Towards nuclear reactions with coupled cluster theory

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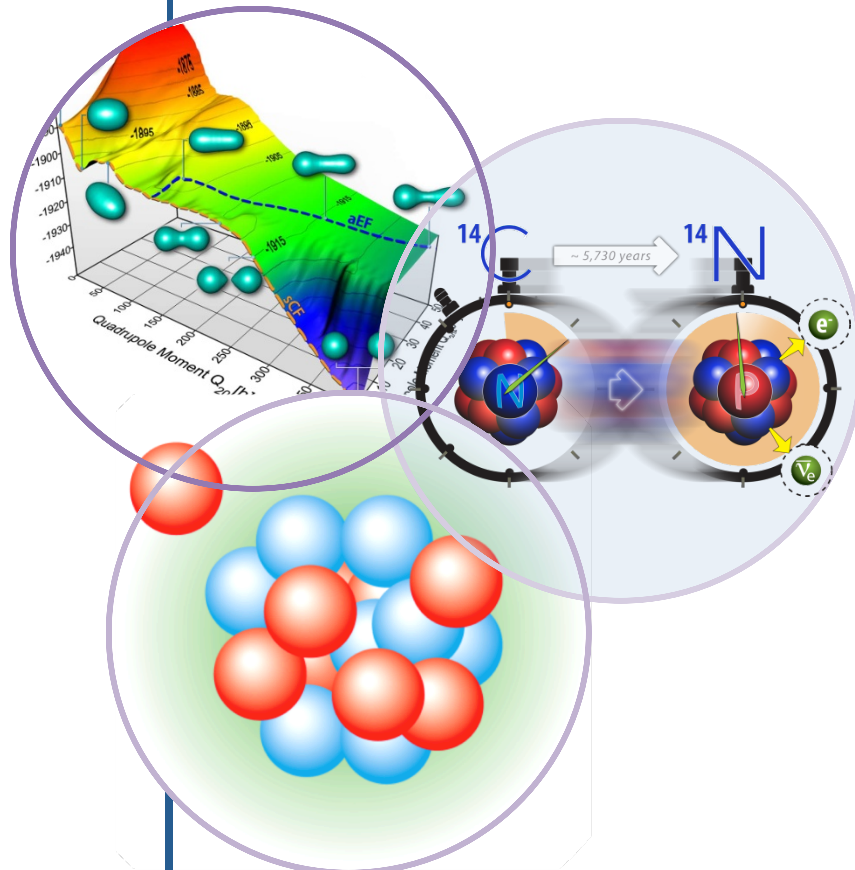
EMMI workshop
GSI, April 26, 2012



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Outline

Questions asked by the organizers:

- What do ab initio structure calculations say about dependence of SFs on Hamiltonians?
- How scale/scheme (or unitary transformation) dependent are long-range correlations?
- How can we investigate this question with ab initio calculations?
- Calculating N-nucleus optical potentials

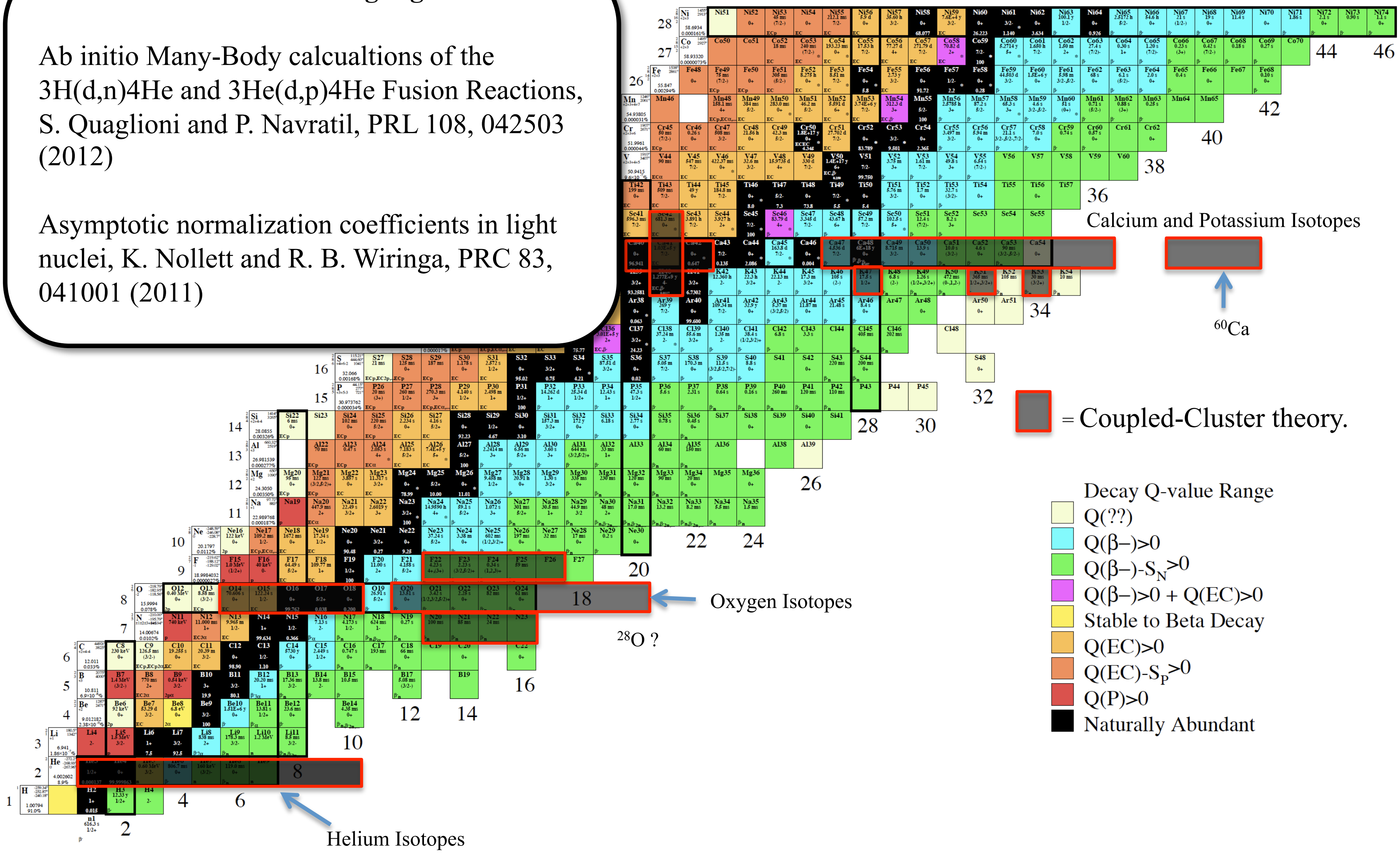
1. General motivation, interactions from chiral EFT and coupled-cluster theory
2. Open-quantum systems: how to describe physics at the edge of stability?
3. Spectroscopic factors from Coupled-Cluster theory: Continuum induced correlations in oxygen isotopes and scale dependence
4. One-nucleon overlap functions and proton elastic scattering
5. Intrinsic densities from coupled-cluster theory as input for reaction theories at the dripline: Resolving the anomalous cross section of ^{23}O.
6. Can ANCs be reliably extracted from intrinsic densities?
7. Coupled-cluster approach to loosely bound and unbound states: The proton halo in ^{17}F and scale dependence.
8. Lorentz Integral Transform from Coupled-Cluster

From light to medium mass neutron rich nuclei

Recent ab-initio reaction highlights:

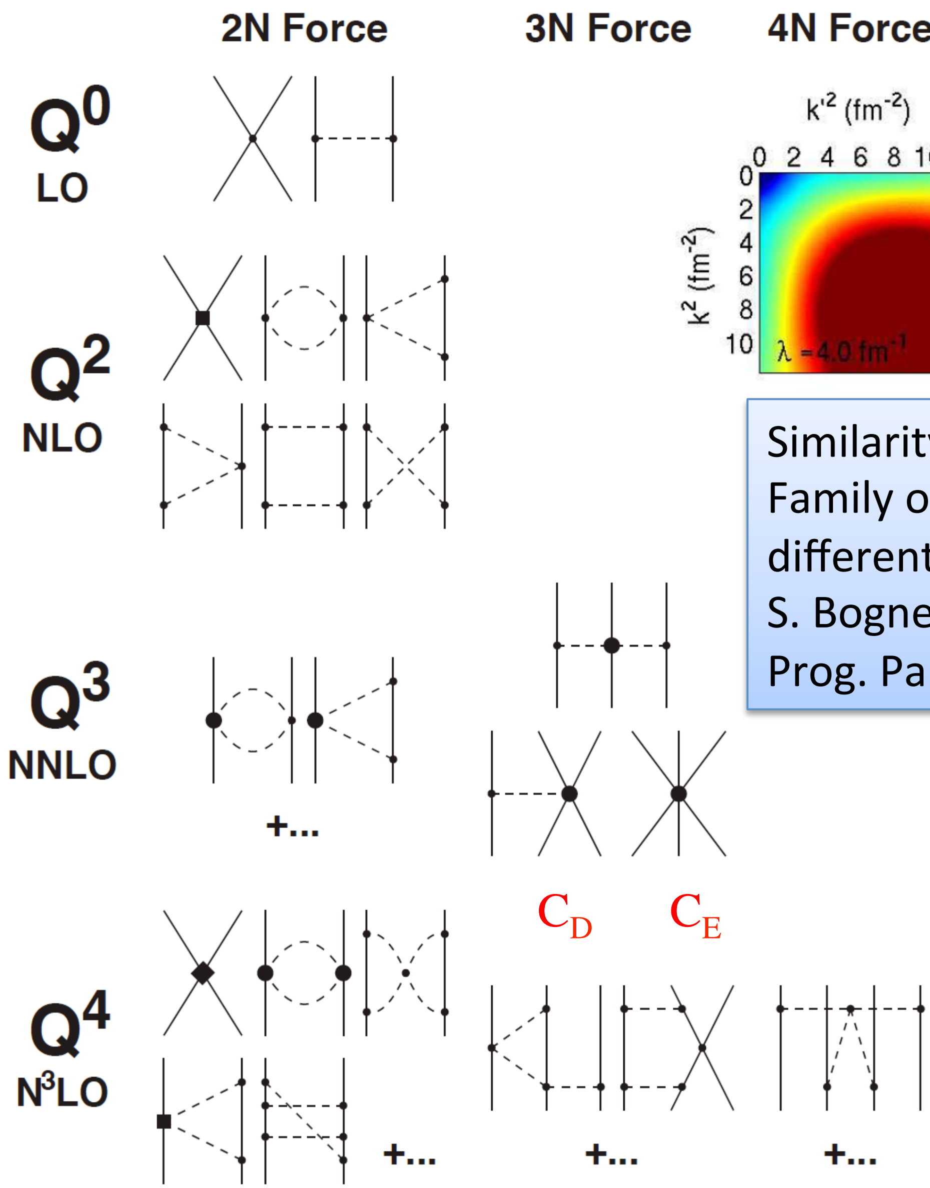
Ab initio Many-Body calcualtions of the 3H(d,n)4He and 3He(d,p)4He Fusion Reactions, S. Quaglioni and P. Navratil, PRL 108, 042503 (2012)

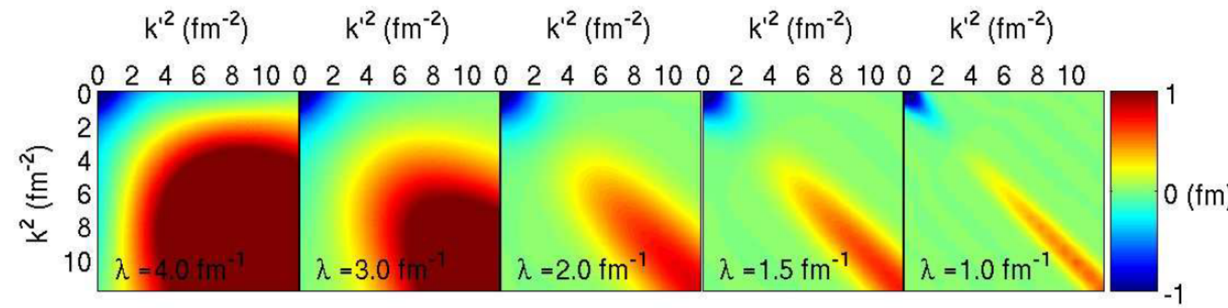
Asymptotic normalization coefficients in light nuclei, K. Nollett and R. B. Wiringa, PRC 83, 041001 (2011)



Nuclear forces from chiral effective field theory

[Weinberg; van Kolck; Epelbaum *et al*.; Entem & Machleidt; …]





Similarity renormalization group for nuclear forces:
Family of phase equivalent potentials at
different resolution scales
S. Bogner, R. J. Furnstahl and A. Schwenk
Prog. Part. Nucl. Phys. 65, 94 (2010)

Low energy constants from fit of NN data, A=3,4 nuclei, or light nuclei.

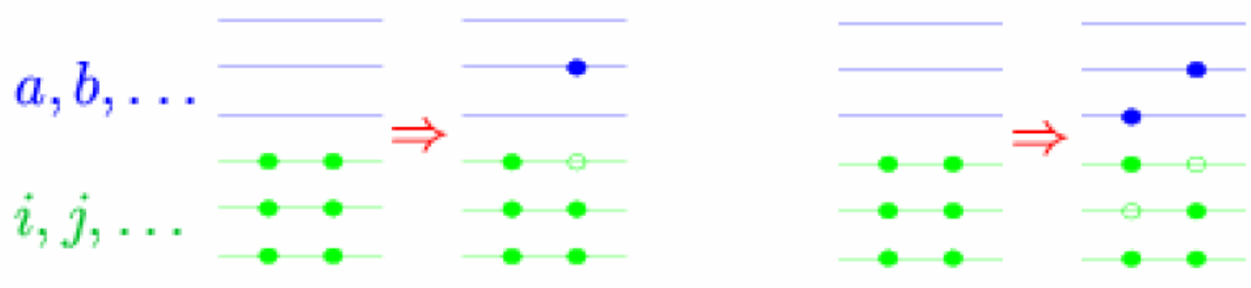
Coupled-cluster method (in CCSD approximation)

Ansatz:

$$
\begin{aligned}
|\Psi\rangle &= e^T|\Phi\rangle \\
T &= T_1 + T_2 + \ldots \\
T_1 &= \sum_{ia} t_i^a a_a^\dagger a_i \\
T_2 &= \sum_{ijab} t_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i
\end{aligned}
$$

- ☺ Scales gently (polynomial) with increasing problem size o^2u^4 .
- ☺ Truncation is the only approximation.
- ☺ Size extensive (error scales with A)
- ☹ Most efficient for doubly magic nuclei

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

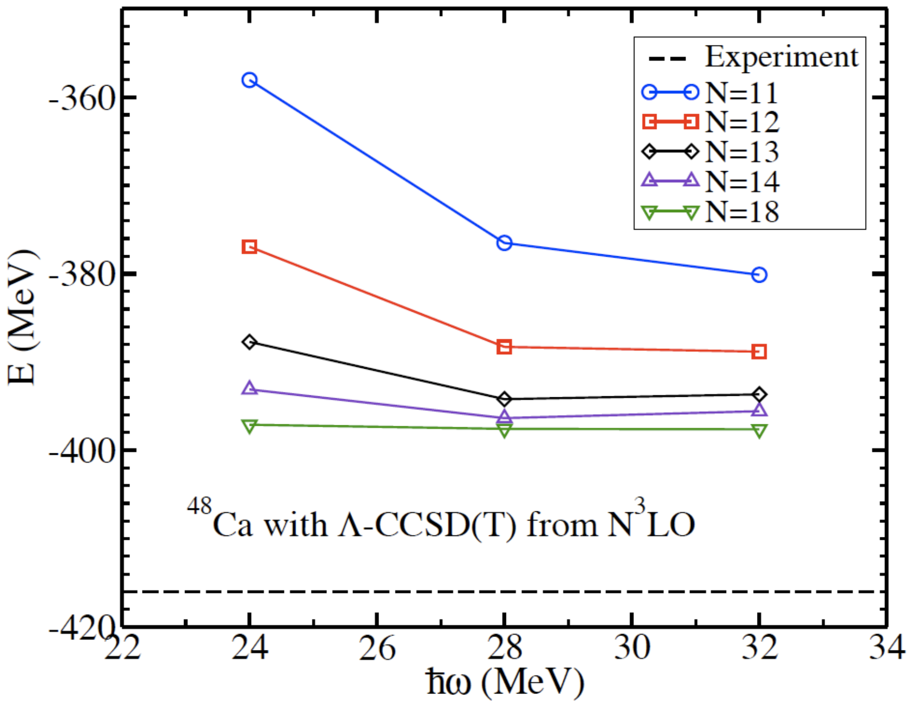


Coupled cluster equations

$$
\begin{aligned}
E &= \langle\Phi|\overline{H}|\Phi\rangle \\
0 &= \langle\Phi_i^a|\overline{H}|\Phi\rangle \\
0 &= \langle\Phi_{ij}^{ab}|\overline{H}|\Phi\rangle \\
\overline{H} &\equiv e^{-T}He^T = \left(He^T\right)_c = \left(H + HT_1 + HT_2 + \frac{1}{2}HT_1^2 + \ldots\right)_c
\end{aligned}
$$

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

Toward medium-mass nuclei
Chiral N^{3}LO (500 MeV) by Entem & Machleidt, NN only



Binding energy per nucleon

Nucleus	CCSD	Λ-CCSD(T)	Experiment
^{4}He	5.99	6.39	7.07
^{16}O	6.72	7.56	7.97
^{40}Ca	7.72	8.63	8.56
^{48}Ca	7.40	8.28	8.67

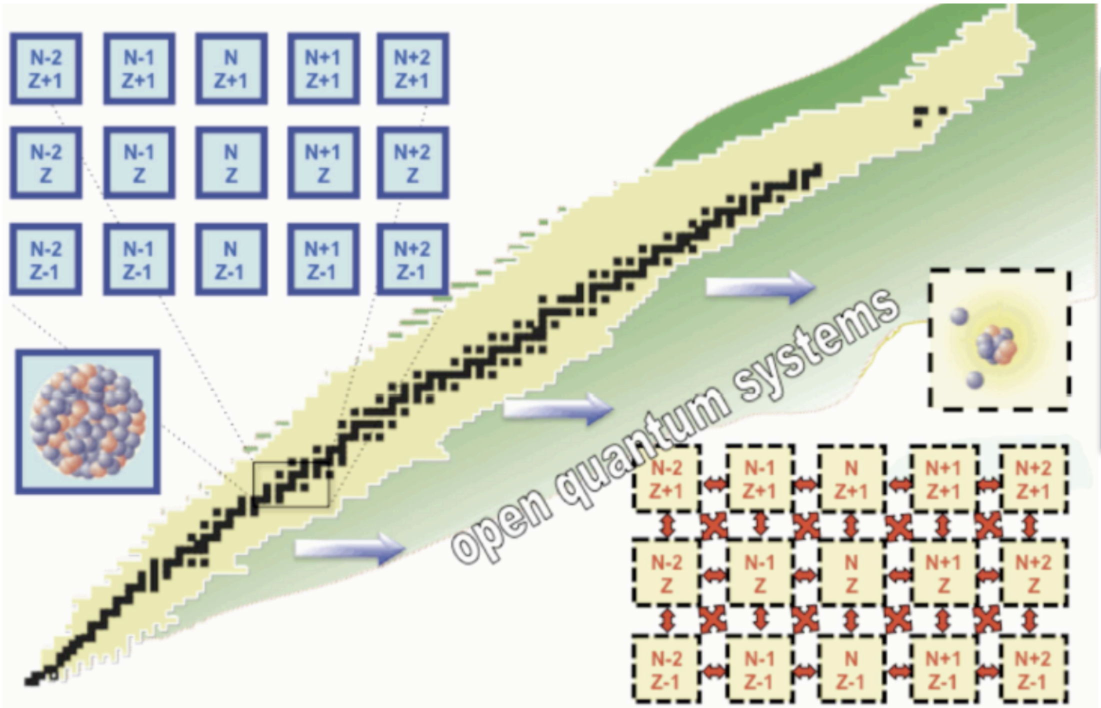
- Chiral NN forces yield saturation, lack about 0.4 MeV per nucleon in binding energy.
- Chiral three-nucleon forces expected to yield 0.4MeV per nucleon?!

Benchmarking different methods:
Our CC results for ^{16}O agree with IT-NCSM (R. Roth et al PRL 107, 072501 (2011)) and UMOA (Fujii et al., Phys. Rev. Lett. 103, 182501 (2009))

	CCM	(IT)-NCSM	UMOA
	E/A	E/A	E/A
^{4}He	-6.39(5)	-6.35	
^{16}O	-7.56(8)	-7.48(4)	-7.47

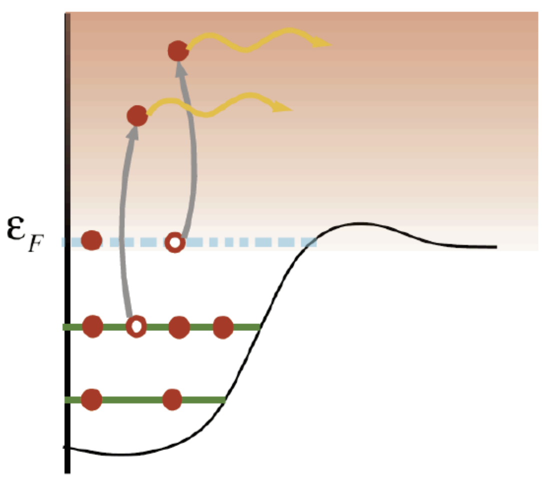
[Hagen, Papenbrock, Dean, Hjorth-Jensen, Phys. Rev. Lett. 101, 092502 (2008)]

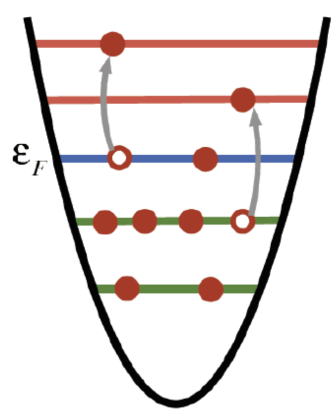
Open Quantum Systems

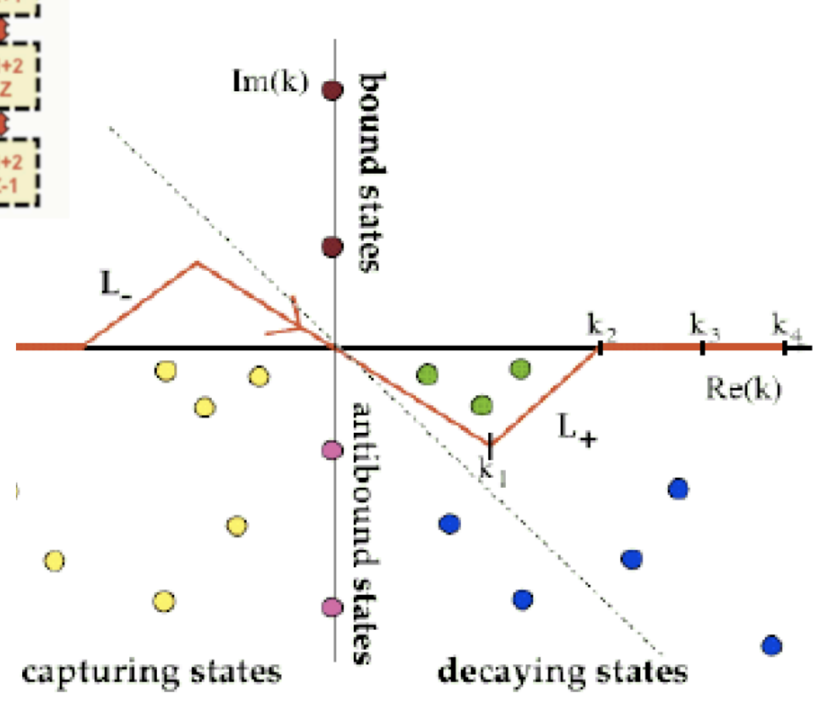


The Berggren completeness treats bound, resonant and scattering states on equal footing.

Has been successfully applied in the shell model in the complex energy plane to light nuclei. For a review see
N. Michel et al J. Phys. G 36, 013101 (2009).

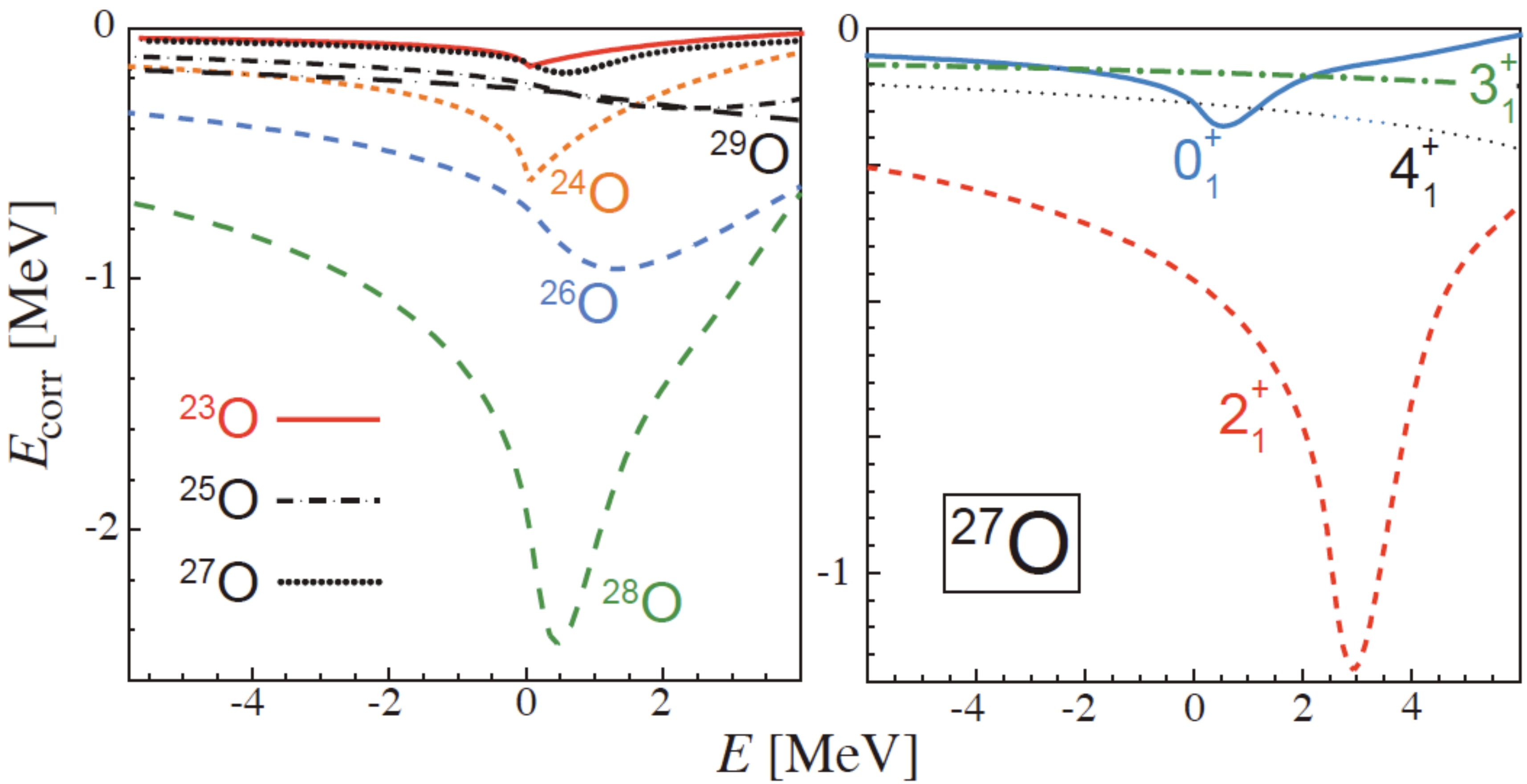






Continuum induced correlations

Continuum shell model calculations of oxygen isotopes. The effect of continuum correlations for nuclei with low neutron emission thresholds can be significant.
N. Michel et al, J. Phys. G **37** 064042 (2010).



Towards nuclear reactions with coupled-cluster theory

One-nucleon overlap functions

Elastic scattering, capture and transfer reactions of a nucleon on/to a target nucleus with mass A is determined by the one-nucleon overlap function

$$O_A^{A+1}(lj;r) = \langle A \| \tilde{a}_{lj}(r) \| A+1 \rangle = \sum_n \langle A \| \tilde{a}_{nlj} \| A+1 \rangle \, \phi_{nlj}(r)$$

Microscopic definition of Spectroscopic Factors

SF is the norm of the overlap function and quantifies the degree of correlations

SFs are not observables and depend on the resolution scale

$$SF = \int_0^\infty dr r^2 \, |O_A^{A+1}(lj;r)|^2$$

Asymptotic properties of the one-nucleon overlap functions

The overlap functions satisfy a one-body Schrodinger like equation, and outside the range of the interaction the overlap function is proportional to a single-particle wave function

$$O_A^{A+1}(lj;r) = C\frac{e^{-\kappa r}}{\kappa r}$$ Bound states

$$O_A^{A+1}(lj;r) = A\left(j_l(kr) - \tan\delta_l n_l(kr)\right)$$ Scattering states

Asymmetry dependence and spectroscopic factors

- Spectroscopic factors are not observables
- They are extracted from a cross section based on a specific structure and reaction model
- Structure and reaction models needs to be consistent!

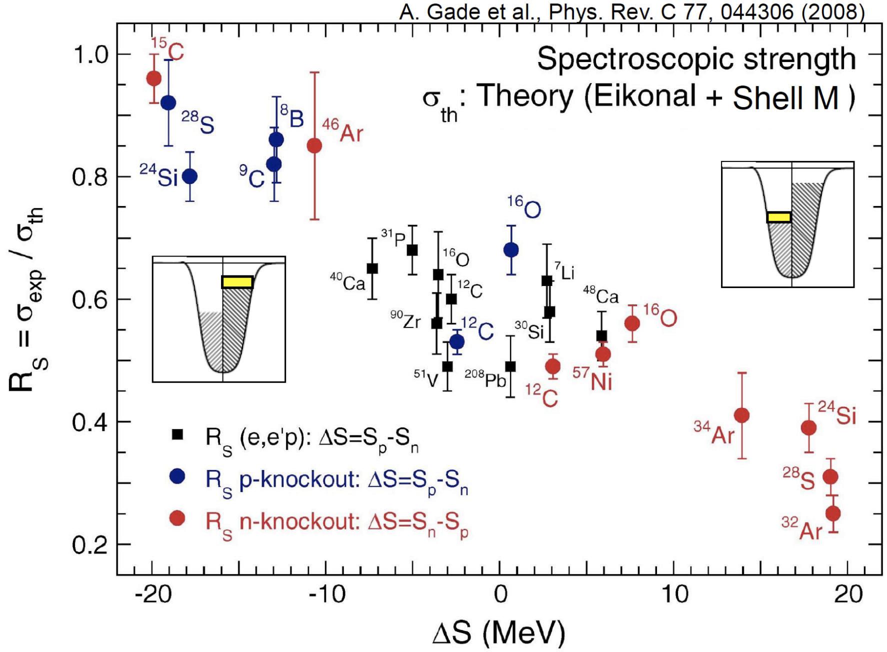
Theoretical cross section:

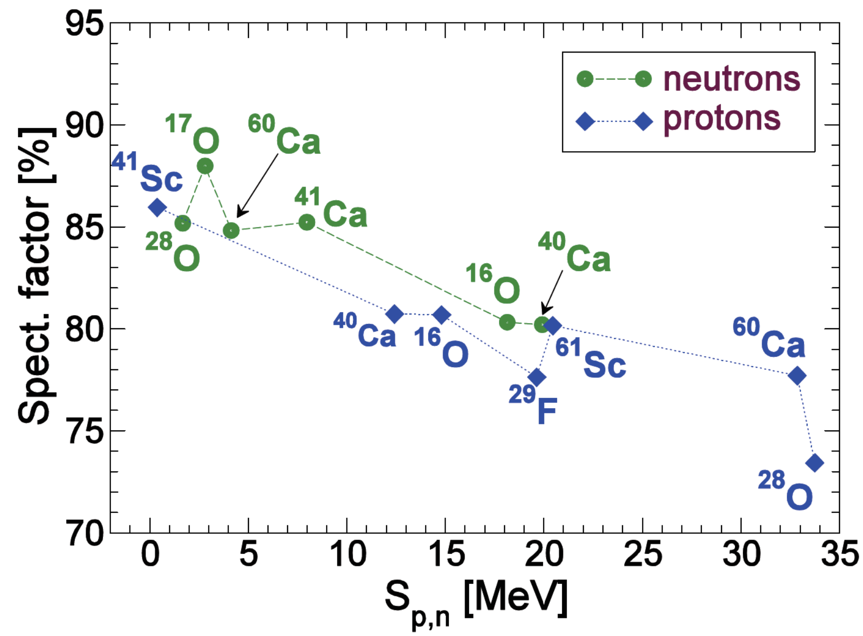
Reaction theory

$$\sigma(j^\pi) = \left(\frac{A}{A-1}\right)^N C^2 S(j^\pi)\sigma_{sp}(j, S_N + E_x[j^\pi])$$

Structure theory

A. Gade et al., Phys. Rev. C 77, 044306 (2008)

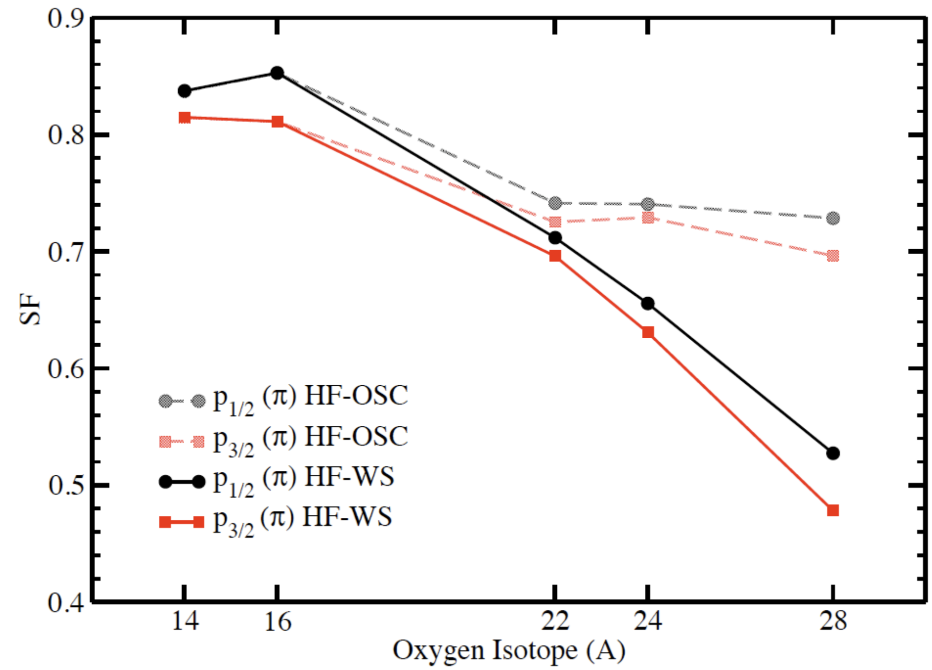




C. Barbieri, W.H.Dickhoff, Int. Jour. Mod. Phys. A24, 2060 (2009).

Self-consistent green's function method show rather weak asymmetry dependence for the spectroscopic factor.

Quenching of spectroscopic factors for proton removal in neutron rich oxygen isotopes

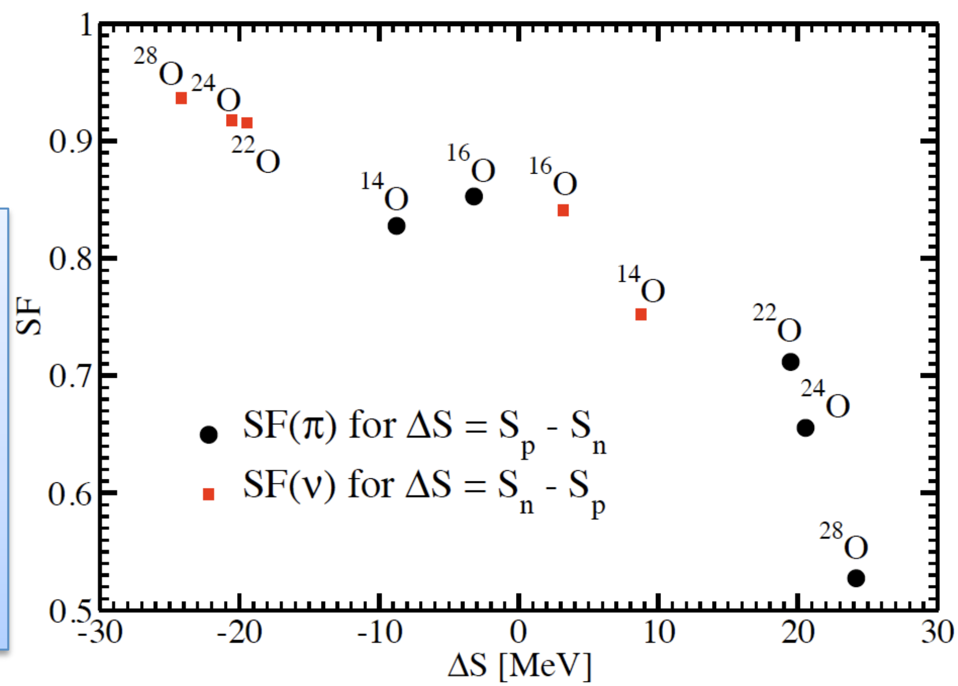


Spectroscopic factor is a useful tool to study correlations towards the dripline.

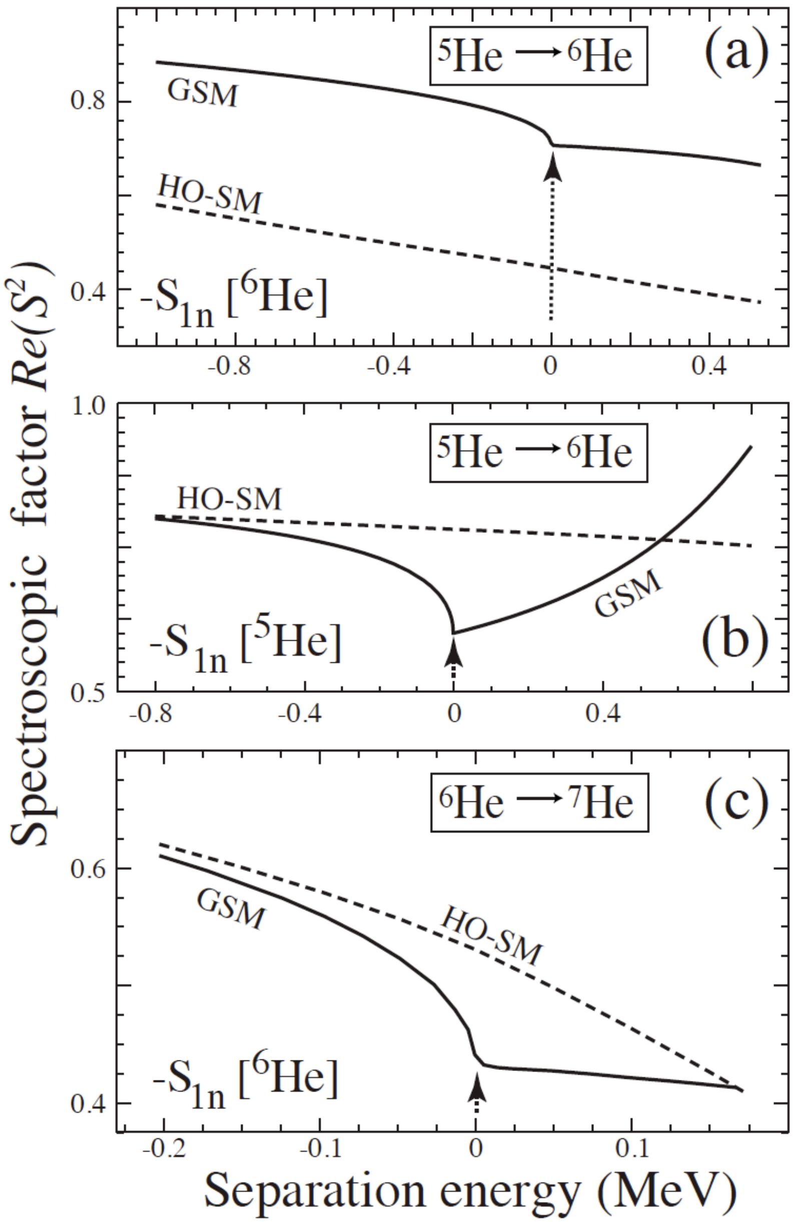
SF for proton removal in neutron rich ^{24}O show strong "quenching" pointing to large deviations from a mean-field like picture.
G. Hagen et al Phys. Rev. Lett. 107, 032501 (2011).

Strong asymmetry dependence on the SF for proton and neutron removal in neutron rich oxygen isotopes.

SF~1 for neutron removal while protons are strongly correlated SF ~0.6-0.7 in ^{22,24,28}O



Threshold effects and spectroscopic factors



Near the scattering threshold for one-neutron decay the spectroscopic factors are Significantly influenced by the presence of The continuum. The standard shell model

$$\langle \Psi_A^{J_A} || a_{n\ell j}^{+} || \Psi_{A-1}^{J_{A-1}} \rangle^2$$

approximation to spectroscopic factors completely fails in this region.

N. Michel et al Phys. Rev. C **75**, 031301 (2007)
N. Michel et al Nucl. Phys. A **794**, 29 (2007)

Top and middle:

$$\langle {}^6\mathrm{He(g.s.)} | [{}^5\mathrm{He(g.s.)} \otimes p_{3/2}]^{0^+} \rangle$$

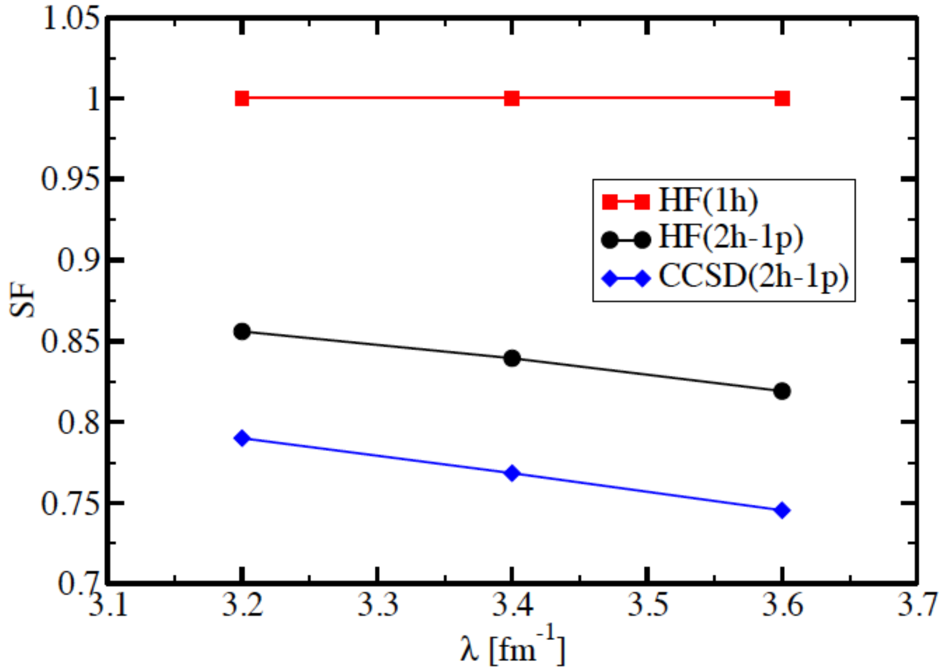
Bottom :

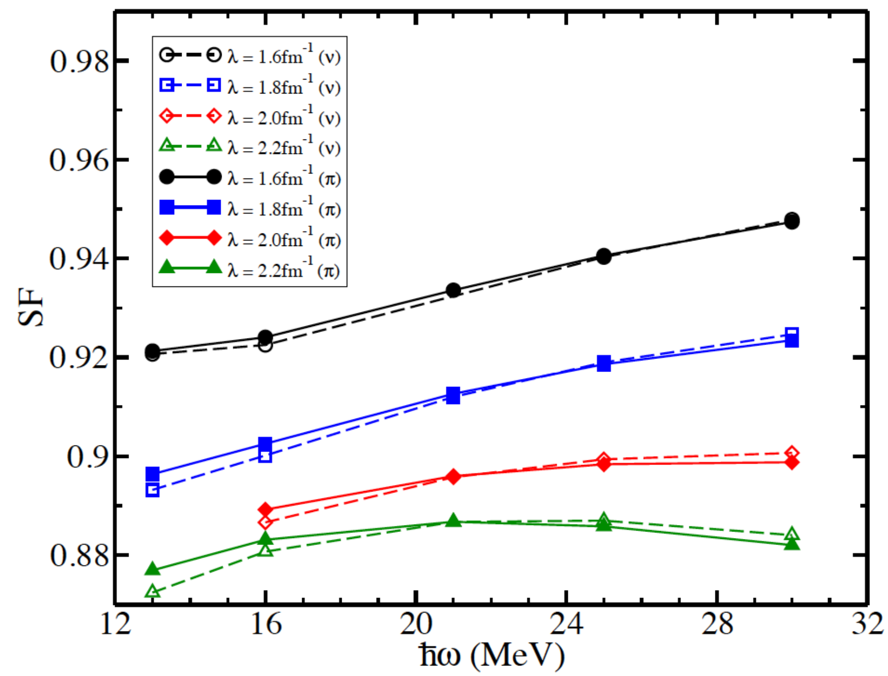
$$\langle {}^7\mathrm{He(g.s.)} | [{}^6\mathrm{He(g.s.)} \otimes p_{3/2}]^{0^+} \rangle$$

Scale and model dependence of spectroscopic factors

$$O^{A}_{A-1}(lj;r) = \sum_{n} \langle A-1 \,\|\, \tilde{a}_{nlj} \,\|\, A \rangle \, \phi_{nlj}(r)$$

$$S^{A}_{A-1}(lj) = \left| O^{A}_{A-1}(lj;r) \right|^{2}$$





Ø. Jensen, G. Hagen, T. Papenbrock, D. J. Dean, J. S. Vaagen, Phys. Rev. C 82, 014310 (2010)

SF for ½$^-$ proton removal in ^{24}O with “bare” chiral interaction (500MeV) = 0.65

<u>**Open problem:**</u>

How will the scale dependence of SFs change with inclusion of (induced) 3NF’s ?

Treatment of long-range Coulomb effects

We diagonalize the one-body shcrodinger equation in momentum space using the off-diagonal method described in **N. Michel Phys. Rev. C 83, 034325 (2011)**

$$h = \frac{\hat{p}^2}{2m} - V_o \left[1 + \exp\left(\frac{r - R_0}{d}\right)\right]^{-1} + U_{Coul}(r)$$

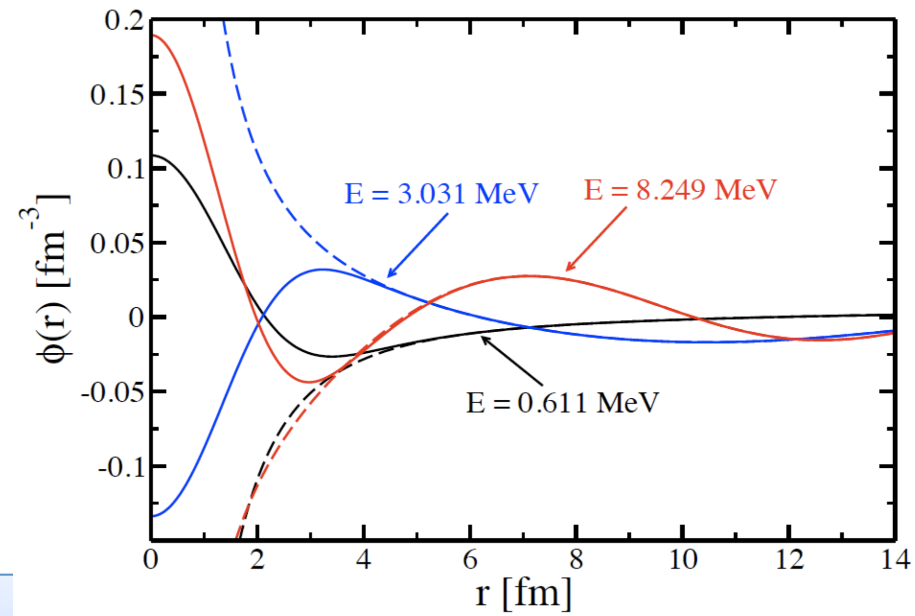
N_{GL}	E cut (MeV)	Γ cut (keV)	E sub (MeV)	Γ sub (keV)	E off-diag (MeV)	Γ off-diag (keV)
15	0.461875	-11.6596	0.464574	9.19011	0.46396	10.2211
30	0.465707	13.4833	0.463777	8.26812	0.463343	8.97219
45	0.463476	8.71097	0.463709	8.33267	0.463334	8.96171
60	0.463307	8.68396	0.463681	8.36454	0.463329	8.96458
75	0.463227	8.70558	0.463667	8.38006	0.463328	8.96595
90	0.46284	8.88896	0.463659	8.3888	0.463327	8.96669
105	0.462952	8.69106	0.463654	8.39421	0.463326	8.96712
120	0.462949	8.62468	0.46365	8.3978	0.463326	8.9674
exact	0.463324	8.96828	0.463324	8.96828	0.463324	8.96828

The many-nucleon Hamiltonian is

$$H = \hat{T} - \hat{T}_{\mathrm{cm}} + \hat{V}_{\mathrm{NN}} + V_{Coul}$$

We write the Coulomb interaction as a sum of two terms:

$$V_{Coul} = U_{Coul}(r) + [V_{Coul} - U_{Coul}(r)]$$



The second term is short range and can be Expanded in Harmonic Oscillator basis. The first term contain the long range Coulomb part.

Elastic proton/neutron scattering on 40Ca

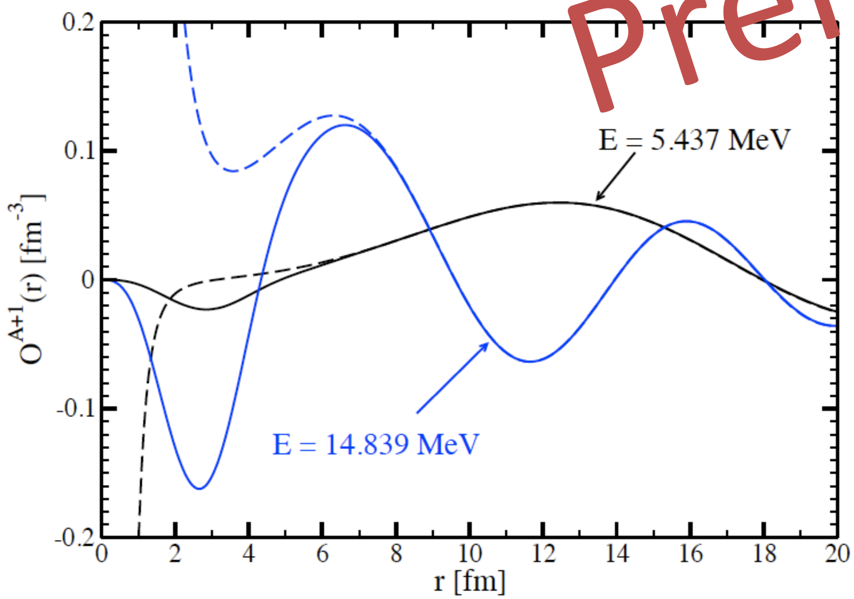
The one-nucleon overlap function: $$O_A^{A+1}(lj;kr) = \sum_n \left\langle A+1 \left\| \tilde{a}^\dagger_{nlj} \right\| A \right\rangle \phi_{nlj}(r).$$

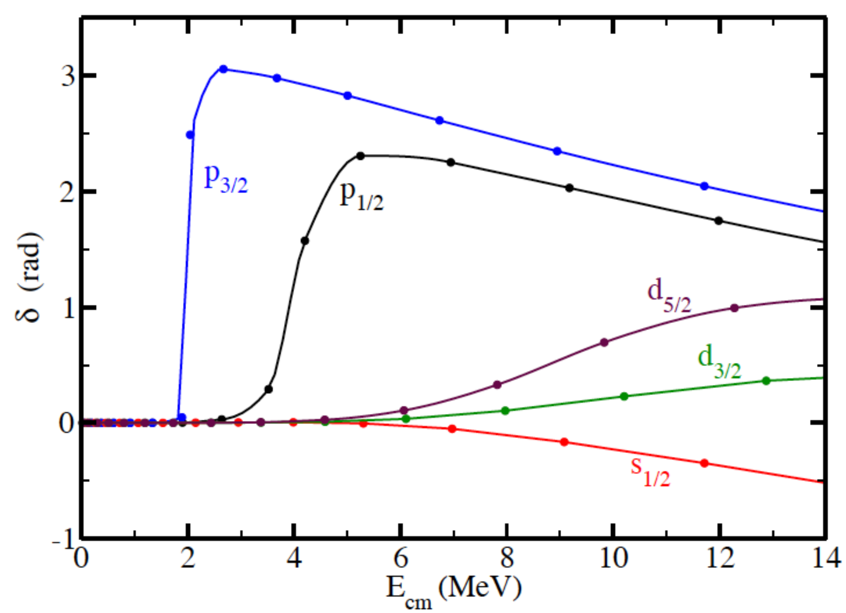
Beyond the range of the nuclear interaction the overlap functions take the form:

$$O_A^{A+1}(lj;kr) = C_{lj}\frac{W_{-\eta,l+1/2}(kr)}{r}, \quad k = i\kappa$$
$$O_A^{A+1}(lj;kr) = C_{lj}\left[F_{\ell,\eta}(kr) - \tan\delta_l(k) G_{\ell,\eta}(kr)\right]$$

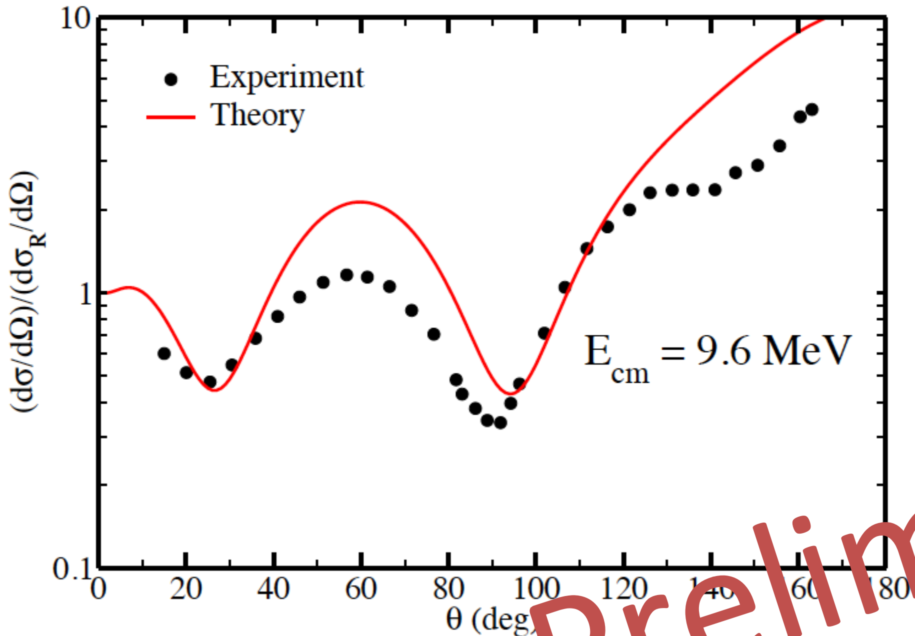
G. Hagen and N. Michel, in preparation (2012).

Preliminary



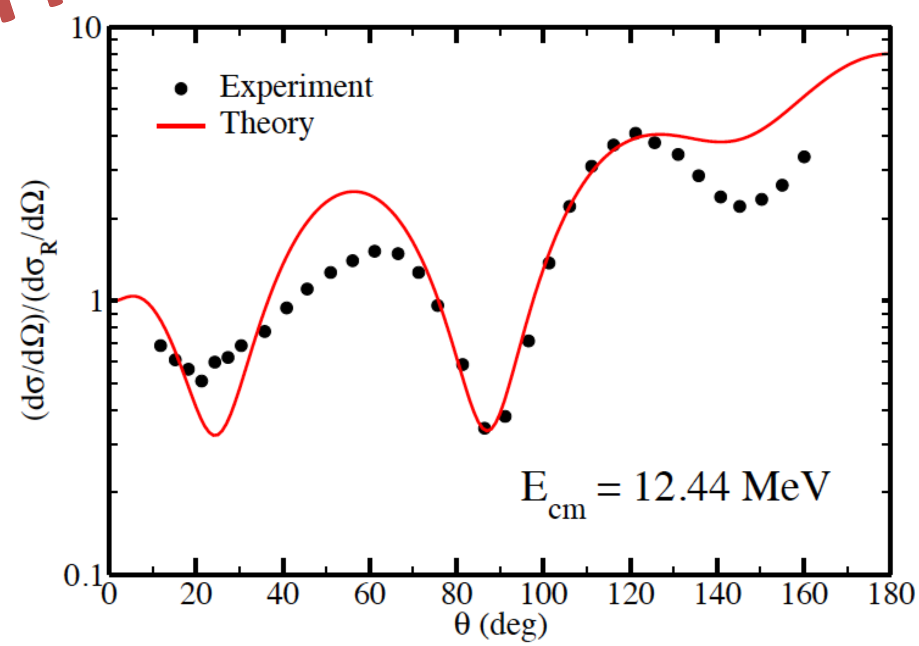


Elastic proton/neutron scattering on 40Ca



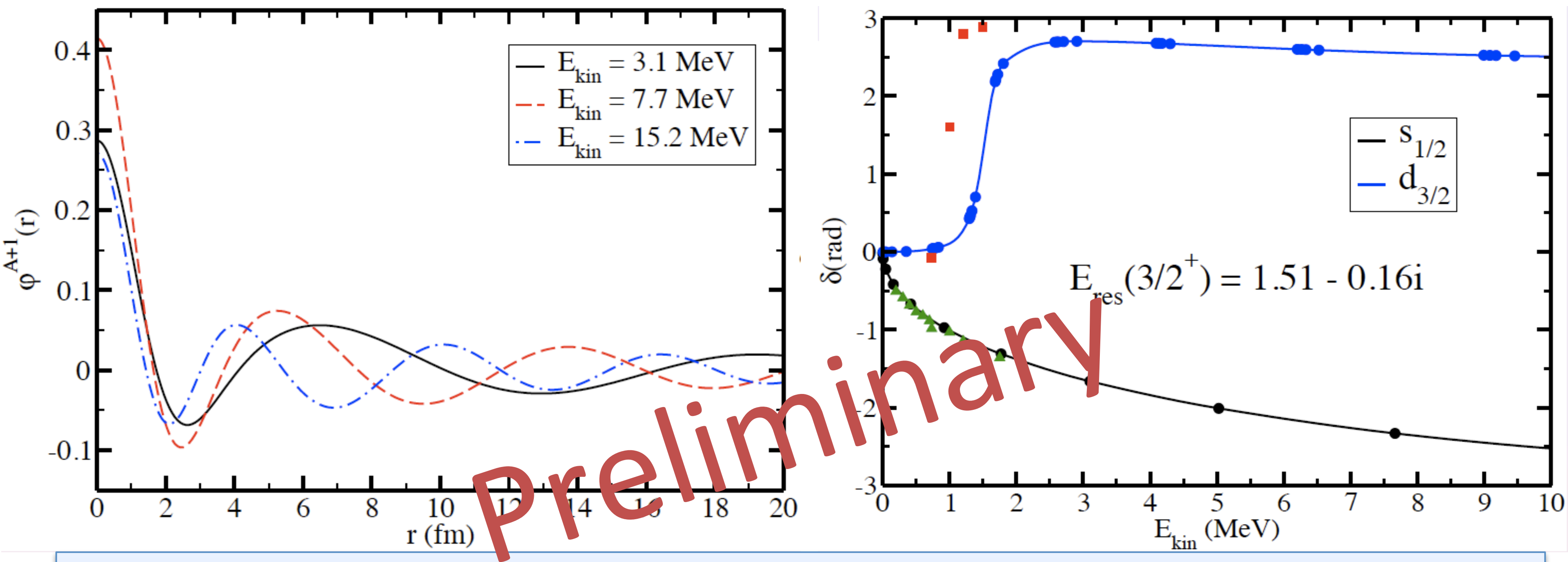
Differential cross section for elastic proton scattering on ^{40}Ca.

Good agreement between theory and Experiment for low-energy scattering.



G. Hagen and N. Michel
In Preparation (2012).

Elastic scattering phase shifts for neutrons on ^{16}O with coupled-cluster theory



<u>Overlap functions provides a simple and intuitive picture of reactions</u>

Left figure: One neutron overlap functions for various J = 1/2+ scattering states in ^{17}O using SRG evolved interaction with cutoff $\lambda = 2.66\ fm^{-1}$

Right figure: By matching the known asymptotic form of the overlap functions to scattering solutions we can extract low-energy elastic scattering phase shifts.

Densities and radii from coupled-cluster theory

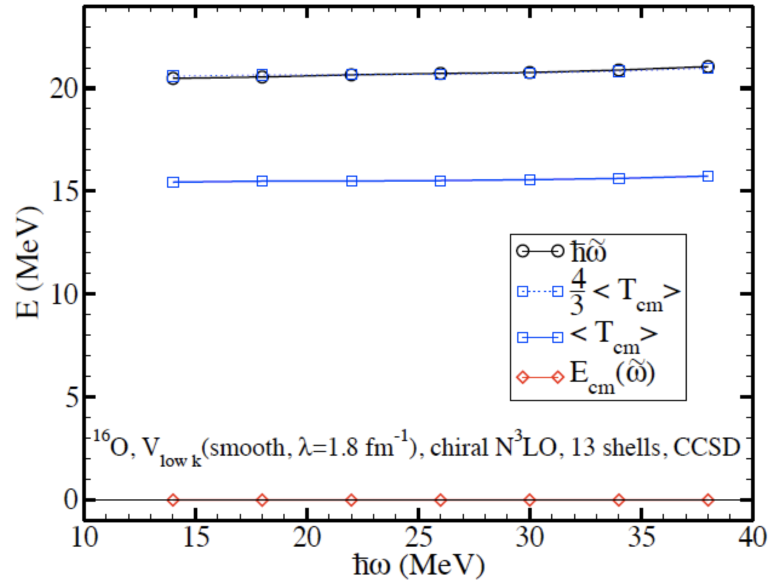
We solve for the right and left ground state of the similarity transformed Hamiltonian

$$e^{-T} H_N e^{T} |\phi_0\rangle = \overline{H_N} |\phi_0\rangle = E_{CC} |\phi_0\rangle \qquad \langle\phi_0| L_0 \overline{H_N} = E_{CC} \langle\phi_0| L_0$$

The density matrix is computed within coupled-cluster method as:

$$\rho_{pq} = \langle\Psi_0| a_p^\dagger a_q |\Psi_0\rangle = \langle\phi_0| L e^{-T} a_p^\dagger a_q e^{T} |\phi_0\rangle = \langle\phi_0| L \overline{a_p^\dagger a_q} |\phi_0\rangle$$

The coupled-cluster wave function factorizes to a good approximation into an intrinsic and center of mass part, $\Psi = \psi_{in}\Gamma$
where the center of mass part is a Gaussian with a fixed oscillator frequency independent of single-particle basis
GH, T. Papenbrock and D. Dean et al, Phys. Rev. Lett. **103**, 062503 (2009)

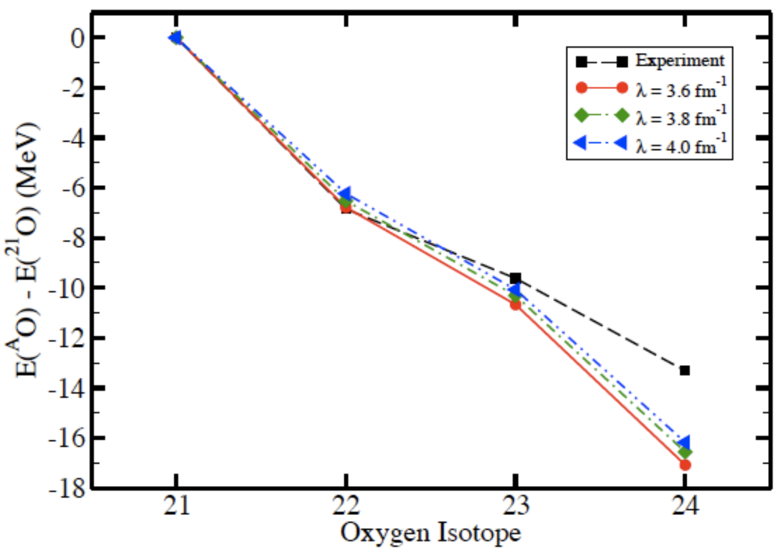


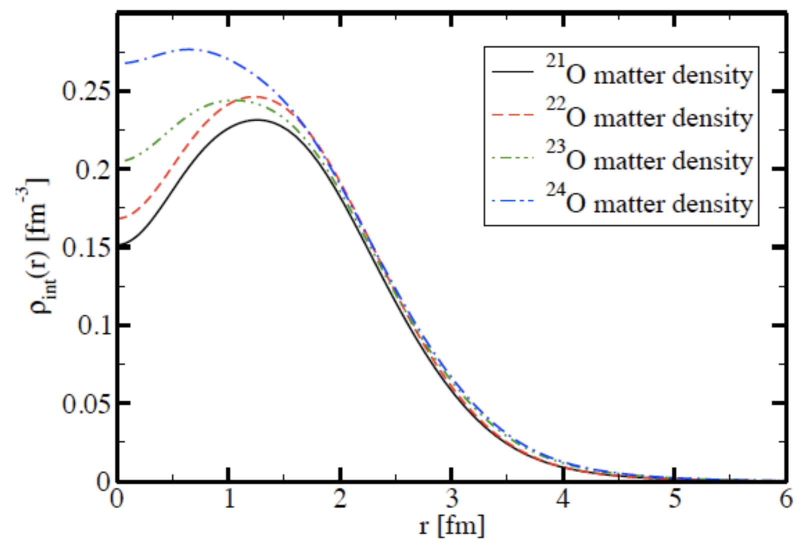
We can obtain the intrinsic density by a deconvolution of the laboratory density
B. G. Giraud, Phys. Rev. C **77**, 014311 (2008)

$$A^{-1}\rho(r) = A^{-1}\int dR\, [\Gamma(R)]^2\, \sigma\left[\frac{A}{A-1}(r-R)\right]$$

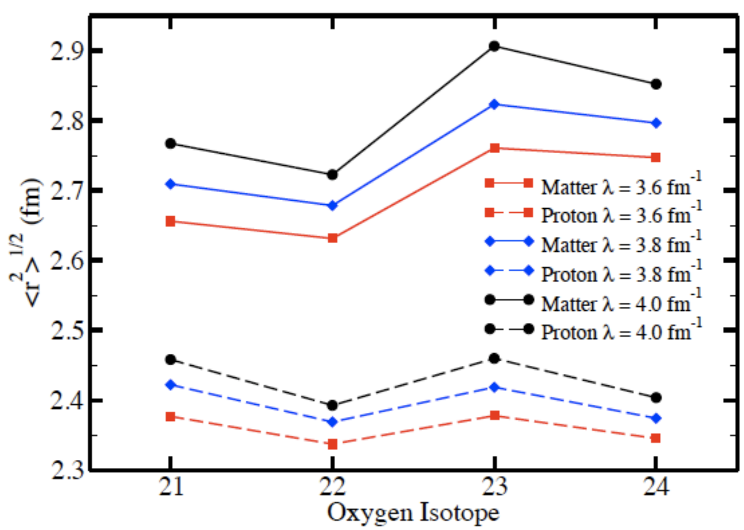
Lab. density   Center of mass part   Intrinsic density

Densities and radii from coupled-cluster theory

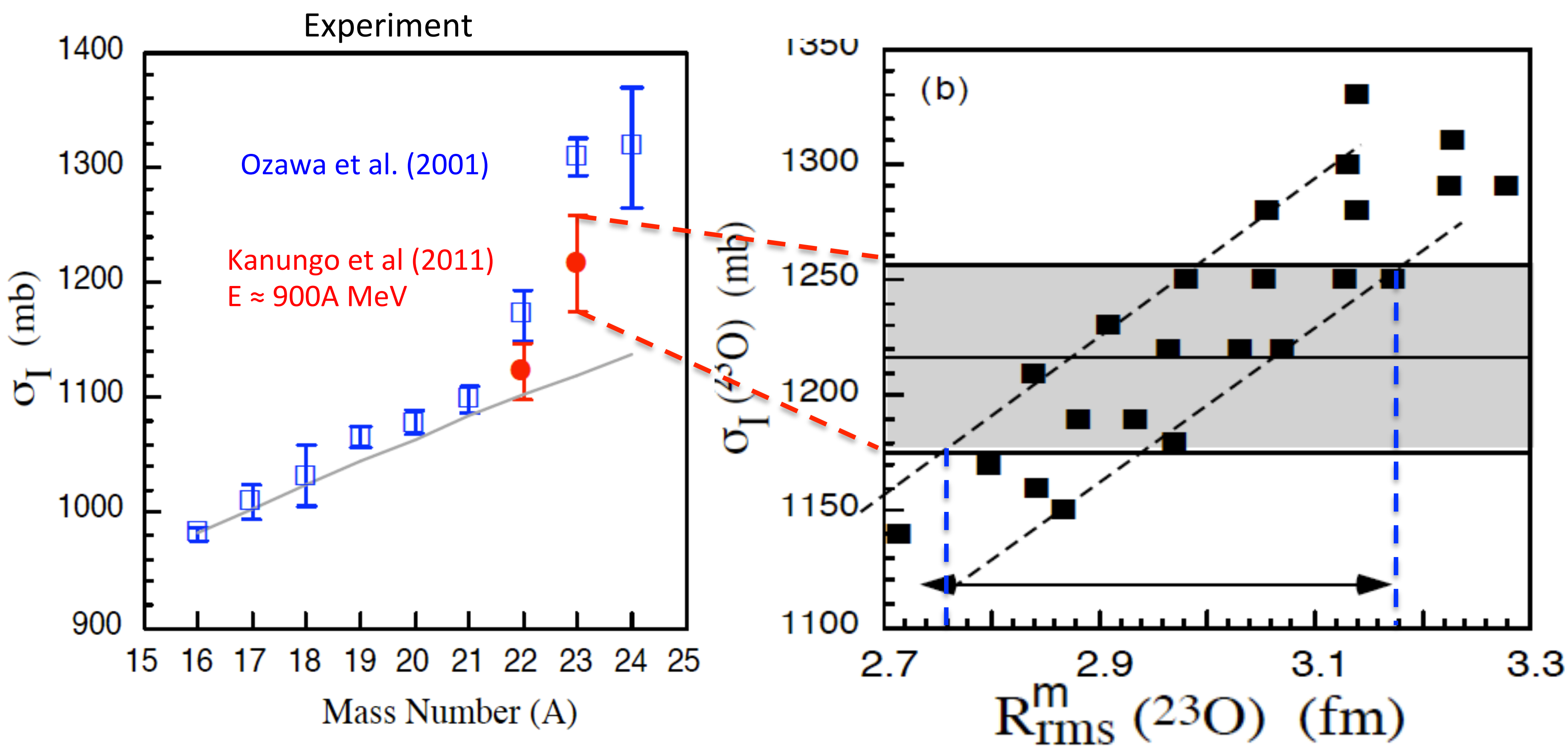




1. Relative energies in $^{21\text{-}24}$O depend weakly on the resolution scale
2. We clearly see shell structure appearing in the matter densities for $^{21\text{-}24}$O
3. Matter and charge radii depend on the resolution scale, however relative difference which is relevant for isotope shift measurements does not

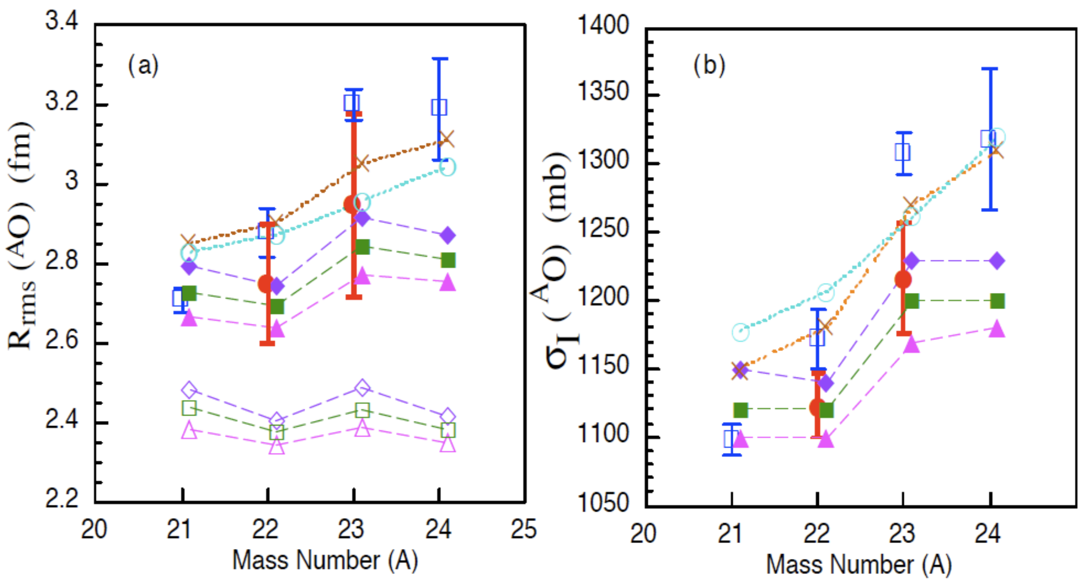


^{23}O interaction cross section (scattering off ^{12}C target @ GSI)



Experimental radii extracted from matter distribution within Glauber model.
Main result of new measurement: ^{23}O follows systematics; interaction cross section consistent with separation energies.
R. Kanungo *et al* Phys. Rev. C **84**, 061304 (2011)

Resolving the anomaly in the cross section of ^{23}O



<u>The anamoly of ^{23}O</u>

New measurements (R. Kanungo) of the ^{23}O cross section and coupled cluster calculations show that ^{23}O is not consistent with a one-neutron halo picture

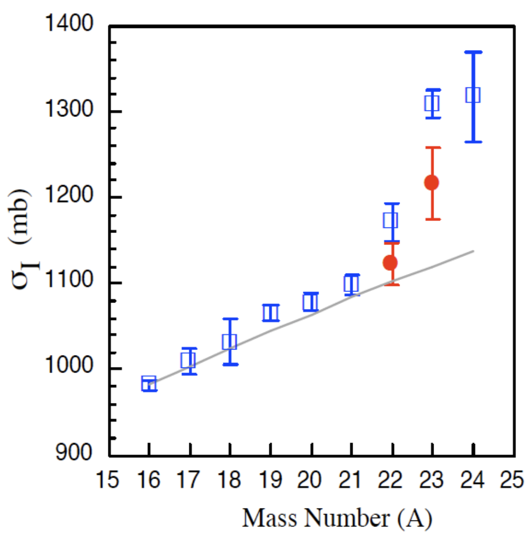


TABLE I: Measured interaction cross sections and the root mean square point matter radii (R^m_{rms}(ex.)) for $^{22-23}O$.

Isotope	$\sigma_I(\Delta\sigma)$ (mb)	$\Delta\sigma$(Stat.) (mb)	$\Delta\sigma$(Syst.) (mb)	R^m_{rms} (ex.) (fm)
^{22}O	1123(24)	18.5	15.3	2.75± 0.15
^{23}O	1216(41)	33.1	24.7	2.95± 0.23

ANC's from microscopic densities

Physics Letters B 314 (1993) 255–259
North-Holland

PHYSICS LETTERS B

On the relationship between single-particle overlap functions, natural orbitals and the one-body density matrix for many-fermion systems

D. Van Neck [1], M. Waroquier [2]
Institute for Nuclear Theory, University of Washington, Seattle, WA 98195, USA and Institute for Nuclear Physics, Proeftuinstraat 86, B-9000 Gent, Belgium

and

K. Heyde
Institute for Theoretical Physics, Proeftuinstraat 86, B-9000 Gent, Belgium

5. Conclusion

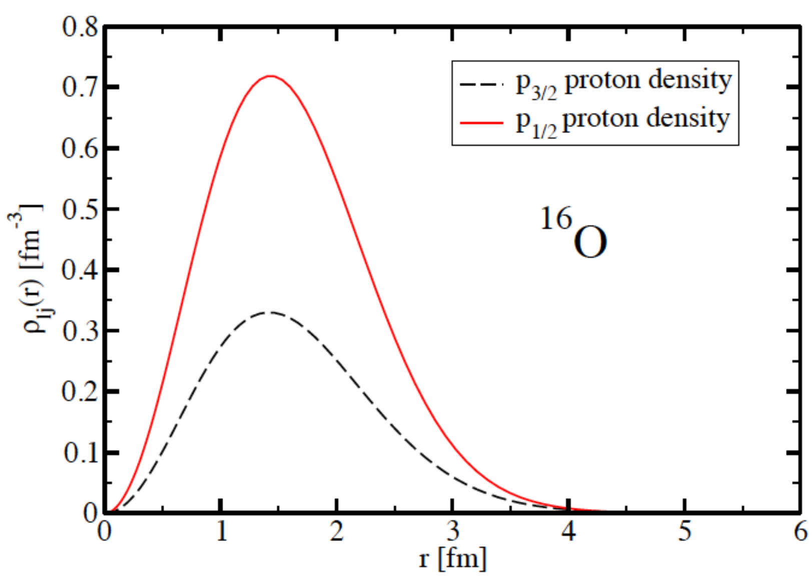
We have shown that, in principle, the overlap functions, spectroscopic factors and separation energies of the bound eigenstates of the $(A-1)$-particle system can be constructed by means of the exact OBDM of the groundstate of the A-particle system.

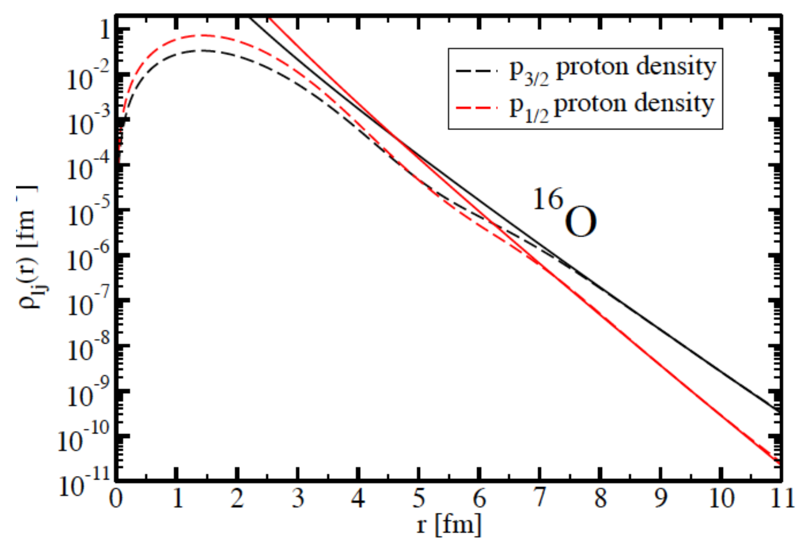
It is rather surprising that the latter quantity contains much of the dynamics in the $(A-1)$ system. The practical applicability is severely limited, however, by the need of a reliable calculation of the full OBDM (diagonal as well as off-diagonal elements) in coordinate space, at large radial distances. This

ANC's from microscopic densities

The density matrix can be written in terms overlap functions between nucleus A and it's a A-1 neighbour

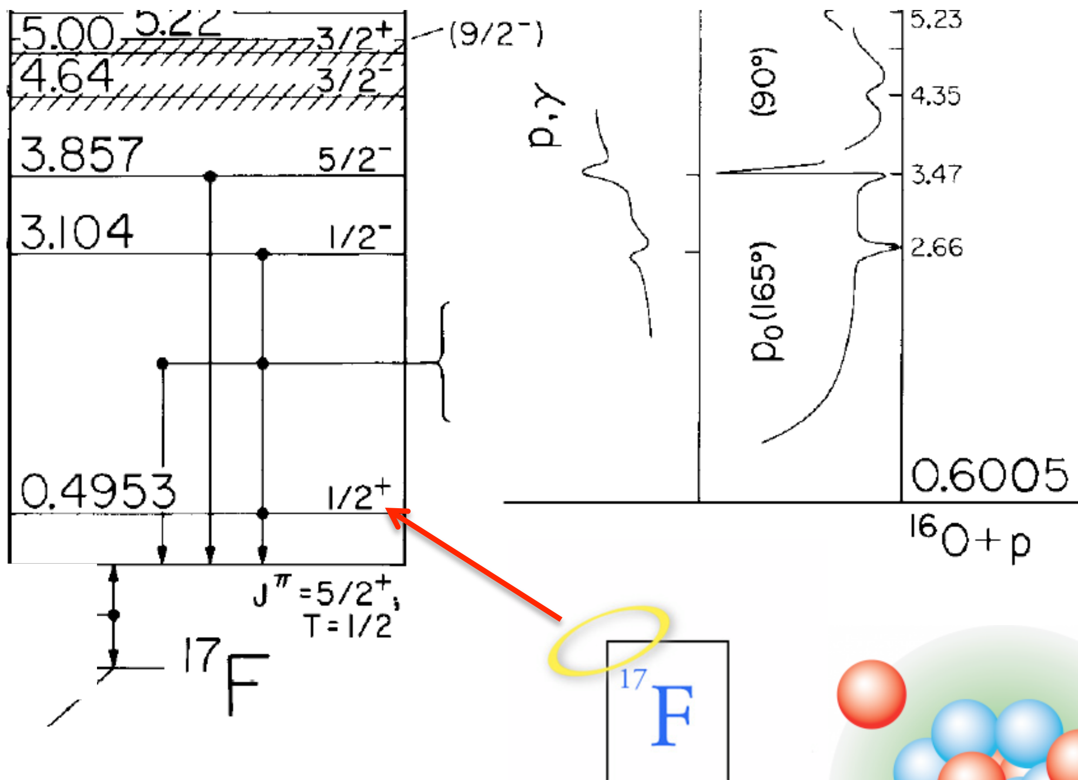
$$\rho^A_{lj}(r) = \sum_\mu \langle A|a_{lj}(r)|A-1\rangle_{\mu\mu}\langle A-1|a^\dagger_{lj}(r)|A\rangle, \quad \rho^A_{lj}(r) \rightarrow |C_{lj}|^2 \frac{e^{-2\kappa_0 r}}{r^2}$$

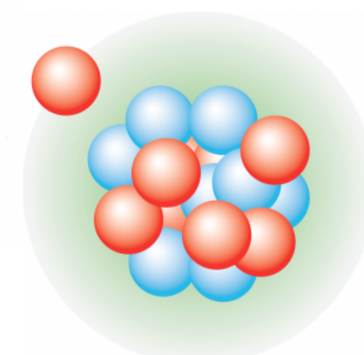




J^π	$E_{CC}(MeV)$	$E_{\rm exp}$ (MeV)	$\|C\|^2_{CC}$ (fm^{-1})	$\|C\|^2_{\rm exp}$ (fm^{-1})
$1/2^-$	17.99	12.13	621.66	529 ($\pm$9)
$3/2^-$	26.60	18.45	4301.17	?

Ab initio description of proton-halo state in ^{17}F

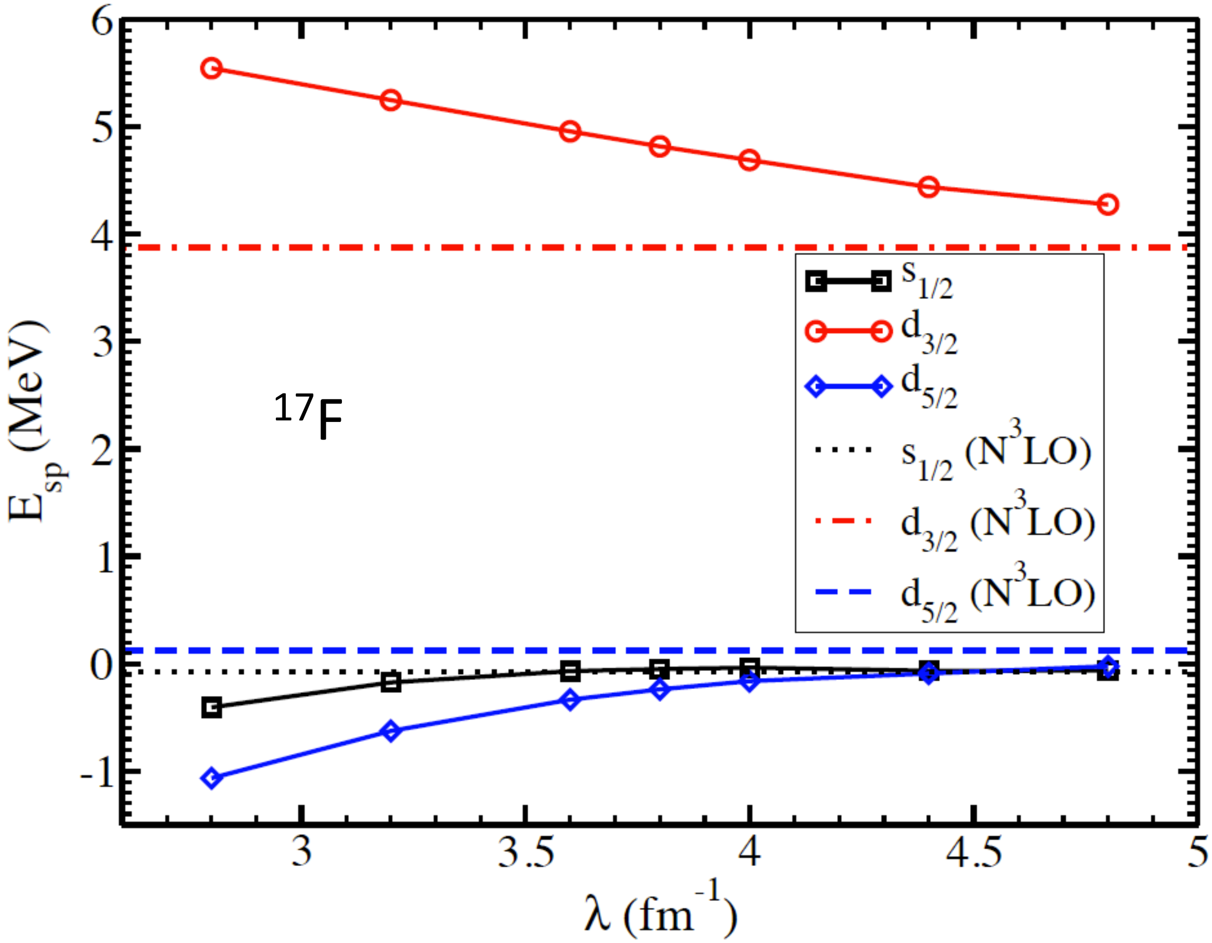




- Separation energy of halo state is only 105 keV
- Continuum has to be treated properly
- Focus is on single-particle states
- Previous study: shell model in the continuum with ^{16}O core

[K. Bennaceur, N. Michel, F. Nowacki, J. Okolowicz, M. Ploszajczak, Phys. Lett. B 488, 75 (2000)]

Variation of cutoff probes omitted short-range forces



- Proton-halo state ($s_{1/2}$) only weakly sensitive to variation of cutoff
- Spin-orbit splitting increases with decreasing cutoff

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

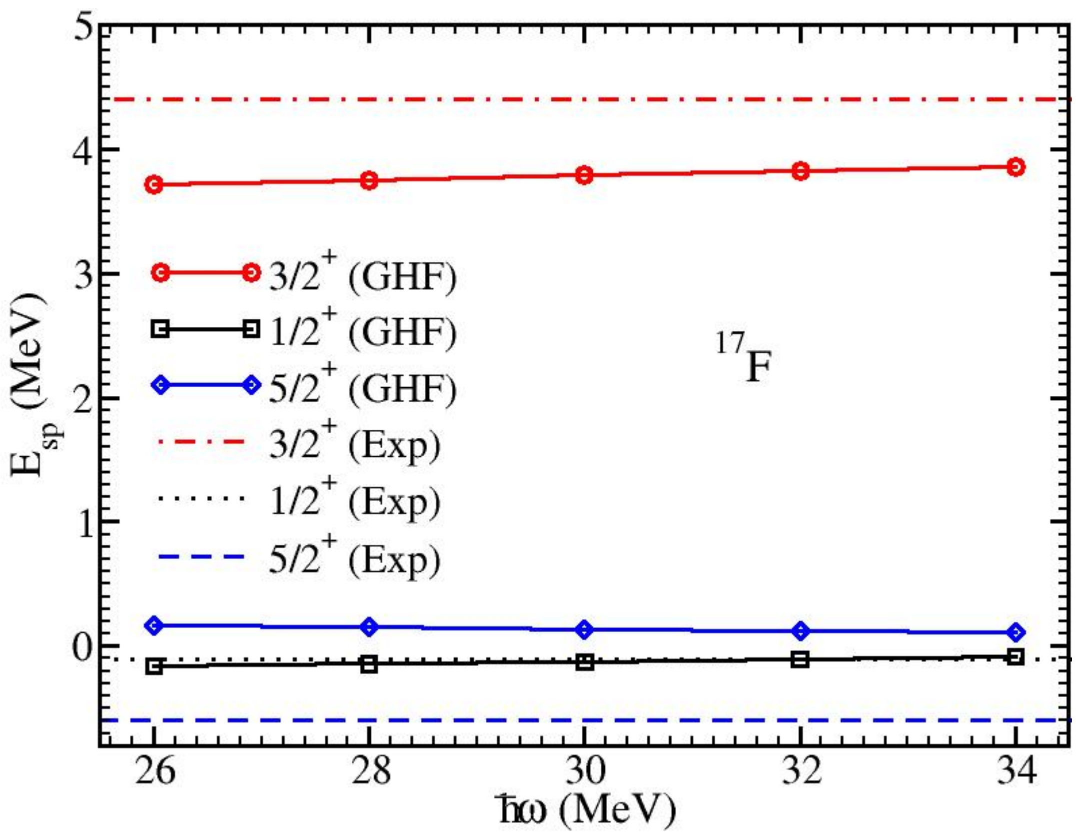
Bound states and resonances in ^{17}F

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"

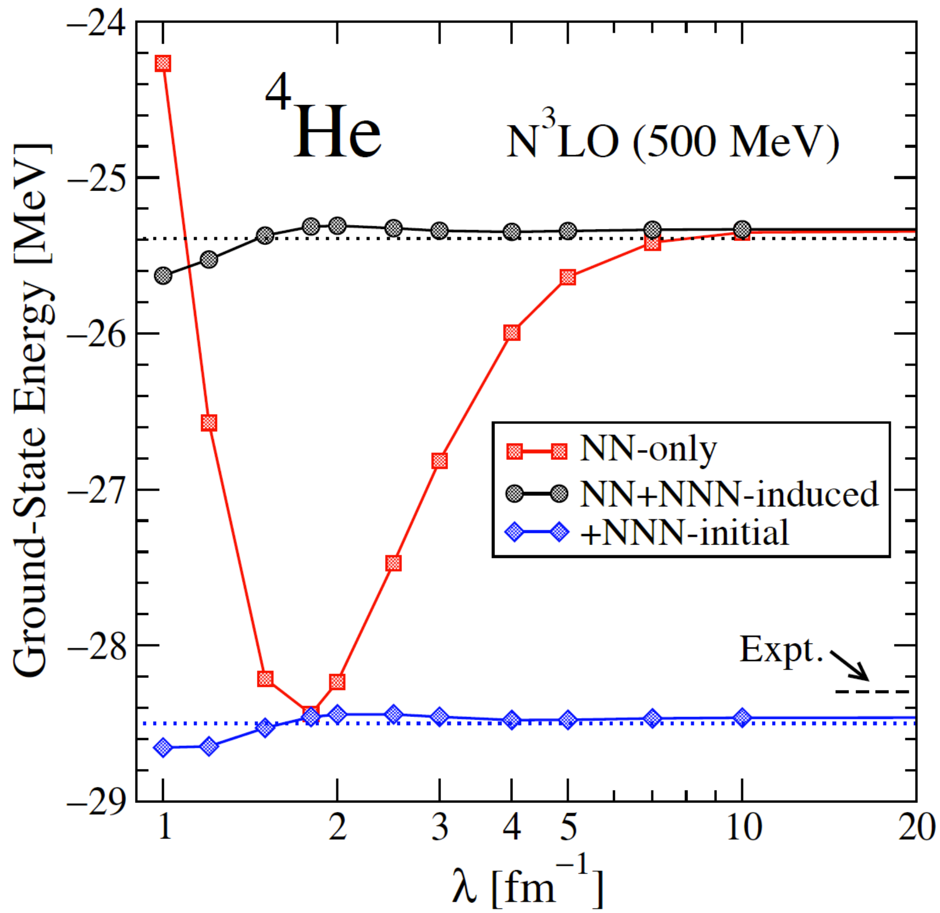
- Excitation operator acting on closed-shell reference
- Here: superposition of one-particle and 2p-1h excitations



- Gamow basis weakly dependent on oscillator frequency
- $d_{5/2}$ not bound; spin-orbit splitting too small
- $s_{1/2}$ proton halo state close to experiment

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

Size of three-nucleon forces from variation of high-momentum (renormalization group)



Similarity RG transformation [S.K. Bogner, R.J. Furnstahl, R.J. Perry, PRC 75, 061001(2007); Hergert & Roth 2007; Wegner 1994; Glazek & Wilson 1994]

- RG transformation of NN force induces NNN
- RG of NN and NNN almost independent of cutoff
- Small cutoff dependence → NNNN forces small

[Jurgenson, Navratil & Furnstahl, Phys. Rev. Lett. 103, 082501 (2009)]

Cutoff-dependence implies missing physics from short-ranged many-body forces.

Coupled-Cluster Lorentz integral transform

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

$$R(\omega) = \sum_f |\langle \Psi_f | \hat{\Theta} | \Psi_0 \rangle|^2 \delta(E_f - E_0 - \omega)$$

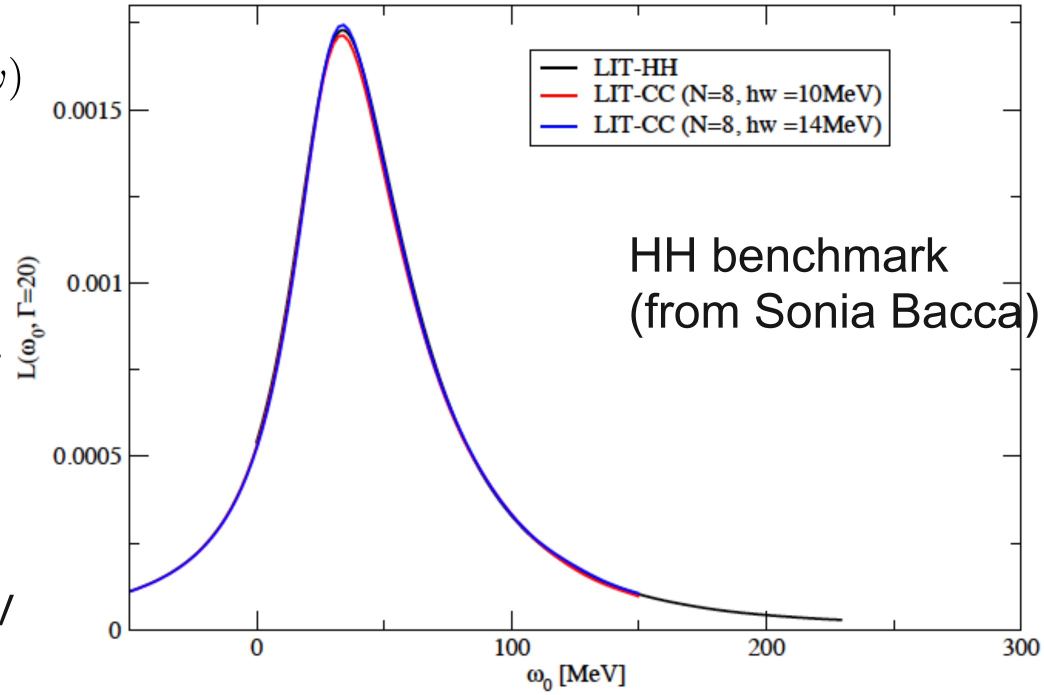
$$L(\omega_0, \Gamma) = \int d\omega \frac{R(\omega)}{(\omega - \omega_0)^2 + \Gamma^2}$$

$$(\hat{H} - E_0 - \omega_0 + i\Gamma)|\widetilde{\Psi}\rangle = \hat{\Theta}|\Psi_0\rangle$$

$$L(\omega_0, \Gamma) = \langle \widetilde{\Psi} | \widetilde{\Psi} \rangle$$

LIT for dipole excitations of ^{4}He

Inelastic peak at high energies 35MeV



HH benchmark
(from Sonia Bacca)

Coupled-Cluster LIT equations

$$|\widetilde{\Phi}_R(z)\rangle = R(z)|\Phi_0\rangle = \left(R_0 + \sum_{ia} R_i^a \hat{c}_a^\dagger \hat{c}_i + \sum_{ia} R_{ij}^{ab} \hat{c}_a^\dagger \hat{c}_b^\dagger \hat{c}_i \hat{c}_j + \dots \right) |\Phi_0\rangle$$

$$\bar{H} R_\mu(z)|\Phi_0\rangle = (z - E_0) R_\mu(z)|\Phi_0\rangle + \bar{\Theta}|\Phi_0\rangle$$

$$\langle \Phi_0 | L_\mu(z) \bar{H} = \langle \Phi_0 | L_\mu(z)(z - E_0) + \langle \Phi_0 | \bar{\Theta}^\dagger$$

$$L(\omega_0, \Gamma) = \langle \Phi_0 | L_\mu(z) R_\mu(z) | \Phi_0 \rangle$$

Summary and outlook

1. Quenching of spectroscopic factors near neutron dripline show role of continuum induced correlations for protons
2. Promising results for elastic nucleon-nucleus scattering on ^{40}Ca and ^{16}O
3. Densities and cross sections from coupled-cluster theory help resolve long-standing anamoly of ^{23}O
4. Isotopic shift in radii of oxygen isotopes well reproduced with chiral NN interactions
5. Proton/neutron halo states well described in CCM with Berggren basis
6. Promising results for Lorentz-Integral Transform based on Coupled-Cluster method.