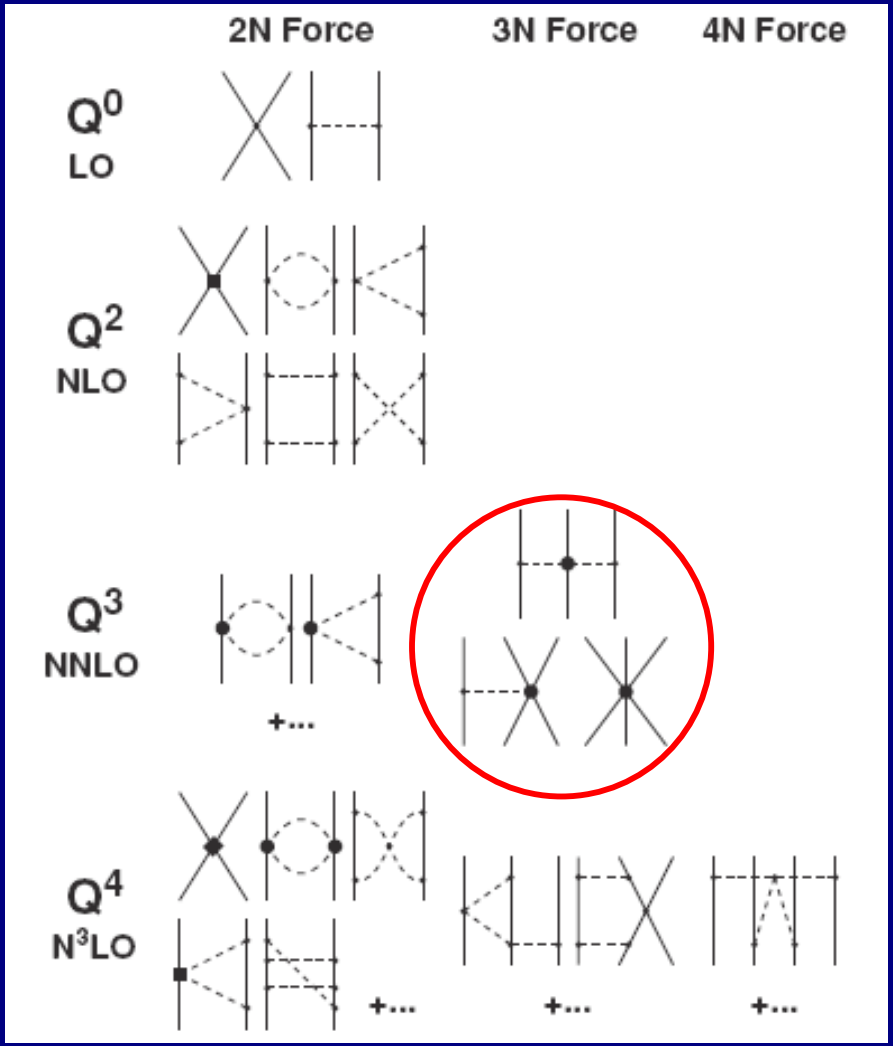
(1) There are no experiments measuring only three-body binding energies and phase shifts that can determine if there are no three-body forces in a three-body system. The question makes no sense. The correct statement is that there may be some systems for which it is possible to find a representation in which three-body forces are not needed.

(2) Different off-shell extensions of two-body forces can be equivalently realized as three-body interactions.

(4) Three-body forces cannot be determined in a manner that is independent of the two-body interaction.

Chiral potential up to order N^{3}LO

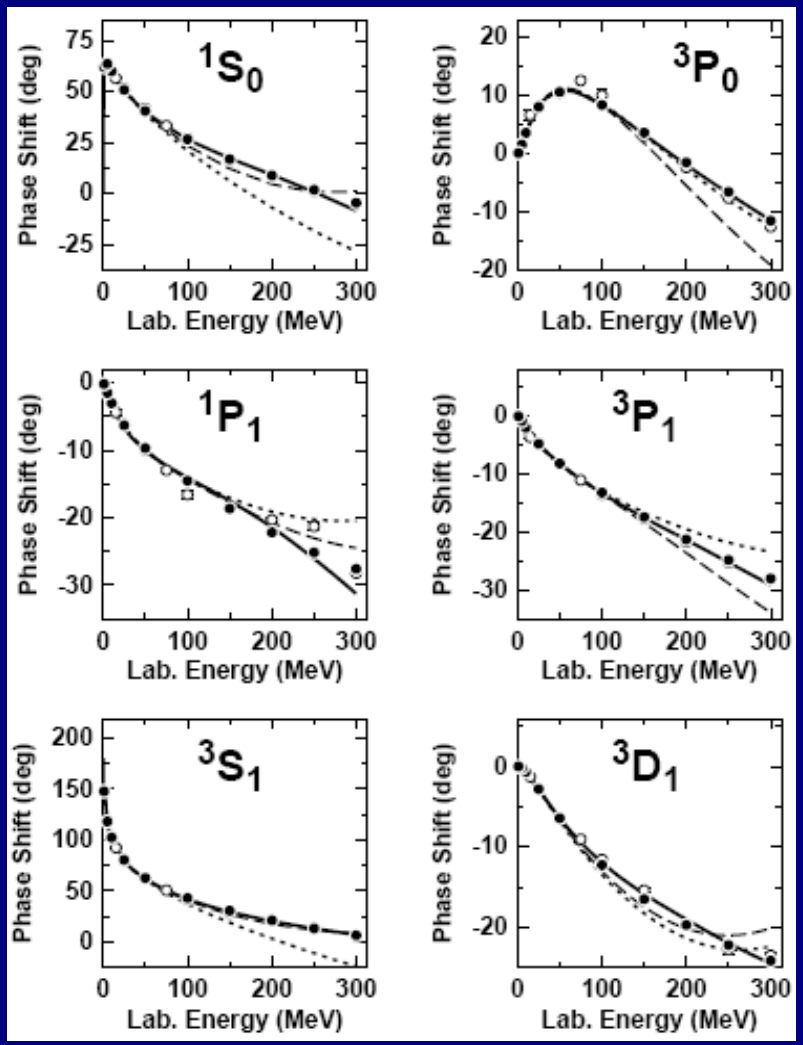
Feynman diagrams



R. Machleidt and D. R. Entem, J. Phys. G 31 (2005) S1235

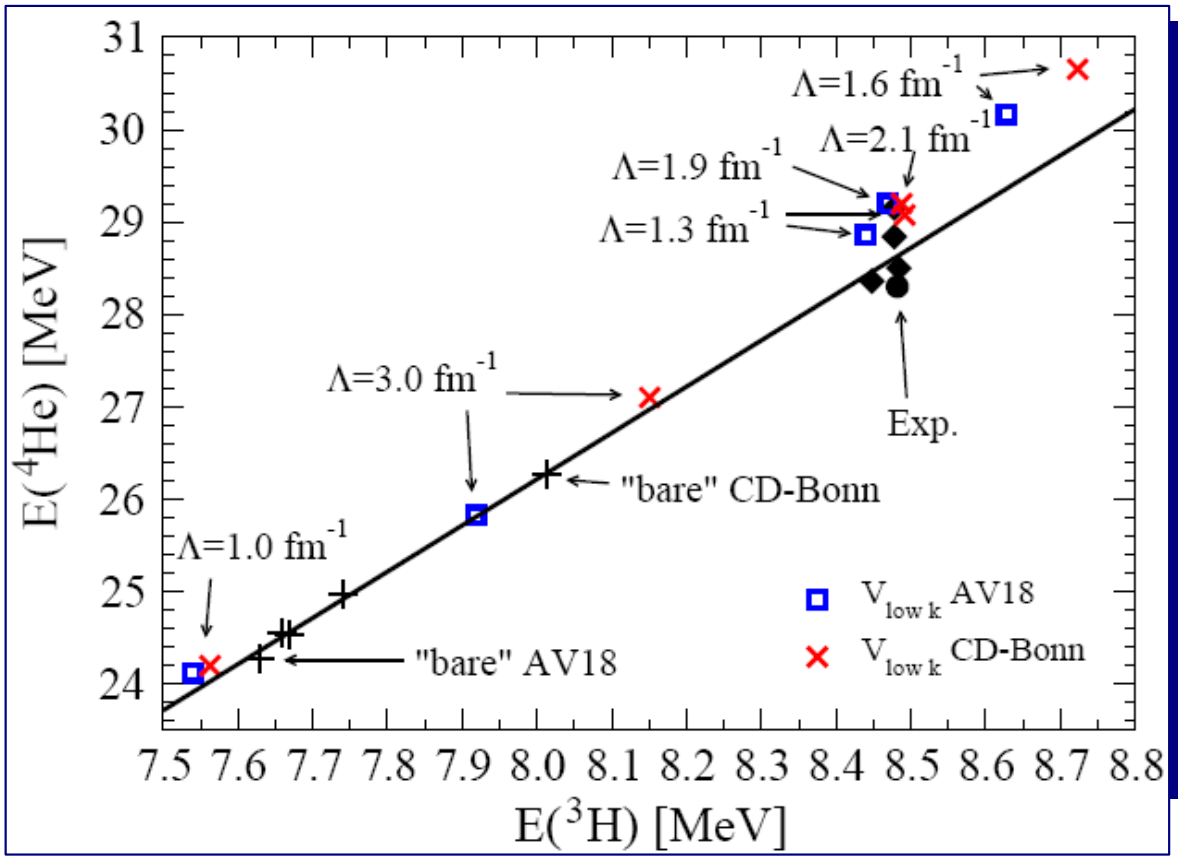
Phase shifts reproduced to χ^2/datum=1

About 24+ parameters



D. R. Entem and R. Machleidt, Phys.Rev. C68 (2003) 041001

Interaction: $V_{low\text{-}k}$ from Av18 + chiral 3NF



As cutoff Λ is varied, motion along Tjon line.

Addition of Λ-dependent three-nucleon force yields agreement with experiment.

Three-nucleon force perturbative at cutoff Λ=1.9 fm^{-1} *for these nuclei.*

A. Nogga, S. K. Bogner, and A. Schwenk, Phys. Rev. C 70 (2004) 061002.

	^{3}H					^{4}He				
Λ [fm^{-1}]	T	$V_{low\,k}$	c-terms	D-term	E-term	T	$V_{low\,k}$	c-terms	D-term	E-term
1.0	21.06	−28.62	0.02	0.11	−1.06	38.11	−62.18	0.10	0.54	−4.87
1.3	25.71	−34.14	0.01	1.39	−1.46	50.14	−78.86	0.19	8.08	−7.83
1.6	28.45	−37.04	−0.11	0.55	−0.32	57.01	−86.82	−0.14	3.61	−1.94
1.9	30.25	−38.66	−0.48	−0.50	0.90	60.84	−89.50	−1.83	−3.48	5.68
2.5(a)	33.30	−40.94	−2.22	−0.11	1.49	67.56	−90.97	−11.06	−0.41	6.62
2.5(b)	33.51	−41.29	−2.26	−1.42	2.97	68.03	−92.86	−11.22	−8.67	16.45
3.0($*$)	36.98	−43.91	−4.49	−0.73	3.67	78.77	−99.03	−22.82	−2.63	16.95

Coupled-cluster theory with three-nucleon forces for ^{4}He

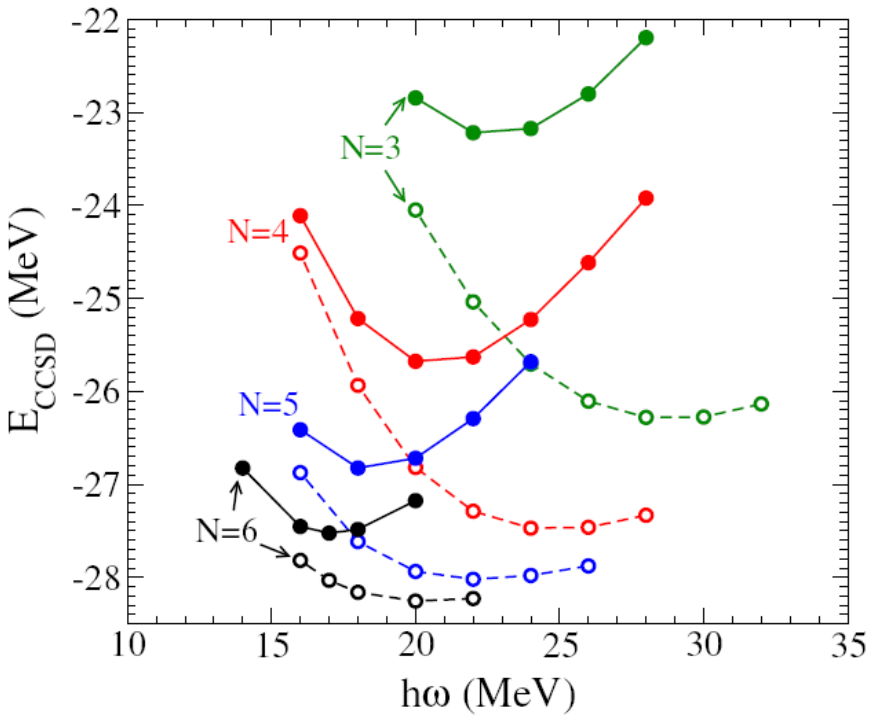


FIG. 5: (Color online) CCSD results for the binding energy of ^{4}He as a function of the oscillator spacing and for model spaces consisting of $N = 3$ to $N = 6$ oscillator shells. The CCSD calculations are based on low-momentum NN and 3N interactions, where the full and dashed lines respectively denote the energy obtained with and without 3NFs.

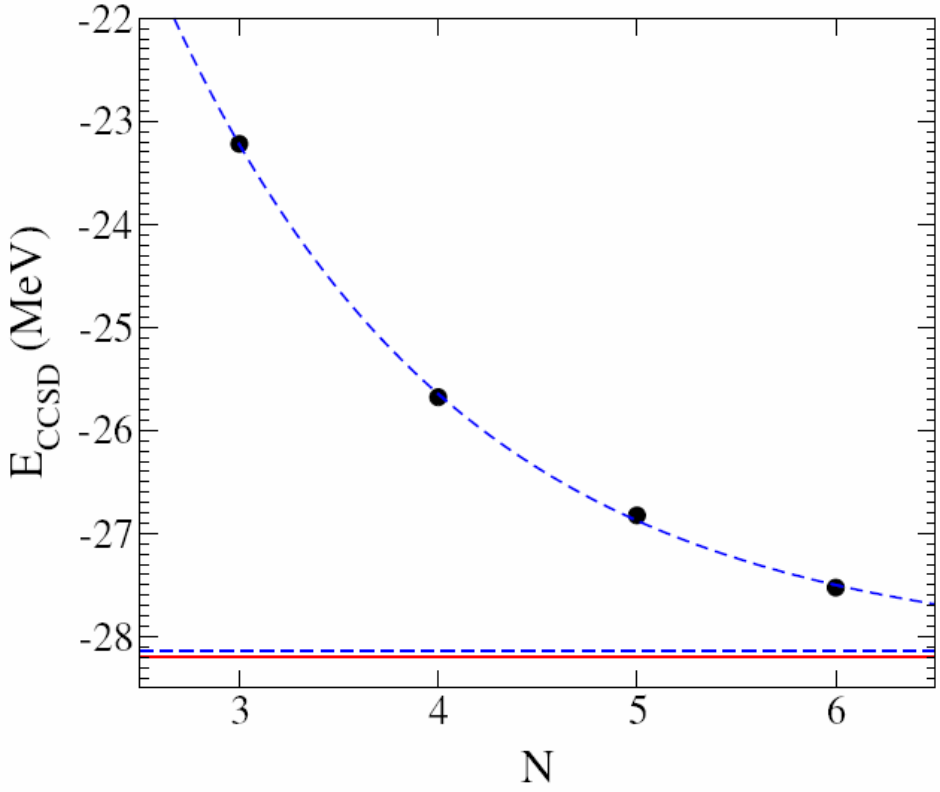


FIG. 6: (Color online) Data points: CCSD results (taken at the $\hbar\omega$ minima) for the binding energy of ^{4}He with 3NFs as a function of the number of oscillator shells. Dashed lines: Exponential fit to the data and asymptote of the fit. Full line: Exact result.

Two-body force: $V_{low\text{-}k}$ with Λ=1.9 fm^{-1} from Argonne V18

Three-body force: Chiral EFT at order N^{2}LO (isospin ½ only)

Main result: Exact result closely matched!

Important (technical) detail: normal-ordered Hamiltonian

The Hamiltonian is normal-ordered w.r.t. the vacuum state |Φ>.

$$\begin{aligned}\hat{H} &= \sum_{pq} \varepsilon_{pq} \hat{a}_p^\dagger \hat{a}_q + \frac{1}{4} \sum_{pqrs} \langle pr||sr\rangle \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_r \hat{a}_s \\ &= \sum_i \varepsilon_{ii} + \frac{1}{2} \sum_{ij} \langle ij||ij\rangle \\ &+ \sum_{ij} \left(\varepsilon_{pq} + \sum_i \langle pi||qi\rangle \right) \{\hat{a}_p^\dagger \hat{a}_q\} + \frac{1}{4} \sum_{pqrs} \langle pq||sr\rangle \{\hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_r \hat{a}_s\}\end{aligned}$$

Similarly, the Hamiltonian of the 3NF becomes

$$\hat{H}_3 = \frac{1}{6} \sum_{ijk} \langle ijk||ijk\rangle + \frac{1}{2} \sum_{ijpq} \langle ijp||ijq\rangle \{\hat{a}_p^\dagger \hat{a}_q\}$$

Vacuum energy and density-dependent one-body terms

$$+\frac{1}{4} \sum_{ipqrs} \langle ipq||irs\rangle \{\hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_s \hat{a}_r\} + \hat{h}_3 \ ,$$

Density-dependent two-body terms

$$\hat{h}_3 \equiv \frac{1}{36} \sum_{pqrstu} \langle pqr||stu\rangle \{\hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_r^\dagger \hat{a}_u \hat{a}_t \hat{a}_s\}$$

Residual three-body terms

Note:

1. The form of the Hamiltonian is different for each nucleus under consideration.
2. Normal-ordering necessary for evaluation of similarity-transformed Hamiltonian.
3. “Density-dependend” terms are coherent sums over two- and three-body matrix elements.

Contributions to the binding energy of ^{4}He

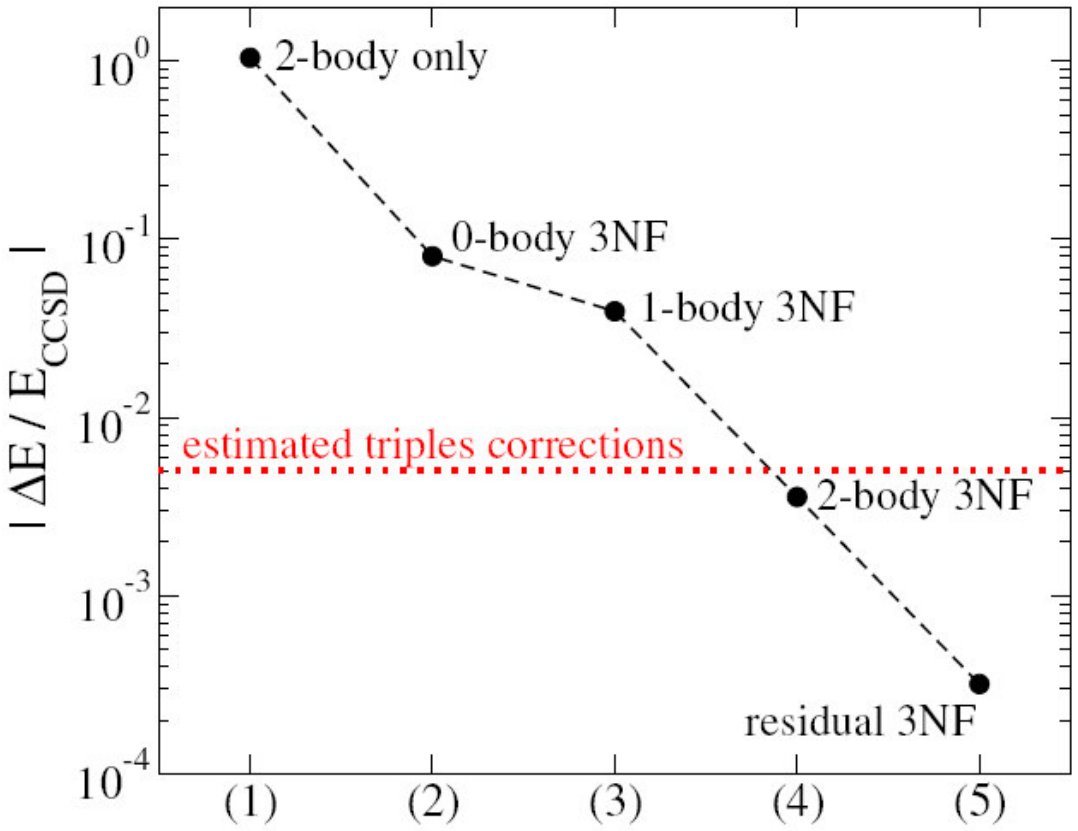


FIG. 7: (Color online) Relative contributions $|\Delta E/E|$ to the binding energy of ^{4}He at the CCSD level. The different points denote the contributions from (1) low-momentum NN interactions, (2) the vacuum expectation value of the 3NF, (3) the normal-ordered one-body Hamiltonian due to the 3NF, (4) the normal-ordered two-body Hamiltonian due to the 3NF, and (5) the residual 3NFs. The dotted line estimates the corrections due to omitted three-particle–three-hole clusters.

Residual 3NF can be neglected!

$$\hat{H}_3 = \frac{1}{6}\sum_{ijk}\langle ijk||ijk\rangle + \frac{1}{2}\sum_{ijpq}\langle ijp||ijq\rangle\{\hat{a}_p^\dagger \hat{a}_q\} + \frac{1}{4}\sum_{ipqrs}\langle ipq||irs\rangle\{\hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_s \hat{a}_r\} + \hat{h}_3 \ ,$$

Main results:

- **Residual 3NF can be neglected.**
- **Enormous reduction of computational effort**
- **"Two-body machinery" can be applied**

Déjà vu …

H. Kümmel, K. H. Lührmann, J. G. Zabolitzky,
Phys. Rep. 36, 1 (1978)

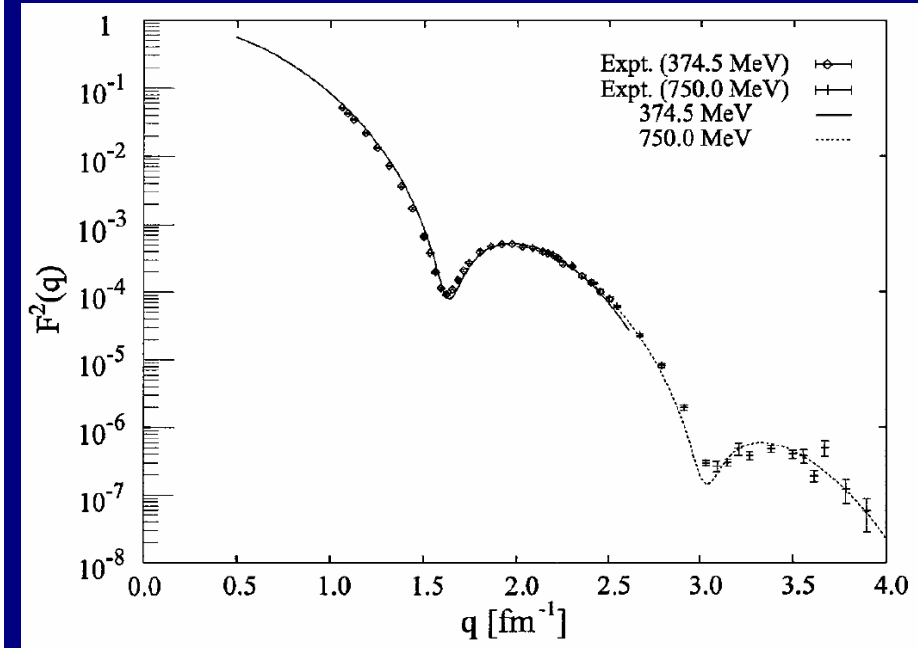
From the abstract:

"For nuclei two body forces as usual do not yield results in agreement with experiments. The introduction of exchange currents into the elastic electron form factor and three body forces greatly improves the situation."

P. Navratil and E. Ormand,
Phys.Rev. Lett. 88, 152502 (2002)

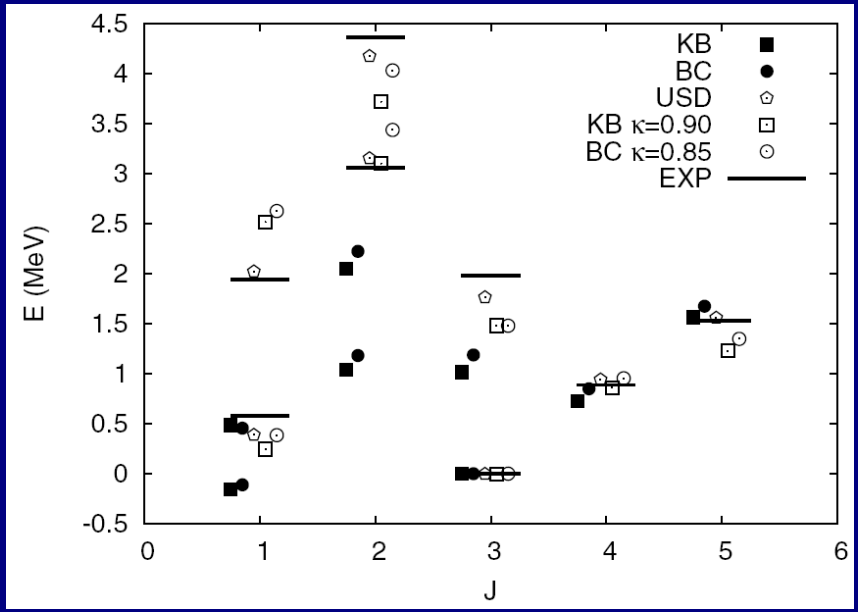
From the conclusion:
"…utilize the interesting feature
that the three-body effective interaction appears to act primarily as a density-dependent two-body interaction."

Form factor for ^{16}O within CC: AV18 + UIX



Mihaila and Heisenberg, PRL 84 (2000) 1403.

Monopole shifts from 3NF as density-dependent NN force (Shown below: Spectrum in ^{22}Na).



A. Zuker, PRL90, 42502 (2003).

Improved CCSD(T) results for ^{4}He: perturbative *3p-3h* clusters

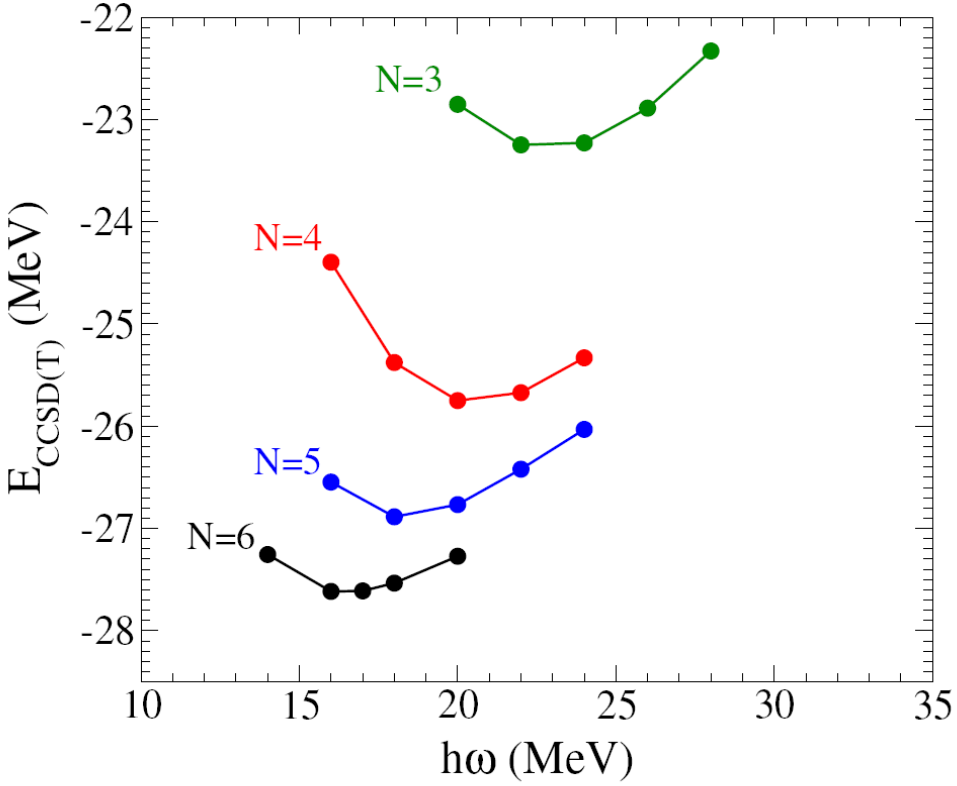


FIG. 8: (Color online) CCSD(T) results for the binding energy of ^{4}He as a function of the oscillator spacing and for model spaces consisting of $N = 3$ to $N = 6$ oscillator shells. The contributions from 3NFs are limited to the density-dependent zero-, one-, and two-body terms and exclude its residual three-body terms.

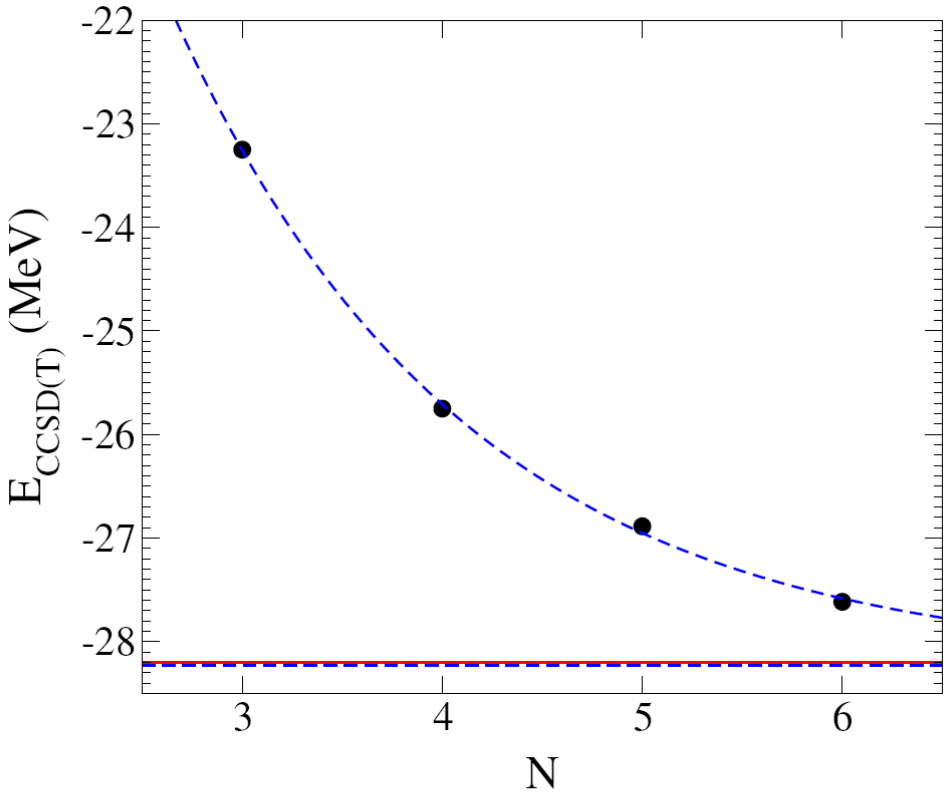


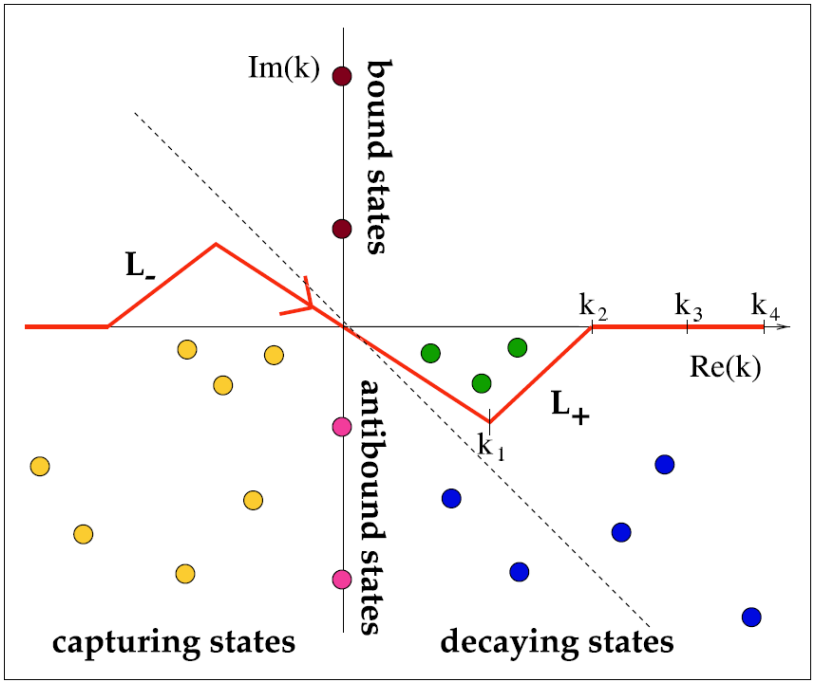
FIG. 9: (Color online) Data points: CCSD(T) results (taken at the $\hbar\omega$ minima) for the binding energy of ^{4}He with 3NFs as a function of the number of oscillator shells. Dashed lines: Exponential fit to the data and asymptote of the fit. Full line: Exact result.

Center-of-mass expectation: 20 keV

Helium isotopes:
weakly bound and unbound quantum systems

Aim: Ab-initio description of weakly bound systems and computation of life times of particle-unstable ^{5,7}He.

Basis set: Single-particle basis of bound, resonance and scattering states: Gamow shell model → complex symmetric Hamiltonian



N. Michel et al, PRC 67, 054311 (2003)

Two new aspects:

1. Particle-unstable nuclei ✔
2. Open-shell nuclei (✔)

Comparison with exact diagonalization

Method	^{3}He	^{4}He	^{5}He	^{6}He
CCSD (OSC)	-6.21	-26.19	-21.53	-20.96
CCSD (RHF)	-6.10	-26.06	-21.55	-20.99
CCSD (SC-RHF)	-6.11	-26.06	-21.55	-21.04
CCSD(T) (OSC)	-6.40	-26.30	-21.91	-22.83
CCSD(T) (RHF)	-6.35	-26.24	-21.90	-22.56
CCSD(T) (SC-RHF)	-6.34	-26.24	-21.91	-22.62
Exact	-6.45	-26.3	-22.1	-22.7

All fine, except ^{6}He (large T corrections); $\langle J^2 \rangle$=0.6

CCSDT yields $\langle J^2 \rangle$ =0.04

Coupled-cluster theory for weakly bound nuclei: He-isotopes

	^{3}He		^{4}He		^{5}He		^{6}He		^{7}He		^{8}He		^{9}He		^{10}He	
lj	Re[E]	Im[E]	Re[E]	Im[E]	Re[E]	Im[E]	Re[E]	Im[E]	Re[E]	Im[E]	Re[E]	Im[E]	Re[E]	Im[E]	Re[E]	Im[E]
$s-p$	-4.94	-0.00	-24.97	-0.00	-20.33	-0.56	-19.07	-0.18	-17.09	-0.25	-17.02	-0.01	-15.44	-0.28	-13.86	-0.14
$s-d$	-6.44	-0.00	-26.61	-0.00	-23.56	-0.20	-23.25	-0.07	-22.22	-0.09	-23.07	-0.00	-21.58	-0.13	-20.69	0.00
$s-f$	-6.82	-0.00	-27.27	-0.00	-24.53	-0.16	-24.69	-0.07	-24.19	-0.10	-25.44	-0.00	-24.16	-0.05	-23.67	-0.00
$s-g$	-6.91	-0.00	-27.35	-0.00	-24.84	-0.15	-25.17	-0.08	-24.90	-0.12	-26.25	-0.00	-25.10	-0.04	-24.77	-0.00
$s-h$	-6.92	-0.00	-27.37	-0.00	-24.90	-0.15	-25.28	-0.09	-25.08	-0.13	-26.45	-0.00	-25.34	-0.03	-25.05	-0.00
$s-i$	-6.92	-0.00	-27.37	-0.00	-24.91	-0.15	-25.31	-0.09	-25.11	-0.13	-26.49	-0.00	-25.38	-0.03	-25.10	-0.00
Expt.	-7.72	0.00	-28.30	0.00	-27.41	-0.33(2)	-29.27	0.00	-28.83	-0.08(2)	-31.41	0.00	-30.14	-0.05(3)	-30.34	-0.09(6)

TABLE II: CCSD calculation of the $^{3-10}$He ground states with the low-momentum N^{3}LO nucleon-nucleon interaction for increasing number partial waves. The energies E are given in MeV for both real and imaginary parts. Experimental data are from Ref. [32]. Our calculated width of ^{10}He is ≈ 0.002MeV.

Interaction: $V_{low\text{-}k}$ with Λ=1.9 fm^{-1} from chiral N^{3}LO potential (no three-body forces)

Main result: Converged ab-initio calculation of decay widths for unbound nuclei!

Summary

NN only:

- Converged results for ^{3}H, ^{4}He, and ^{16}O.
- Almost converged results for ^{40}Ca (1% error estimate)
- Approaches that are not size extensive problematic if size matters!
- Description of weakly bound He isotopes with Gamow states

3NFs:

- Developed CCSD for 3NF.
- Found that 0-, 1-, and 2-body parts of 3NF are dominant (in ^{4}He).
- ☺ Residual 3-body part of 3NF can be neglected.

Outlook

1. Densities and response to external potentials for comparison with DFT
   → UNEDF

2. Revisit helium isotopes, study neutron-rich oxygen isotopes with 3NF

3. Spherical CC approach: Ca, Ni isotopes, “bare” interactions, comparison with AFMC
   → CCSD on a laptop