Coupled-Cluster Theory for Nuclei

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Outline

1. Effective interactions
   - N-N forces from chiral EFT
   - Low-momentum NN interactions
2. Coupled Cluster approach to nuclear structure
   - Coupled-Cluster theory and the role of size extensivity
   - Application to light and medium mass nuclei
   - CCSD in J-coupled scheme
   - Coupled Cluster approach with three-body Hamiltonians
3. Conclusion and Perspectives

N-N force from Chiral perturbation theory

"If you want more accuracy, you have to use more theory (more orders)"

Effective Lagrangian → obeys QCD symmetries (spin, isospin, chiral symmetry breaking)

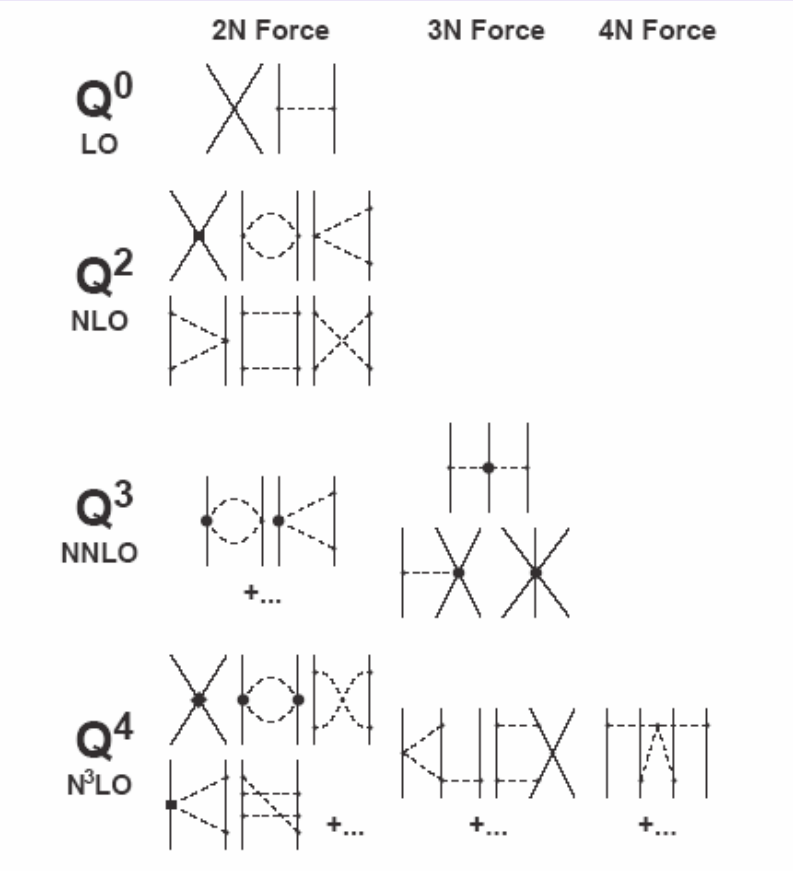
Lagrangian
→ infinite sum of Feynman diagrams.

Expand in $O(Q/\Lambda_{QCD})$

Weinberg, Ordonez, Ray, van Kolck

NN amplitude uniquely determined by two classes of contributions: contact terms and pion exchange diagrams.

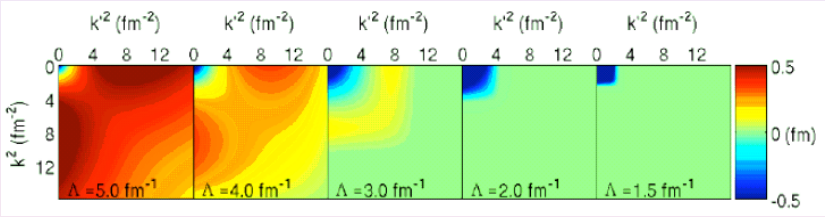
24 paramters (rather than 40 from meson theory) to describe 2400 data points with

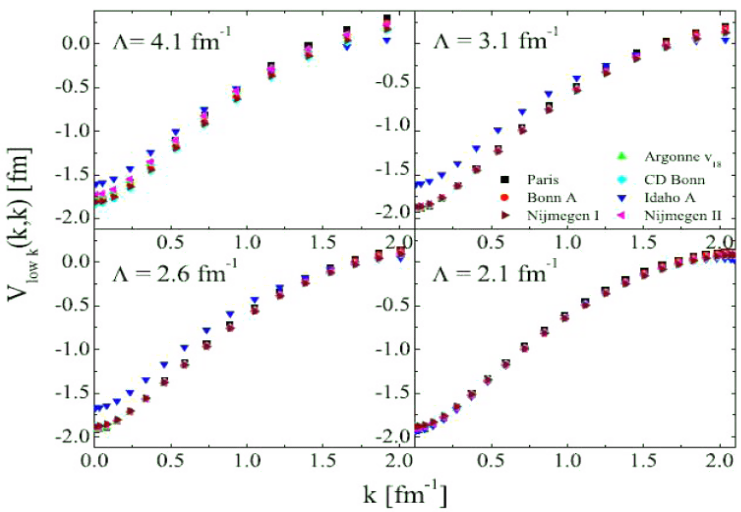


Low-momentum nucleon-nucleon interaction: $V_{\mathrm{low}-k}$

A-body nuclear Hamiltonian

$$H^A = T - T_{CM} + V_2(\Lambda) + V_3(\Lambda) + \cdots V_A(\Lambda) \approx T - T_{CM} + V_2(\Lambda) + V_3(\Lambda)??$$





Different high-precision potentials

Universal low-momentum potential

Ref.: S. K. Bogner, T. T. S. Kuo, and A. Schwenk, Phys. Rep. 386 (2003) 1

Coupled Cluster approach to medium mass nuclei

1. Coupled Cluster Theory is fully microscopic .
2. Coupled Cluster is size extensive. No unlinked diagrams enters, and error scales linearly with number of particles.
3. Low computational cost (CCSD scales as $n_o^2 n_u^4$).
4. Capable of systematic improvements.
5. Amenable to parallel computing.

Computational Chemistry: 100's of publications in any year (Science Citation Index) for applications and developments.

Coupled Cluster Theory

Exponential Ansatz for Ψ

$$|\Psi\rangle = e^{\hat{T}}|\Phi_0\rangle, \quad \hat{T} = \hat{T}_1 + \hat{T}_2 + \ldots + \hat{T}_A$$

$$\hat{T}_1 = \sum_{i,a} t_i^a \hat{a}_a^\dagger \hat{a}_i, \; \hat{T}_2 = \frac{1}{2} \sum_{i<j,a<b} t_{ij}^{ab} \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i.$$

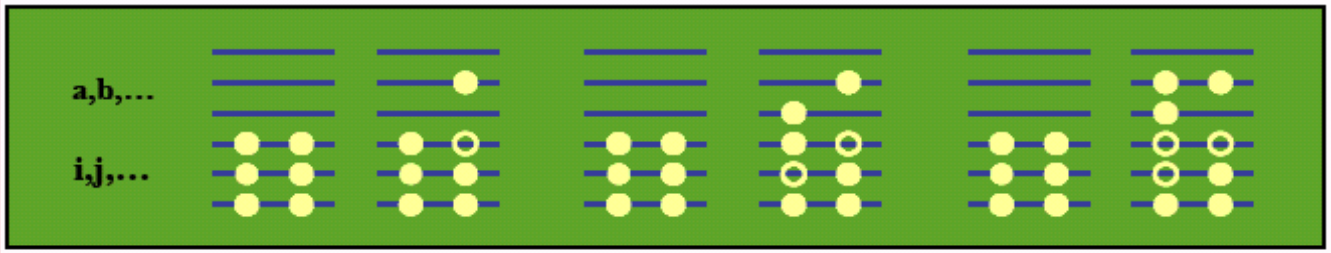
Coupled Cluster Equations

$$\Delta E = \langle \Phi_0 | \left(H_N exp(T)\right)_C | \Phi_0 \rangle$$

$$0 = \langle \Phi_p | \left(H_N exp(T)\right)_C | \Phi_0 \rangle$$

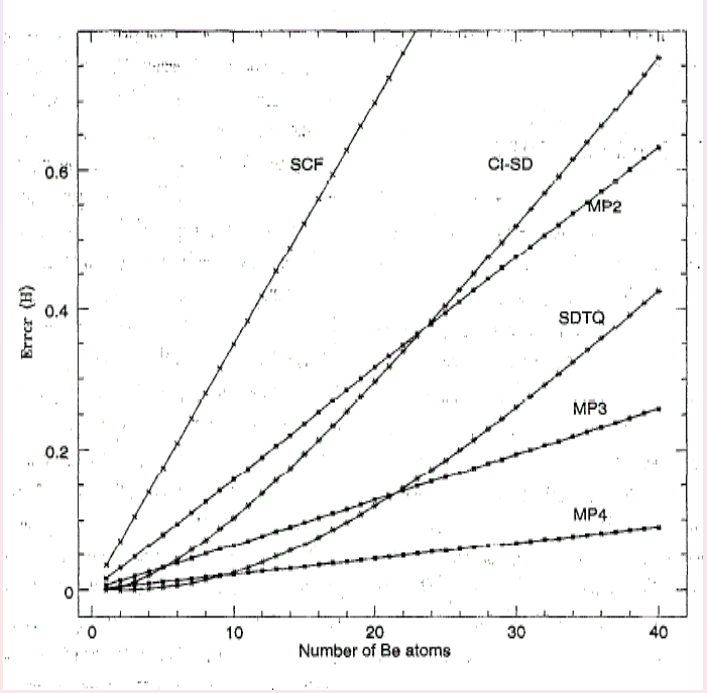
$$\bar{H} = \left(H_N exp(T)\right)_C$$

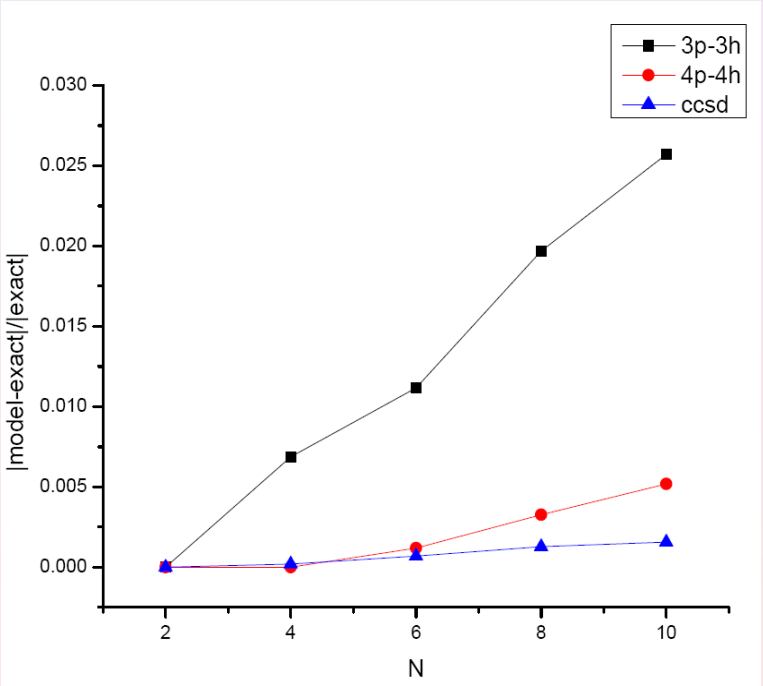
$$T_1 = \sum_{\substack{i \\ a}} t_i^a \left| \Phi_i^a \right\rangle, \quad T_2 = \sum_{\substack{i>j \\ a>b}} t_{ij}^{ab} \left| \Phi_{ij}^{ab} \right\rangle, \quad T_3 = \sum_{\substack{i>j>k \\ a>b>c}} t_{ijk}^{abc} \left| \Phi_{ijk}^{abc} \right\rangle$$



Size Matters! Role of size-extensivity

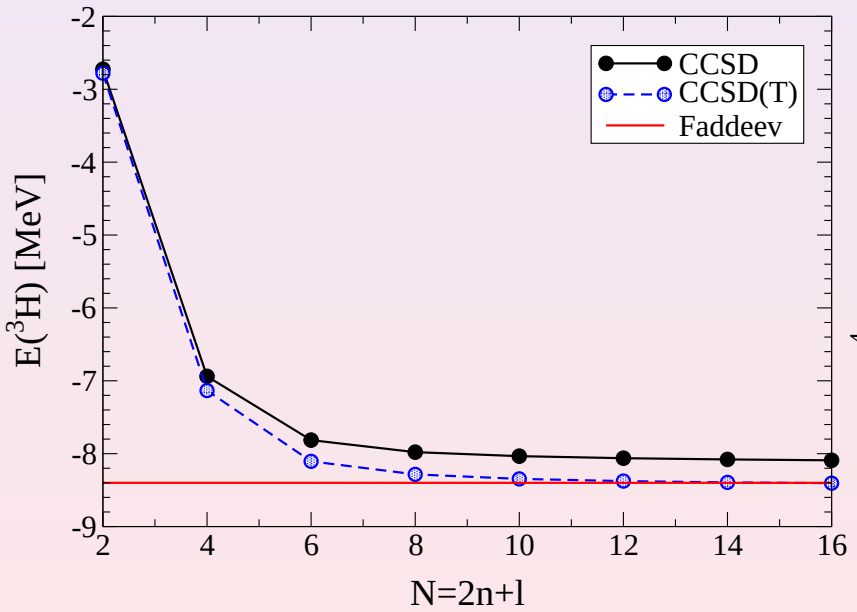
Disconnected diagrams in truncated shell model/CI models (CISD, CISDT,...) leads to wrong scaling of energy with increasing number of particles.

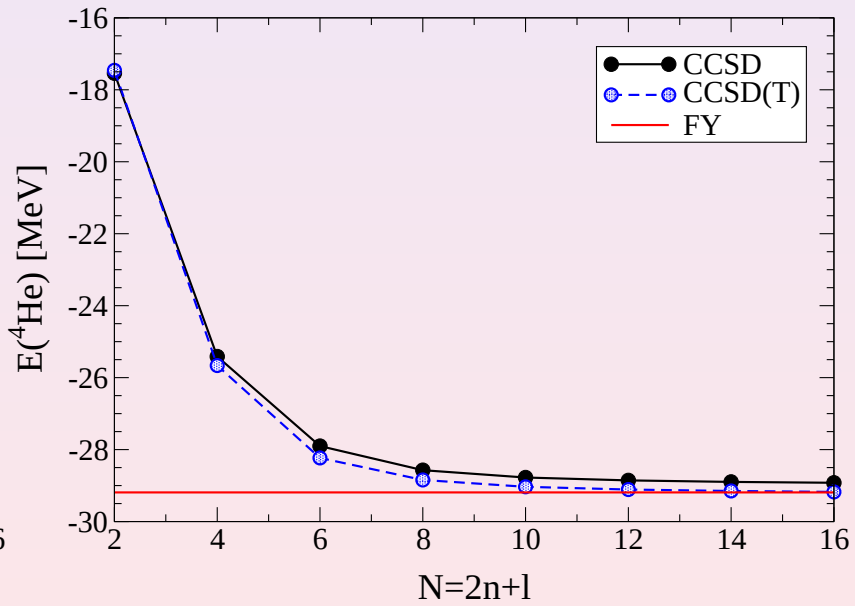




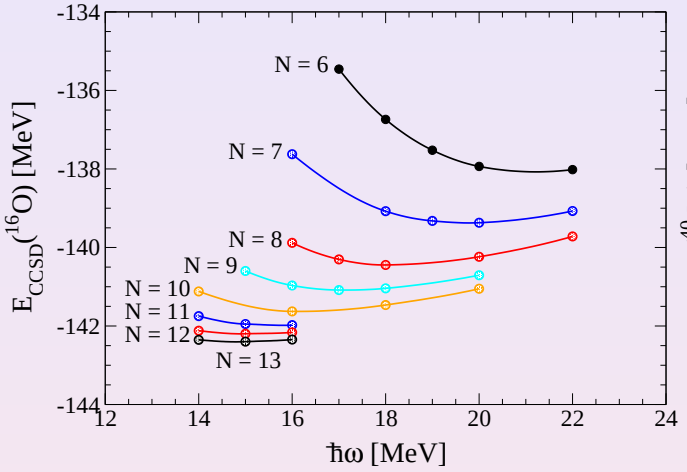
Coupled Cluster meets benchmarks of ^{3}H and ^{4}He!

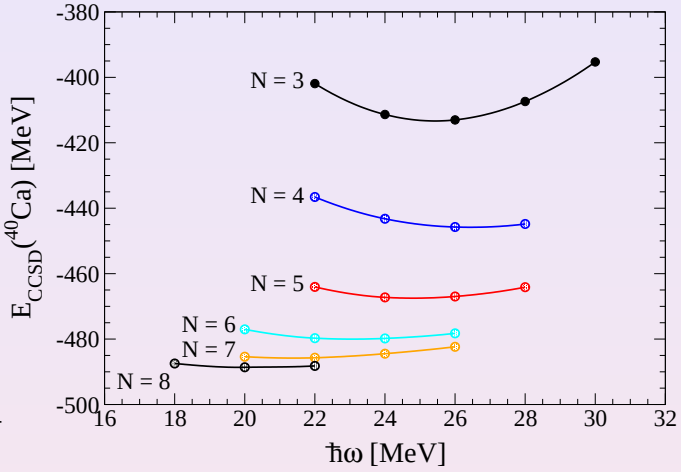
CCSD(T) and Faddeev (-Yakubovsky) results for ^{3}H and ^{4}He using $V_{\mathrm{low}-k}$ from AV18 with $\Lambda = 1.9\mathrm{fm}^{-1}$. **CCSD(T) are within the errors (50 keV) of the Faddeev results!**





Benchmarking ^{16}O and ^{40}Ca





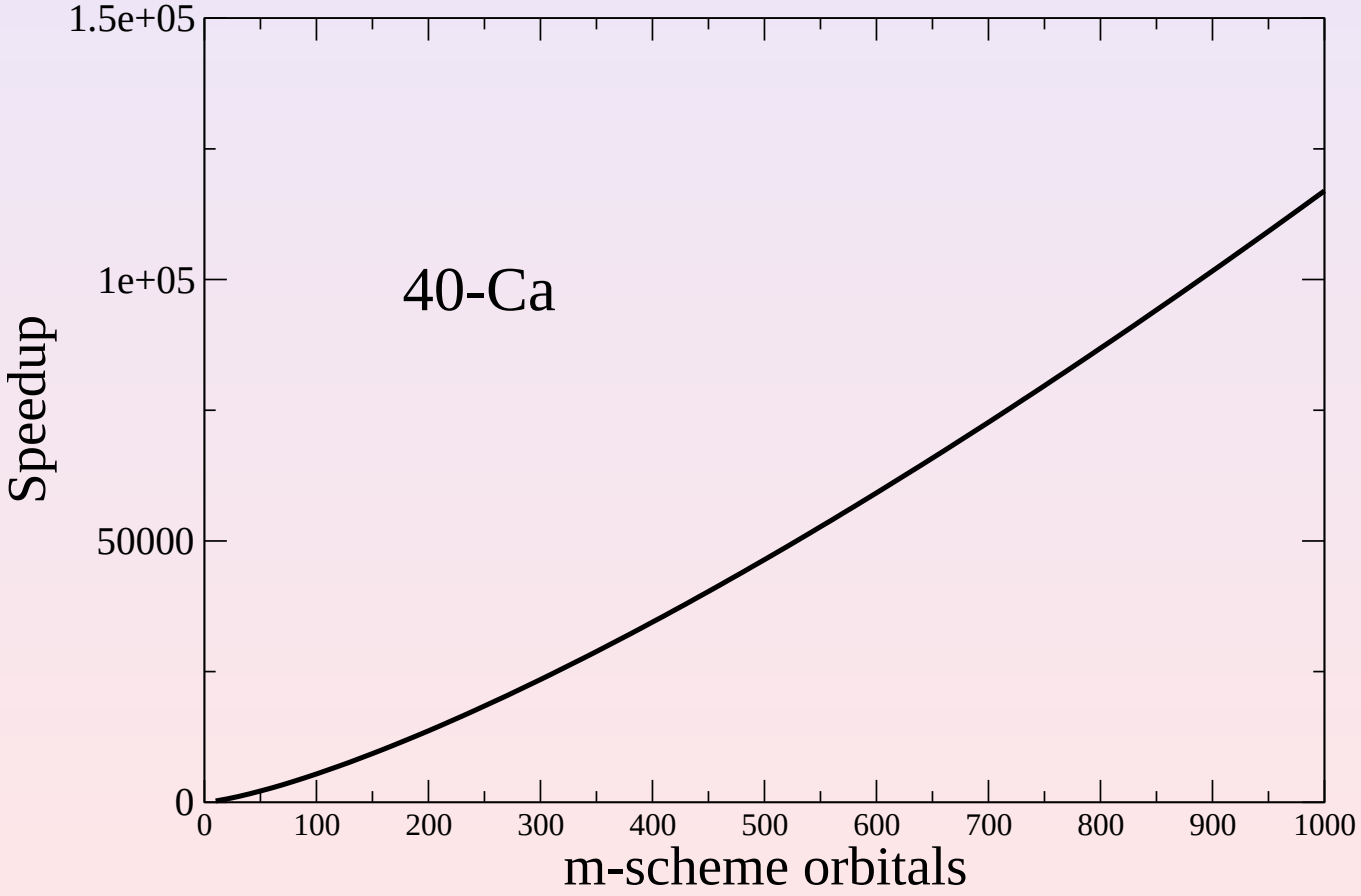
	^{4}He	^{16}O	^{40}Ca
E_0	-11.815	-60.204	-347.474
ΔE_{CCSD}	-17.107	-82.576	-143.736
$\Delta E_{\mathrm{CCSD(T)}}$	-0.253	-5.450	-11.699
$E_{\mathrm{CCSD(T)}}$	-29.175	-148.232	-502.908
exact (FY)	-29.19(5)		

^{40}Ca converged within 1% !

Roth and Navratil PRL 99, 092501 (2007) E_{CISDT} = -462.7MeV. Our comment: arXiv:0709.0449

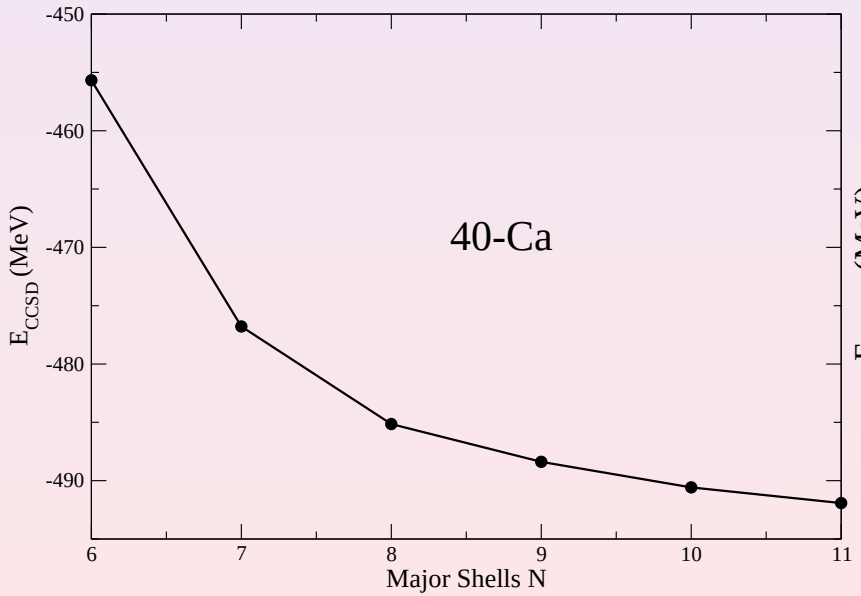
Speedup of J-coupled CCSD code for ^{40}Ca

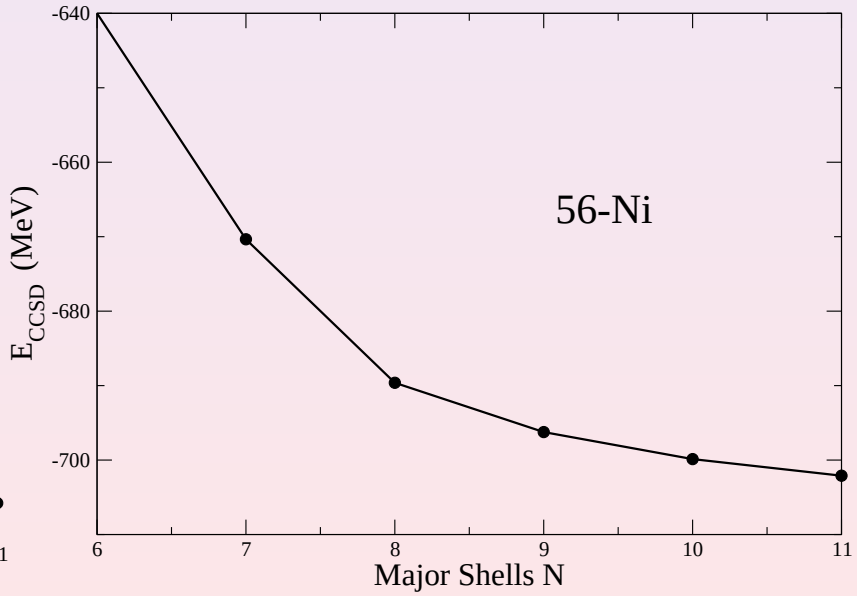
Speedup of J-coupled CCSD code for ^{40}Ca as compared to m-scheme CCSD code.



CCSD results for ^{40}Ca and ^{56}Ni using $V_{\mathrm{low}-k}$.

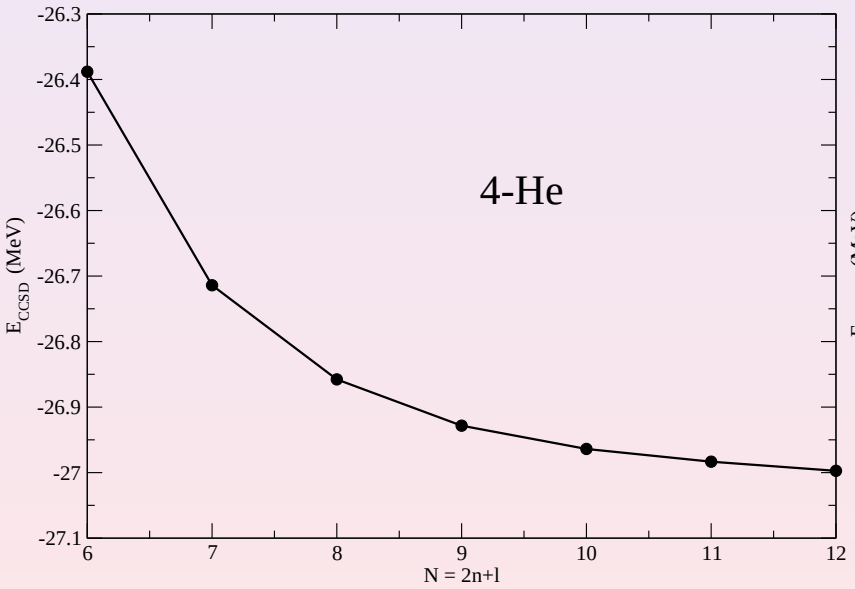
- We have derived and implemented CCSD in a J-coupled scheme.
- Computational cost drastically reduced, from $n_o^2 n_u^4$ to $n_o^{4/3} n_u^{8/3}$.
- Converged CCSD results for ^{40}Ca and ^{56}Ni on your laptop!

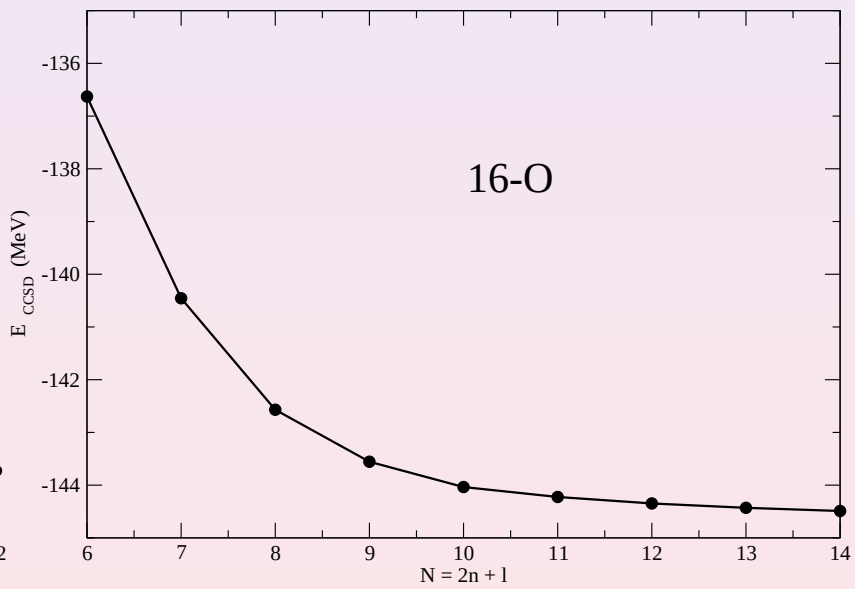




CCSD results for ^{4}He and ^{16}O using V-SRG

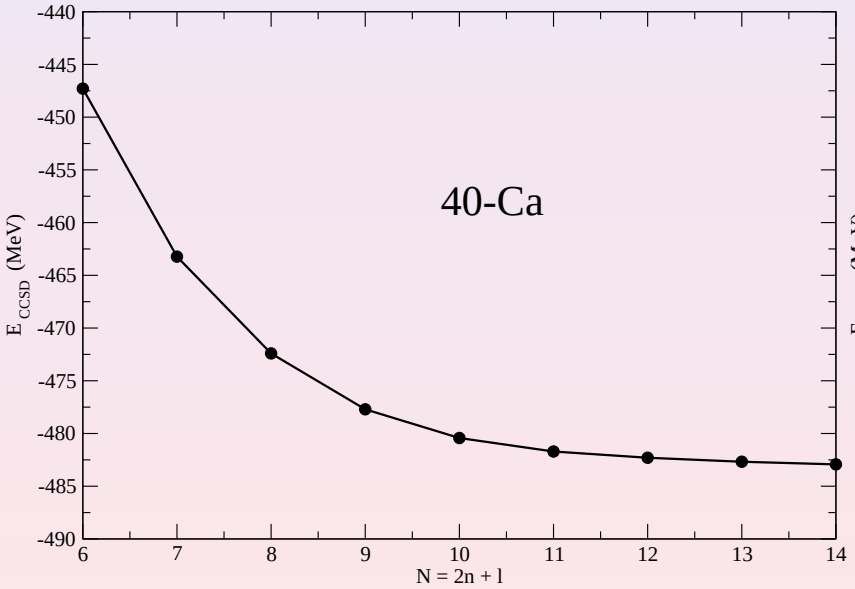
Converged results for ^{4}He and ^{16}O, using N^{3}LO evolved down to $\lambda = 2.5\mathrm{fm}^{-1}$ from similarity renormalization group (SRG) theory.

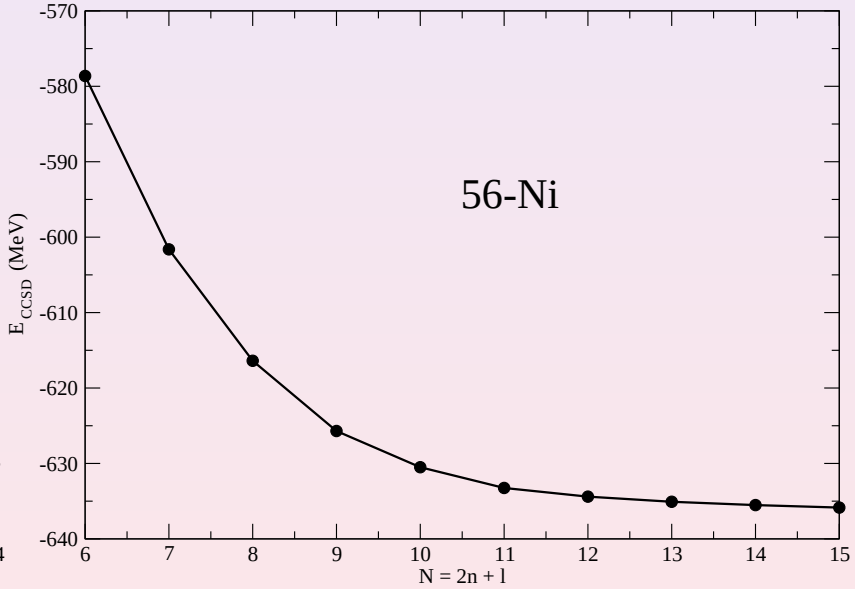




CCSD results for ^{40}Ca and ^{56}Ni using V-SRG

Converged results for ^{40}Ca and ^{56}Ni, using N^{3}LO evolved down to $\lambda = 2.5\mathrm{fm}^{-1}$ from similarity renormalization group theory.





CCSD results using the "bare" N3LO interaction

CCSD results using N^3LO at 500 MeV cutoff.

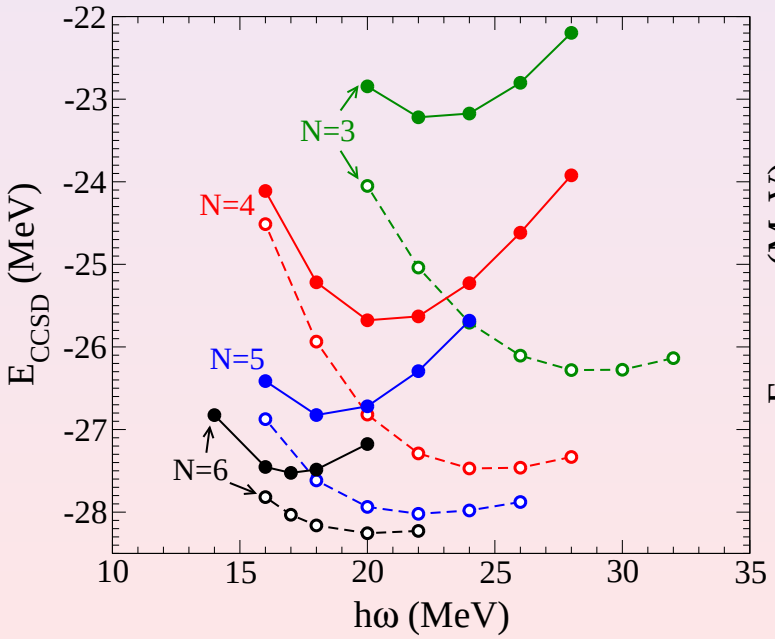
N	^{16}O	^{12}C	^{14}C	^{28}S	^{40}Ca	^{48}Ca	^{56}Ni
10	-99.73	-48.44	-71.97	-142.50	-275.09	-292.05	-246.73
11	-100.67	-49.19	-72.78	-145.24	-281.48	-305.46	-269.63
12	-100.82	-49.29	-72.90	-147.62	-286.54	-310.86	-276.33
13	-101.08	-49.56	-73.15	-148.06	-287.77	-314.65	-283.81
14	-101.12	-	-	-	-289.72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

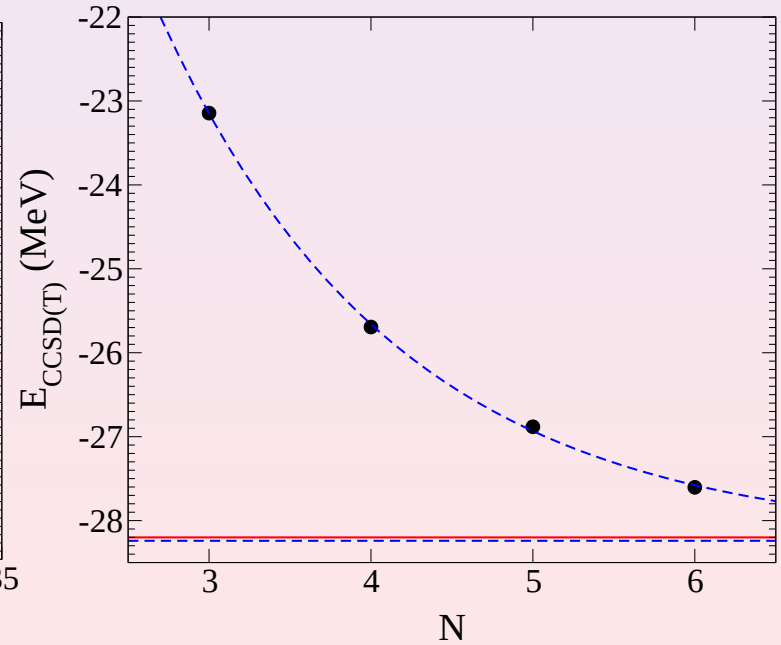
Coupled Cluster Theory with 3NF

- We have derived and implemented Coupled Cluster equations for three-body Hamiltonians.
- Probe cutoff dependence of $V_{\mathrm{low}-k}$ with three nucleon force in light and medium heavy nuclei.
- Does 3NF provide the necessary repulsion/attraction needed to approach experimental mass values ?
- *" Coupled-cluster theory for three-body Hamiltonians "* G. Hagen et al., PRC (76) 034302 (2007).

Coupled Cluster Results for ^{4}He with 3NF

- $V_{\mathrm{low}-k}$ from AV18 with $\Lambda = 1.9\mathrm{fm}^{-1}$.
- 3NF brings in repulsion as expected !
- CCSD and CCSD(T) with 3NF meets Faddeev-Yakubovsky benchmark ! $E_{\mathrm{CCSD(T)}} \approx -28.24$ MeV. F-Y $E = -28.20(5)$MeV.

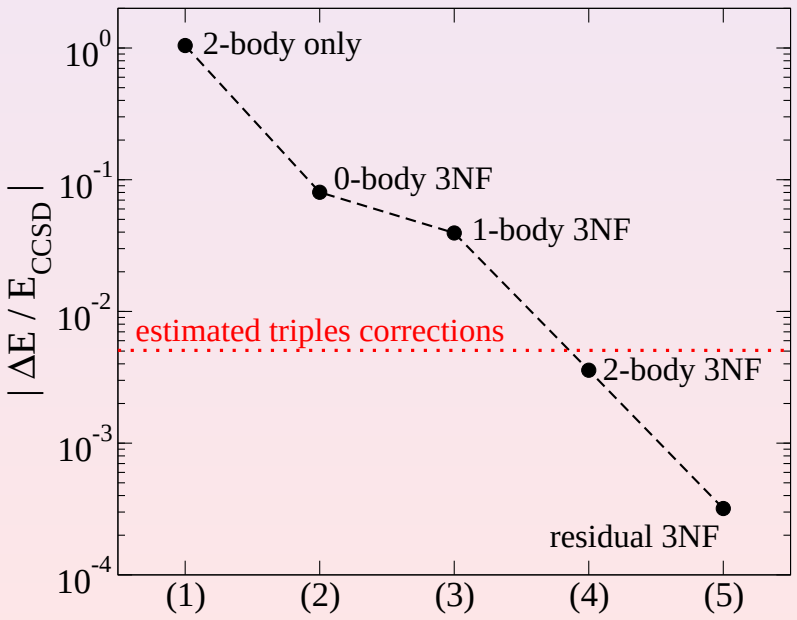




Different contributions to E_{CCSD} from 3NF in ^{4}He

Three-body Hamiltonian in normal ordered form:

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



Really good news!

- The "density dependent" terms of 3NF are dominant!
- ϵ from residual 3NF costs $1-\epsilon$ of work !
- "2-body" machinery can be used.
- **Residual three-nucleon force can be neglected!**

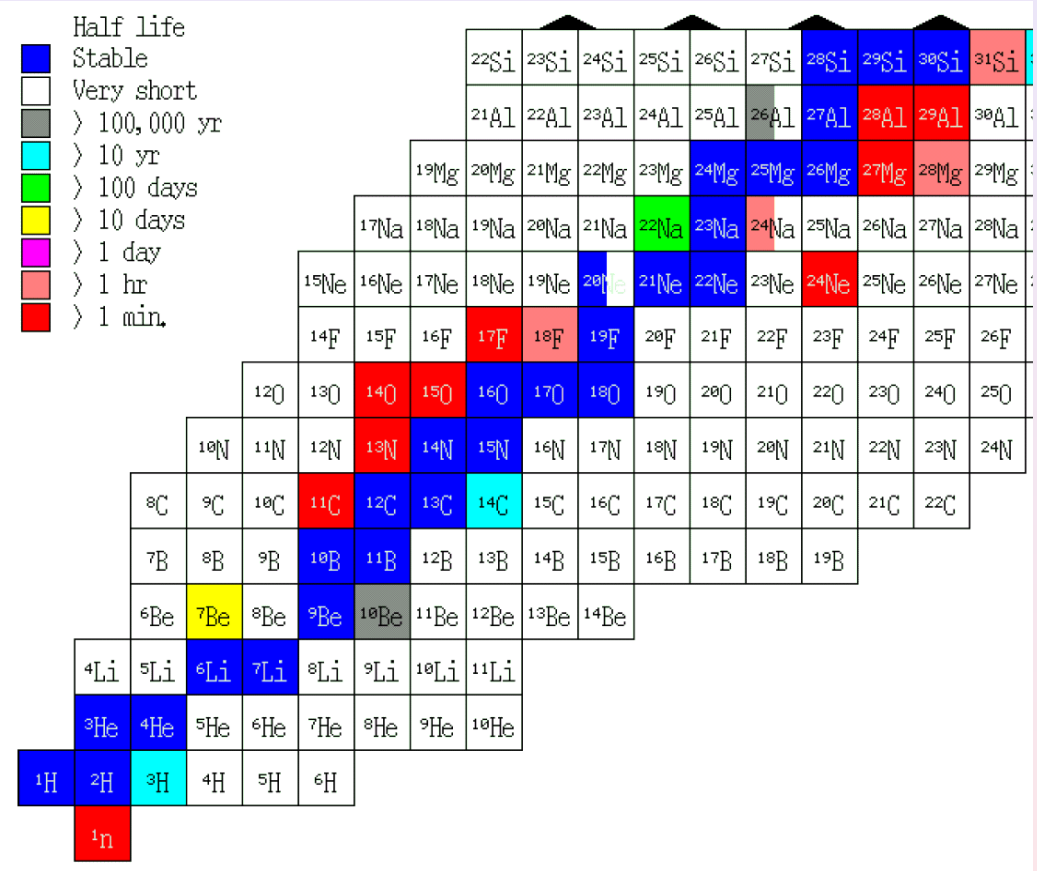
Conclusion

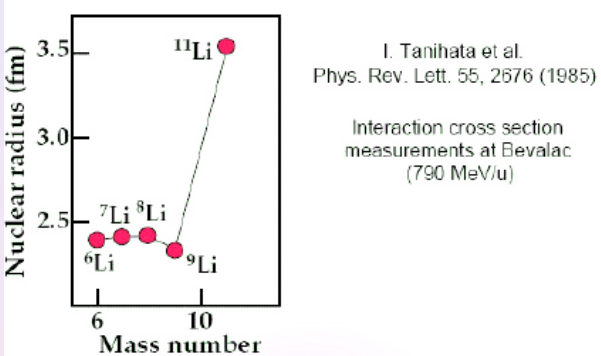
- Coupled Cluster meets few-body benchmark calculations; we have benchmarked ^{16}O and ^{40}Ca.
- J-coupled CCSD code has been derived and implemented. Calculate ^{40}Ca and ^{56}Ni on your laptop!
- Coupled Cluster theory with 3NF has been derived and implemented. Benchmarks of ^{4}He has been met.
- Density dependent zero-, one- and two-body parts of 3NF give the major contributions. Interesting perspective for heavier systems.
- CCM has been succesfully applied to the description of open-quantum systems.
- We have a tool to attack the structure and properties of medium mass nuclei !

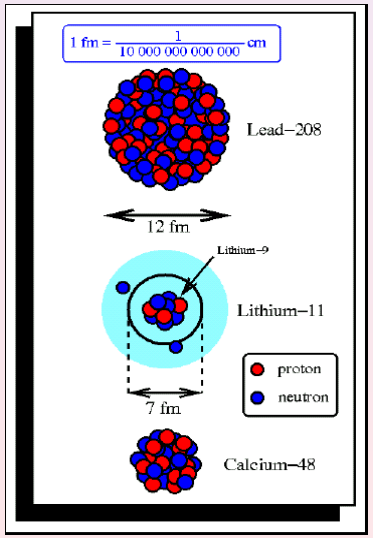
Future perspectives

- Linking DFT with CCM; matter densities, currents and response to external fields. Within the SciDAC-UNEDF program.
- Provide information on how the density functional looks like ?
- Location of dripline in the Oxygen chain ?
- Revisit Helium chain with 3NF. Spin-orbit splitting in He7 and He9.
- Inclusion of full triples for truly open-shell nuclei.
- Excited states and matter densities for dripline nuclei.
- We are developing a J-coupled CCSDT code. Virtual exact solutions of ^{56}Ni and ^{100}Sn within a year!

Ab-initio approach to light and medium mass nuclei







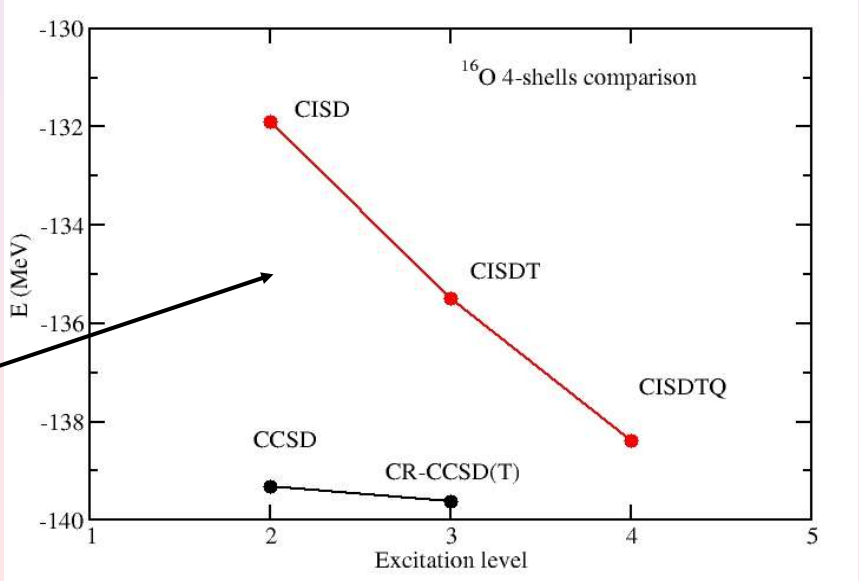
Comparison with Shell Model/Configuration Interaction

In Shell Model approach a linear excitation operator is used instead of an exponential. $\Psi = (1 + B_1 + B_2 + ...)\Phi_0$

- Any particle-hole truncation introduces unlinked diagrams, and it is therefore not size extensive.
- Dimension increases dramatically with number of active particles.

Comparison of CC with CI at given excitation level.

Nuclear Example (Kowalski et al PRL 2004).



Relationship between shell model and CC amplitudes

$$B_1 = T_1$$

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

$$B_3 = T_3 + T_2 T_1 + \frac{1}{6} T_1^3$$

$$B_4 = T_4 + T_3 T_1 + \frac{1}{2} T_2^2 + \frac{1}{2} T_2 T_1^2 + \frac{1}{24} T_1^4$$

$$\ldots$$

CCSD

CCSDT

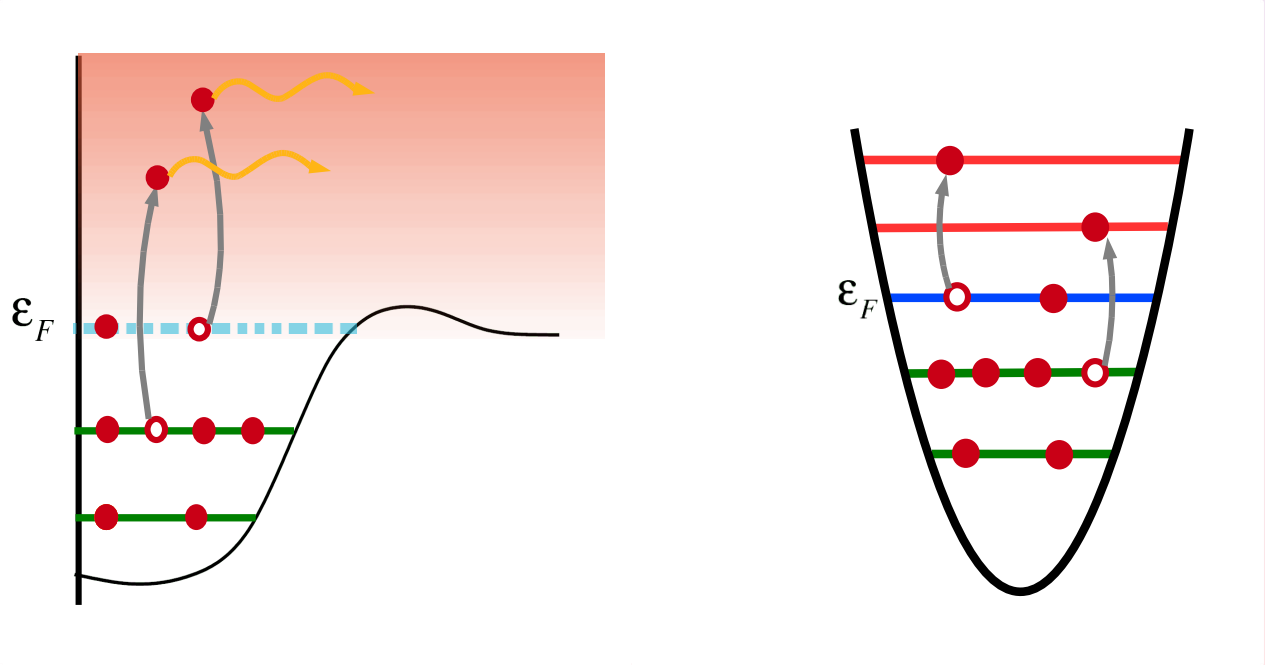
Disconnected quadruples

Connected quadruples

Coupled Cluster for open quantum systems

Open Quantum System.
Coupling with continuum taken into account.

Closed Quantum System.
No coupling with external continuum.

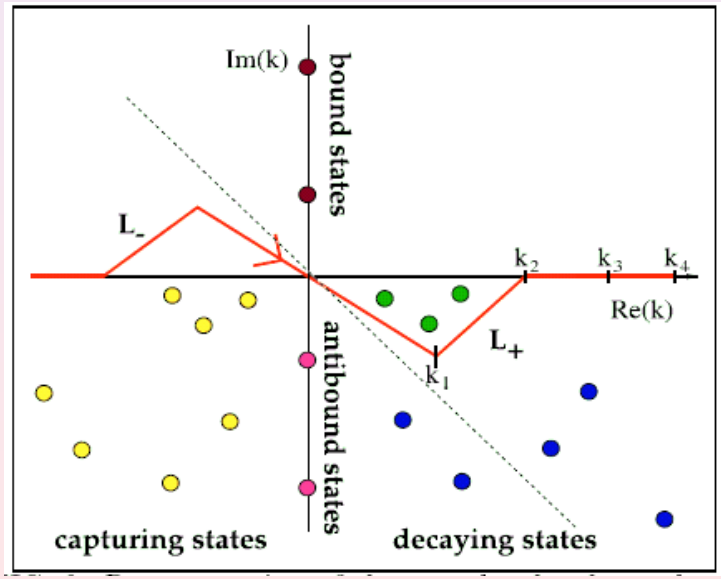


Berggren Single-particle basis

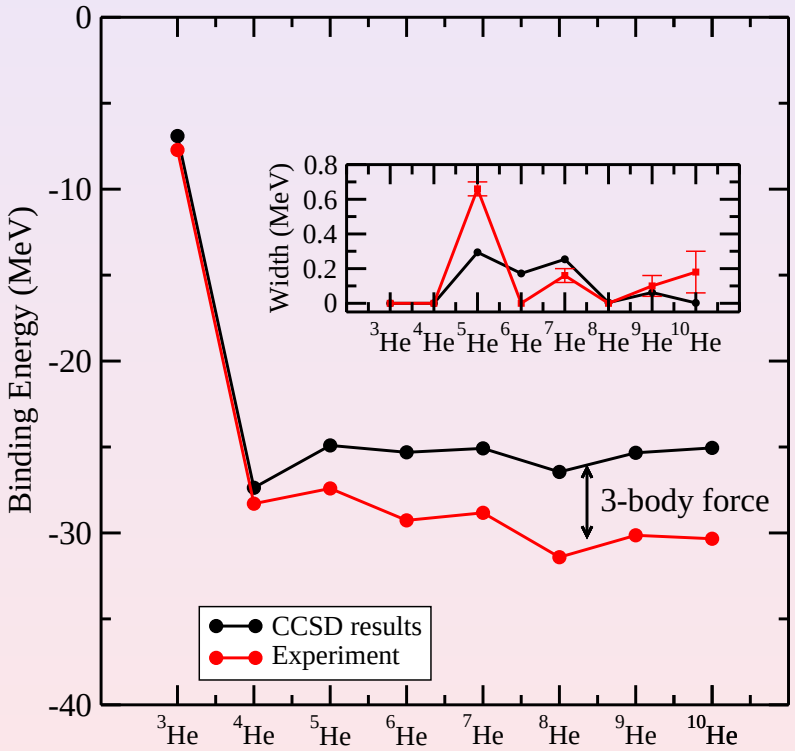
Complex energies requires a generalized completeness relation

$$|\Psi(\mathbf{r},t)|^2 = |\Phi(\mathbf{r})|^2 exp(-\frac{\Gamma}{\hbar}t), \;\; E = E_r - i\Gamma/2.$$

$$\mathbf{1} = \sum_{n=b,d} |\psi_l(k_n)\rangle\langle\tilde{\psi}_l(k_n)| + \int_{L^+} dk\; k^2 |\psi_l(k)\rangle\langle\tilde{\psi}_l(k)|.$$



CCSD results for Helium chain using $V_{\mathrm{low}-k}$

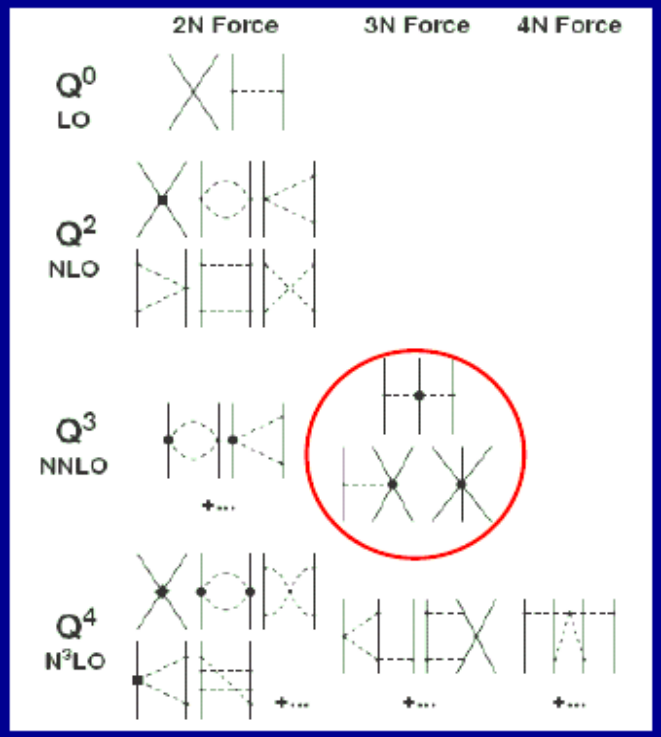


- $V_{\mathrm{low}-k}$ from N3LO with $\Lambda = 1.9\mathrm{fm}^{-1}$.
- G. Hagen et al., Phys. Lett. B 656, 169 (2007). arXiv:nucl-th/0610072.

- First *ab-initio* calculation of decay widths !
- CCM unique method for dripline nuclei.
- ~ 1000 active orbitals
- Underbinding hints at missing 3NF

3NF from Chiral perturbation theory

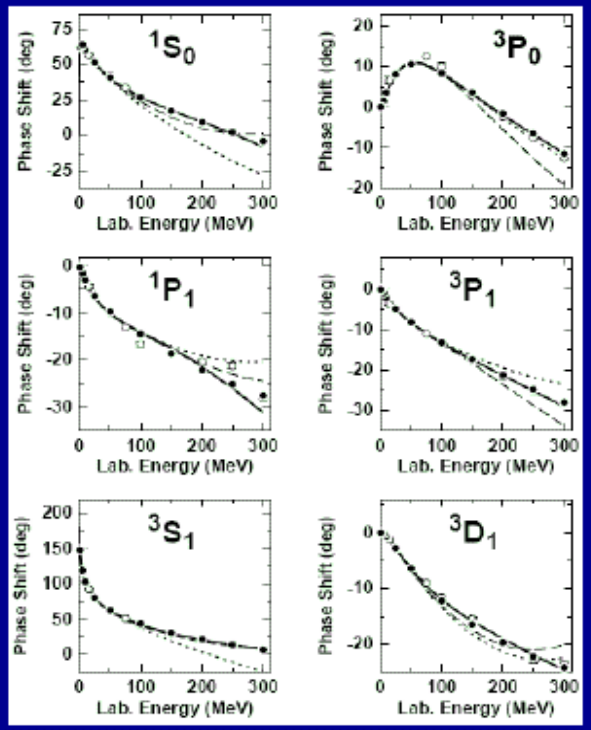
Feynman diagrams



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

Phase shifts reproduced to χ^2/datum=1

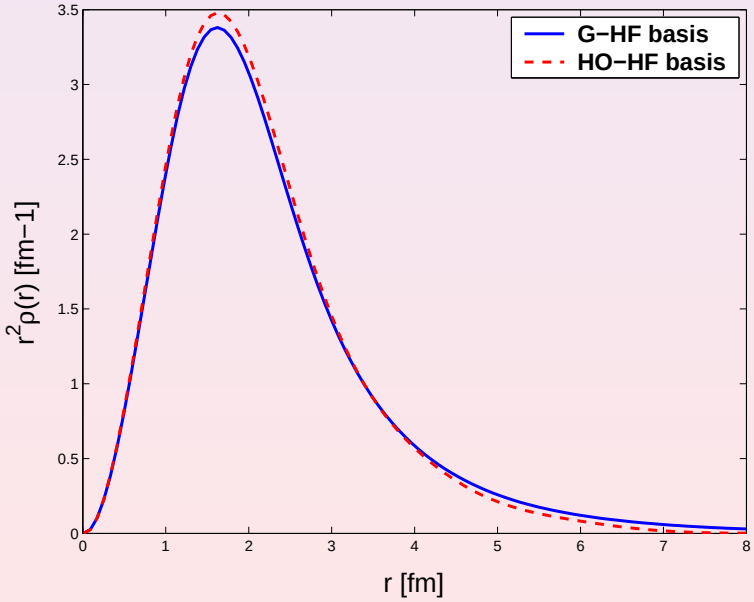
About 24+ parameters

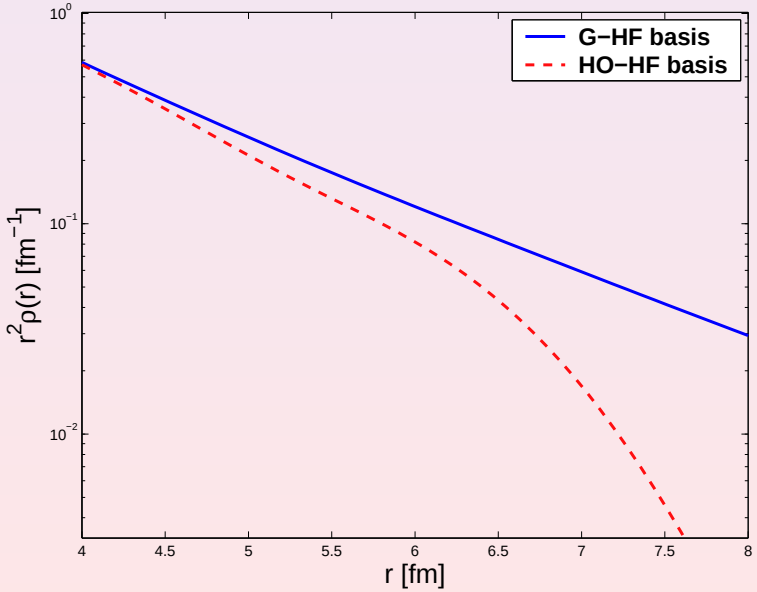


D. R. Entem and R. Machleidt, Phys.Rev. C68 (2003) 041001

Properties of weakly bound nuclei

- Single-particle density in loosely bound ^{8}He.
- Gamow-Hartree-Fock basis has correct asymptotics.
- Hartree-Fock from oscillator basis has bad asymptotics and slow convergence.





CCM vs. exact calculations for open-shell nuclei.

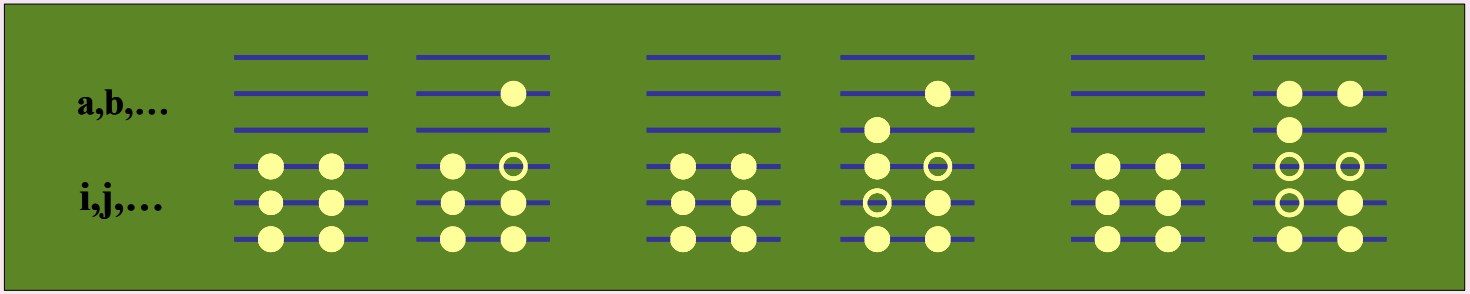
Various Coupled Cluster approaches to the $^{3-6}$He ground states. Single reference Coupled-Cluster methods works!

Method	^{3}He	^{4}He	^{5}He	^{6}He	$\langle J \rangle$, ^{6}He
CCSD	-6.21	-26.19	-21.53	-20.96	0.61
CCSD(T)	-6.40	-26.27	-21.88	-22.60	0.65
CCSDT-1	-6.41	-28.27	-21.89	-22.85	0.29
CCSDT-2	-6.41	-28.26	-21.89	-22.78	0.25
CCSDT-3	-6.42	-26.27	-21.92	-22.90	0.26
CCSDT	-6.45	-26.28	-22.01	-22.52	0.04
Exact	-6.45	-26.3	-22.1	-22.7	0.00

Coupled Cluster in pictures

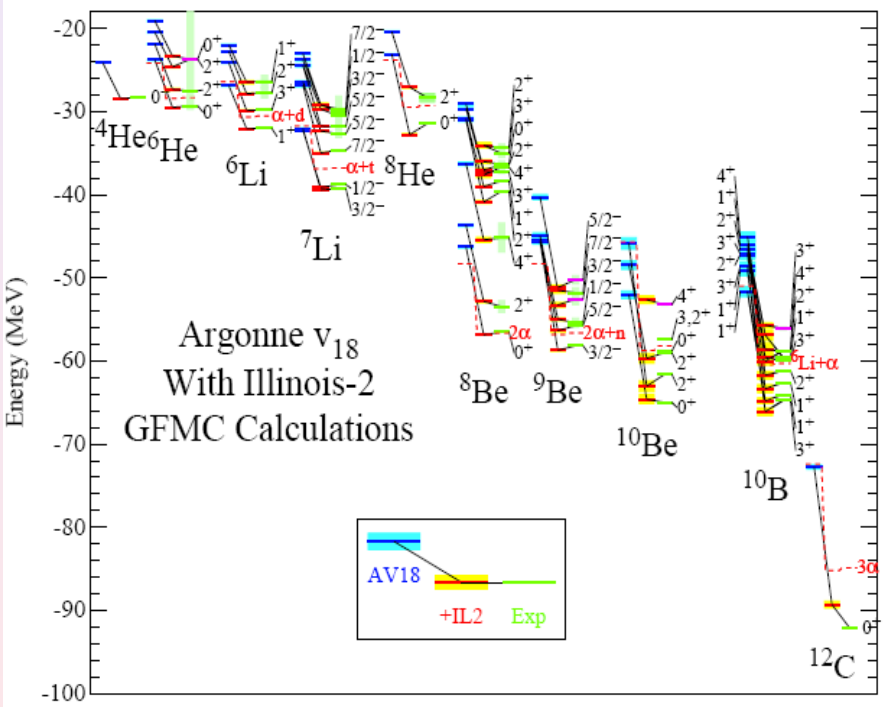
$$\left|\Psi\right\rangle = e^{T^{(A)}}\left|\Phi\right\rangle, \quad T^{(A)} = \sum_{k=1}^{m_A} T_k$$

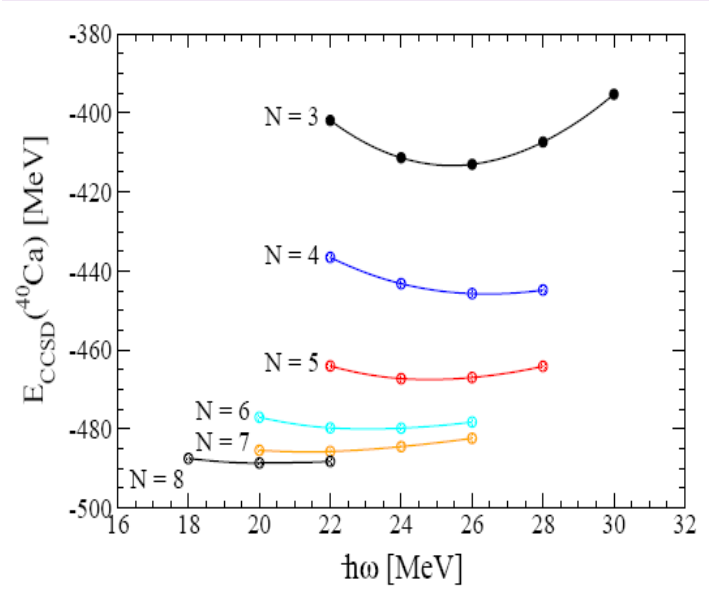
$$T_1 = \sum_{\substack{i \\ a}} t_i^a \left|\Phi_i^a\right\rangle, \quad T_2 = \sum_{\substack{i>j \\ a>b}} t_{ij}^{ab} \left|\Phi_{ij}^{ab}\right\rangle, \quad T_3 = \sum_{\substack{i>j>k \\ a>b>c}} t_{ijk}^{abc} \left|\Phi_{ijk}^{abc}\right\rangle$$



Extending the ab-initio program to medium mass nuclei

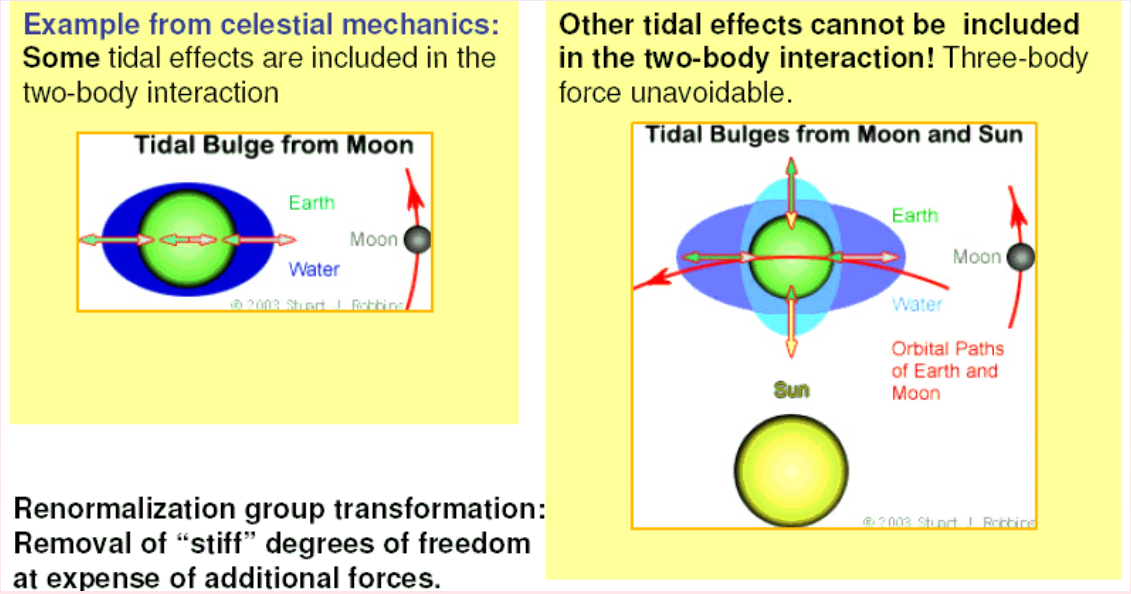
Two-body forces alone are not sufficient to describe the spectra of nuclei





Why three-nucleon forces?

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



Gamow-Shell-Model calculation of ^{6}He

Separable expansion of $V_{\mathrm{low}-k}$ in a finite oscillator basis.
G. Hagen, M. Hjorth-Jensen and N. Michel, Phys.Rev. C73, 064307 (2006)

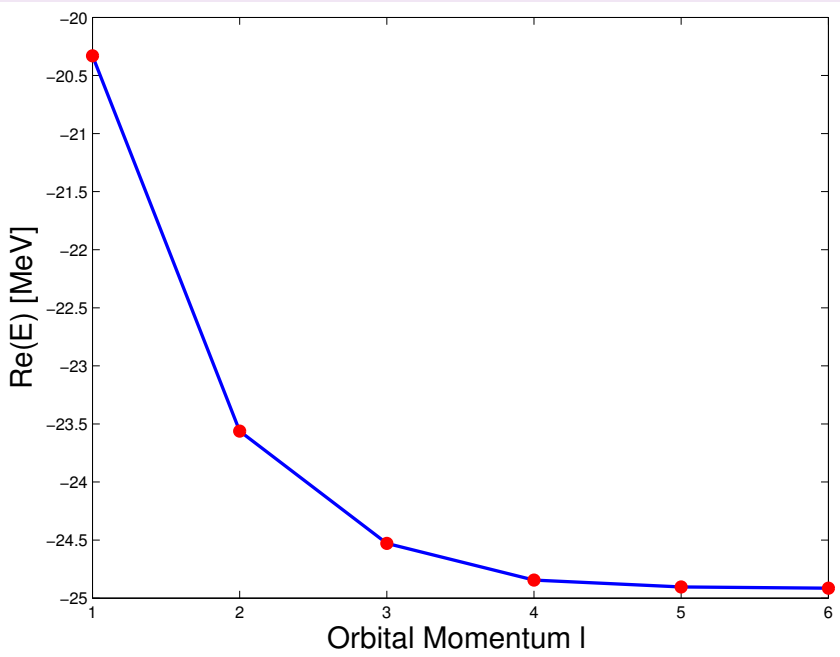
$$\langle ab|V_{\mathrm{osc}}|cd\rangle \approx \sum_{\alpha\leq\beta}^{N}\sum_{\gamma\leq\delta}^{N}\langle ab|\alpha\beta\rangle\langle\alpha\beta|V_{\mathrm{low-k}}|\gamma\delta\rangle\langle\gamma\delta|cd\rangle,$$

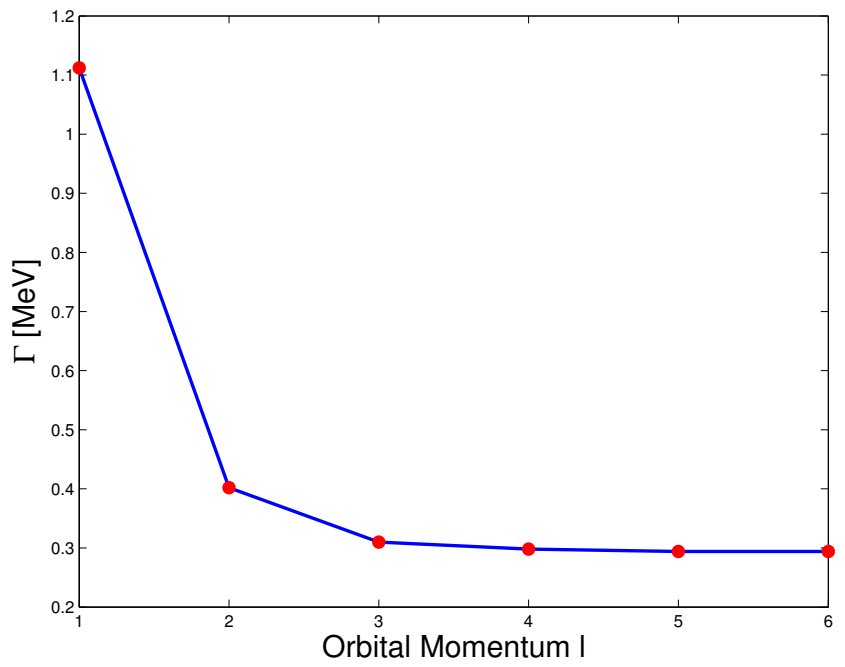
- Calculations done in a Gamow-Hartree-Fock basis.
- $V_{\mathrm{low}-k}$ from N^{3}LO with $\Lambda = 1.9\mathrm{fm}^{-1}$.
- Energies/density converge with $n_{\mathrm{max}} \sim 4-6$.

	$J^\pi = 0_1{}^+$		$J^\pi = 2_1{}^+$	
n_{max}	Re[E]	Im[E]	Re[E]	Im[E]
4	-0.4760	0.0000	0.9504	-0.0467
8	-0.4719	0.0000	0.9597	-0.0453
12	-0.4721	0.0000	0.9600	-0.0452
16	-0.4721	0.0000	0.9601	-0.0453
Exp.	-0.98	0.00	0.82	-0.06

Convergence of CCSD results

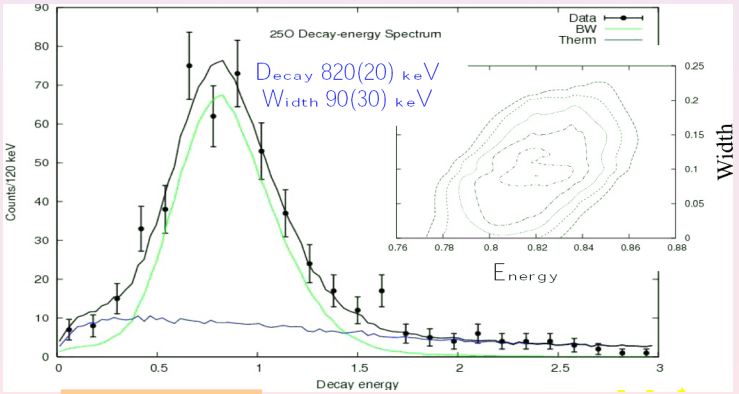
Convergence of ^{5}He ground state energy with increasing number of partial waves in the basis.



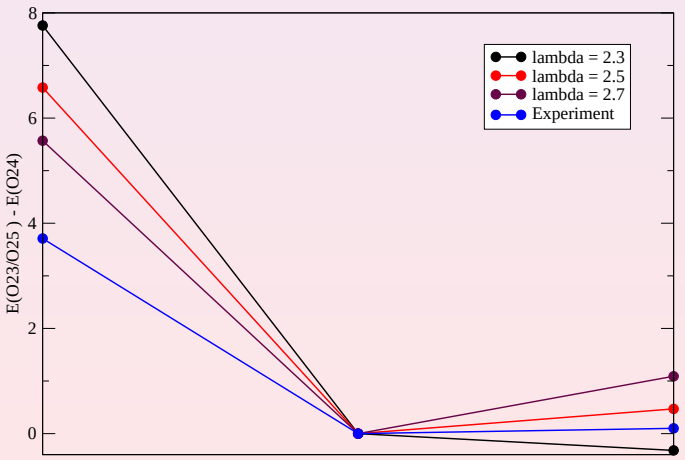


First attempt at Oxygen isotopes

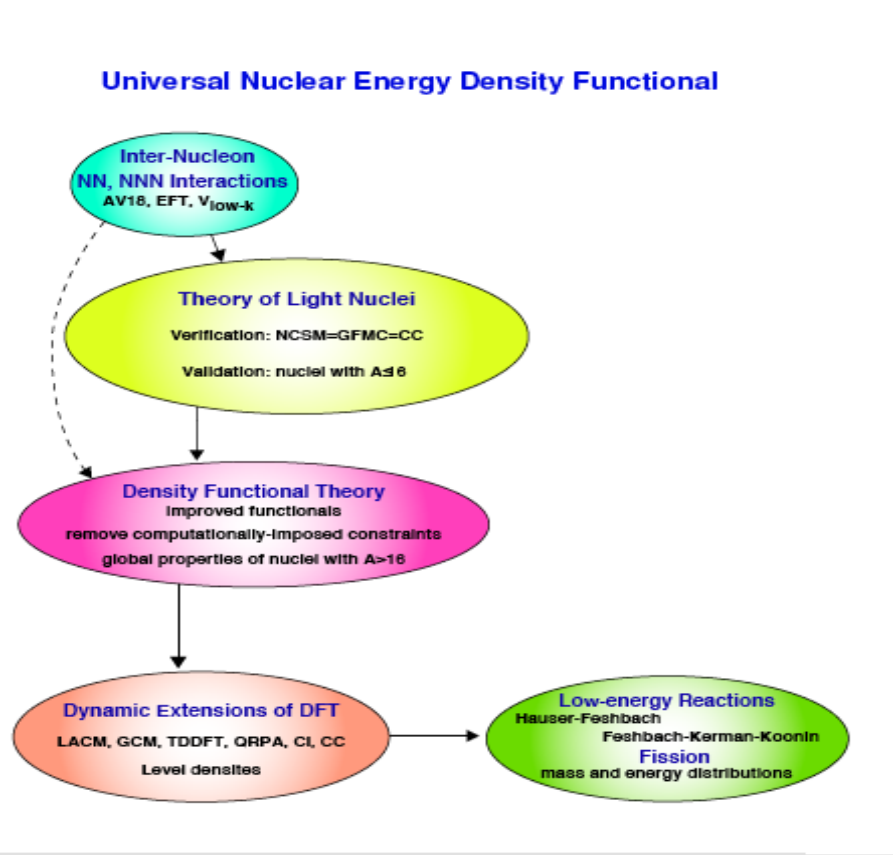
- There has been experimental evidence at MSU, that ^{24}O is the last stable oxygen isotope.
- Understand shell evolution for neutron-rich nuclei.
- Evidence for a new magic number at N=16



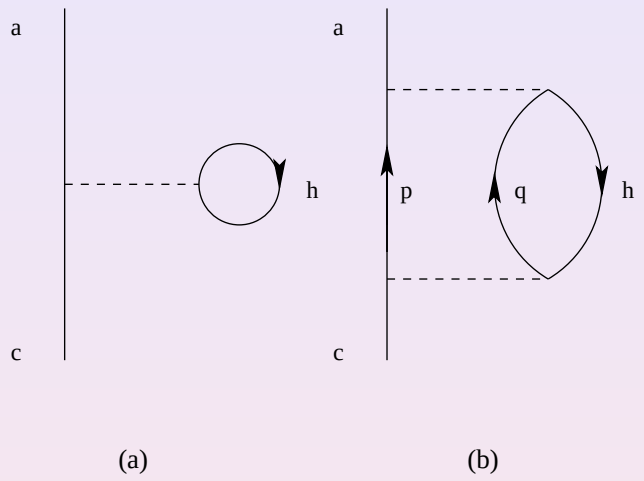
From Calem Hoffman



CC within UNEDF



Gamow-Hartree-Fock calculation of ^{4}He.



The analytically continued momentum-space Hartree-Fock equation

$$\int_{L^+} dk'\, k'^2 \langle k|T + V_{HF}|k'\rangle\langle k'|\psi_\alpha\rangle = E_\alpha \langle k|\psi_\alpha\rangle$$

Gamow-HF calculations of neutron single-particle energies in ^{4}He using low-momentum N^{3}LO NN interaction.

	$\Lambda = 1.8\mathrm{fm}^{-1}$		$\Lambda = 1.9\mathrm{fm}^{-1}$		$\Lambda = 2.0\mathrm{fm}^{-1}$		Expt.	
lj	Re[E]	Im[E]	Re[E]	Im[E]	Re[E]	Im[E]	Re[E]	Im[E]
$s_{1/2}$	-25.73	0.00	-24.54	0.00	-23.08	0.00	-20.58	0.00
$p_{3/2}$	0.82	-0.33	1.04	-0.48	1.29	-0.67	0.89	-0.32
$p_{1/2}$	2.50	-3.70	2.51	-3.78	2.65	-4.03	2.16	-2.79

N-N interactions in Bergren-represenation

Separable expansion of $V_{\mathrm{low}-k}$ in a finite oscillator basis.
G. Hagen, M. Hjorth-Jensen and N. Michel, Phys.Rev. C73, 064307 (2006)

$$\langle ab|V_{\mathrm{osc}}|cd\rangle \approx \sum_{\alpha\leq\beta}^{N}\sum_{\gamma\leq\delta}^{N}\langle ab|\alpha\beta\rangle\langle\alpha\beta|V_{\mathrm{low-k}}|\gamma\delta\rangle\langle\gamma\delta|cd\rangle,$$

- Two-body states $|ab\rangle$ in lab-system via vector-bracket transformation $\rightarrow$ complicated !
- Expand the interaction in a two-body oscillator basis - simple analytical continuation in the complex plane.
- Expansion coefficients from Brody-Moshinsky transformation.
- Two-body overlaps $\langle ab|\alpha\beta\rangle$ needed. Converge everywhere in the complex plane of phsyical importance.

Gamow-Shell-Model calculation of ^{6}He

- Calculations done in a Gamow-Hartree-Fock basis.
- $V_{\mathrm{low}-k}$ from N^{3}LO with $\Lambda = 1.9\mathrm{fm}^{-1}$.
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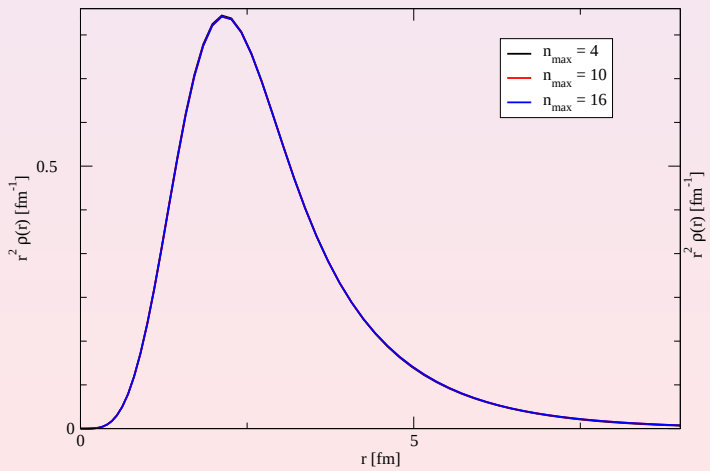
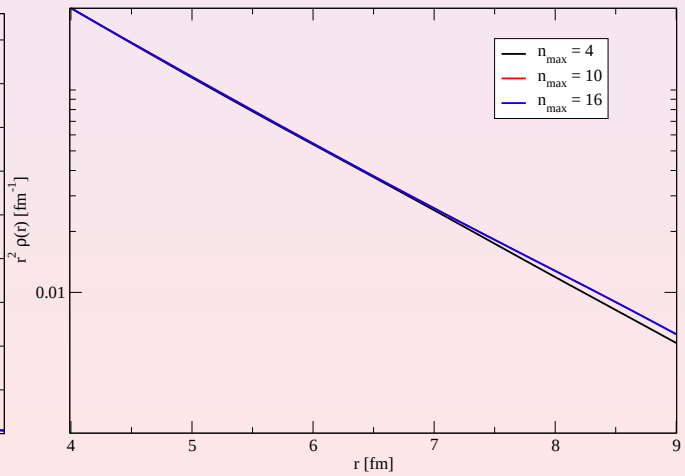




Expectation values in CCM

Expectation values in CCM

$$\langle\Psi|\tilde{O}|\Psi\rangle = \langle\Phi_0|e^{T^\dagger}\tilde{O}e^{T}|\Phi_0\rangle$$

Expectation values are non-terminating series in T

- Equation of motion (EOM)
- Hellmann-Feynman Theorem.

Properties by energy derivatives:

$$\langle\Psi|\tilde{O}|\Psi\rangle = \left.\frac{d\mathrm{E}}{d\lambda}\right|_{\lambda=0} - (\mathrm{non-HFT})$$

non-HFT contains contributions from higher T amplitudes not included in Ψ.
Hellmann-Feynmann effectively fulfilled.

Computational cost in full CI vs. CCSD

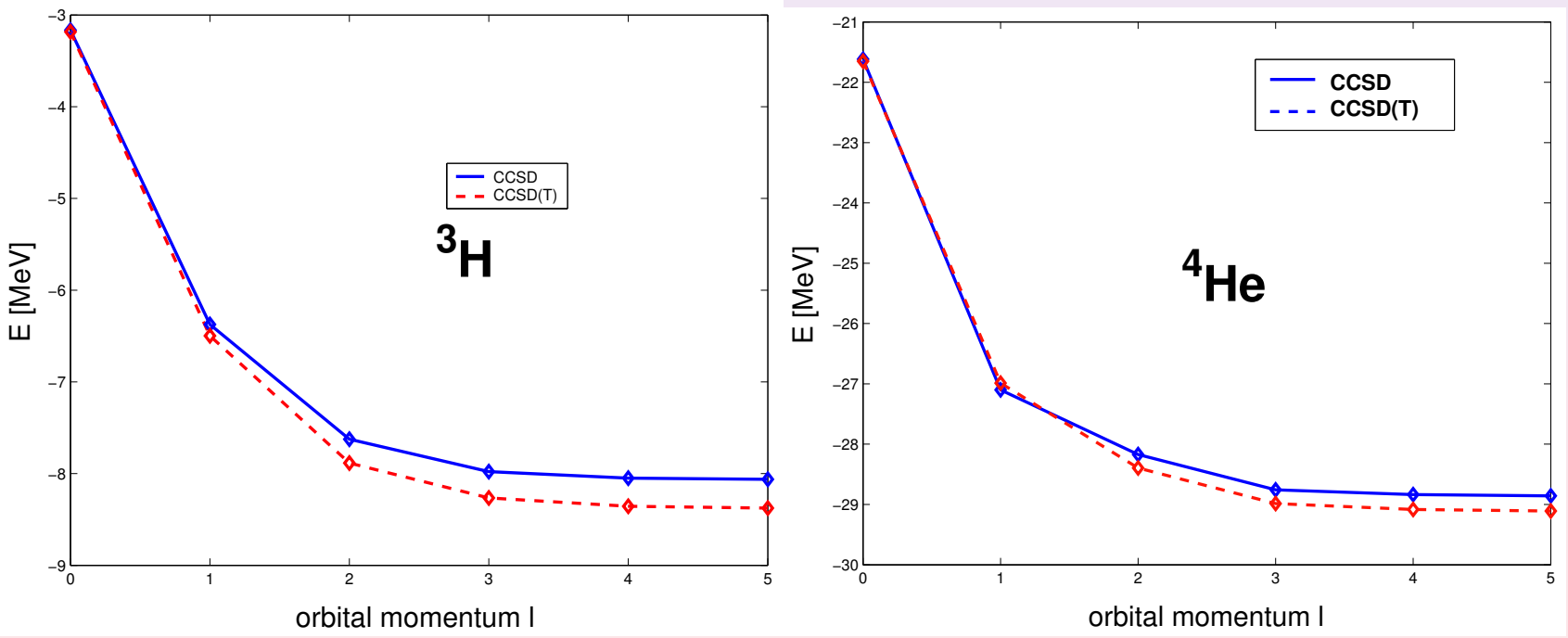
- In our largest Coupled Cluster calculations of the He-chain we employed ~ 400 proton and $\sim 500 - 550$ neutron orbitals.
- Large scale shell model codes can reach dimensions: $d \sim 1E10$
- Monte-Carlo based shell model codes can reach dimensions: $d \sim 1E15$

Nucleus	^{4}He	^{6}He	^{8}He	^{9}He	^{10}He
Dim	8E+9	1E+14	1E+18	2E+20	1E+22

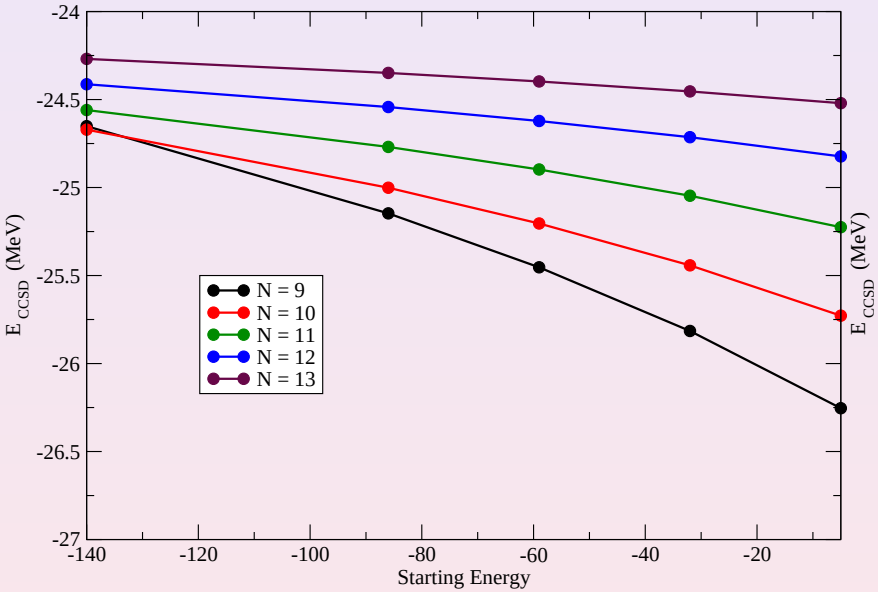
Results for ^{3}H and ^{4}He using $V_{\mathrm{low}-k}$

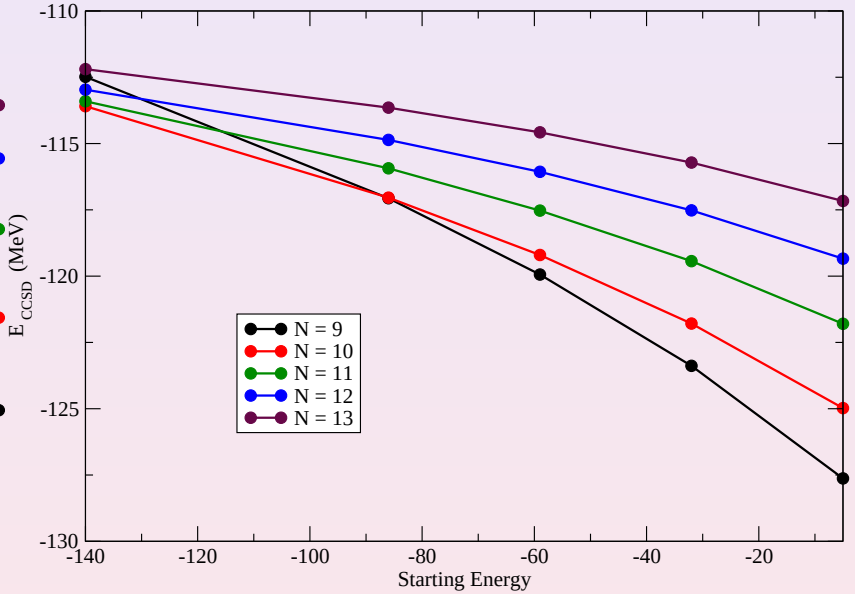
Cusp of $V_{\mathrm{low}-k}$ at cutoff momentum Λ requires a large number of nodes in the basis. Can we truncate orbital momentum l at lower values ?

$V_{\mathrm{low}-k}$ from AV18 with $\Lambda = 1.9\mathrm{fm}^{-1}$.



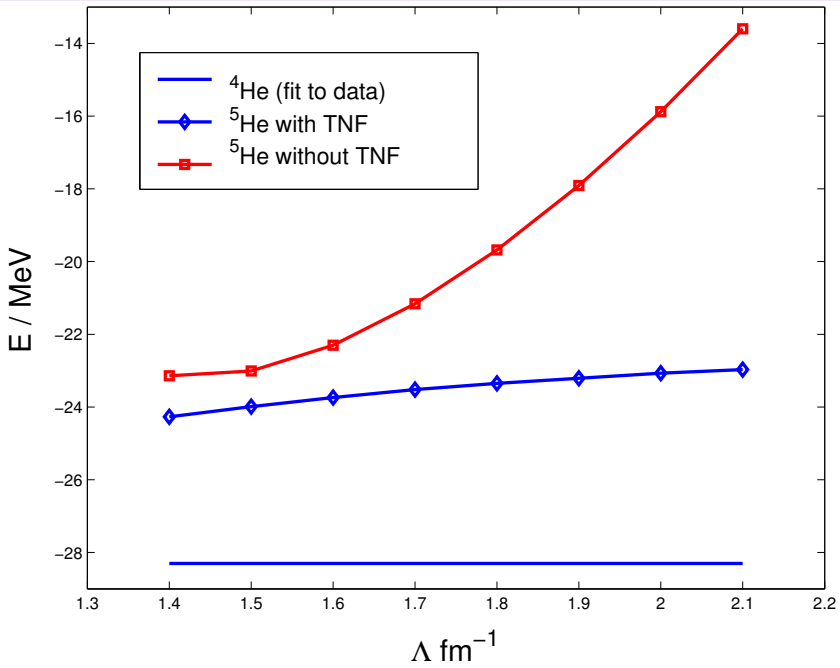
CCSD results with G-matrix

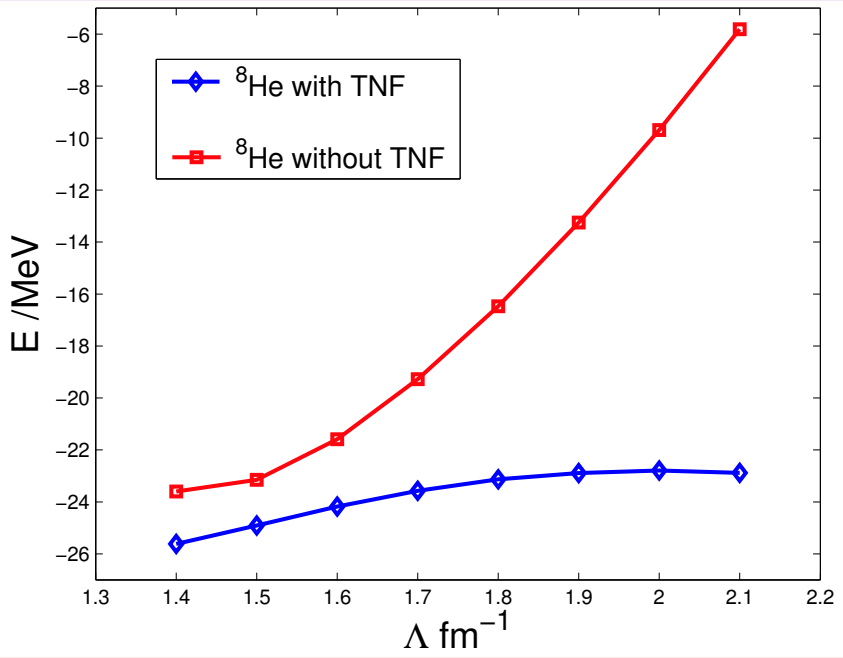




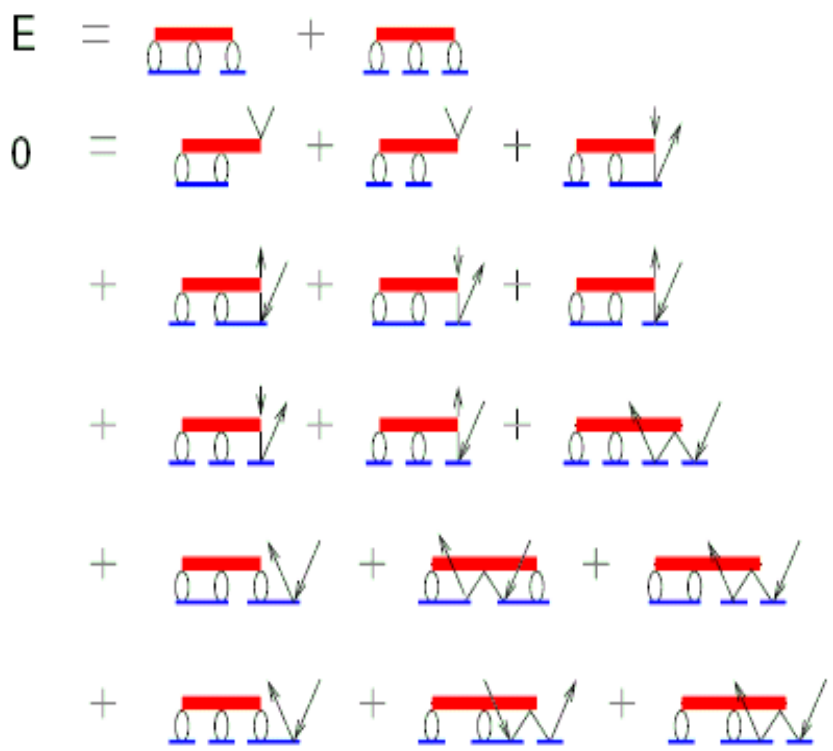
Coupled Cluster Results for Helium isotopes with 3NF

CC results with $V_{\mathrm{low}-k}$ from N3LO NN-interaction. Rather limited model-space $N = 3$. Only contact term at NN2LO is retained in the three nucleon force. 3NF fitted to reproduce binding energy of ^{4}He.





3NF contribution to the $\hat{T}_1$ cluster equation



Energy and 1p-1h equation as examples.

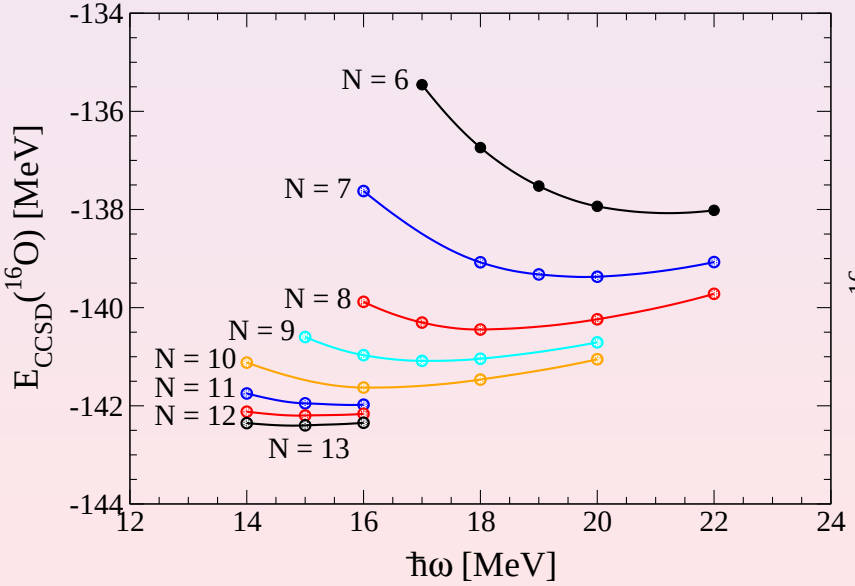
Factorization of diagrams very useful!

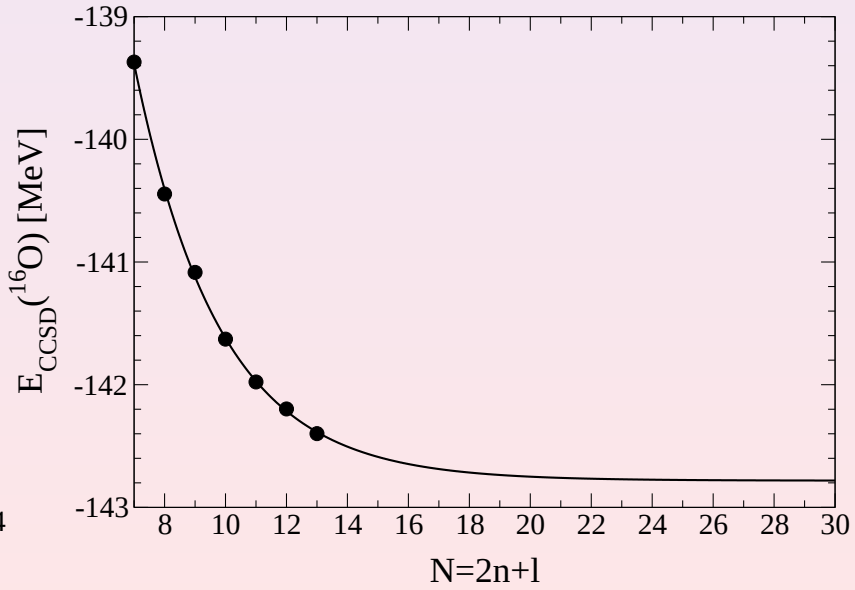
1p-1h: 15 diagrams

2p-2h: 51 diagrams

Benchmarking ^{16}O with Coupled Cluster Theory

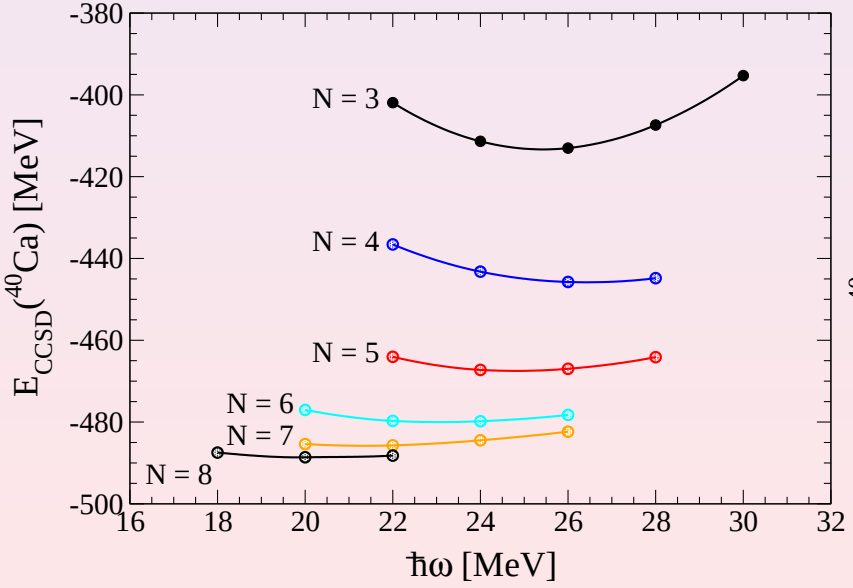
- $V_{\mathrm{low}-k}$ from AV18 with $\Lambda = 2.1\mathrm{fm}^{-1}$.
- 16 active particles and 1008 single particle orbitals $\rightarrow$ shell model dimension: $10E33$!
- An exponential fit to the energy minima yields $E \approx -142.782$MeV. Large overbinding due to missing 3NF!

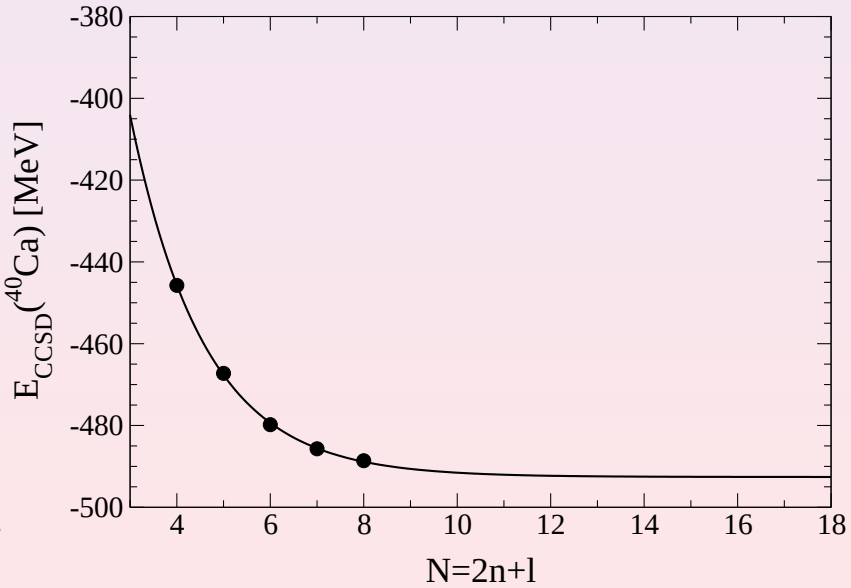


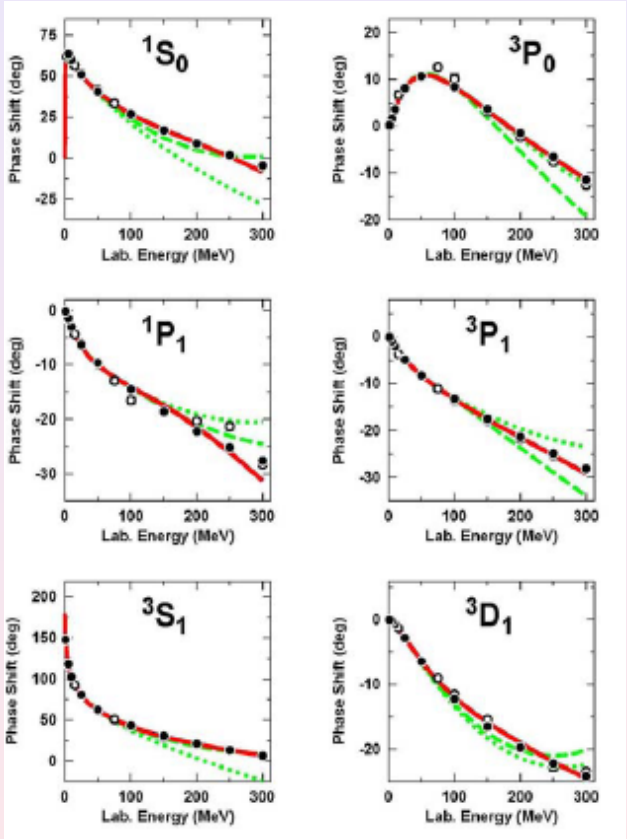


Benchmarking ^{40}Ca with Coupled Cluster Theory

- $V_{\mathrm{low}-k}$ from AV18 with $\Lambda = 2.1\mathrm{fm}^{-1}$.
- 40 active particles and 660 single particle orbitals $\rightarrow$ shell model dimension: $10E63$!
- An exponential fit to the energy minima yields $E \approx -491.21$MeV.
- G. Hagen et al., Phys. Rev. C 76, 044305 (2007). arXiv:0707.1516





N-N phase shifts order by order in Chiral EFT

N-N phase shifts up to 300 MeV from NLO, N2LO and N3LO interactions.
Red line from Entem&Machleidt, PRC 68, 041001 (2003),
green lines from Epelbaum et. al.,
Eur. Phys. J. A15, 543 (2002).