

Coupled-Cluster theory for Nuclei

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Effective Field Theories and the Many-Body Problem
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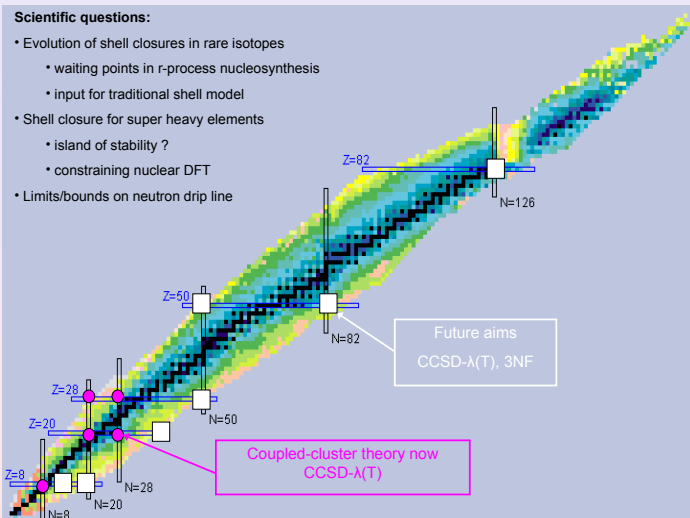
Outline

- 1 Status and goals in microscopic nuclear structure approaches
- 2 Coupled Cluster approach to nuclear structure
- 3 Coupled-Cluster in J-coupled scheme
 - CCSD and Λ CCSD(T) results with “bare” chiral interactions applied to $^{16-28}\text{O}$, ^{40}Ca , ^{48}Ca and ^{48}Ni
- 4 Coupled Cluster for open quantum systems
 - CCSD calculation of Helium chain
 - Charge radii and densities in ^4He and ^8He
- 5 Conclusion and Perspectives

Ab-initio approaches to light and medium mass nuclei

Scientific questions:

- Evolution of shell closures in rare isotopes
 - waiting points in r -process nucleosynthesis
 - input for traditional shell model
- Shell closure for super heavy elements
 - island of stability ?
 - constraining nuclear DFT
- Limits/bounds on neutron drip line



N-N force from Chiral perturbation theory

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

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

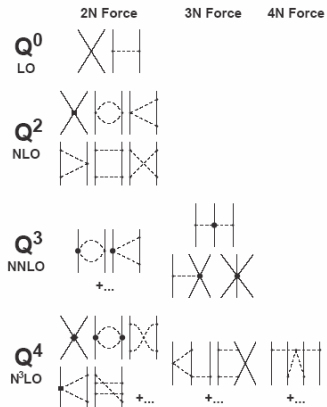
Lagrangian \rightarrow infinite sum of Feynman diagrams.

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

Weinberg, Ordonez, Ray, van Kolck

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

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



Coupled Cluster Theory

Exponential Ansatz for Ψ

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

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

Coupled Cluster Equations

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

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

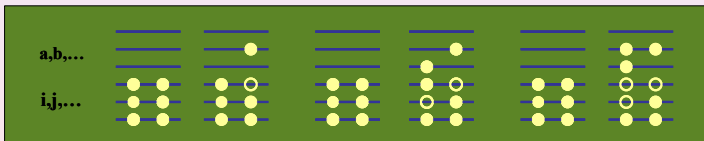
$$\bar{H} = (H_N \exp(T))_C$$

- 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.

Coupled Cluster in pictures

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

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

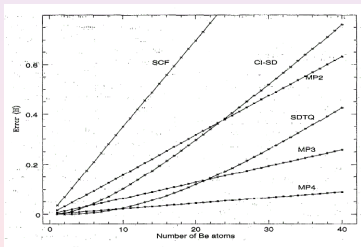


Size Matters! Role of size-extensivity

Goldstone's linked cluster theorem (1955)

Formal diagrammatic proof of Brueckner's conjecture that perturbation theory is size extensive. 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.



- **Size extensive theories:** Many-body perturbation theory, Full Configuration Interaction (FCI) and Coupled-cluster theory
- **Non-size extensive theories:** Particle-hole truncated shell-model (CISD, CISDT...)

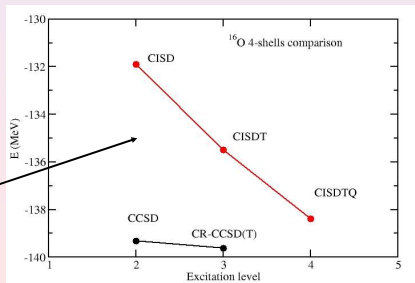
Comparison with Shell Model/Configuration Interaction

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

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

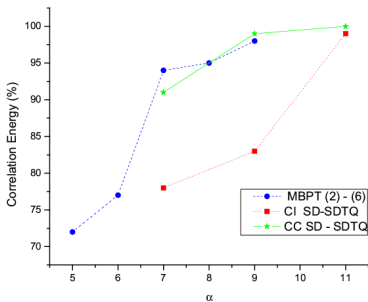
Comparison of CC with CI
at given excitation level.

Nuclear Example (Kowalski et al PRL 2004).



Comparison with Shell Model/Configuration Interaction

Performance of theories for the correlation energy in small molecules.
To facilitate comparisons, the ordinate gives the size-scaling parameter
of the approximation, $\alpha = \alpha_n + \alpha_N + \alpha_H$ in the computational
cost function $n^{\alpha_n} N^{\alpha_N} N_H^{\alpha_H}$.



Relationship between shell model and CC amplitudes

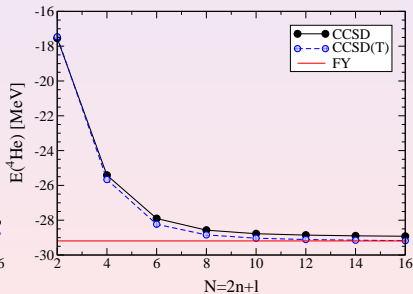
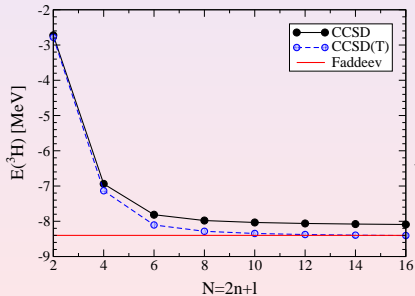
$$\begin{aligned}
 B_1 &= T_1 \\
 B_2 &= T_2 + \frac{1}{2} T_1^2 \\
 B_3 &= T_3 + T_2 T_1 + \frac{1}{6} T_1^3 \\
 B_4 &= T_4 + T_3 T_1 + \frac{1}{2} T_2^2 + \frac{1}{2} T_2 T_1^2 + \frac{1}{24} T_1^4 \\
 &\dots
 \end{aligned}$$

CCSD
CCSDT

↖ Disconnected quadruples
↖ Connected quadruples

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

CCSD(T) and Faddeev (-Yakubovsky) results for ^3H and ^4He using $V_{\text{low}-k}$ from AV18 with $\Lambda = 1.9\text{fm}^{-1}$. **CCSD(T) are within the errors (50 keV) of the Faddeev results!** (G. Hagen et al., Phys. Rev. C 76, 044305 (2007))



Disagreement between CCM and IT-NCSM for ^{40}Ca

	Coupled-Cluster	IT-NCSM
^{16}O	-142.8 (CCSD)	
	-148.2 (CCSD(T))	-137.8 (4p-4h)
^{40}Ca	-491.2 (CCSD)	-461.8 (3p-3h)
	-502.9 (CCSD(T))	-471.0 (4p-4h)

- Coupled-Cluster theory **size extensive**, energy scales correctly with size
- IT-NCSM is **not size extensive**. Can not judge the quality of a calculation of large system from the quality of a small (light) system.

Refs.:

1. Roth and Navratil PRL 99, 092501 (2007)
2. Hagen, Dean, Hjorth-Jensen, Papenbrock, Schwenk PRC 76, 044305 (2007)
3. Dean, Hagen, Hjorth-Jensen, Papenbrock, Schwenk PRL. 101, 119201 (2008) (comment)
4. Roth and Navratil, arxiv:0801.1484 (reply)

Spherical Coupled-Cluster Approach

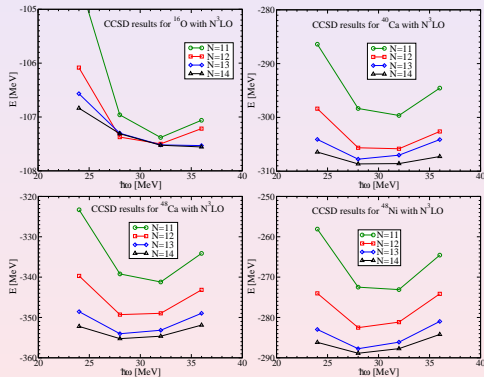
- 1 Possible for nuclei with closed sub-shell (or $cs \pm 1$)
- 2 Relatively simple since similarity transformed Hamiltonian is two-body (CCSD) or three-body (CCSDT) at most
- 3 Enormous computational reduction: $n_o + n_u \rightarrow (n_o + n_u)^{2/3}$ (naive estimate)
 CCSD(T) for ^{40}Ca and ^{48}Ca on a single CPU (now)
 CCSDT for ^{48}Ca on many CPUs (future)
 CCSD(T) for ^{100}Sn and ^{132}Sn with “bare” chiral interactions on many CPUs.

$$\hat{T}_1 = \sum_{j_i, j_a} t_{j_i}^{j_a} (a_{j_a}^\dagger \times \tilde{a}_{j_i})^{(0)},$$

$$\hat{T}_2 = \sum_{j_i, j_j, j_a, j_b, J} t_{j_i, j_j}^{j_a, j_b}(J) (a_{j_a}^\dagger \times a_{j_b}^\dagger)^{(J)} \cdot (\tilde{a}_{j_j} \times \tilde{a}_{j_i})^{(J)}.$$

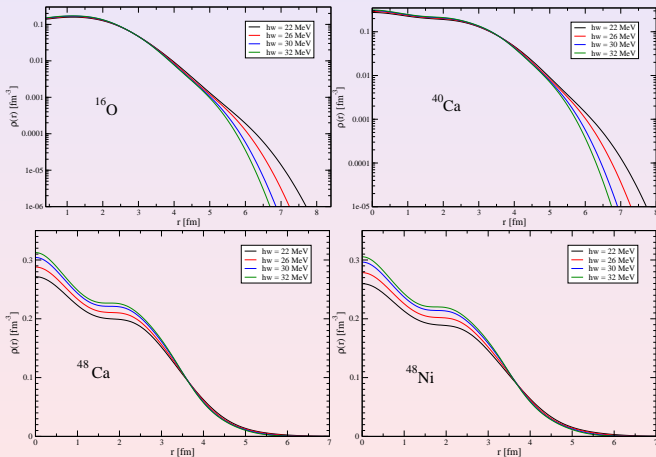
j_i and j_a denote the spin of the occupied and unoccupied subshells.

^{16}O , ^{40}Ca , ^{48}Ca and ^{48}Ni with “bare” chiral interactions



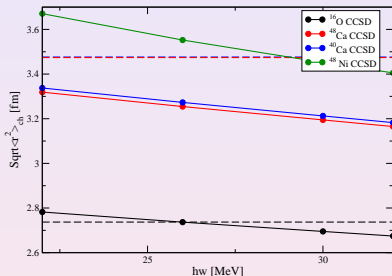
Medium-Mass Nuclei from Chiral Nucleon-Nucleon Interactions,
 G. Hagen et. al, Phys. Rev. Lett. 101, 092502 (2008)

^{16}O , ^{40}Ca , ^{48}Ca and ^{48}Ni ground state densities



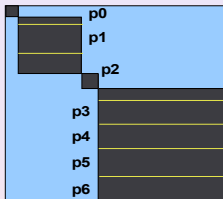
Charge and matter radii/Summary of results

- Mirror nuclei ^{48}Ca and ^{48}Ni differ by 1.38 MeV/A \rightarrow close to mass table predictions.
- 3NF and triples expected to yield $\sim 1\text{MeV/A}$?
- Radii and densities stronger model space dependence.



Nucleus	E/A	V/A	Q	$\Delta E/A$	$\langle r^2 \rangle_{ch}^{1/2}$	$\langle r^2 \rangle_{ch}^{1/2}$ (Exp)
^4He	-5.99	-22.75	0.90	1.08		1.673(1)
^{16}O	-6.72	-30.69	1.08	1.25	2.72(5)	2.737(8)
^{40}Ca	-7.72	-36.40	1.18	0.84	3.25(9)	3.4764
^{48}Ca	-7.40	-37.97	1.21	1.27	3.24(9)	3.4738
^{48}Ni	-6.02	-36.04	1.20	1.21	3.52(15)	?

Parallelization of coupled-cluster code



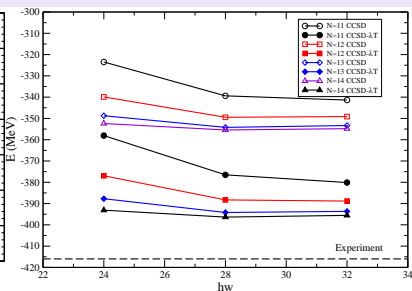
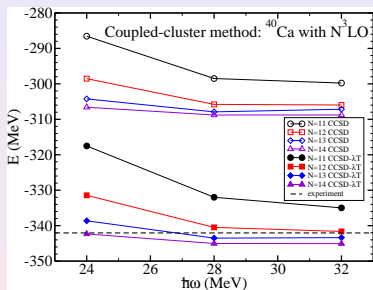
Computational challenges

- Inclusion of three-nucleon force
- Needs coding in current J-coupled scheme
- Generation of matrix elements
- Approximation possible ?

Computational details

- 350 cpu hours per point ($N=14$)
- $N = 14$ requires 20Gb of memory
- Triples correction factor 20 more expensive
- MPI code with distributed matrix elements of interaction and intermediates.
- BLAS routines for (some) computationally expensive tasks
- Weak scaling expected

Triples correction to ground state energies

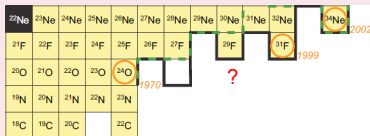


- \bullet $\sim 400\text{keV}/A$ missing for ^{16}O and ^{48}Ca .
- \bullet Interesting isospin behavior of three-body force in Calcium isotopes.

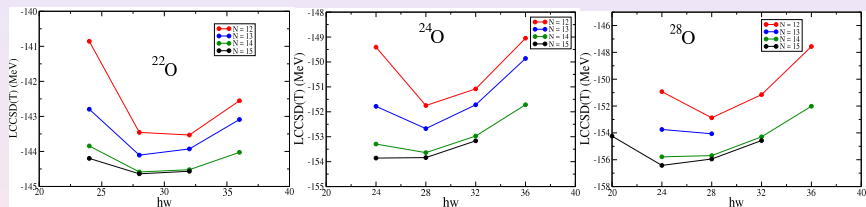
Nucleus	CCSD		Λ CCSD(T)	
	E/A	$\Delta E/A$	E/A	$\Delta E/A$
^{16}O	-6.72	1.25	-7.56	0.41
^{40}Ca	-7.72	0.84	-8.63	-0.08
^{48}Ca	-7.40	1.27	-8.26	0.40

Dripline in Oxygen isotopes

- Evidence of new magic numbers in oxygen isotopes $N = 14$ and $N = 16$.
- Does ^{28}O exist ? ^{28}O is a doubly magic nucleus.
- All shell model calculation in the $s - d$ shell with realistic NN interactions predicts dripline beyond ^{28}O .
- Preliminary results from Otsuka et al. with inclusion of 3NF predicts ^{28}O unstable.
- Adding one more proton binds 6 more neutrons in fluorine isotopes.
- Can Ab-initio theory answer this question ?

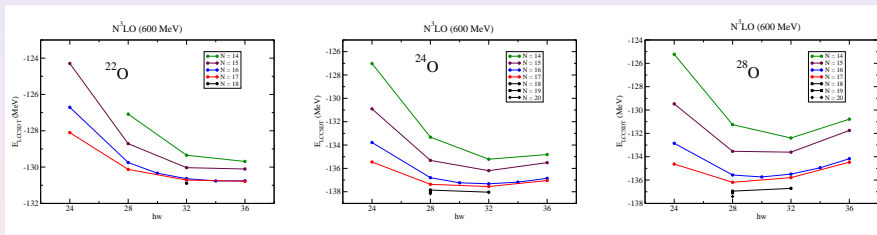


^{22}O , ^{24}O , and ^{28}O with $N^3\text{LO}$ (500 MeV)



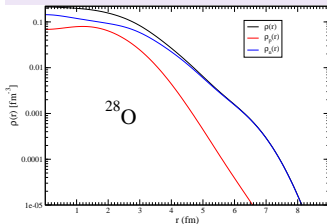
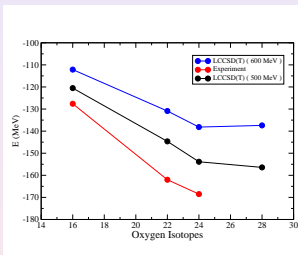
	^{22}O	^{24}O	^{28}O
E_0	50.37	56.19	71.58
ΔE_{CCSD}	-175.79	-190.39	-207.67
$\Delta E_{\text{CCSD}-\lambda T}$	-19.22	-19.64	-19.85

^{22}O , ^{24}O , and ^{28}O with $N^3\text{LO}$ (600 MeV)



	^{22}O	^{24}O	^{28}O
E_0	46.33	52.94	68.57
ΔE_{CCSD}	-156.51	-168.49	-182.42
$\Delta E_{\text{CCSD}-\lambda T}$	-20.71	-22.49	-22.86

Is ^{28}O stable ?



- Ab-initio Coupled-Cluster calculations can not rule out the existence of ^{28}O .
- Cutoff variation indicates that three-nucleon forces will play a crucial role in the determination of the neutron dripline.

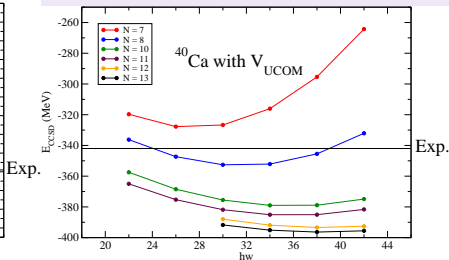
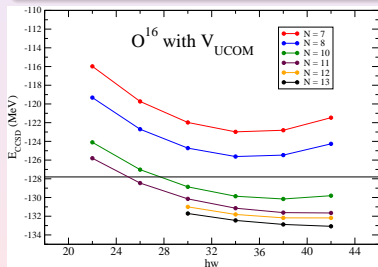
Cutoff dependence and summary of results for Oxygen isotopes

N ³ LO (500 MeV)					
Nucleus	CCSD		Λ CCSD(T)		$\langle r^2 \rangle^{1/2}$
	E/A	$\Delta E/A$	E/A	$\Delta E/A$	
¹⁶ O	-6.72	1.25	-7.53	0.44	
²² O	-5.72	1.64	-6.59	0.77	2.82
²⁴ O	-5.58	1.42	-6.42	0.58	2.89
²⁸ O	-4.86	?	-5.57	?	3.06

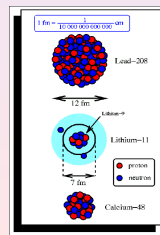
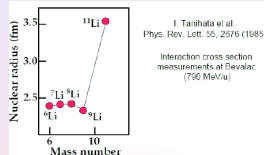
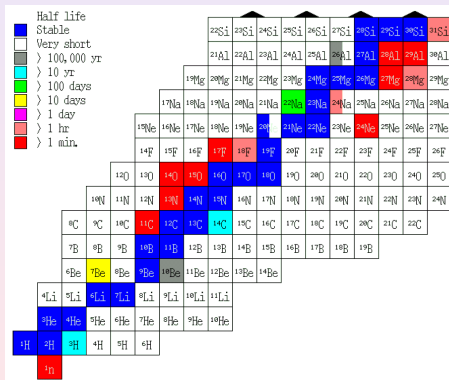
N ³ LO (600 MeV)					
Nucleus	CCSD		Λ CCSD(T)		$\langle r^2 \rangle^{1/2}$
	E/A	$\Delta E/A$	E/A	$\Delta E/A$	
¹⁶ O	-6.06	1.92	-7.01	0.97	
²² O	-5.01	2.36	-5.95	1.45	2.93
²⁴ O	-4.84	2.18	-5.76	1.26	3.08
²⁸ O	-4.11	?	-4.90	?	3.30

^{16}O , ^{40}Ca with V_{UCOM}

V_{UCOM} overbinds and converge slowly for medium mass nuclei.



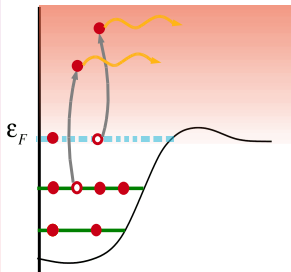
Ab-initio approach weakly bound and unbound nuclear states



Coupled Cluster for open quantum systems

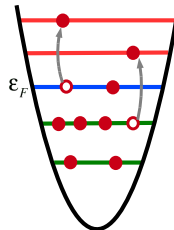
Open Quantum System.

Coupling with continuum taken into account.



Closed Quantum System.

No coupling with external continuum.

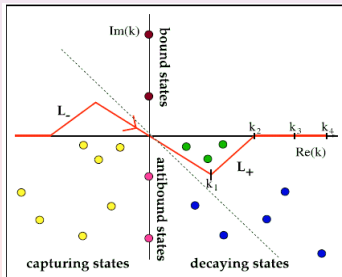


Berggren Single-particle basis

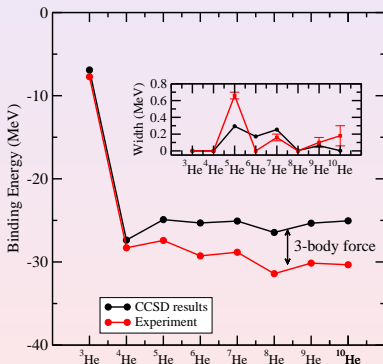
Complex energies requires a generalized completeness relation

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

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



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

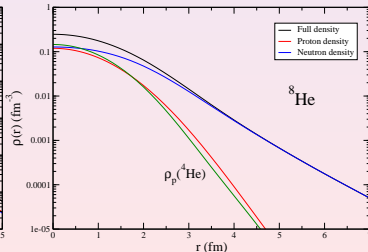
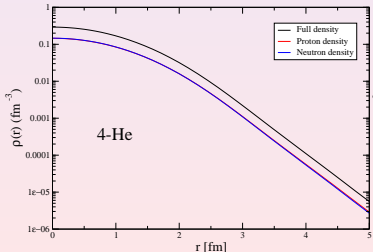


- $V_{\text{low}-k}$ from N3LO with $\Lambda = 1.9\text{fm}^{-1}$.
- G. Hagen et al., Phys. Lett. B 656, 169 (2007). arXiv:nucl-th/0610072.

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

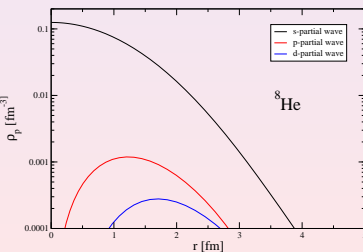
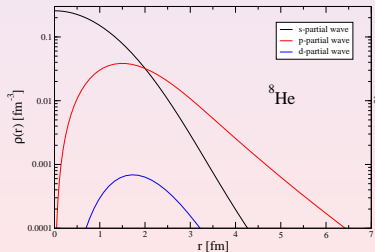
^4He and ^8He density distributions with V-srg

- Single-particle density in ^4He and ^8He .
- Gamow-Hartree-Fock basis has correct asymptotics.
- N^3LO evolved down to $\lambda = 2.0\text{fm}^{-1}$ from similarity renormalization group theory.



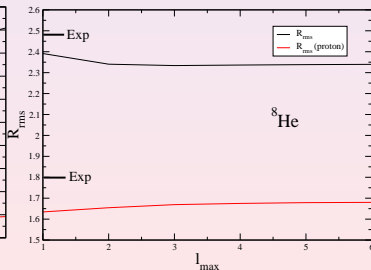
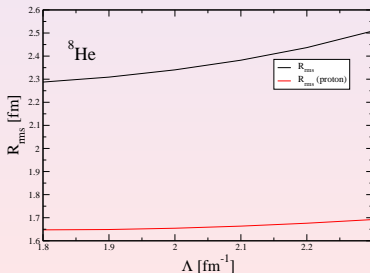
Partial wave decomposition of ^8He density

- $N^3\text{LO}$ evolved down to $\lambda = 2.0\text{fm}^{-1}$ from similarity renormalization group theory.
- Neutron skin in ^8He is mainly built from s - and p -partial waves. Protons are mainly occupying s - partial waves.



Matter and charge radii of ^8He using V-srg

- Λ dependence on ^8He charge and matter radii indicates missing 3NF.
- Hamiltonians with two-body renormalized interactions (SRG/low-k) underestimates matter and charge radii.



Conclusion

- Coupled Cluster meets few-body benchmark calculations.
- J-coupled CCSD and Λ CCSD(T) code has been derived and implemented. **Coupled cluster approach to medium mass and driplines with bare interactions!**
- Derived and implemented Equation of Motion CCM; calculation of density distributions and radii.
- CCM has been successfully applied to the description of weakly bound and unbound helium isotopes.
- We have a tool to attack the structure and properties of dripline and medium mass nuclei !

Future perspectives

- Revisit Helium chain with 3NF. Spin-orbit splitting in He7 and He9.
- Matter and charge radii of ^{11}Li .
- Excited states and matter densities for dripline nuclei.
- Coupled Cluster approach to nuclear matter.
- Construction of effective interaction for shell-model calculations.
- Coupled-Cluster approach to nuclear reactions; CC-LIT and construction of optical potentials from folding procedures.
- We are developing a J-coupled CCSDT code.
- **Ab-initio description of ^{56}Ni , ^{100}Sn and ^{208}Pb within reach!**

Coupled-Cluster method and the Center of Mass

- 1 Our implementation of CCM does not preserve translational invariance.
- 2 In oscillator basis $\langle H_{CM} \rangle \sim 200\text{keV}$ for ^{40}Ca with vlowk and $N = 8$.
In HF basis energies are expected to be much better than wave functions.

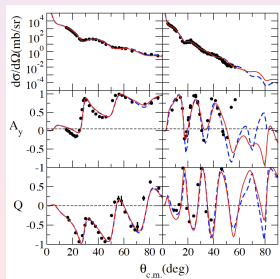
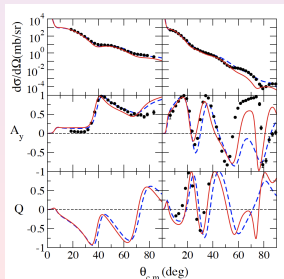
Compare two methods

- 1 Exact diagonalization (CI) of intrinsic Hamiltonian in all A-body states built from this s.p. basis \rightarrow Variational but breaks translational invariance, result $:E_{CI}$
- 2 NCSM in $N\hbar\Omega$ space spanned by this basis \rightarrow Variational keeps translational invariance, result E_{NCSM}

$$E_{EXACT} \leq E_{CI} \leq E_{NCSM}$$

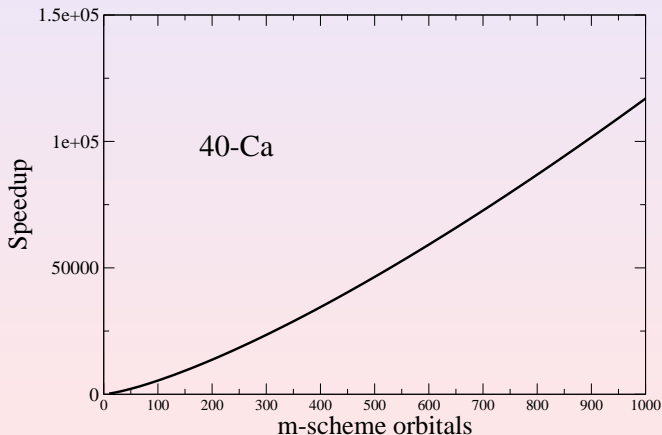
Elastic scattering of protons from ^{16}O and ^{40}Ca

- g -folding optical potential model with realistic one-body density matrices from ab-initio Coupled-Cluster calculations. With K. Amos (To be submitted for publication in Phys. Rev. C)
- Elastic scattering of protons from ^{16}O (left figure) and ^{40}Ca (right figure) at 65 MeV and 200 MeV.



Spherical Coupled-Cluster Approach

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



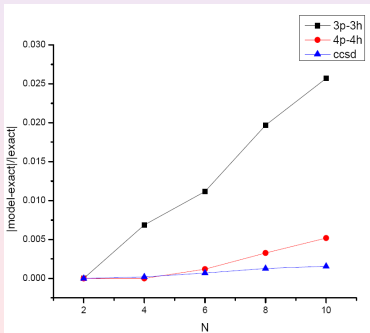
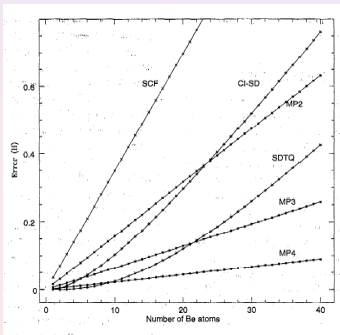
How well does SR-CC describe open-shell nuclei?

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

Method	^3He	^4He	^5He	^6He	$\langle J^2 \rangle, ^6\text{He}$
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
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CCSDT-3	-6.42	-26.27	-21.92	-22.90	0.26
CCSDT	-6.45	-26.28	-22.01	-22.52	0.04
FCI	-6.45	-26.3	-22.1	-22.7	0.00

Size Matters! Role of size-extensivity

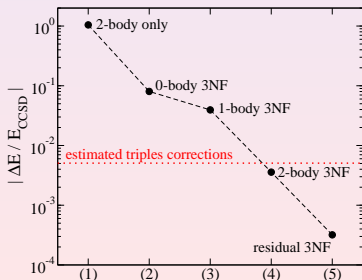
Disconnected diagrams in truncated shell model/CI models (CISD, CISDT,...) leads to wrong scaling of energy with increasing number of particles.



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

Three-body Hamiltonian in normal ordered form:
 (G. Hagen et al., PRC (76) 034302 (2007))

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

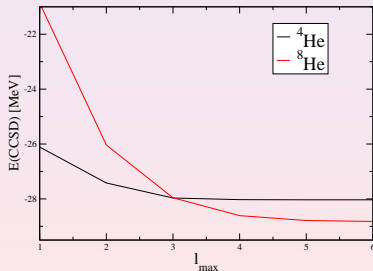


Really good news!

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

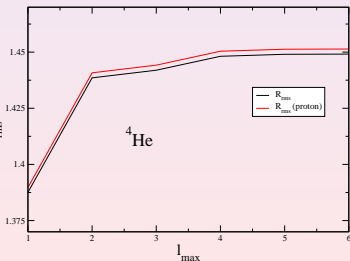
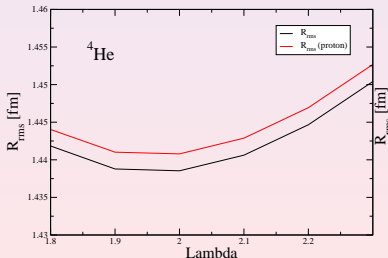
Properties of weakly bound nuclei

Convergence of ${}^4\text{He}$ and ${}^8\text{He}$ ground state energies with increasing number of partial waves in the basis.



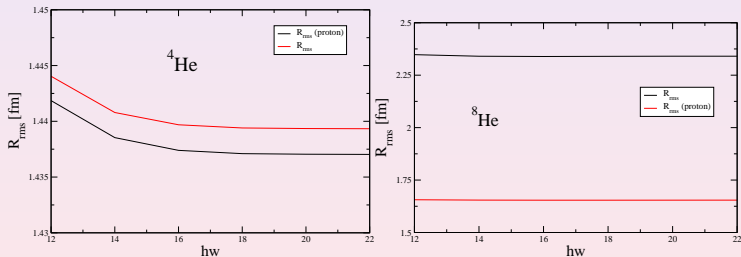
Matter and charge radii of ^4He using V-srg

- Λ dependence on ^4He charge and matter radii indicates missing 3NF.
- Hamiltonians with two-body renormalized interactions (SRG/low-k) underestimates matter and charge radii.



Properties of weakly bound nuclei

$\hbar\omega$ dependence on ${}^4\text{He}$ and ${}^8\text{He}$ charge and matter radii.



Coupled Cluster Theory

Exponential Ansatz for Ψ

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

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

Coupled Cluster Equations

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

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

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

Iterative CCSDT-n approximations to full CCSDT

$$\text{CCSDT} - 1 \quad 0 = \langle \Phi_{ijk}^{abc} | (F_N T_3 + H_N T_2)_C | \Phi_0 \rangle$$

$$\text{CCSDT} - 2 \quad 0 = \langle \Phi_{ijk}^{abc} | \left(F_N T_3 + H_N T_2 + H_N T_2^2/2 \right)_C | \Phi_0 \rangle$$

$$\text{CCSDT} - 3 \quad 0 = \langle \Phi_{ijk}^{abc} | (F_N T_3 + H_N \exp(T_1 + T_2))_C | \Phi_0 \rangle$$

$$\text{CCSDT} \quad 0 = \langle \Phi_{ijk}^{abc} | (H_N \exp(T_1 + T_2 + T_3))_C | \Phi_0 \rangle$$

Coupled Cluster Theory with 3NF

- We have derived and implemented Coupled Cluster equations for three-body Hamiltonians.
- Probe cutoff dependence of $V_{\text{low-}k}$ 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).

N-N force from Chiral perturbation theory

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

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

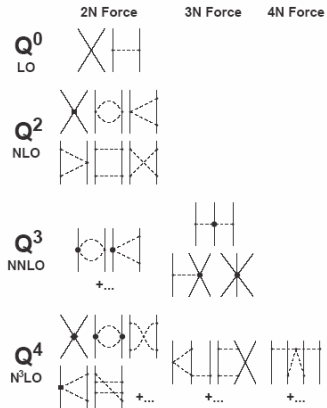
Lagrangian
 \rightarrow infinite sum of Feynman diagrams.

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

Weinberg, Ordonez, Ray, van Kolck

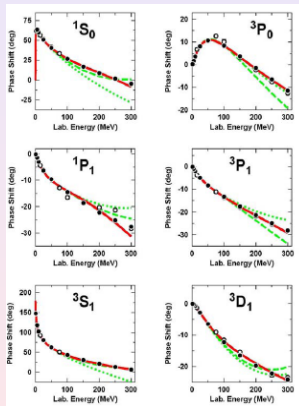
NN amplitude uniquely determined by two classes of contributions: contact terms and pion exchange diagrams.

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



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).



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

$$\begin{aligned}
 E &= \text{diagram 1} + \text{diagram 2} \\
 0 &= \text{diagram 3} + \text{diagram 4} + \text{diagram 5} \\
 &+ \text{diagram 6} + \text{diagram 7} + \text{diagram 8} \\
 &+ \text{diagram 9} + \text{diagram 10} + \text{diagram 11} \\
 &+ \text{diagram 12} + \text{diagram 13} + \text{diagram 14} \\
 &+ \text{diagram 15} + \text{diagram 16} + \text{diagram 17}
 \end{aligned}$$

Energy and 1p-1h equation
 as examples.

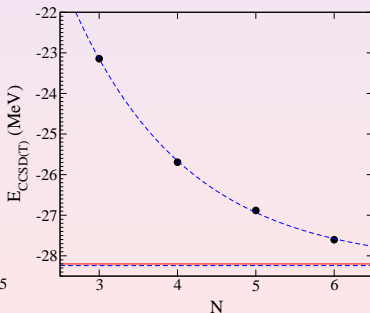
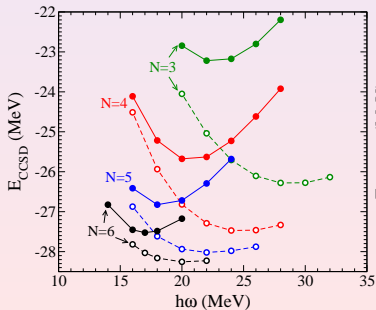
Factorization of diagrams
 very useful!

1p-1h: 15 diagrams

2p-2h: 51 diagrams

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

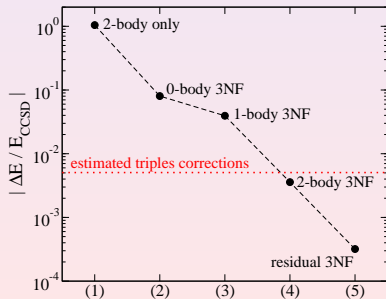
- $V_{\text{low}-k}$ from AV18 with $\Lambda = 1.9\text{fm}^{-1}$.
- 3NF brings in repulsion as expected !
- CCSD and CCSD(T) with 3NF meets Faddeev-Yakubovsky benchmark !
 $E_{\text{CCSD(T)}} \approx -28.24 \text{ MeV}$. F-Y $E = -28.20(5)\text{MeV}$.



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

Three-body Hamiltonian in normal ordered form:

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



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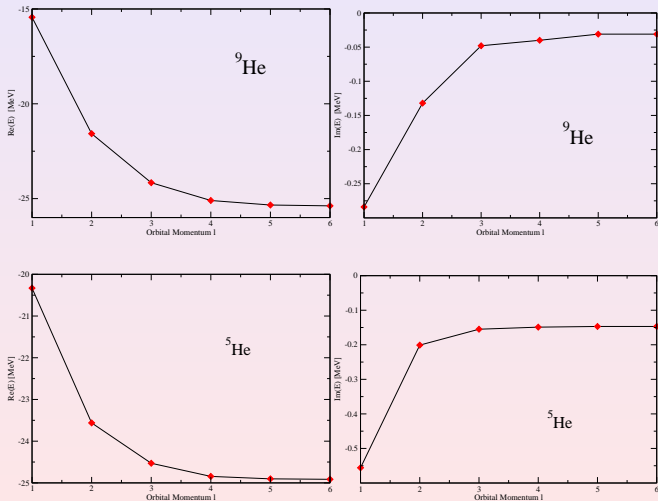
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- “2-body” machinery can be used.
- **Residual three-nucleon force can be neglected!**

CCM vs. exact calculations for open-shell nuclei.

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

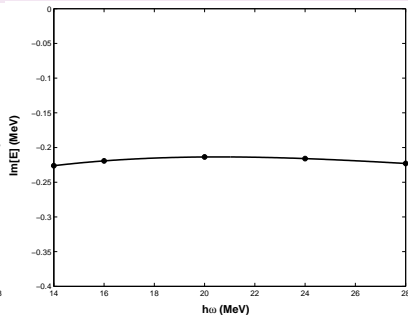
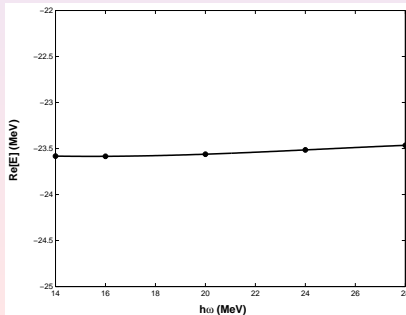
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Convergence of CCSD results



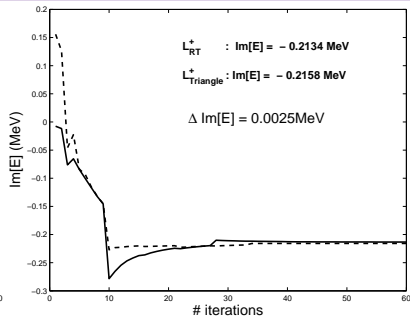
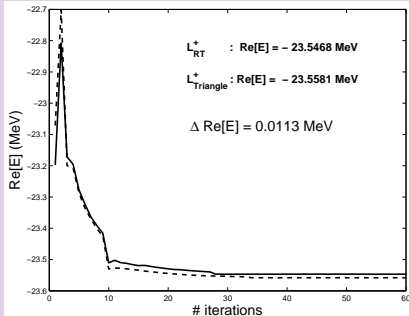
Convergence of CCSD energy with $2n + l \leq 10$ truncation.

- ^5He ground state energy starting with oscillator bases given for different $\hbar\omega$ values.
- Weak $\hbar\omega$ dependence, Results are well converged.
 $\Delta\text{Re}[E] \sim 0.1\text{MeV}$, $\Delta\text{Im}[E] \sim 0.01\text{MeV}$



Convergence of CCSD energy.

CCSD convergence of ${}^5\text{He}$ ground state energy for the $s - d$ space (300 orbitals) using $n = 20$ discretization points for L^+ . The calculation was performed using two very different L^+ contours



Coupled Cluster Results for Helium isotopes with TNF

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

