Coupled-cluster theory within UNEDF

Thomas Papenbrock

and OAK RIDGE NATIONAL LABORATORY

UNEDF: G. Hagen (ORNL), J. Holt, T. Lesinski (UT/ORNL)

CS support: H. A. Nam, B. Velamur Asokan (ORNL)

External collaborators: K. Amos (Melbourne), S. Bacca (TRIUMF), N. Barnea (Jerusalem), D. J. Dean (ORNL), M. Hjorth-Jensen (Oslo)

1. Main accomplishments since last meeting
2. Status regarding high-performance computing
3. Roadmap for remainder of year 4 and for year 5

Annual UNEDF collaboration meeting

East Lansing, MI, June 21-25 2010

Research partly funded by the US Department of Energy

Main accomplishments since last meeting

Science:

1. Computation of proton halo state and resonances in A=17 nuclei
2. Computation of spectroscopic factors
3. Long article on nuclear structure with NN interactions from chiral EFT and from $V_{low\ k}$ and SRG
4. Progress on interfacing with DFT and reactions (unpublished)
5. Moving toward reactions (optical potentials via g-folding models from ab initio densities; Lorentz integral transform)
6. Inclusion of 3NF (normal ordered contributions to NN within HF basis)

Computing / algorithm developments:

1. Inclusion of continuum effects within the spherical coupled-cluster code (rationale: description of open quantum systems)
2. Implementation of spherical equation-of-motion methods for computation of A±1 nuclei (from closed shell nucleus A)

Publication Summary

Submitted articles

1. *Ab initio coupled-cluster approach to nuclear structure with modern nucleon-nucleon interactions*, G. Hagen, T. Papenbrock, D. J. Dean, and M. Hjorth-Jensen, arXiv: 1005.2627, submitted to Phys. Rev. C.
2. *Computation of spectroscopic factors with the coupled-cluster method*, O. Jensen, G. Hagen, T. Papenbrock, D. J. Dean, and J. S. Vaagen, arXiv:1004.2611, accepted for publication in Phys. Rev. C. (2010).

Published since July 2009

1. *Solution of the center-of-mass problem in nuclear structure calculations*, G. Hagen, T. Papenbrock, and D. J. Dean, Phys. Rev. Lett. 103, 062503 (2009).
2. *Ab-initio computation of neutron-rich oxygen isotopes*, G. Hagen, T. Papenbrock, D. J. Dean, M. Hjorth-Jensen, and B. Velamur Asokan, Phys. Rev. C 80, 021306(R) (2009).
3. *Gamow shell-model calculations of drip-line oxygen isotopes*, K. Tsukiyama, M. Hjorth-Jensen, and G. Hagen, Phys. Rev. C 80, 051301 (2009).
4. *Ab initio computation of the 17F proton-halo state and resonances in A = 17 nuclei*, G. Hagen, T. Papenbrock, and M. Hjorth-Jensen, Phys. Rev. Lett. 104, 182501 (2010).
5. *Many-body interactions and nuclear structure*, M. Hjorth-Jensen, D. J. Dean, G. Hagen and S. Kvaal, J. Phys. G: Nucl. Part. Phys. 37, 064035 (2010).

Talks

1. *Coupled cluster theory for medium mass nuclei*, ECT* workshop “Linking Nuclei, Molecules, and Condensed Matter: Computational Quantum Many-Body Approaches,” Trento, Italy, July 6-10, 2009. (TP)
2. *Ab-initio approach to nuclei beyond the valley of stability*, ECT Workshop on Confrontation and Convergence in Nuclear Theory, ECT, Trento, Italy, July 27-31, 2009 (GH)
3. *Nuclear structure from chiral effective field theory*, “19th International IUPAP Conference on Few-Body Problems in Physics,” Bonn, Germany, Aug. 31 - Sept. 5, 2009. (TP)
4. *Coupled Cluster Approach to Nuclear Structure*, Internal nuclear physics seminar at the University of Tokyo,Tokyo, Japan, November 10, 2009 (GH)
5. *Three-Nucleon Forces for Medium-Mass Nuclei Towards the Dripline*. Nuclear Theory Seminar University of Tokyo Tokyo, Japan; November 16, 2009 (JH)
6. *Three-Nucleon Forces in Neutron-Rich Nuclei*, Nuclear Physics Seminar RIKEN Nishina Center for Accelerator-Based Science Wako, Saitama, Japan; November 18, 2009 (JH)
7. *Coupled Cluster Approach to Nuclear Structure*, Nuclear physics seminar at RIKEN, Waco, Japan, November 18, 2009 (GH)
8. *Ab initio calculations of neutron-rich oxygen isotopes*, “JUSTIPEN-EFES Workshop on Unstable nuclei,” RIKEN, Wakoshi, Dec. 7-9 2009 (TP)
9. *Coupled-Cluster theory for medium mass and neutron rich nuclei*, ECT Workshop on Many-Body Open Quantum Systems: From Atomic Nuclei to Quantum Dots, ECT, Trento, Italy, February 24, 2010 (GH)
10. *Coupled-cluster theory for nuclei*, INT workshop “Weakly-bound systems in atomic and nuclear physics,” Seattle, March 8-12, 2010. (TP)
11. *Role of the Continuum in Coupled Cluster Theory*, INT workshop on Weakly Bounds Systems in Atomic and Nuclear Physics, INT, Seattle, March 8 - 12, 2010 (GH)
12. *Ab-initio Coupled Cluster Approach to Medium-mass and Neutron-rich Nuclei*, The 4th LACM-EFES-JUSTIPEN Workshop, Oak Ridge, Tennessee, March 16, 2010 (GH)
13. *Three-Nucleon Forces and Nuclear Structure in Neutron-Rich Calcium Isotopes*. The 4th LACM-EFES-JUSTIPEN Workshop Joint Institute for Heavy Ion Research Oak Ridge, TN; March 17, 2010 (JH)
14. *Ab initio coupled cluster computations of nuclei*, 6th ANL/MSU/JINA/INT FRIB Theory Workshop “Computational Forefront in Nuclear Theory: Preparing for FRIB,” ANL, March 23-26, 2010. (TP)
15. *Three-Nucleon Forces for Medium-Mass Nuclei Towards the Dripline*, New Quests in Nuclear Structure 10th International Spring Seminar on Nuclear Physics Vietri Sul Mare, Italy; May 22, 2010 (JH)
16. *Coupled Cluster Approach to Medium Mass and Neutron Rich Nuclei*, 10th International spring seminar on nuclear physics, new quests in nuclear structure, Italy, Vietri Sul Mare, May 22, 2010 (GH)
17. *Three-Nucleon Forces and Fully Microscopic Description of Neutron-Rich Nuclei*, Nuclear Physics Seminar Yukawa Institute for Theoretical Physics; University of Kyoto Kyoto, Japan; June 13, 2010 (JH)
18. *Three-Nucleon Forces and Nuclear Structure in Neutron-Rich Calcium Isotopes*. Second EMMI-EFES Workshop on Neutron-Rich Nuclei RIKEN Nishima Center for Accelerator-Based Research Wako, Saitama, Japan; June 17, 2010 (JH)

Personnel

UNEDF collaborators: G. Hagen, J. Holt, (T. Lesinski → UW), T. Papenbrock

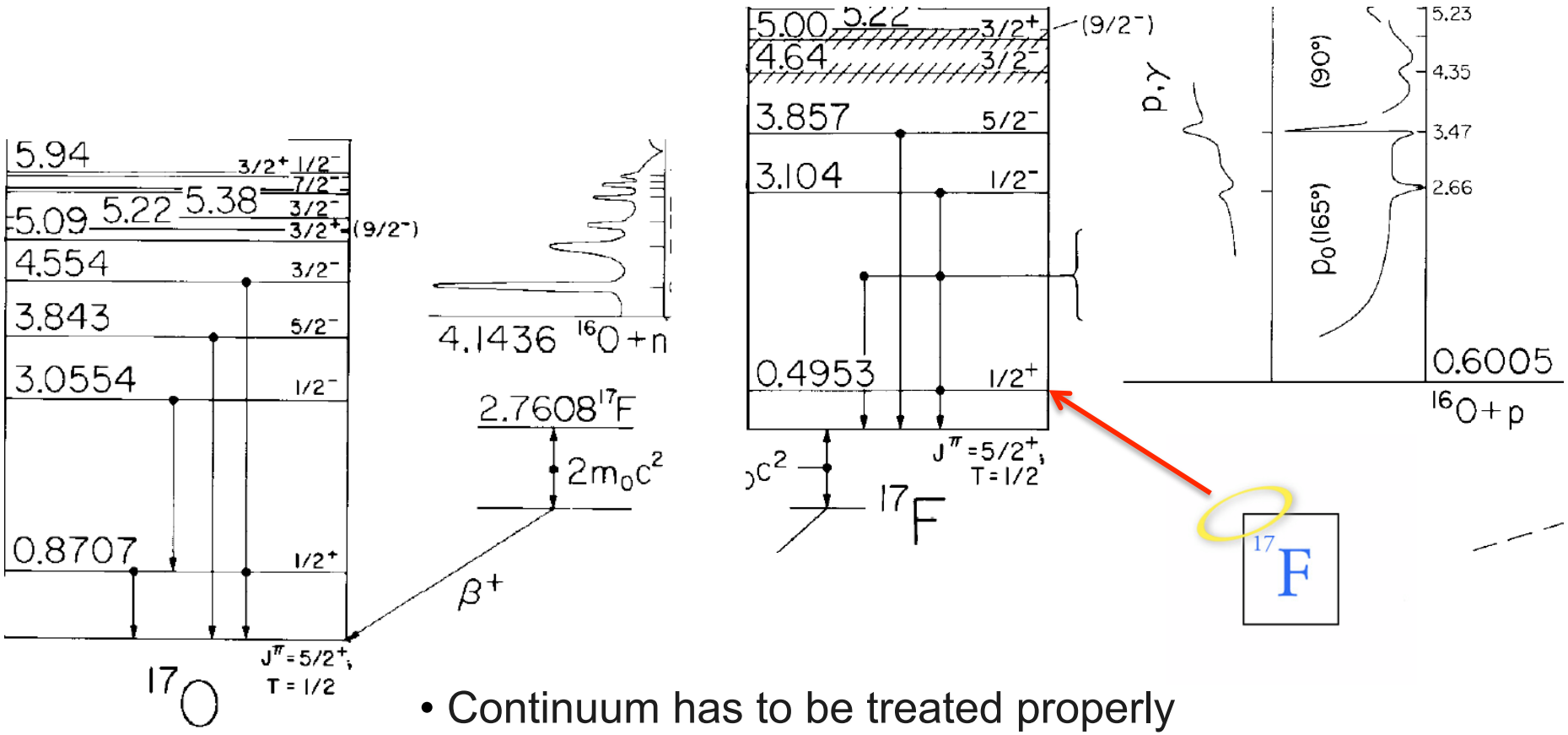
CS support: Hai Ah Nam (ORNL)

Development of coupled-cluster method with relevance for UNEDF (by students supervised by Hjorth-Jensen and Hagen)

Øyvind Jensen (student at University of Bergen; spectroscopic factors)

Gustav Jansen (student at University of Oslo; closed shell ±2 nucleons)

Low lying states in A=17 nuclei



- Continuum has to be treated properly
- Our focus is on single-particle states
- Previous study: shell model in the continuum with ^{16}O core

[Bennaceur et al Phys. Lett. B 488, 75 (2000)]

Bound states and resonances in ^{17}F and ^{17}O

Single-particle basis consists of bound, resonance and scattering states

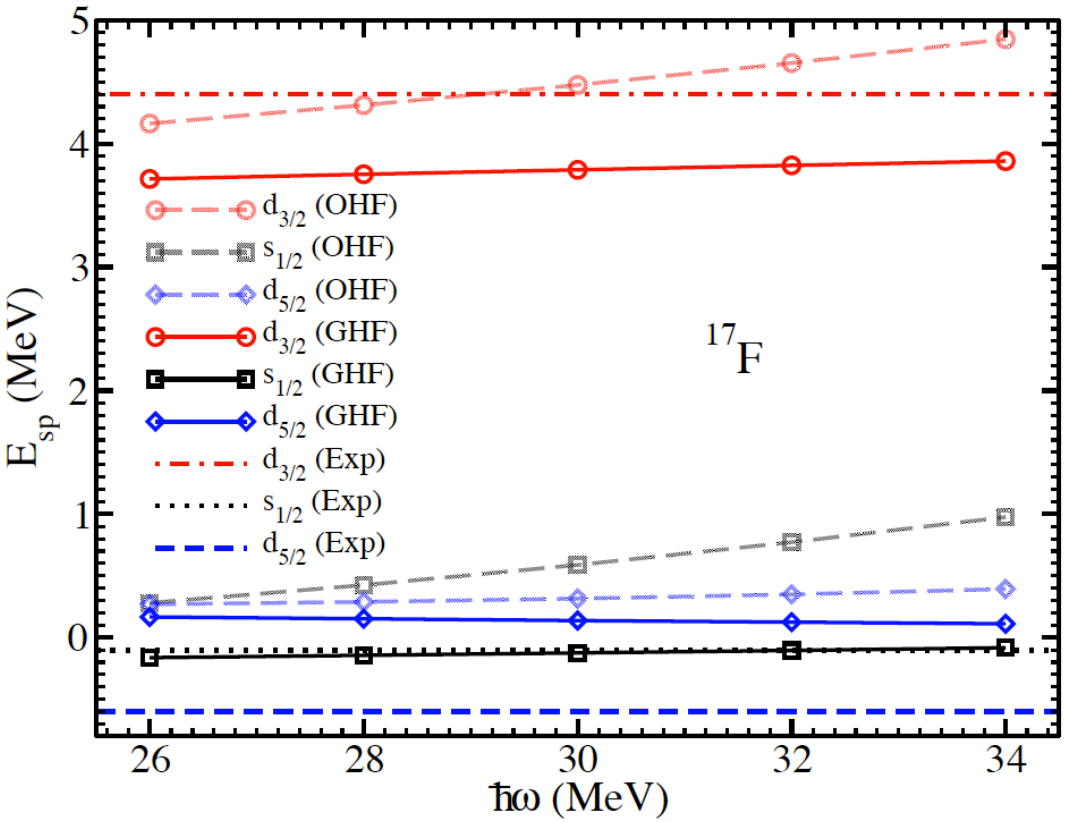
- Gamow basis for $s_{1/2}$ $d_{5/2}$ and $d_{3/2}$ single-particle states
- Harmonic oscillator states for other partial waves

Computation of single-particle states via "Equation-of-motion CCSD"

- Excitation operator acting on closed-shell reference
- Here: superposition of one-particle and 2p-1h excitations

$$R_\mu = r^a a_a^\dagger + \frac{1}{2} r_j^{ab} a_a^\dagger a_b^\dagger a_j$$

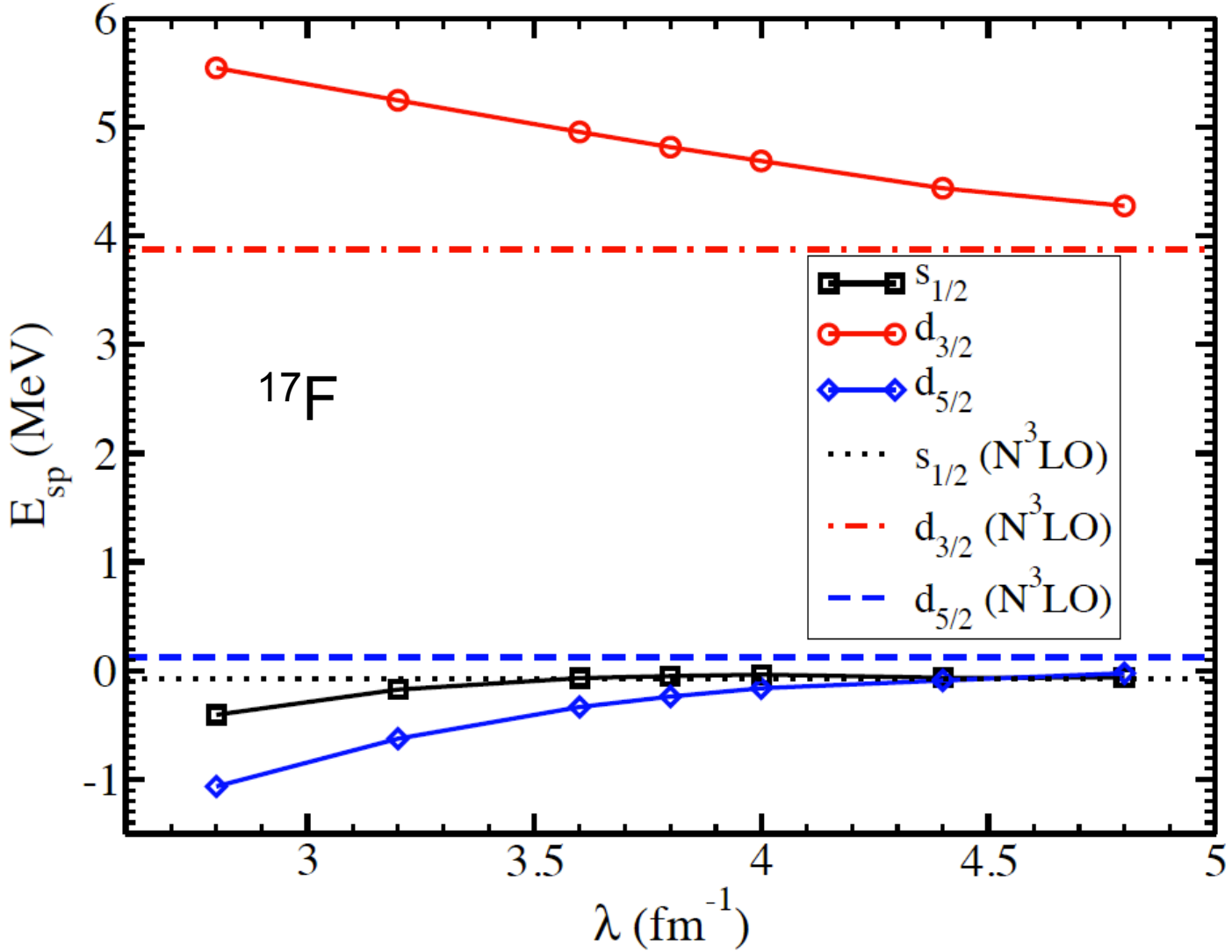
$$\left[\overline{H}, R_\mu\right] |\phi_0\rangle = \omega_\mu R_\mu |\phi_0\rangle$$



- Gamow basis weakly dependent on oscillator frequency
- d5/2 not bound; spin-orbit splitting too small
- s1/2 proton halo state close to experiment

G. Hagen, TP, M. Hjorth-Jensen,
Phys. Rev. Lett. 104, 182501 (2010)

Variation of cutoff probes omitted short-range forces



- Proton-halo state (s1/2) very weakly sensitive to variation of cutoff
- Spin-orbit splitting increases with decreasing cutoff

CCM results with a chiral N^{3}LO (NN only)

	CCSD		Λ-CCSD(T)	
Nucleus	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

[Hagen, TP, Dean, Hjorth-Jensen, arXiv:1005.2627]

Main results

1. Well converged CCSD results with respect to size of model space (< 1% change in binding energy when going from 14 to 15 oscillator shells.
2. Λ-triples correction adds 0.8MeV per nucleon in binding energy.
3. Three-nucleon force and triples corrections expected to yield 0.4MeV additional binding?

Research proposed at **last** UNEDF meeting
Future plans (remainder of year 3 and for year 4)

1. Interface with DFT (response of density to external potentials, check DME)
2. Toward ab-initio reactions
    1. Spectroscopic factors
    2. CC densities as microscopic input for optical potentials / g-folding methods
    3. Lorentz integral transform
3. Role of three-nucleon forces in medium-mass nuclei

DFT – coupled cluster interface

(Hagen, Holt, Lesinski,TP)

Aim: expansion of density functional up to quadratic terms around CCSD density for a given nucleus.

- Zeroth order: ground-state energy
- 1st order: Kohn Sham potentials reproduce CCSD densities for non interacting nucleons.
- 2nd order: add small external potentials and extract second derivative of functional from response of density (near future).

$$\mathbf{J}(\mathbf{r}) = -i \sum_i \rho_i \, \phi_i^\dagger(\mathbf{r}) \boldsymbol{\sigma} \times \boldsymbol{\nabla} \phi_i(\mathbf{r})$$

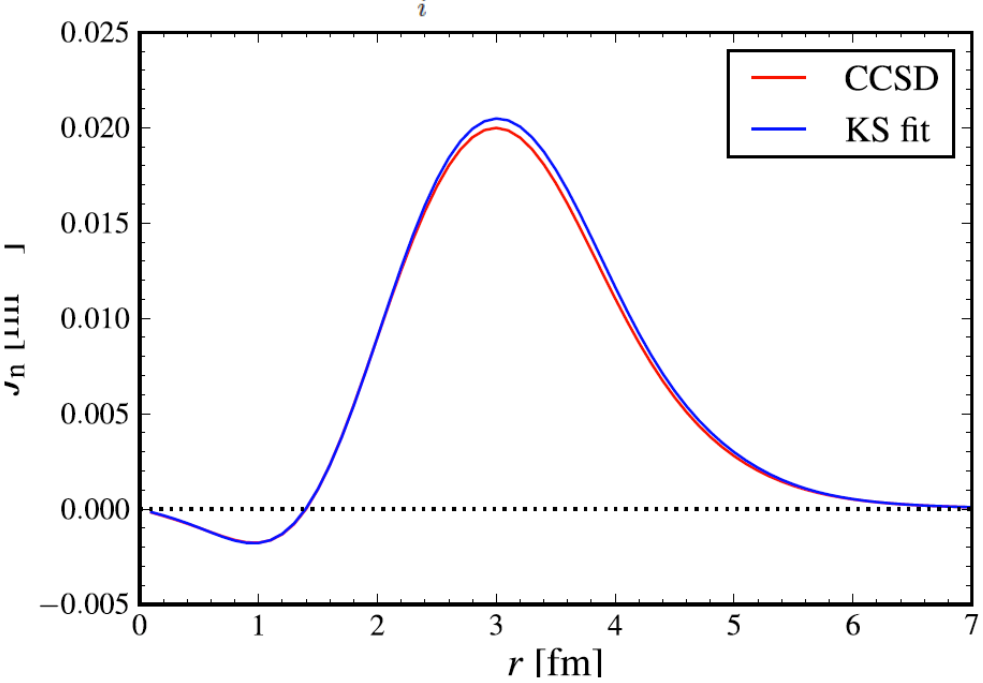


FIG. 2. Spin-orbit neutron density in ^{48}Ca from CCSD and the fit of an external KS potential.

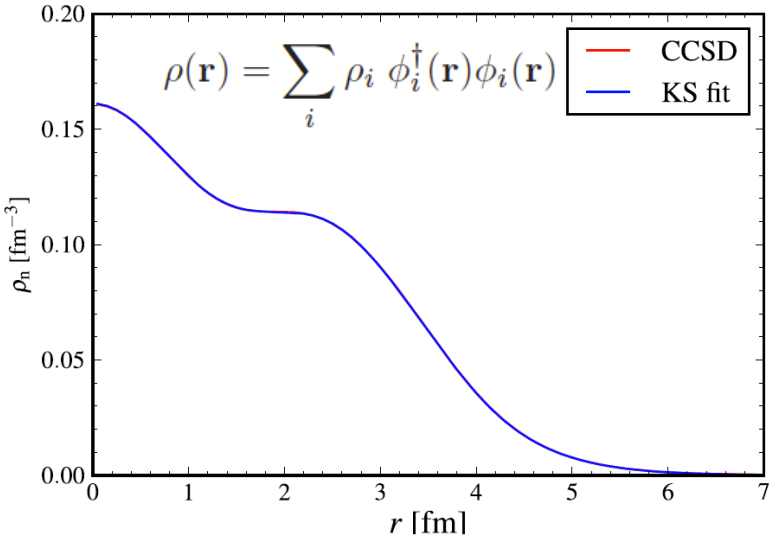


FIG. 1. Local neutron density in ^{48}Ca from CCSD and the fit of an external KS potential.

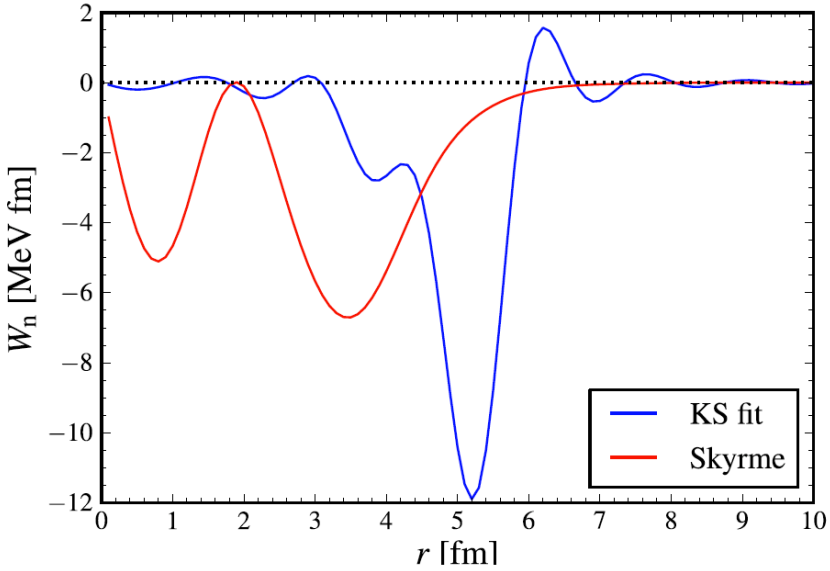


FIG. 3. Neutron spin-orbit field ^{48}Ca the fit of an external KS potential on CCSD results and a naive Skyrme density-gradient shape.

Spectroscopic factors within CCM

nucleon removal from ^{16}O

$$S^A_{A-1}(lj) = \sum_n |\langle A-1||\tilde{a}_{nlj}||A\rangle|^2$$

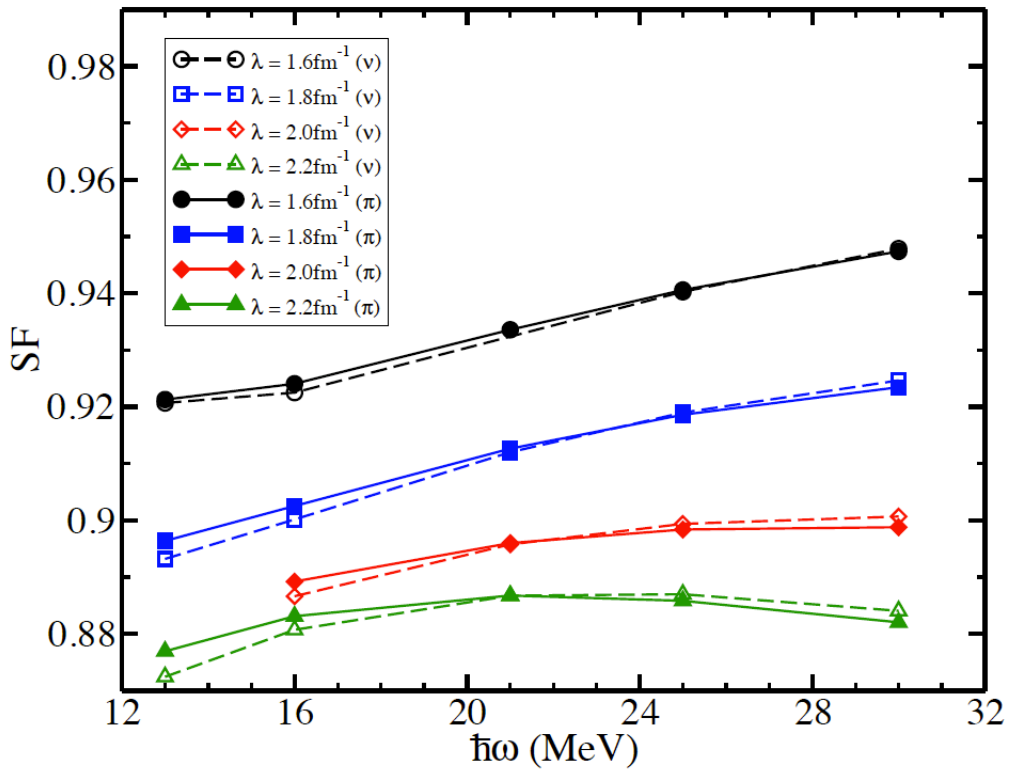
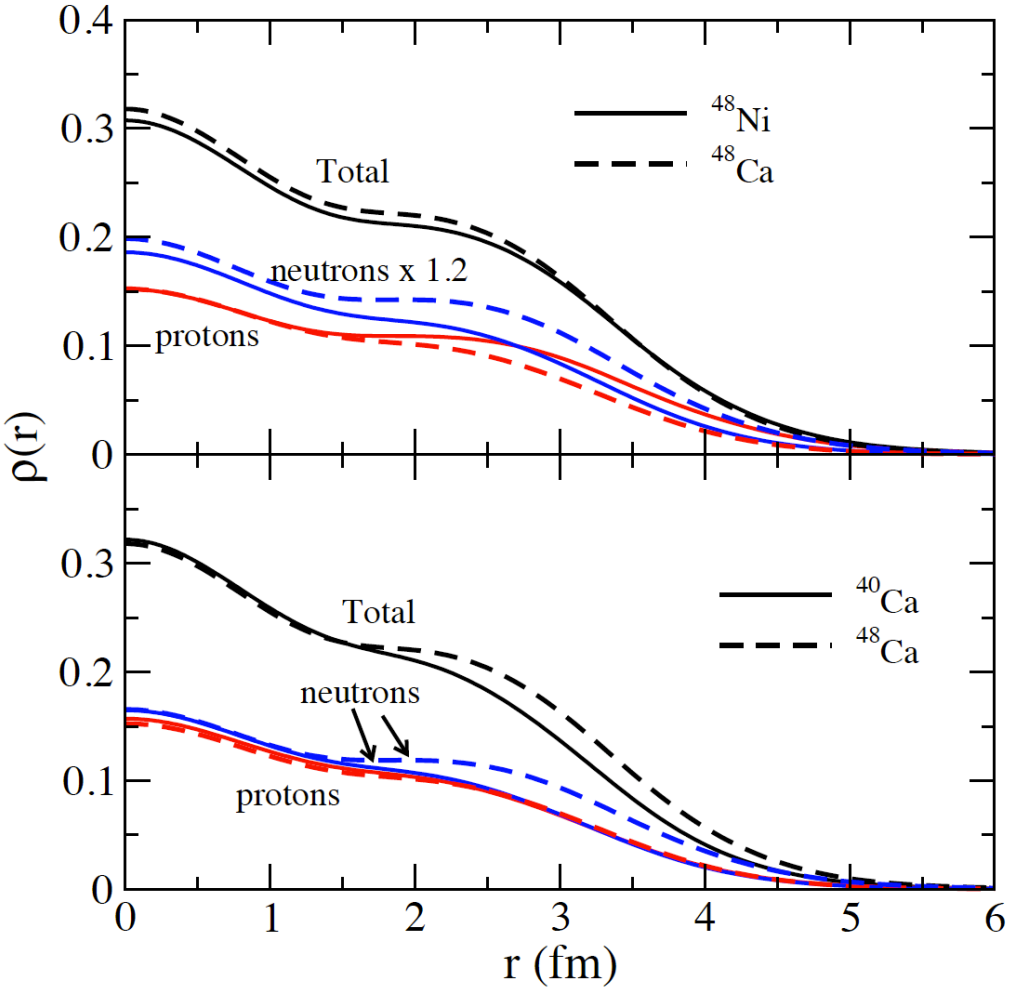


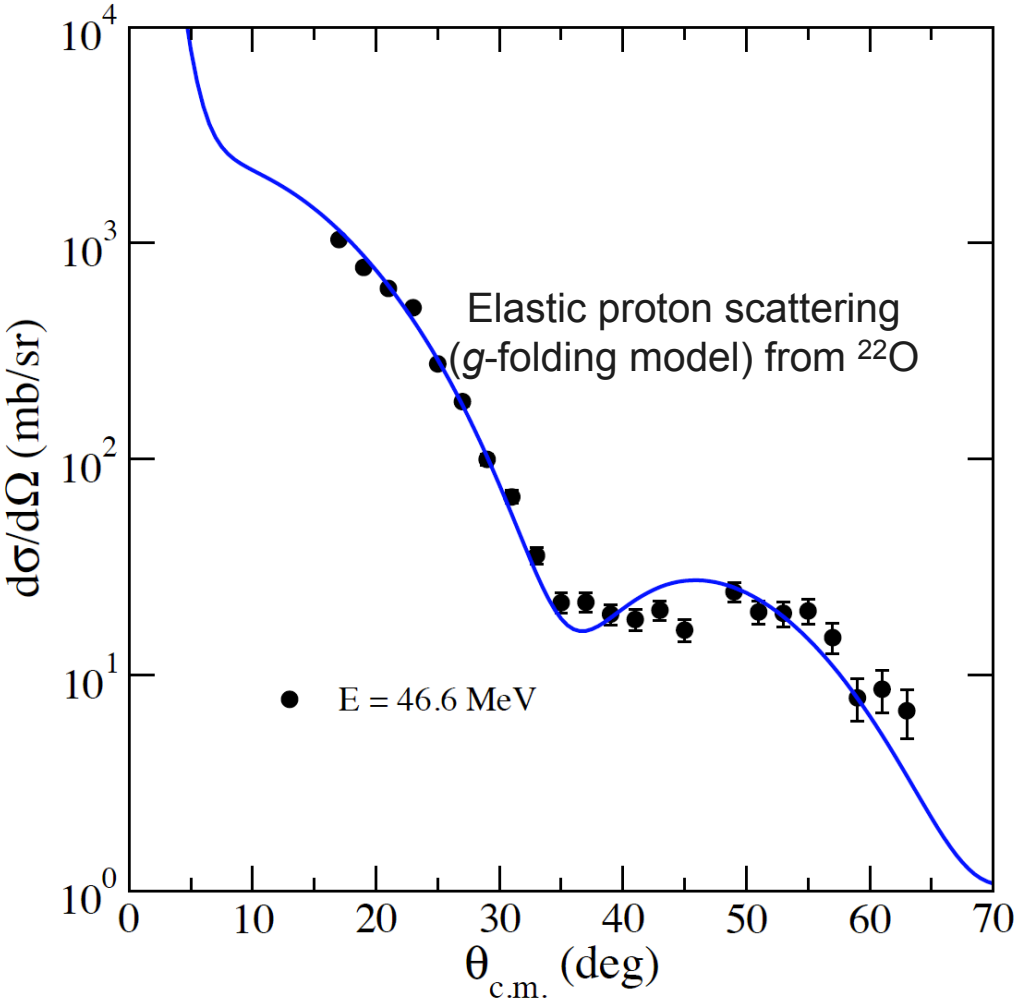
FIG. 4: (Color online) Spectroscopic factor SF$(1/2^-)$ for neutron and proton removal as a function of the oscillator spacing $\hbar\omega$ for nucleon-nucleon interactions with different cutoffs in a model space with $N = 6$.

Ø. Jensen, G. Hagen, TP, D. J. Dean, and J.S. Vaagen, arXiv:1004.2611

Densities and elastic reaction cross sections

(in collaboration with Ken Amos; figures by Ken Amos)





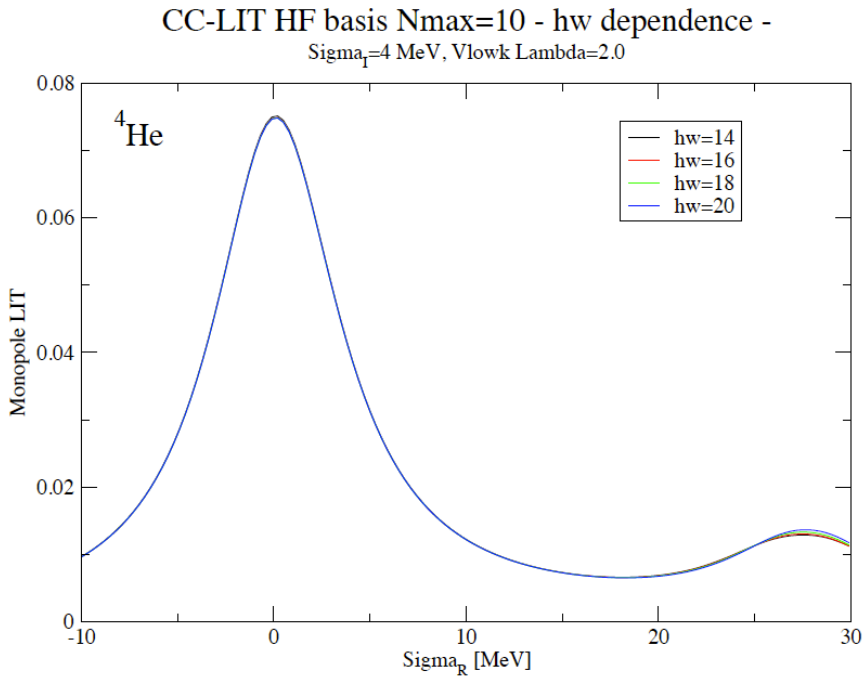
Densities based on one-body density matrix – no center-of-mass correction yet.

- Optical potential based on CC density computed with an N^{3}LO potential.
- *g*-folding model employs different potential (coordinate space; Yukawa terms)

[K. Amos *et al.*, Adv. Nucl. Phys. 25, 275 (2000)]

Lorentz integral transform – preliminary results

(in collaboration with S. Bacca and N. Barnea)

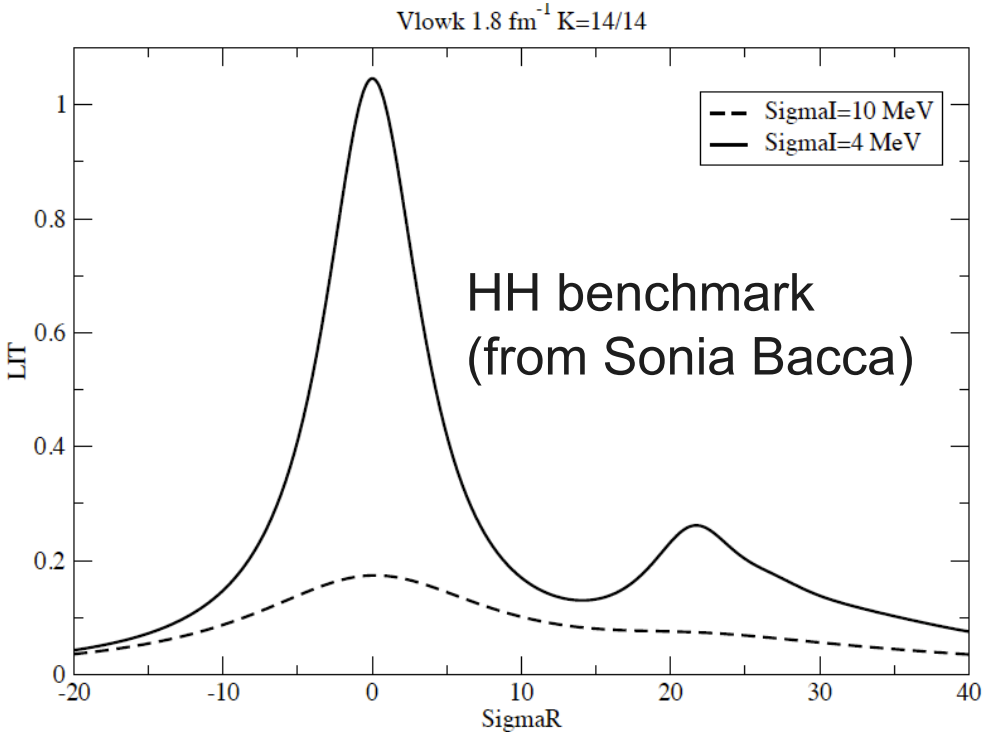


$$R(\omega) = \sum_f |\langle f|\Theta|0\rangle|^2 \delta(E_f - E_0 - \omega)$$

$$\mathcal{L}(\sigma_R, \sigma_I) = \int d\omega \frac{R(\omega)}{(\omega - \sigma_R)^2 + \sigma_I^2}$$

$$\mathcal{L}(\sigma_R, \sigma_I) = \langle \tilde{\Psi}|\tilde{\Psi}\rangle$$

$$(H - E_0 - \sigma_R - i\sigma_I)|\tilde{\Psi}\rangle = \Theta|0\rangle$$



Cross section for monopole excitations of ^{4}He

- Artificial broadening by 4MeV
- Elastic peak around zero frequency
- Inelastic peak at high energies 20-30MeV

To do

- Role of center-of-mass corrections
- dipole excitations

Computational status

Data organization

- Interaction spread across processors
- cluster amplitudes stored locally
- oxygen-16 in 20 shells ~ 1500 processor hours per model space
- proton halo state in ^{17}F: total cost of about 100,000 CPU hours on Jaguar.

Challenge

- Number of j-coupled matrix elements of interactions fluctuate strongly for given sets of quantum numbers
- load balancing non-trivial: Calculation of estimated computational cost → distribution of data
- scaling (load-balancing) up to few hundred processors

Progress for years 3-4

Proposed work	**Status**
Interface with DFT: response of energy and density to external potentials	First results available
Spectroscopic factors	^{15}O, ^{15}N (*m*-scheme) In progress: spherical scheme
Employ densities for optical potentials (with Ken Amos)	First results
Lorentz integral transform (w/ Sonia Bacca and Nir Barnea)	First results (monopole excitations)
Role of three-nucleon forces in medium-mass nuclei (w Sonia Bacca and Achim Schwenk)	**Hartree-Fock transformation with 3NF implemented**
Equation-of-motion techniques for computation of A ±1 nuclei from closed-shell nucleus A	Implemented: ^{17}F, ^{17}O

Project is reasonably well on track

Future plans (remainder of year 4 and for year 5)

1. Interface with DFT, and toward ab initio reactions
    1. Intrinsic ground-state densities (w/ CoM corrections)
    2. CC densities as microscopic input for optical potentials / *g*-folding methods
    3. Lorentz integral transform (proof of principle)

2. Role of three-nucleon forces in medium-mass nuclei

    → Ab initio computation of ^{48}Ca with 3NF as possible highlight

3. Toward ab-initio reactions
    1. Spectroscopic factors in j-coupled code
    2. Lorentz integral transform (applications)
4. Nuclear matter (PhD student Gustav Baardsen from UiO)