Role of the continuum in Coupled-Cluster theory

Gaute Hagen[1]
Collaborators : T. Papenbrock, D. Dean, M. Hjorth-Jensen, S. Bacca and A. Schwenk

[1]Oak Ridge National Laboratory, Physics Division, E-mail: hageng@ornl.gov

Weakly-Bound Systems in Atomic and Nuclear Physics
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Outline

1. The driplines - the limit of nuclear existence
2. Coupled Cluster approach to nuclear structure
   - Single-Reference Coupled-Cluster theory
   - Coupled-Cluster approach to open quantum systems and Helium isotopes
3. Equation-of-Motion Coupled-Cluster approach to open-shell nuclei
   - Equation-of-Motion Coupled-Cluster theory
   - Microscopic description of resonances and halo states in ^{17}F and ^{17}O
   - Low-lying states in ^{17}O and the Center of Mass
   - Shell evolution in the oxygen and fluorine isotopes
4. Conclusion and Perspectives

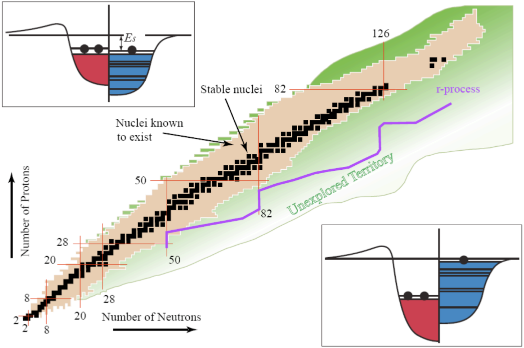
Peculiarities at the nuclear driplines

~ 300 stable nuclei

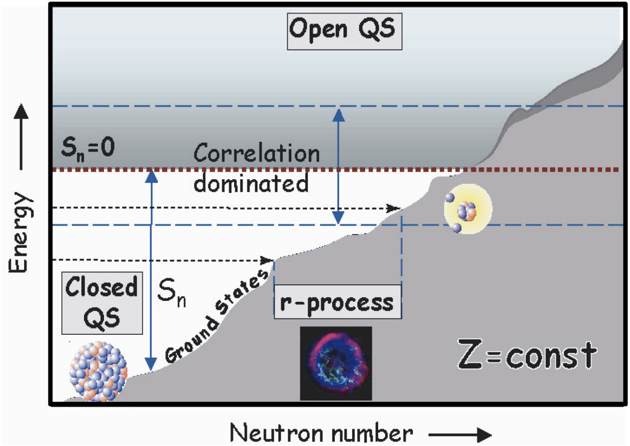
N/Z~1 for light nuclei

N/Z~1.5 for ^{208}Pb

~4000-6000 unstable nuclei
decay by α, β, 1p, 2p,
1n, cluster emission, fission...



Peculiarities at the nuclear driplines



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)

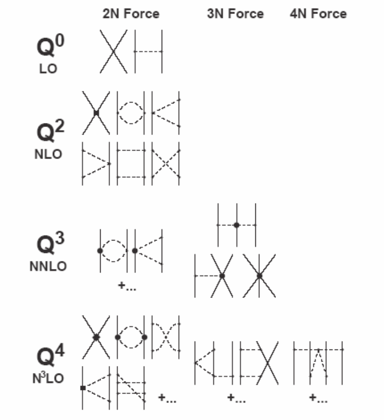
Lagrangian
→ infinite sum of Feynman diagrams.

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.

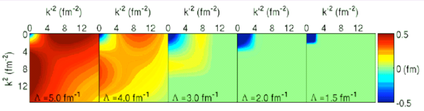
24 paramters (rather than 40 from meson theory) to describe 2400 data points with

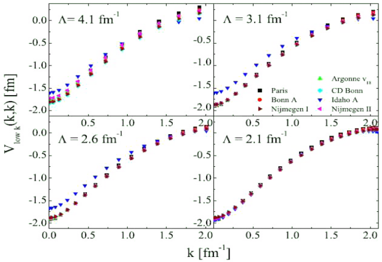


Low-momentum nucleon-nucleon interaction: $V_{\mathrm{low}-k}$

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

Single-Reference 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

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

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

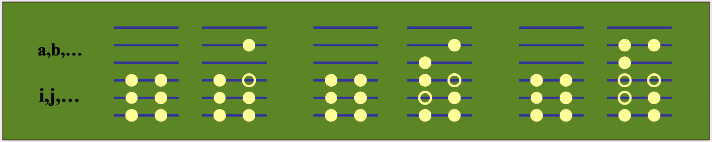
$$\bar{H} = \left(H_N exp(T) \right)_C$$

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

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

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

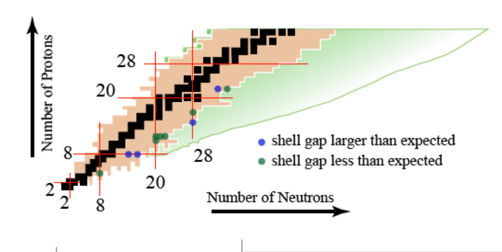


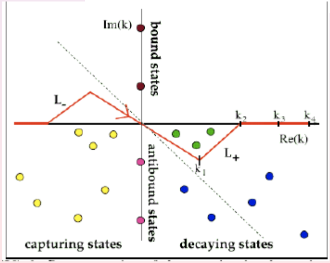
How well does SR-CC describe open-shell nuclei?

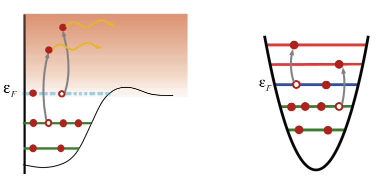
Various Coupled Cluster approaches to the $^{3-6}$He ground states. Single reference Coupled-Cluster methods works.

Method	^{3}He	^{4}He	^{5}He	^{6}He	$\langle J^2 \rangle$, ^{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
FCI	-6.45	-26.3	-22.1	-22.7	0.00

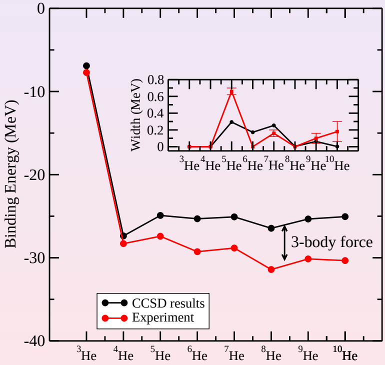
Coupled-cluster approach to open quantum systems







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

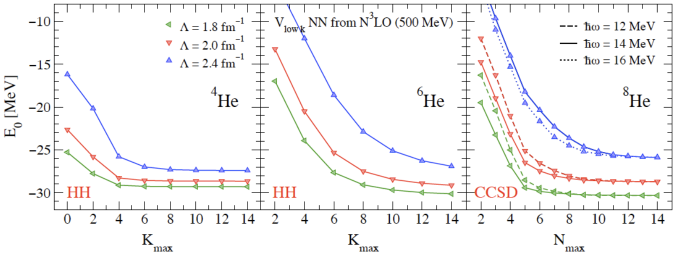


- $V_{\mathrm{low}-k}$ from N3LO with $\Lambda = 1.9\mathrm{fm}^{-1}$.
- G. Hagen et al., Phys. Lett. B 656, 169 (2007). arXiv:nucl-th/0610072.

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

Helium isotopes with V_{low-k}

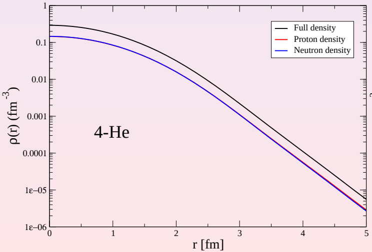
S. Bacca, A. Schwenk, G. Hagen, T. Papenbrock, Eur. Phys. J. A **42**, 553 (2009).

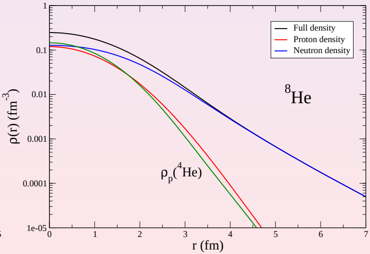


Λ [fm^{-1}]	$E_0(^4\text{He})$	$E_0^\infty(^6\text{He})$ [$E_0(K_{\max}=14)$]	$E_0(^8\text{He})$ Λ-CCSD(T) [CCSD]
1.8	−29.30(2)	−30.28(3) [−30.13]	−31.21 [−30.33]
2.0	−28.65(2)	−29.35(13) [−29.13]	−29.84 [−28.72]
2.4	−27.40(2)	−27.62(19) [−26.91]	−27.54 [−25.88]
experiment	−28.296	−29.268 [44]	−31.395 [4]

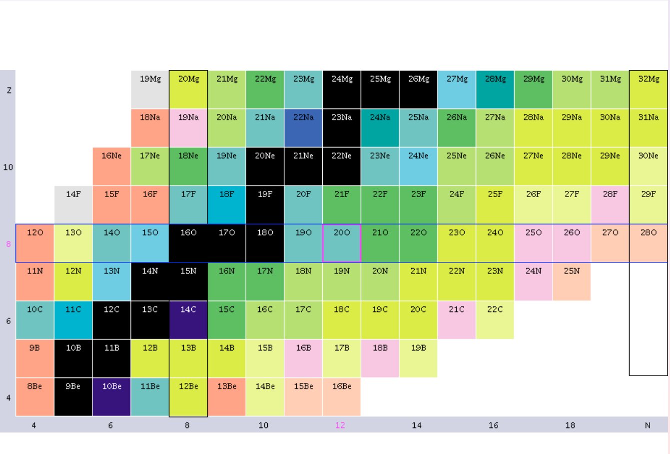
^{4}He and ^{8}He density distributions with V-srg

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





Most nuclei are open-shell. How to access these nuclei with coupled-cluster method?



Single-reference or Multi-reference Coupled-Cluster theory?

Single-Reference CC

- Single-Reference Coupled-Cluster (SR CC) theory can in principle be applied to open-shell nuclei.
- SR CC can not define a unique reference function.
- SR CC breaks rotational invariance for truly open shell systems like ^{6}He.
- SR CC requires uncoupled basis (m-scheme), must use soft interactions due to explosion of basis states.

Equation-of-Motion (Multi-Reference) CC:

- Equation-of-Motion provides us with a consistent approach to open-shell nuclei.
- Equation-of-Motion can be implemented in a spherical scheme, can apply basis sets large enough to accomodate “bare” interactions

Equation-of-Motion CC for open-shell nuclei

Equation-of-Motion Coupled-Cluster theory

The idea of Equation-of-Motion Coupled-Cluster theory is to calculate ground- and excited states of system B by acting with a excitation operator Ω_k on the ground state of system A

$$|\psi_k^B\rangle = \Omega_k|\psi_0^A\rangle, \;\; |\psi_0^A\rangle = \exp(T)|\phi_0^A\rangle$$

Define the non-particle conserving excitation operators $\Omega_k = R_k^{(A\pm1)}$

$$R_k^{(A+1)} = r^a a_a^\dagger + \frac{1}{2} r_j^{ab} a_a^\dagger a_b^\dagger a_j + \dots,$$

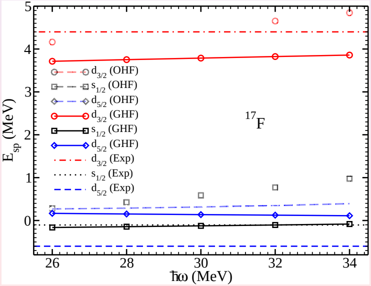
$$R_k^{(A-1)} = r_i a_i + \frac{1}{2} r_{ij}^{b} a_b^\dagger a_i a_j + \dots,$$

Particle-Attached/Removed EOM-CC equations

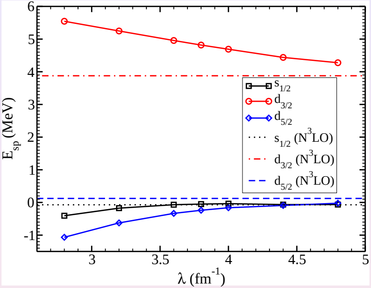
$$\left[\overline{H}, R_k^{(A\pm1)}\right]|\phi_0\rangle = \left(\overline{H} R_k^{(A\pm1)}\right)_C |\phi_0\rangle = \omega_k R_k^{(A\pm1)}|\phi_0\rangle,$$

Low-lying states in ^{17}F and the role of continuum

- Low-lying single-particle states in ^{17}F using a Gamow-Hartree-Fock basis (GHF) and a Oscillator-Hartree-Fock (OHF) basis.
- Very weak dependence on the oscillator frequency $\hbar\omega$ for calculations done in a GHF basis.
- Significant effect of continuum coupling on the $1/2^+$ and $3/2^+$ states in ^{17}F.



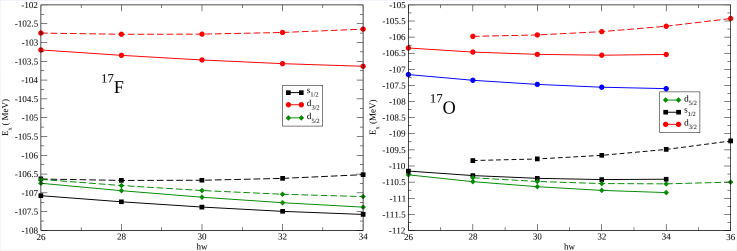
Cutoff dependence on Low-lying states in ^{17}F



- Cuttoff dependence on the low-lying states in ^{17}F.
- Spin-orbit splitting increases between the $d_{5/2}$-$d_{3/2}$ orbitals with decreasing cutoff λ.
- $s_{1/2}$ state show very weak dependence on the cutoff.
- The $1/2^+$ state is a *halo* state which extends far beyond the range of the interaction. Renormalizing the interaction by integrating out high momentum modes does not alter the long range physics.

Low-lying states in ^{17}O and ^{17}F

- Low-lying states in ^{17}F and ^{17}O using a Gamow-Hartree-Fock basis and a Oscillator-Hartree-Fock basis.



Summary of results for ^{17}O and ^{17}F

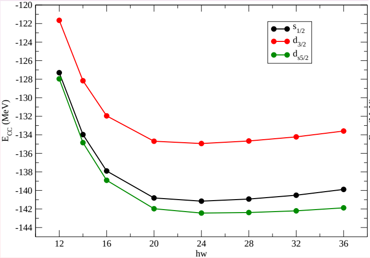
- Our calculations for the $1/2^+$ states in ^{17}F and ^{17}O agree remarkably well with experiment.
- Spin-orbit splitting between $d_{5/2}$-$d_{3/2}$ orbitals too compressed without three-nucleon forces.
- Our calculations of the widhts of the $3/2^+$ resonant states compare reasonably well with experiment.

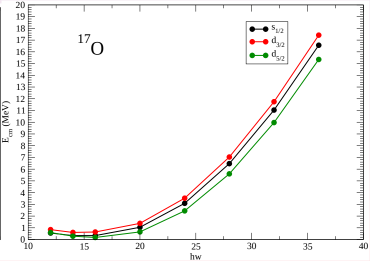
	^{17}O			^{17}F		
	$(1/2)^+_1$	$(5/2)^+_1$	$E_{s.o.}$	$(1/2)^+_1$	$(5/2)^+_1$	$E_{s.o.}$
OHF	-1.888	-2.955	4.891	0.976	0.393	4.453
GHF	-2.811	-3.226	4.286	-0.082	0.112	3.747
Exp.	-3.272	-4.143	5.084	-0.105	-0.600	5.000

	^{17}O $(3/2)^+_1$		^{17}F $(3/2)^+_1$	
	Re[E_{sp}]	Γ	Re[E_{sp}]	Γ
PA-EOMCCSD	1.059	0.014	3.859	0.971
Experiment	0.942	0.096	4.399	1.530

Low-lying states in ^{17}O with V_{srg} (2.8/fm) and the center of mass

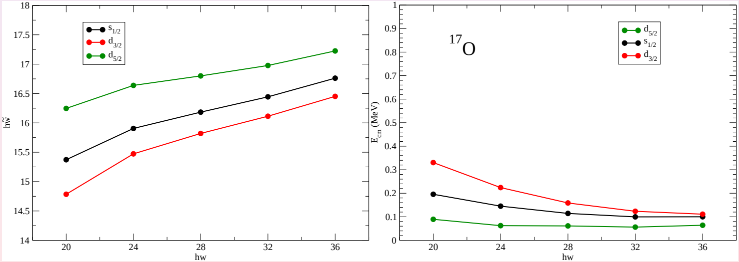
- Low-lying $1/2^+, 3/2^+ and 5/2^+$ states in ^{17}O calculated using PA-EOM-CCSD in 13 major oscillator shells.
- The expectation value of $H_{cm}(\omega) = T_{cm} + \frac{1}{2}mA\omega^2 R_{cm}^2 - \frac{3}{2}\hbar\omega$ meassures to what degree the CoM is a Gaussian with oscillator frequency ω.



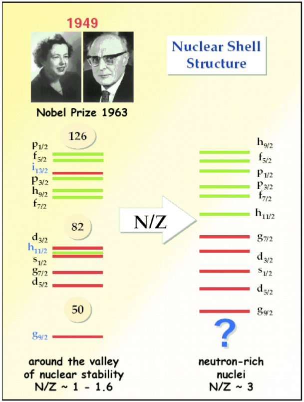


Coupled-Cluster wave function factorizes: $\psi_{int}\psi_{cm}$

- Assumption: CoM wave function is always a gaussian (approximately).
- Take expectation value of the generalized CoM Hamiltonian $H_{cm}(\tilde{\omega}) = T_{cm} + \frac{1}{2}mA\tilde{\omega}^2R_{cm}^2 - \frac{3}{2}\hbar\tilde{\omega}$.
- CC wave function factorizes and the CoM wave function is a Gaussian with almost constant width $\hbar\tilde{\omega} \sim 16MeV$ for all different $\hbar\omega$ values of the basis.



Shell evolution towards the drip line



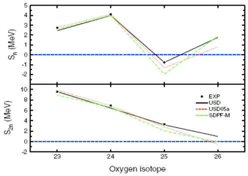
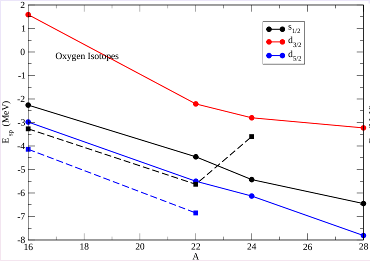


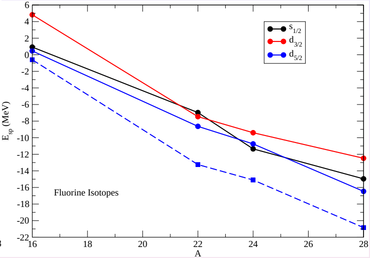
FIG. 4 (color online). The experimental [25,26] (data points) and theoretical [13–15] (lines) one- and two-neutron separation energies for the $N = 15$–18 oxygen isotopes. The experimental error is shown if it is larger than the symbol size.

25O neutron separation energy: -820 keV
the width was measured to be 90(30) keV
giving a lifetime of t ~ 7x10-21 sec

C. Hoffman PRL 100 (2008) 152502

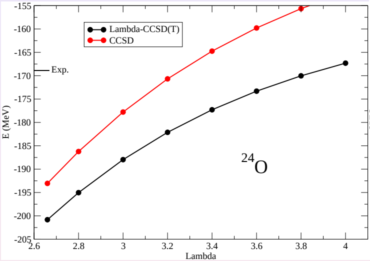
Shell evolution in oxygen and fluor

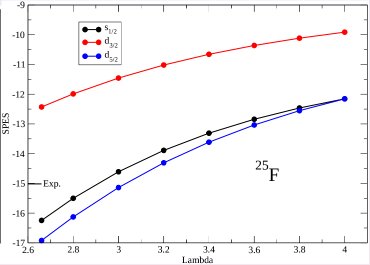




- Low lying states in oxygen and fluorine isotopes calculated using PA/PR-EOMCCSD with “bare” chiral interactions.
- Model space consists of 15 major harmonic oscillator shells with fixed oscillator frequency $\hbar\omega = 32$MeV.
- ^{25}O is stable with respect to neutron emission. Interesting inversion of ground state in ^{25}F.
- What is the role of continuum and three-body forces ?

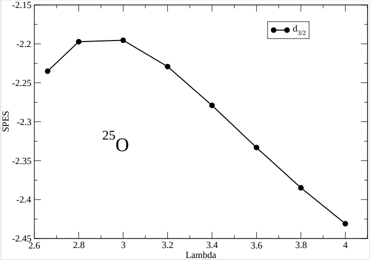
Cutoff dependence in ^{24}O and ^{25}F





- Variation of the cutoff as a tool to probe the effects of missing many-body forces.
- No unique cutoff that will reproduce data in ^{24}O and ^{25}F simultaneously.
- Three-nucleon forces are needed. Continuum coupling might bring additional binding in the low-lying states in ^{25}F.

Cutoff dependence in ^{25}O



- Cuttoff dependence on the $3/2^+$ state in ^{25}O.
- Calculations done in 15 major oscillator shells with fixed oscillator frequency $\hbar\omega = 32$MeV.
- There are no two-body forces within the family of phase-equivalent low-momentum interactions derived from N^{3}LO that will make ^{25}O unstable.
- Three-nucleon forces are needed to match theory with experiment in ^{25}O!

Conclusion

- Coupled-Cluster theory has been successfully applied to weakly bound and unbound helium isotopes.
- Derived and implemented Equation of Motion CCM; calculation of open-shell systems, excited states, density distributions and radii.
- PA-EOM Coupled-cluster method has been succesfully applied to the description of weakly bound and unbound states in ^{17}O and ^{17}F.
- Coupling to the continuum plays a significant role on states close to the particle emission threshold.
- PR/PA-EOM Coupled-Cluster theory allows for *ab initio* calculations of single-particle states and the study of shell-evolution in neutron rich nuclei.
- Provide realistic single-particle energies for shell-model calculations with a core.

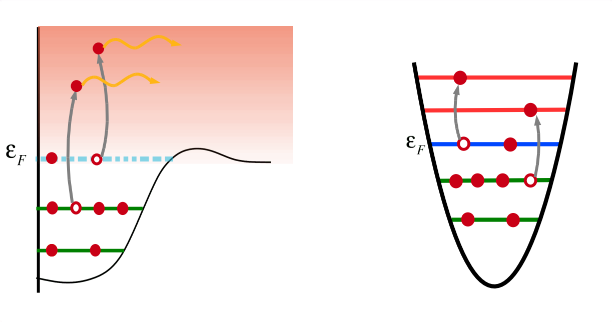
Future perspectives

- 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.
- Ab-initio description of ^{56}Ni, ^{100}Sn and ^{208}Pb within reach.

Coupled Cluster for open quantum systems

Open Quantum System.
Coupling with continuum taken into account.

Closed Quantum System.
No coupling with external continuum.

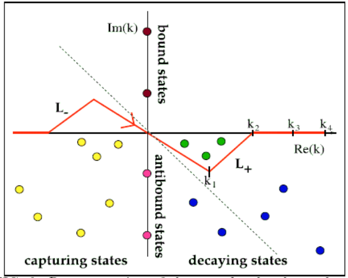


Berggren Single-particle basis

Complex energies requires a generalized completeness relation

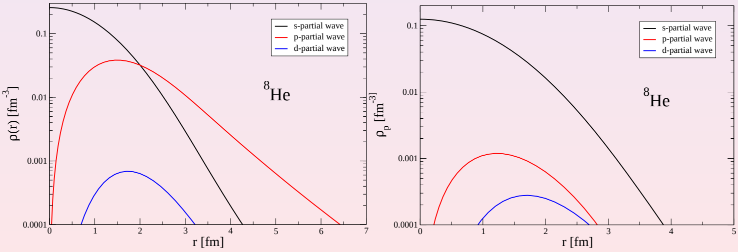
$$|\Psi(\mathbf{r},t)|^2 = |\Phi(\mathbf{r})|^2 exp(-\frac{\Gamma}{\hbar}t), \quad E = E_r - i\Gamma/2.$$

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



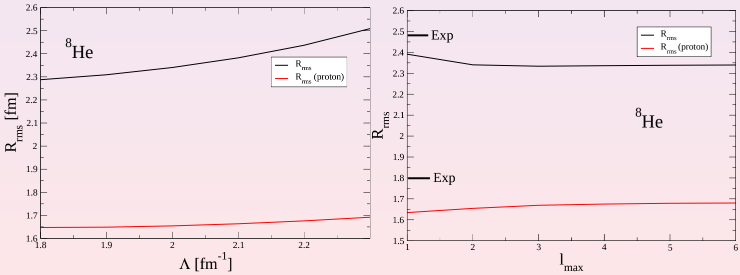
Partial wave decomposition of ^{8}He density

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



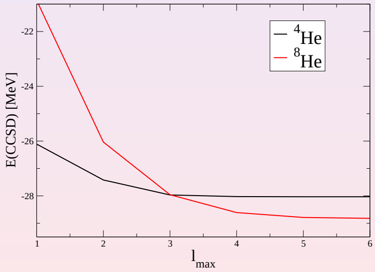
Matter and charge radii of ^{8}He using V-srg

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



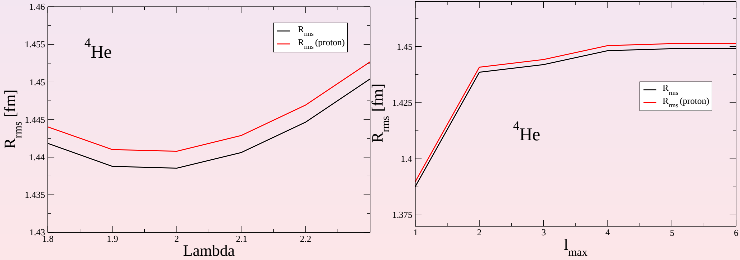
Properties of weakly bound nuclei

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



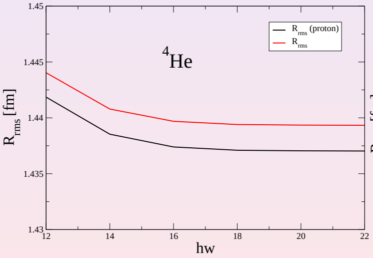
Matter and charge radii of ^{4}He using V-srg

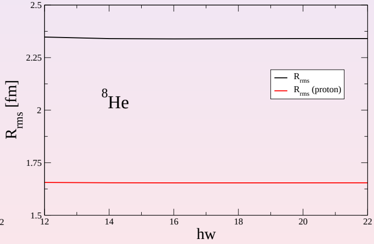
- Λ dependence on ^{4}He charge and matter radii indicates missing 3NF.
- Hamiltonians with two-body renormalized interactions (SRG/low-k) underestimates matter and charge radii.



Properties of weakly bound nuclei

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

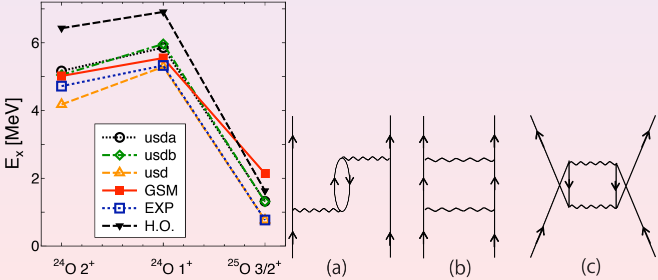




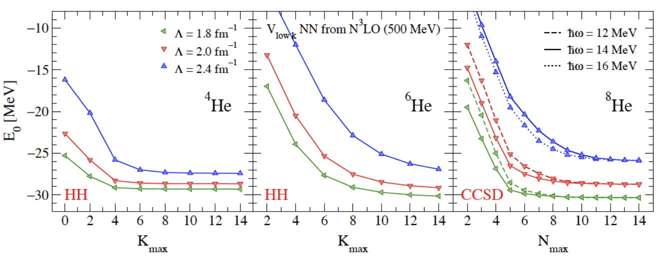
The role of continuum in calculations of oxygen isotopes

- Shell model calculations of oxygen isotopes using two-body effective interactions and second order perturbation theory.
- Calculations starting from a ^{16}O core gives ^{25}O bound.
- Starting from a ^{22}O core gives ^{25}O unbound in both HO and Gamow basis.
- Inclusion of many-body effects crucial, continuum plays a role in the description of excited states.

K. Tsukiyama, M. Hjorth-Jensen, G. Hagen, Phys. Rev. C(R) 80, 051301 (2009)

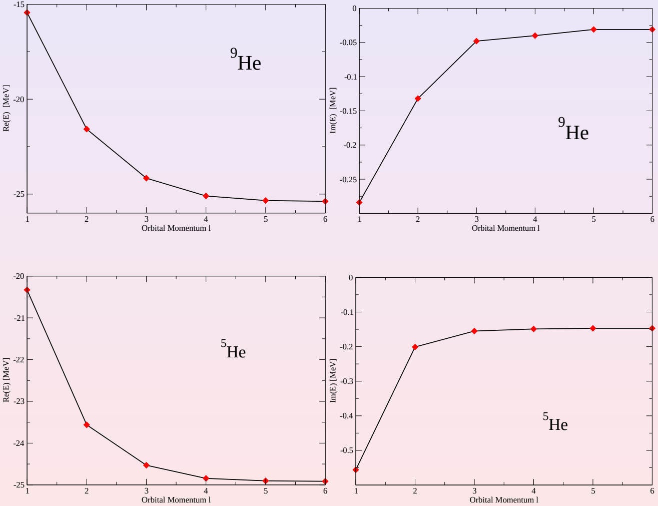


$^{4-8}$He with smooth v-lowk



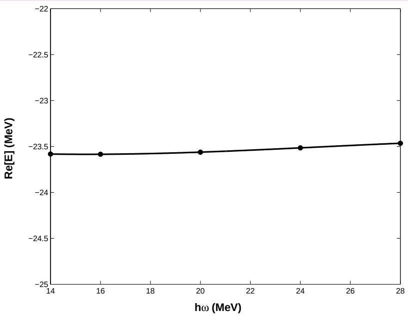
Λ [fm^{-1}]	$E_0(^4\mathrm{He})$	$E_0^\infty(^6\mathrm{He})$ $[E_0(K_{\max}=14)]$	$E_0(^8\mathrm{He})$ Λ-CCSD(T) [CCSD]
1.8	−29.30(2)	−30.28(3) [−30.13]	−31.21 [−30.33]
2.0	−28.65(2)	−29.35(13) [−29.13]	−29.84 [−28.72]
2.4	−27.40(2)	−27.62(19) [−26.91]	−27.54 [−25.88]
experiment	−28.296	−29.268 [44]	−31.395 [4]

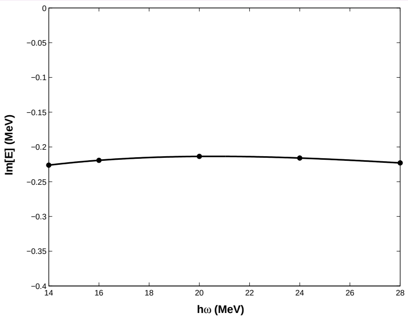
Convergence of CCSD results



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

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





Convergence of CCSD energy.

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