

# Coupled-cluster theory for medium-mass nuclei



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# Overview

1. Coupled-cluster theory
2. Consistent scaling with system size – size (extensivity) matters  
[Dean, Hagen, Hjorth-Jensen, TP, Schwenk, arxiv:0709.0449]
3. Benchmark calculations  
[Hagen, Dean, Hjorth-Jensen, TP, Schwenk, Phys. Rev. C **76** (2007) 044305]
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, Phys. Lett. B 656 (2007) 169]
6. J-coupled scheme: much reduced computational effort, “harder” interactions, larger model spaces, heavier nuclei...

# Motivation

“Exact” ab-initio methods like GFMC and NCSM (in their present forms) are limited to p-shell nuclei.

- GFMC: Spin-isospin configurations  $\sim 4^A$
- NCSM: Configuration space  $\sim M! / [(M-A)! A!]$ , and  $M$  increases with  $A$

**Need theoretical approach that scales more favorable!**

**(Moore’s law is not compatible with above scaling relations)**



**Coupled-cluster theory (CCSD) scales like  $(M-A)^4 A^2$**

# Coupled-cluster theory (CCSD)

Ansatz:  $|\Psi\rangle = e^T |\Phi\rangle$

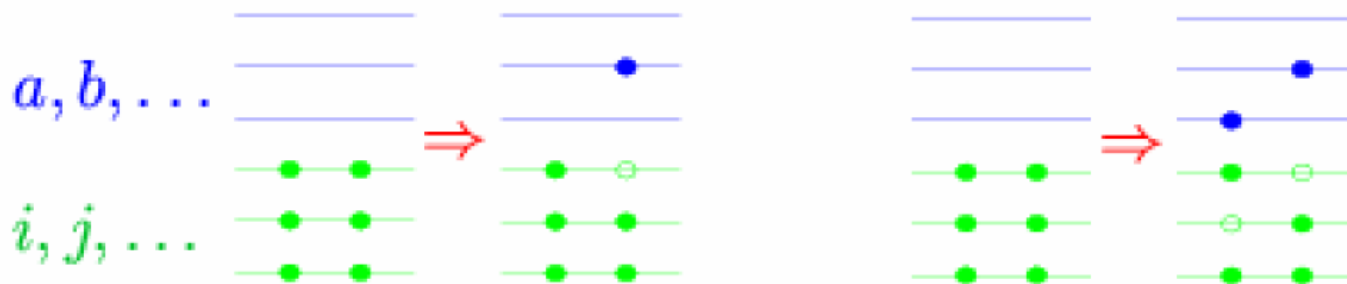
$$T = T_1 + T_2 + \dots$$

$$T_1 = \sum_{ia} t_i^a a_a^\dagger a_i$$

$$T_2 = \sum_{ijab} t_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i$$

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

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



Coupled cluster equations

$$E = \langle \Phi | \bar{H} | \Phi \rangle$$

$$0 = \langle \Phi_i^a | \bar{H} | \Phi \rangle$$

$$0 = \langle \Phi_{ij}^{ab} | \bar{H} | \Phi \rangle$$

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

$$\bar{H} \equiv e^{-T} H e^T = (H e^T)_c = \left( H + H T_1 + H T_2 + \frac{1}{2} H T_1^2 + \dots \right)_c$$



All you ever wanted to know about size extensivity and never dared to ask

**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"):

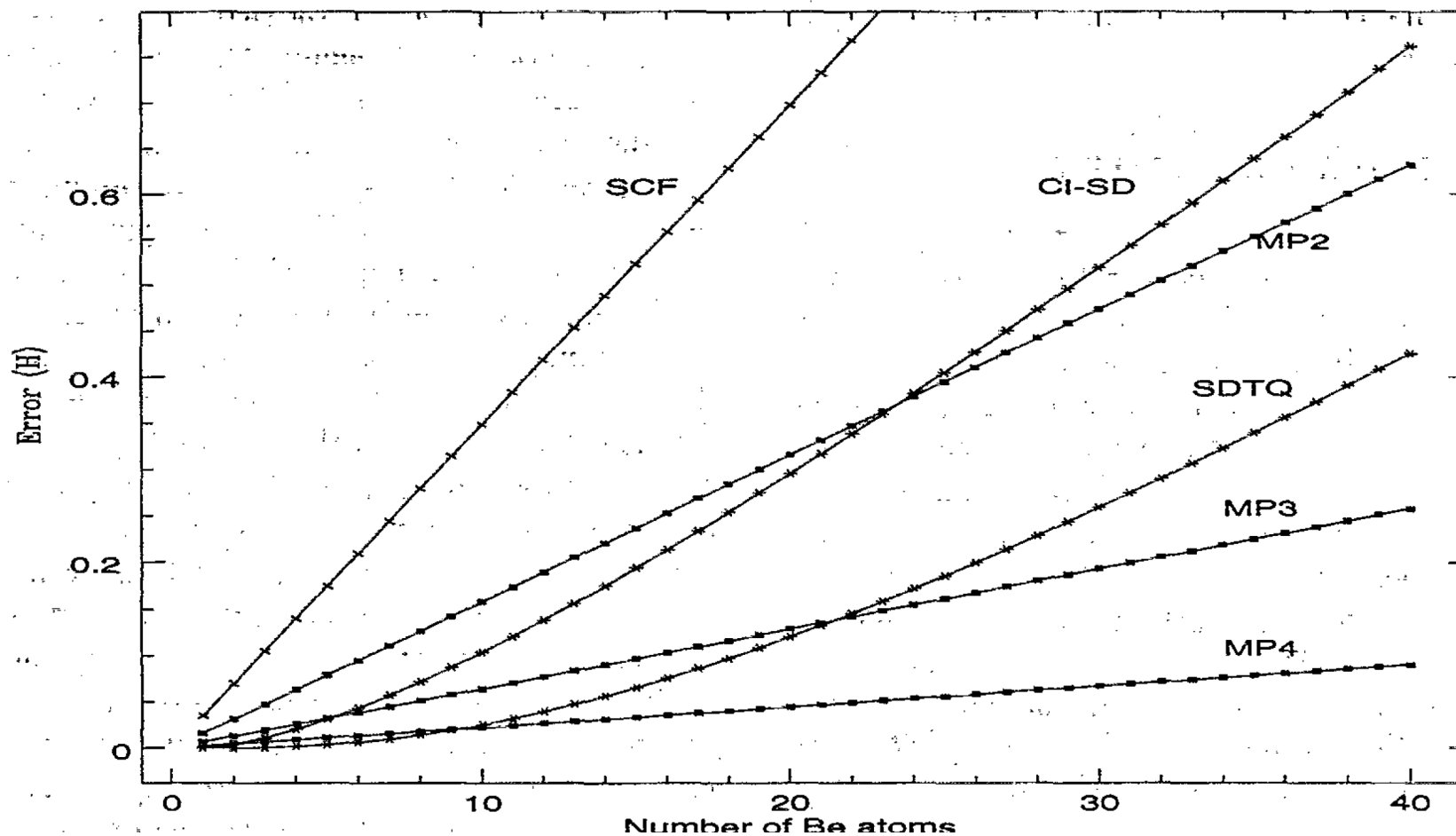
- ☺ Many-body perturbation theory
- ☺ "Exact" methods like matrix diagonalization within a full model space
- ☺ Coupled-cluster theory (CCSD, CCSDT, ...)

Theoretical approaches that are not size extensive:

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

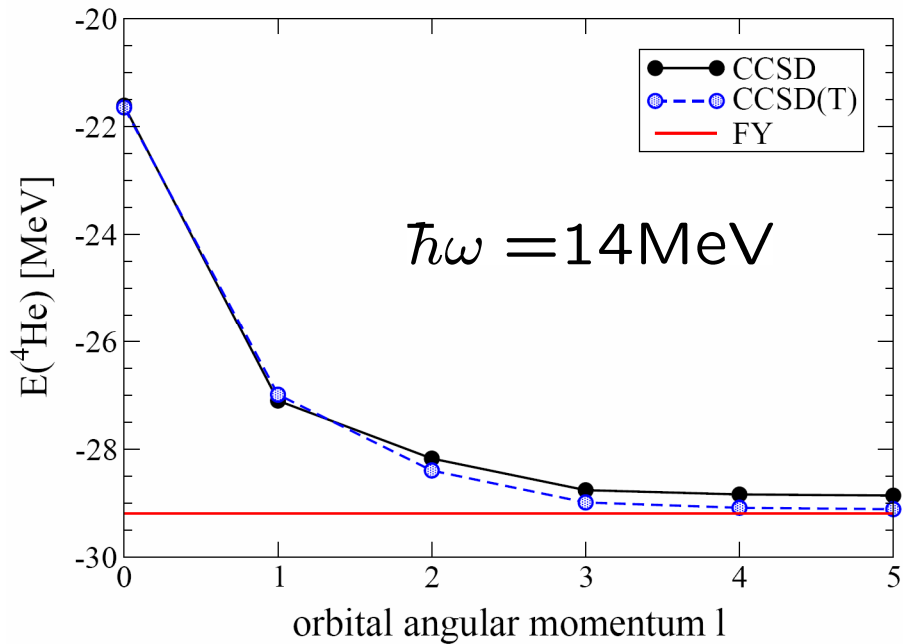
# Size extensivity matters for large systems

Size extensive theories produce a result (and an error) that scale as  $A$ .

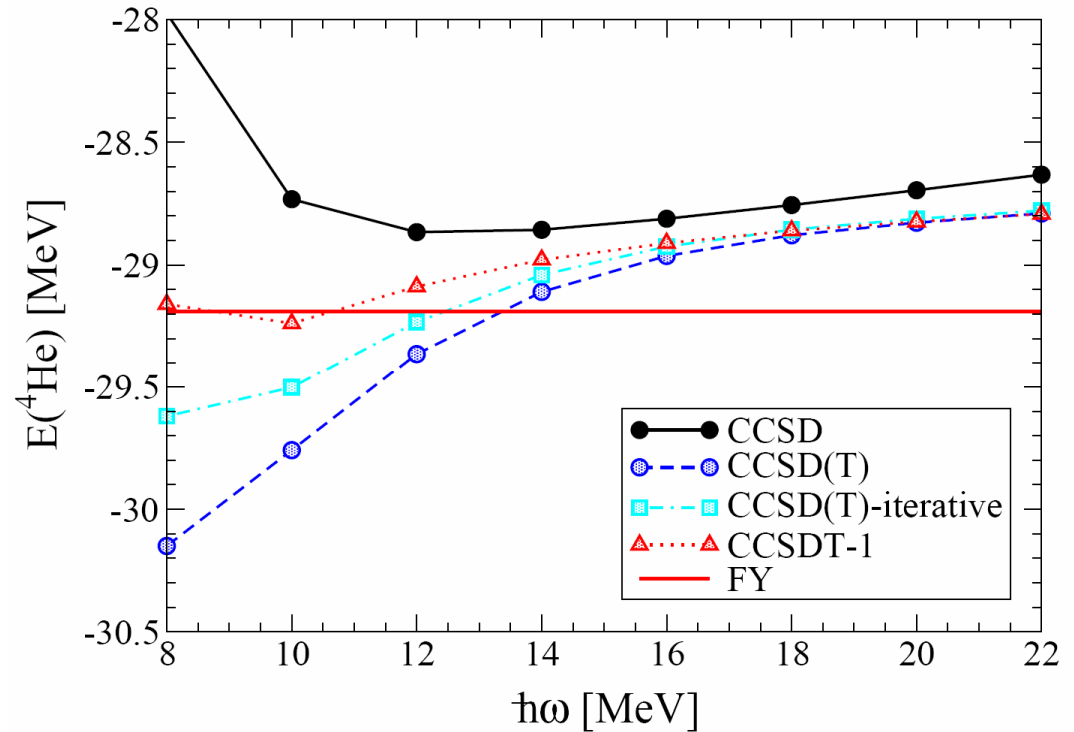


[Duch and Diercksen, J. Chem. Phys. 101 (1994) 3018]

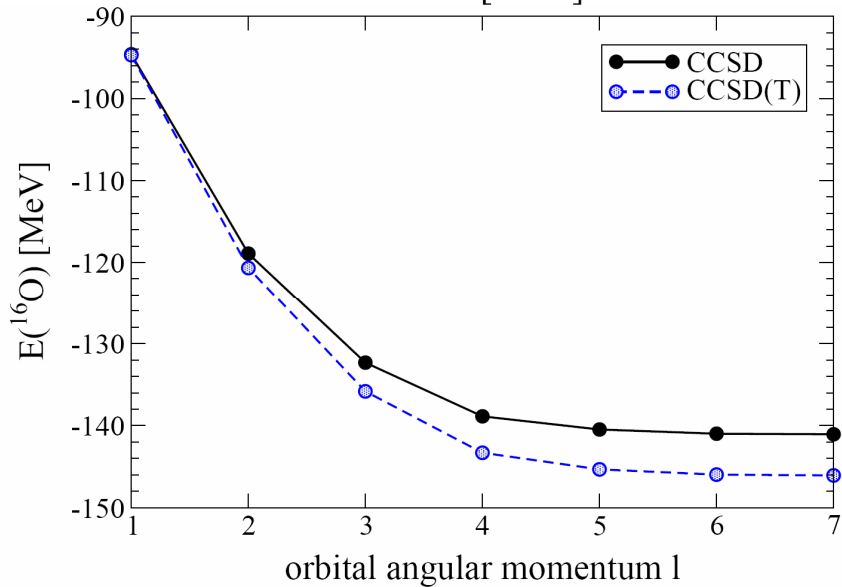
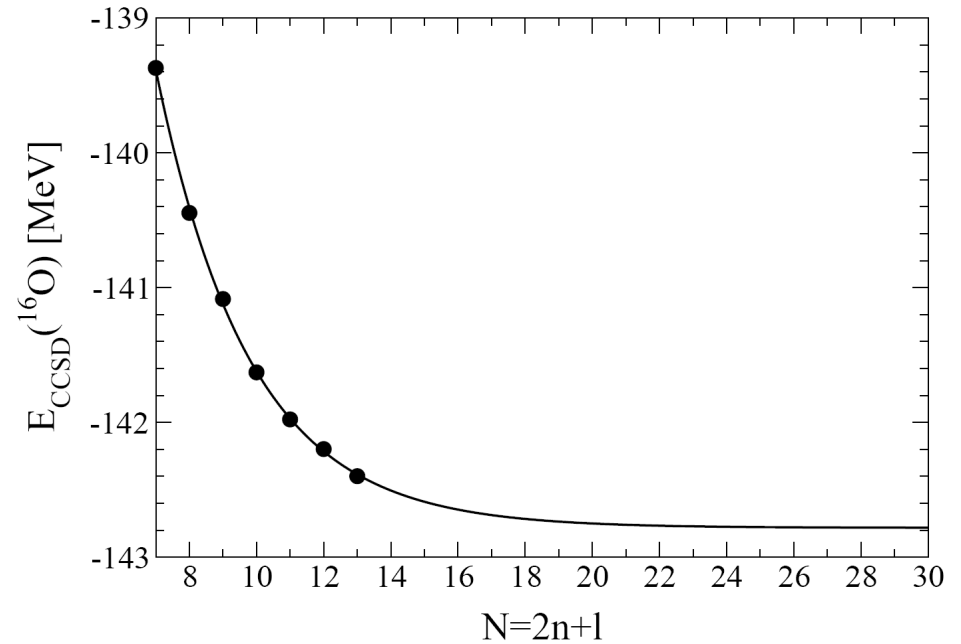
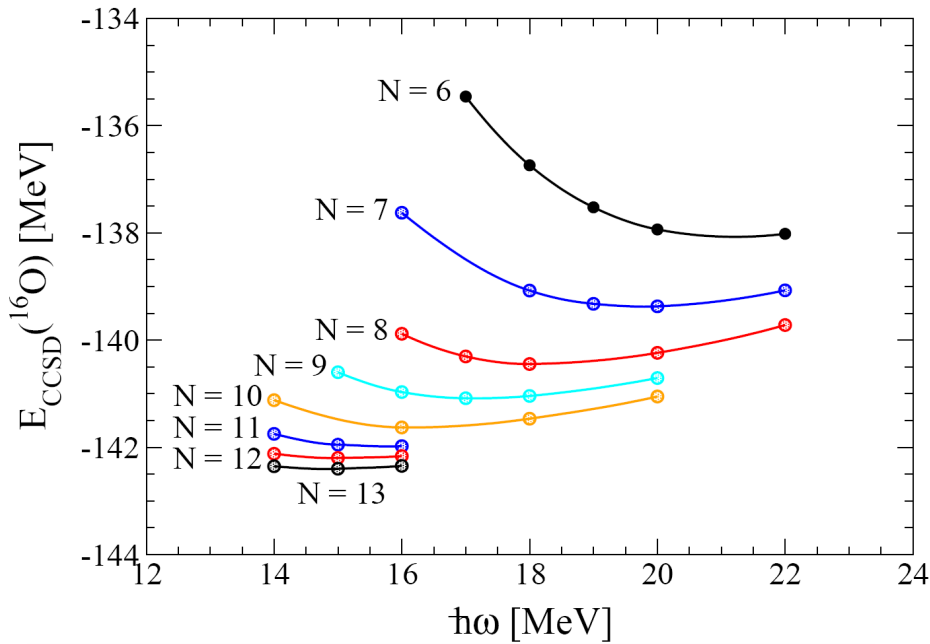
# Convergence and $\hbar\omega$ -dependence for ${}^4\text{He}$



Perturbative and non-iterative triples correction diverge at small  $\hbar\omega$ . Self-consistent corrections perform better.



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

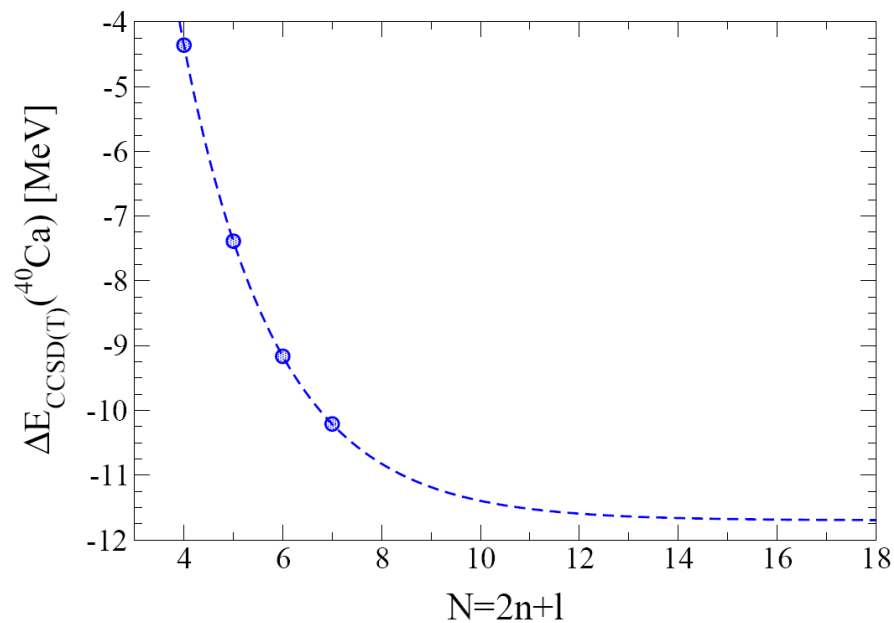
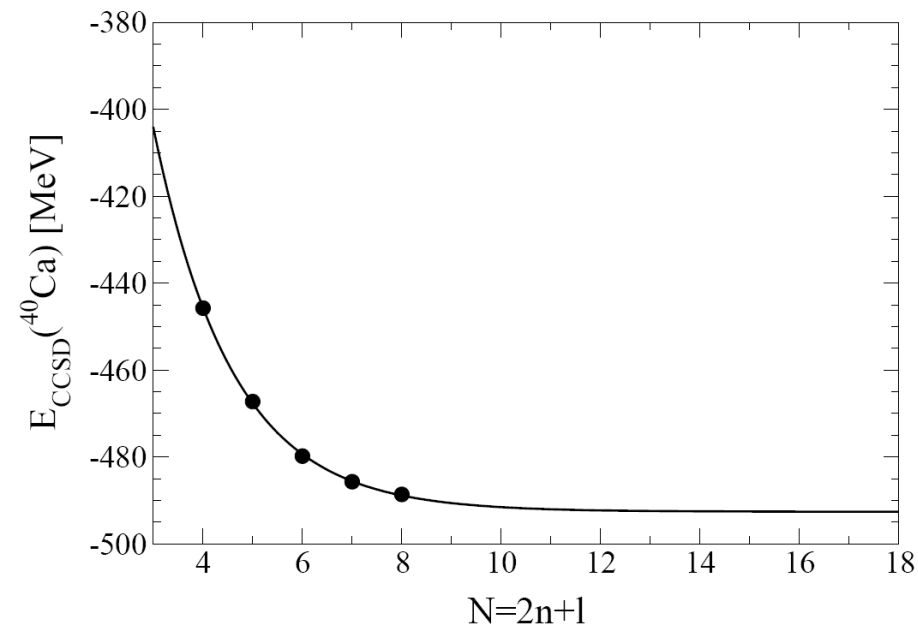
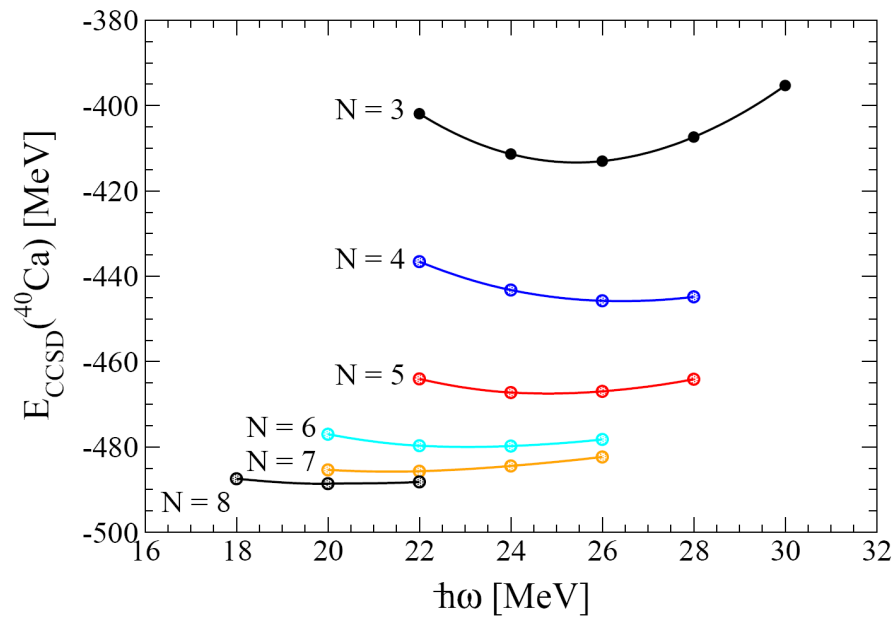


Interaction:  $V_{\text{low-k}}$  with  $\Lambda=1.9 \text{ fm}^{-1}$  from Argonne V18 (no three-body forces)

Model space: about 1000 single-particle orbitals

**Main result: accuracy estimate about 1%**

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



Accuracy estimate: 1% level.

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

# $^{40}\text{Ca}$ : Coupled clusters vs. truncated shell model

	$^{16}\text{O}$	$^{40}\text{Ca}$
CCSD(T)	-142.8 -148.2	-391.2 (CCSD) -502.9 (CCSD(T))
NCSM	-137.8	-461.8 (3p3h) -471.0 (4p4h)

Unfortunately, no exact result is yet available, and two ab-initio approaches disagree. (Model spaces also differ)

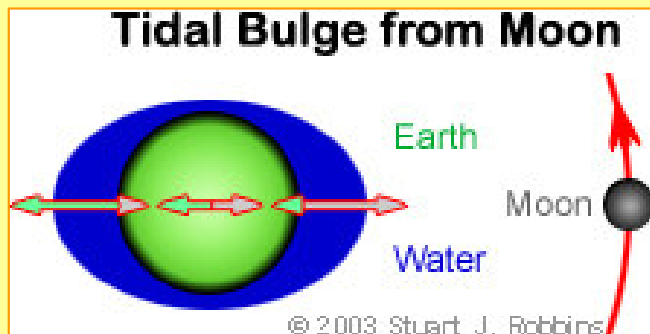
	Translational invariance	Rotational invariance	Variational principle	Size extensivity
Coupled cluster	$\langle T_{\text{cm}} \rangle \approx 200\text{keV}$	☺	no	☺
NCSM	☺	☺	☺	☺
p-h truncation	$\langle T_{\text{cm}} \rangle \approx 100\text{keV}$	☺	☺	no
importance sampling	$\langle T_{\text{cm}} \rangle \approx 100\text{keV}$	broken at truncation level	☺	no
Davidson correction			no	☺

# Three-nucleon forces: Why?

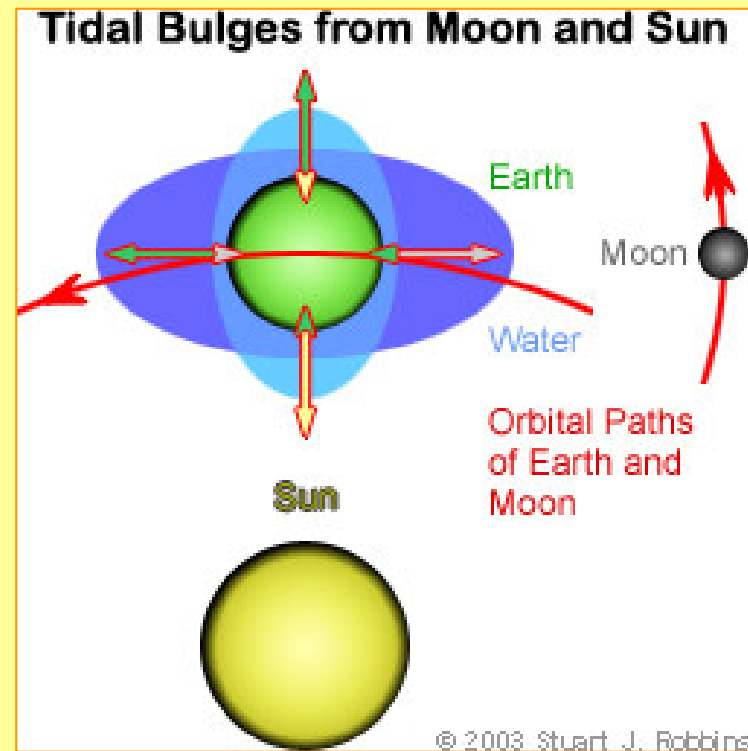
- Nucleons are not point particles (i.e. not elementary).
- We neglected some internal degrees of freedom (e.g.  $\Delta$ -resonance, “polarization effects”, ...), and unconstrained high-momentum modes.

## 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*

$$H_{ij} = H_i + H_j + V_{ij} \quad \text{and} \quad \bar{H}_{ij} = H_i + H_j + \bar{V}_{ij} \quad (1.1)$$

*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*

$$H = H_1 + H_2 + H_3 + V_{12} + V_{23} + V_{31} \quad (1.2)$$

*and*

$$\bar{H}' = \bar{H} + W \quad (1.3)$$

*with*

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

*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*

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

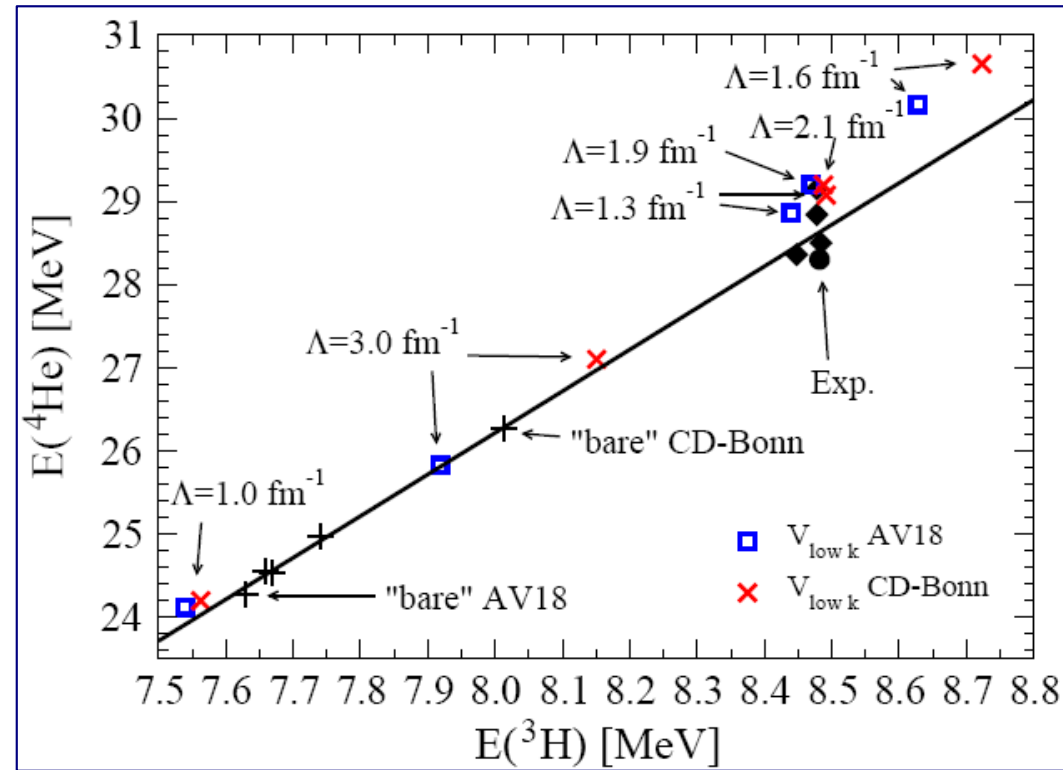
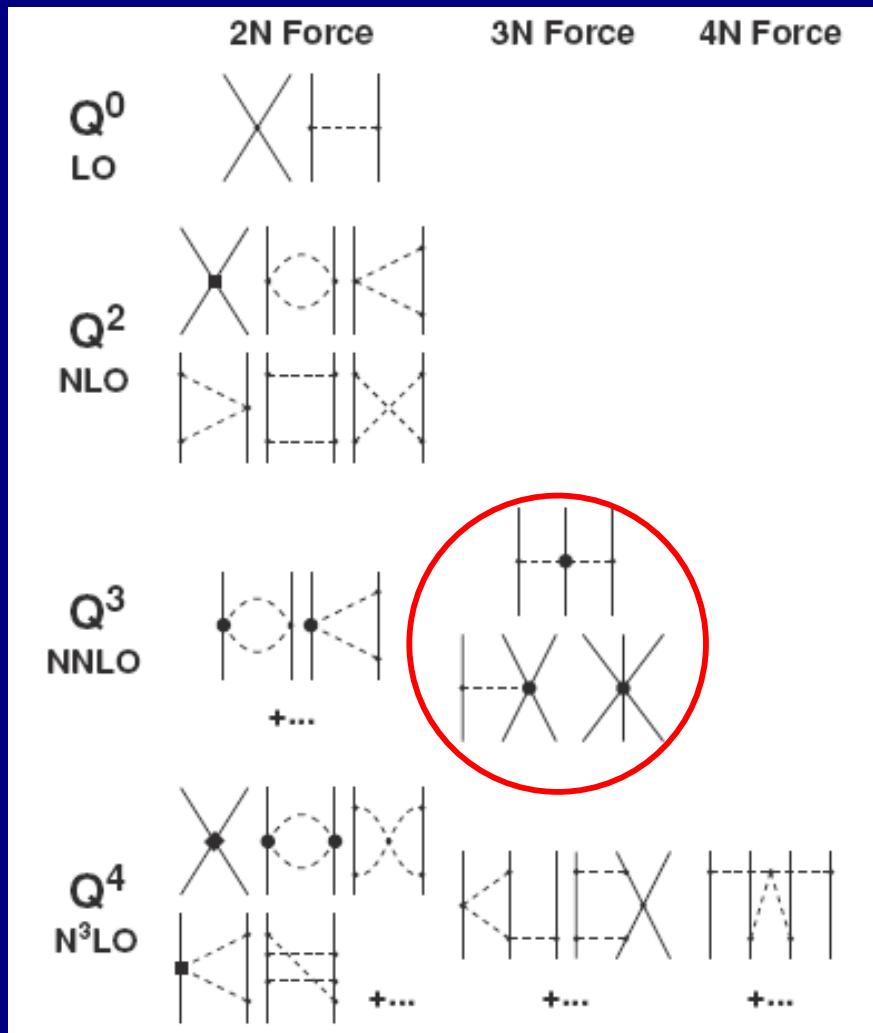
*have the same binding energies and scattering matrix.*

## 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.

# NN from Vlowk with chiral 3NF

EFT: B. van Kolck, E. Epelbaum, ...



- Tjon line is mapped out as cutoff is varied
- 3NF perturbatively small at cutoff  $1.9 \text{ fm}^{-1}$

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

# Coupled-cluster theory with three-nucleon forces for ${}^4\text{He}$

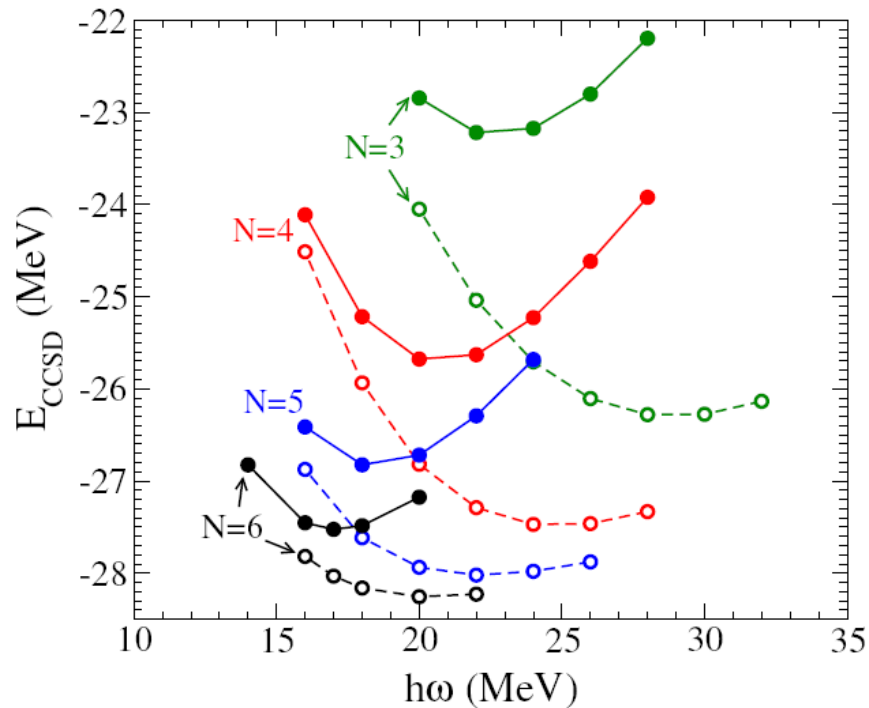


FIG. 5: (Color online) CCSD results for the binding energy of  ${}^4\text{He}$  as a function of the oscillator spacing and for model spaces consisting of  $N = 3$  to  $N = 6$  oscillator shells. The CCSD calculations are based on low-momentum NN and 3N interactions, where the full and dashed lines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

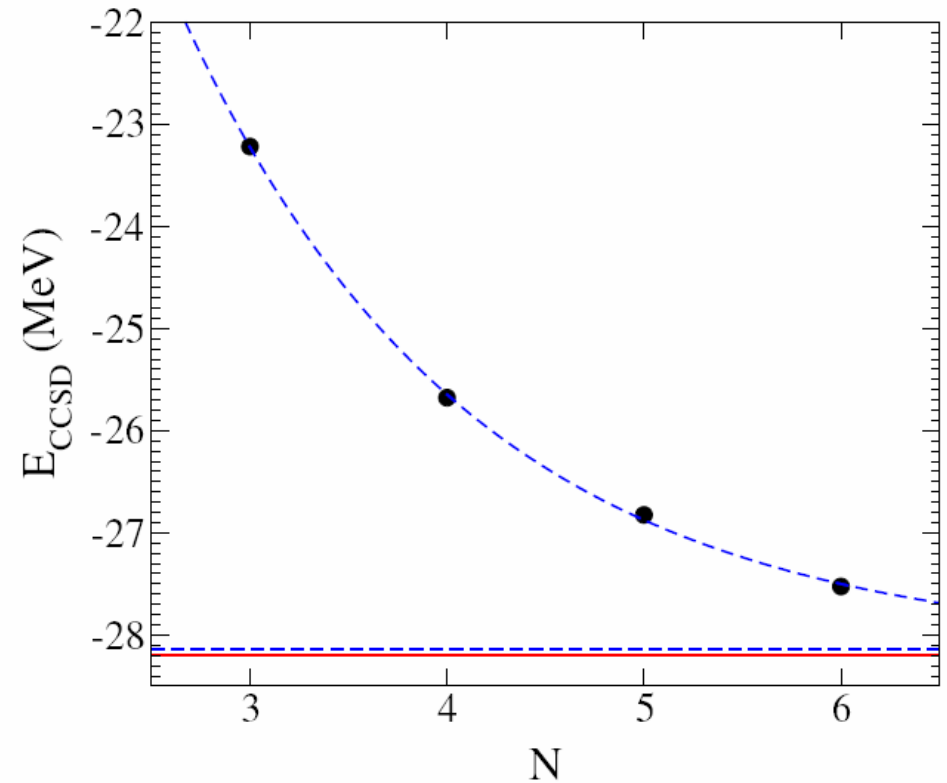


FIG. 6: (Color online) Data points: CCSD results (taken at the  $\hbar\omega$  minima) for the binding energy of  ${}^4\text{He}$  with 3NFs as a function of the number of oscillator shells. Dashed lines: Exponential fit to the data and asymptote of the fit. Full line: Exact result.

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

Three-body force: Chiral EFT at order  $N^2\text{LO}$  (isospin  $1/2$  only)

Main result: Exact result closely matched!

# Important (technical) detail: normal-ordered Hamiltonian

The Hamiltonian is normal-ordered w.r.t. the vacuum state  $|\Phi\rangle$ .

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

Similarly, the Hamiltonian of the 3NF becomes

$$\begin{aligned}\hat{H}_3 &= \frac{1}{6} \sum_{ijk} \langle ijk || ijk \rangle + \frac{1}{2} \sum_{ijpq} \langle ijp || ijq \rangle \{ \hat{a}_p^\dagger \hat{a}_q \} && \text{Vacuum energy and density-dependent one-body terms} \\ &\quad + \frac{1}{4} \sum_{ipqrs} \langle ipq || irs \rangle \{ \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_s \hat{a}_r \} + \hat{h}_3, && \text{Density-dependent two-body terms} \\ \hat{h}_3 &\equiv \frac{1}{36} \sum_{pqrst} \langle pqr || stu \rangle \{ \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_r^\dagger \hat{a}_t \hat{a}_s \} && \text{Residual three-body terms}\end{aligned}$$

- 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 ${}^4\text{He}$

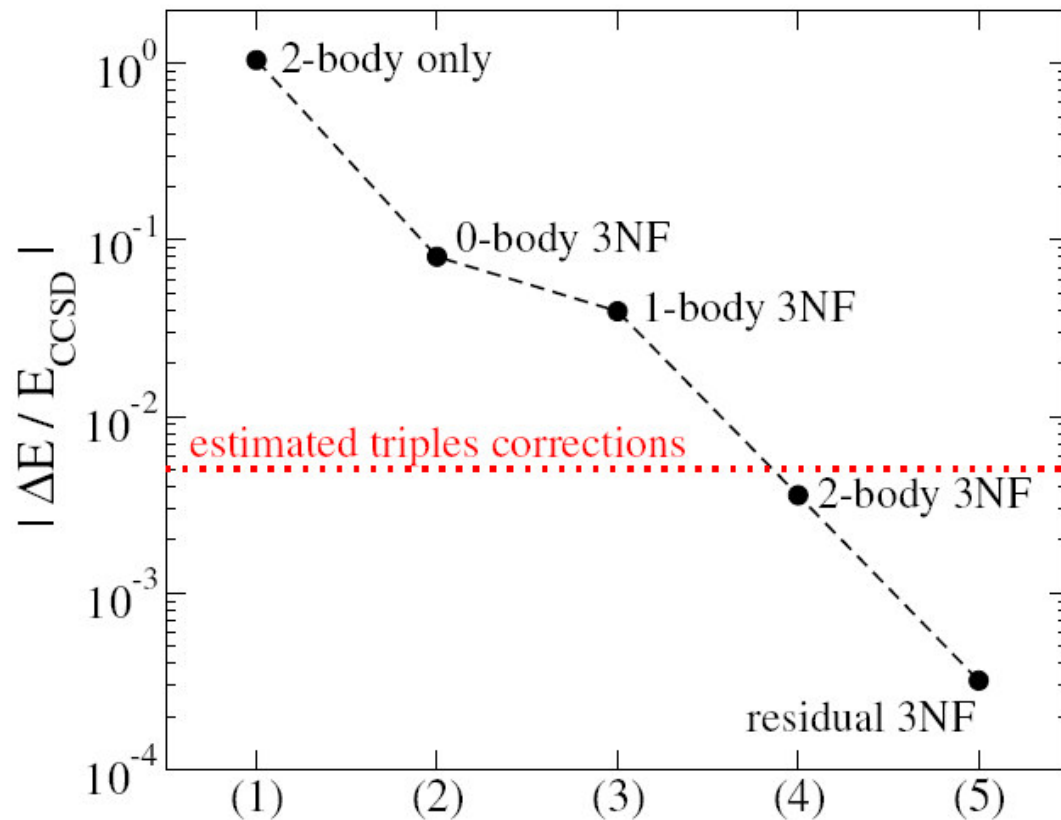


FIG. 7: (Color online) Relative contributions  $|\Delta E/E|$  to the binding energy of  ${}^4\text{He}$  at the CCSD level. The different points denote the contributions from (1) low-momentum NN interactions, (2) the vacuum expectation value of the 3NF, (3) the normal-ordered one-body Hamiltonian due 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**

# Improved CCSD(T) results for ${}^4\text{He}$ : perturbative $3p$ - $3h$ clusters

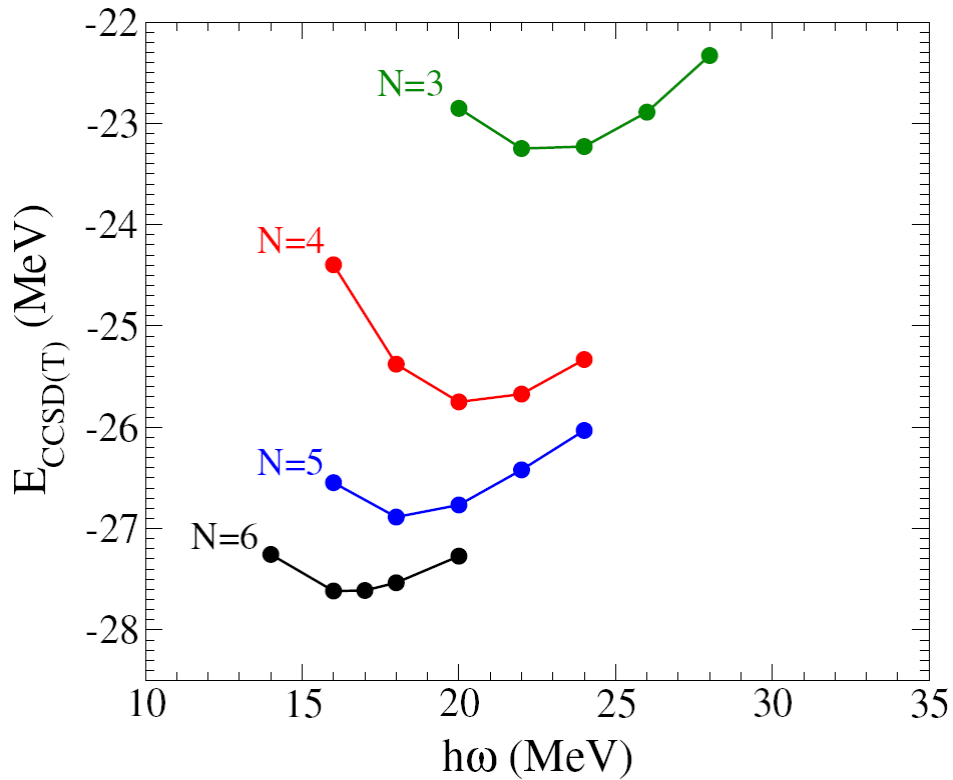


FIG. 8: (Color online) CCSD(T) results for the binding energy of  ${}^4\text{He}$  as a function of the oscillator spacing and for model spaces consisting of  $N = 3$  to  $N = 6$  oscillator shells. The contributions from 3NFs are limited to the density-dependent zero-, one-, and two-body terms and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

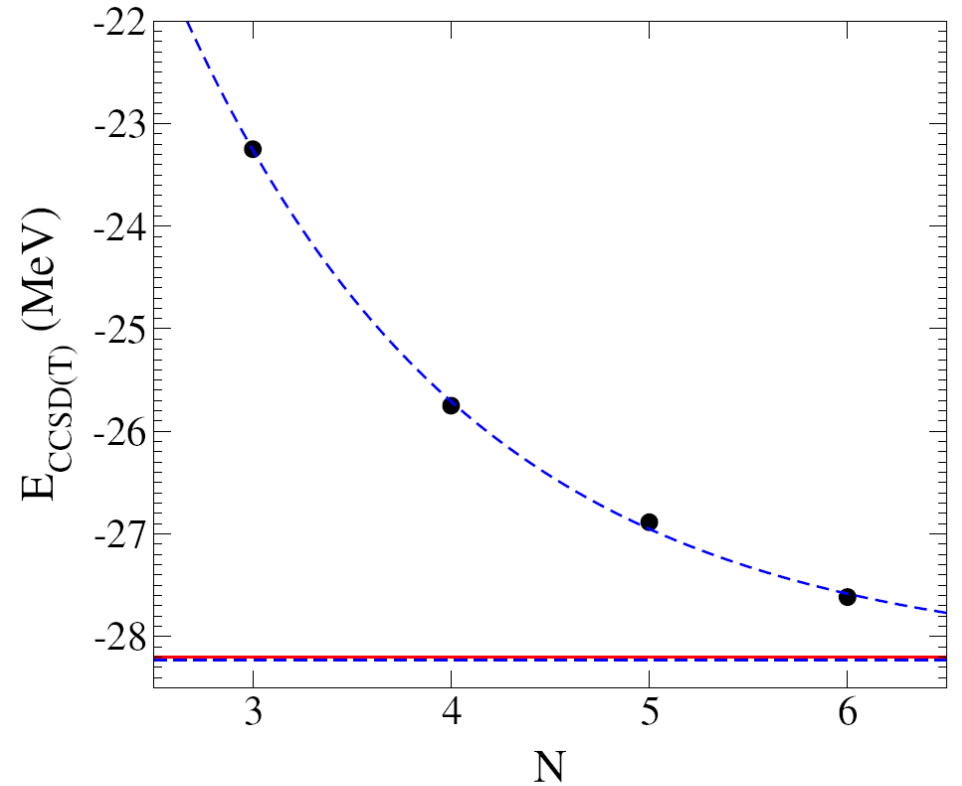


FIG. 9: (Color online) Data points: CCSD(T) results (taken at the  $\hbar\omega$  minima) for the binding energy of  ${}^4\text{He}$  with 3NFs as a function of the number of oscillator shells. Dashed lines: Exponential fit to the data and asymptote of the fit. Full line: Exact result.

Center-of-mass expectation: 20 keV

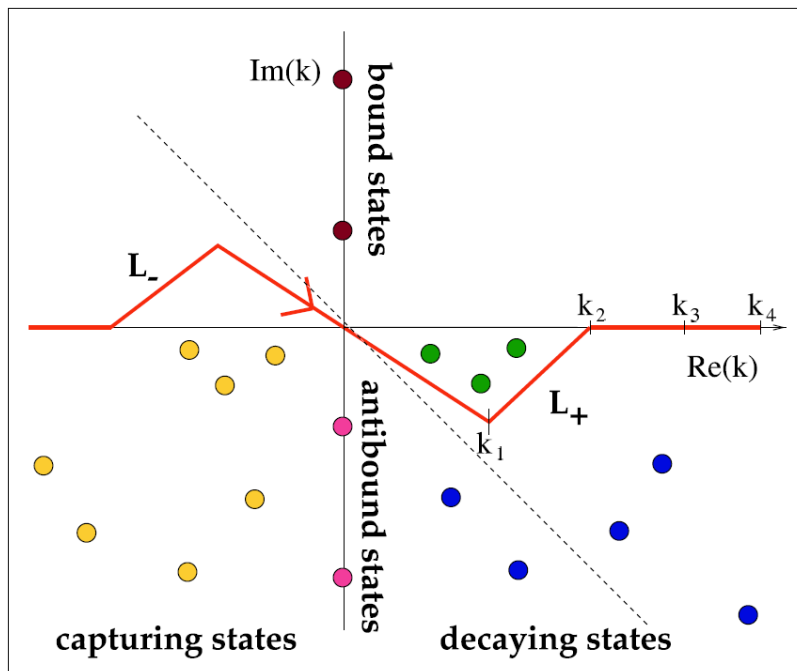
# Helium isotopes: weakly bound and unbound quantum systems

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

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

Two new aspects:

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



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

## Comparison with exact diagonalization

Method	${}^3\text{He}$	${}^4\text{He}$	${}^5\text{He}$	${}^6\text{He}$
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  ${}^6\text{He}$  (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

	<sup>3</sup> He		<sup>4</sup> He		<sup>5</sup> He		<sup>6</sup> He		<sup>7</sup> He		<sup>8</sup> He		<sup>9</sup> He		<sup>10</sup> He	
<i>lj</i>	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]
<i>s - p</i>	-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
<i>s - d</i>	-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
<i>s - f</i>	-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
<i>s - g</i>	-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
<i>s - h</i>	-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
<i>s - i</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 <sup>3-10</sup>He ground states with the low-momentum N<sup>3</sup>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 <sup>10</sup>He is  $\approx 0.002$ MeV.

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

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

# Spherical (j-coupled) coupled-cluster approach

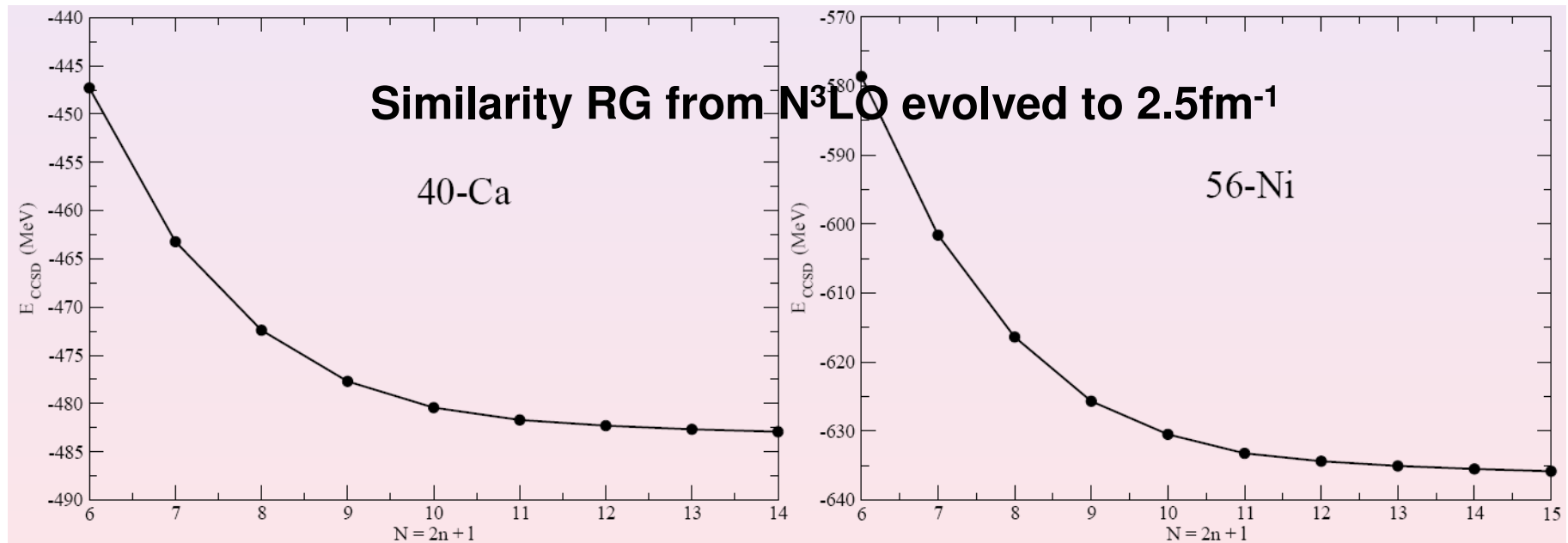
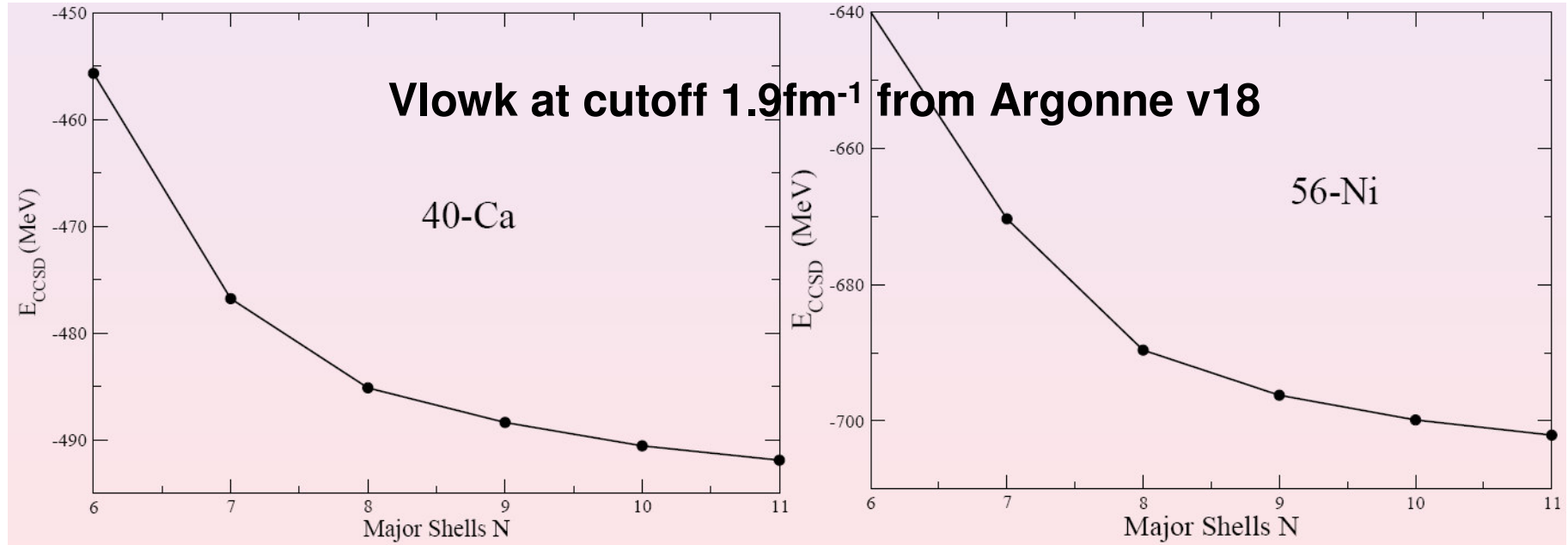
Reformulate coupled-cluster theory and exploit spherical symmetry

1. Possible for nuclei with closed sub-shell (or cs +/- 1)
2. Relatively simple since similarity-transformed Hamiltonian is two-body (CCSD) or three-body (CCSDT) at most
3. Enormous computational reduction:  $o^2u^4 \rightarrow (o^2u^4)^{2/3}$ 
  - CCSD for  $^{40}\text{Ca}$  on a laptop (now)
  - CCSDT for medium-mass nuclei via super computers (near future)

Preliminary CCSD results:  $N^3\text{LO}$  (oscillator basis with  $hw=34\text{MeV}$ )

N	$^{16}\text{O}$	$^{12}\text{C}$	$^{14}\text{C}$	$^{28}\text{S}$	$^{40}\text{Ca}$	$^{48}\text{Ca}$	$^{56}\text{Ni}$
10	-99.73	-48.44	-71.97	-142.50	-275.09	-292.05	-246.73
11	-100.67	-49.19	-72.78	-145.24	-281.48	-305.46	-269.63
12	-100.82	-49.29	-72.90	-147.62	-286.54	-310.86	-276.33
13	-101.08	-49.56	-73.15	-148.06	-287.77	-314.65	-283.81
14	-101.12	-	-	-	-289.72	-316.42	-285.82

# Preliminary results $^{40}\text{Ca}$ and $^{56}\text{Ni}$ in j-coupled scheme



# Summary

NN only:

- Converged results w.r.t. model space and cluster truncation for  $^3\text{H}$ ,  $^4\text{He}$ , and  $^{16}\text{O}$ .
- Almost converged results for  $^{40}\text{Ca}$  (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  $^4\text{He}$ ).
- ☺ Residual 3-body part of 3NF can be neglected.

J-coupled code:

- Preliminary CCSD results for  $^{40,48}\text{Ca}$ ,  $^{56}\text{Ni}$  for soft and hard interactions

# Outlook

- Densities and response to external potentials for comparison with DFT  
→ SciDAC project UNEDF
- Revisit helium isotopes, study neutron-rich oxygen isotopes with 3NF, ab-initio studies of  $^9,^{11}\text{Li}$
- Spherical CC approach: medium-mass nuclei, “bare” interactions  
→ CCSD on a laptop  
→ CCSDT (“gold standard”) on supercomputers
- m-scheme CC approach for open-shell problems, time-dependent phenomena, fusion