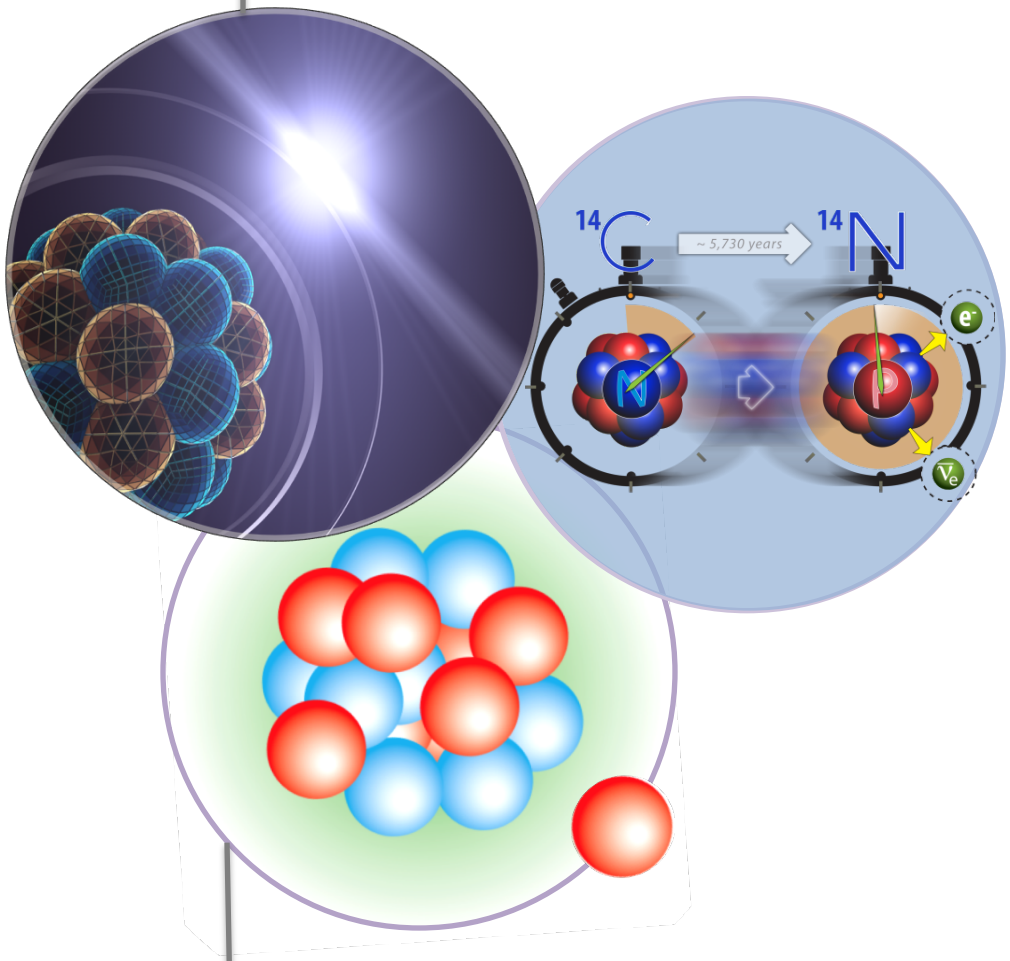
Nuclear structure and reactions from coupled-cluster theory



Gaute Hagen

Oak Ridge National Laboratory

INT, March 29th, 2017

U.S. DEPARTMENT OF ENERGY

NUCLEI
Nuclear Computational Low-Energy Initiative

BSF
United States – Israel
Binational Science Foundation

OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

Collaborators

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@ Chalmers: **B. Carlsson**, A. Ekström, C. Forssén

@ Hebrew U: N. Barnea, D. Gazit

@ MSU/ U Oslo: M. Hjorth-Jensen

@ Trento: G. Orlandini

@ TRIUMF: S. Bacca, J. Holt, **M. Miorelli**, P. Navratil, **S. R. Stroberg**

@ TU Darmstadt: **C. Drischler**, **C. Stumpf**, K. Hebeler, R. Roth, A. Schwenk, **J. Simonis**

@ LLNL: **K. Wendt**

Outline

- Optical potentials from coupled-cluster theory
- The neutron skin and dipole polarizability of ^{48}Ca and ^{68}Ni
- Structure of ^{78}Ni
- Structure and decay of ^{100}Sn

Overlap with key topics of the workshop:

•**Integrated structure and reaction *ab initio* modeling: Addressing the challenge of heavier nuclei, continuum, and multiple reaction channels.**
Ab initio approaches carry predictive power, which is critical for studying short-lived isotopes inaccessible by experiment, but are currently limited to light nuclei. Following the development of *ab initio* structure models that exhibit a better scaling, the program will discuss and guide the development of *ab initio* reaction theory for medium-mass nuclei.

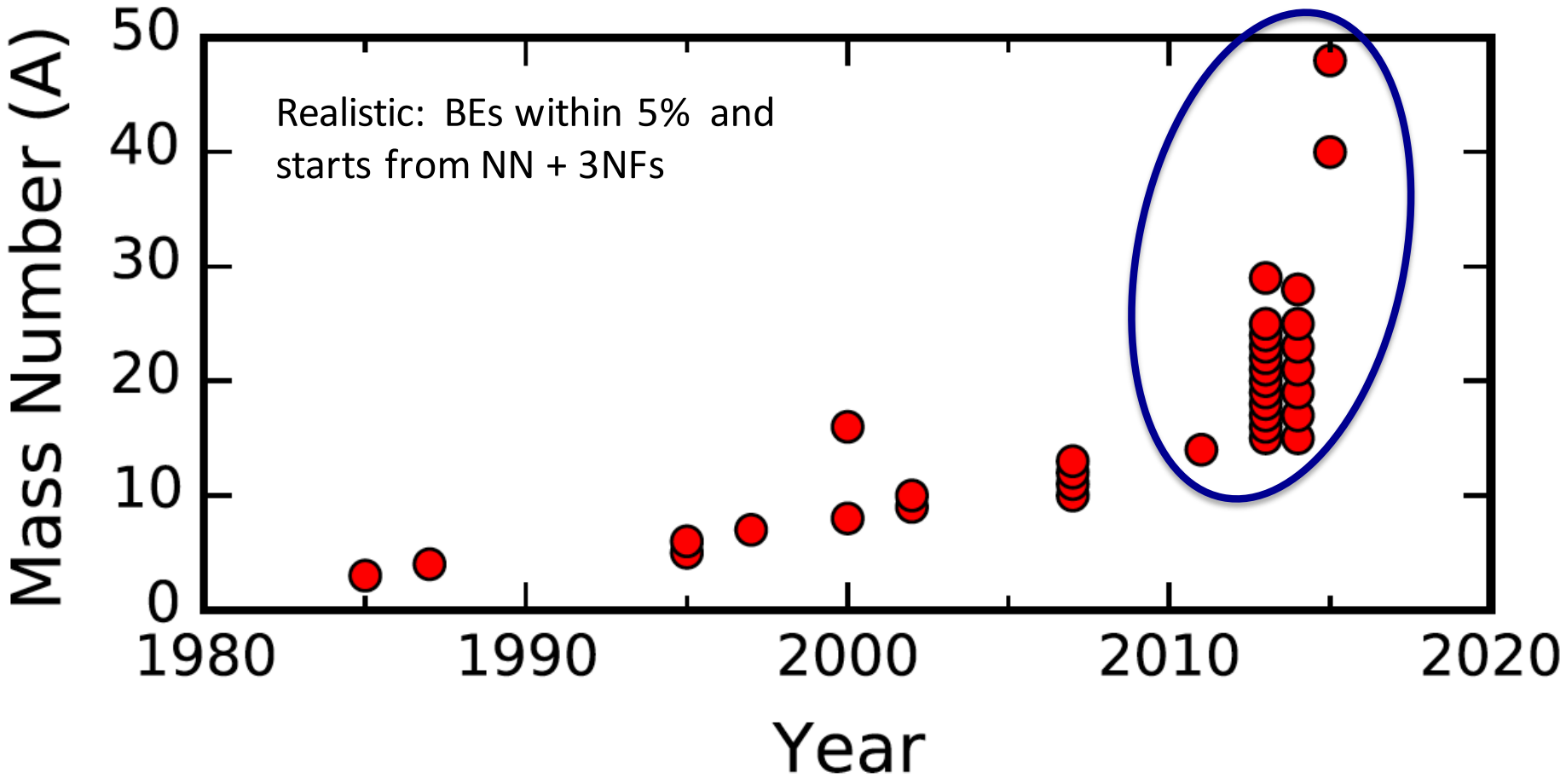
•**Effective interactions in reaction calculations.**
Effective interactions (optical potentials) have to enter reaction descriptions when possible reaction channels are eliminated from explicit consideration. The program will address the challenge of developing effective interactions that have predictive power in the regime of exotic nuclei, where data is scarce, and seek strategies for anchoring these interaction in *ab initio*, microscopic, or effective theories.

•**Improving structure inputs to reaction approaches.**
To achieve more reliable predictions for unstable nuclei, it is important that *ab initio* theories inform/replace current microscopic models for medium-mass systems, while microscopic methods need to replace the phenomenology used for heavier systems. The program will review recent developments in nuclear structure theory and identify avenues for integrating improved structure information into new and existing reaction theories and codes.

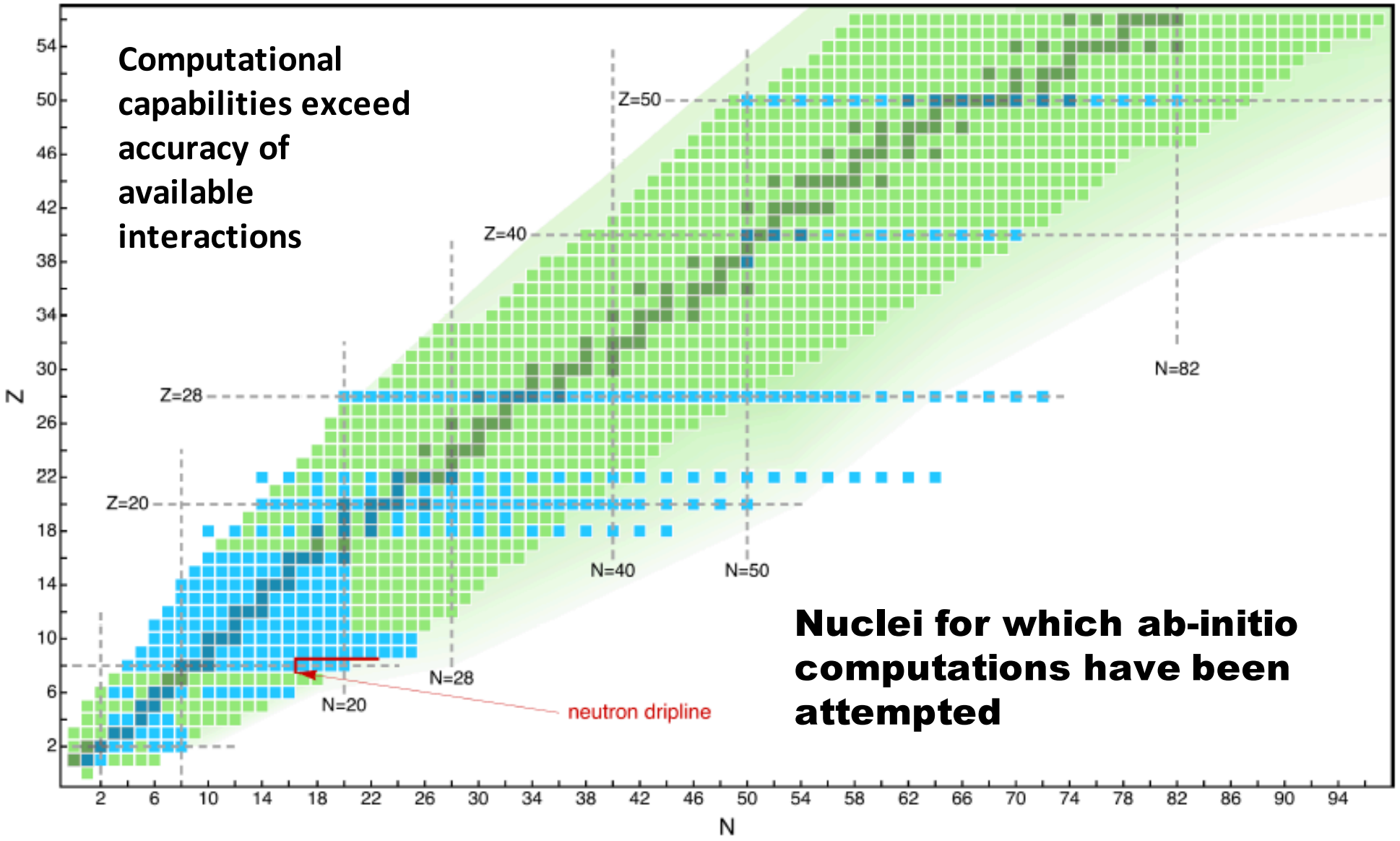
Trend in realistic ab-initio calculations

Explosion of many-body methods (Coupled clusters, Green's function Monte Carlo, In-Medium SRG, Lattice EFT, MCSM, No-Core Shell Model, Self-Consistent Green's Function, UMOA, …)

Application of ideas from EFT and renormalization group (V_{low-k}, Similarity Renormalization Group, …)



Reach of ab-initio computations of nuclei



H. Hergert *et al*, Physics Reports 621, 165-222 (2016)

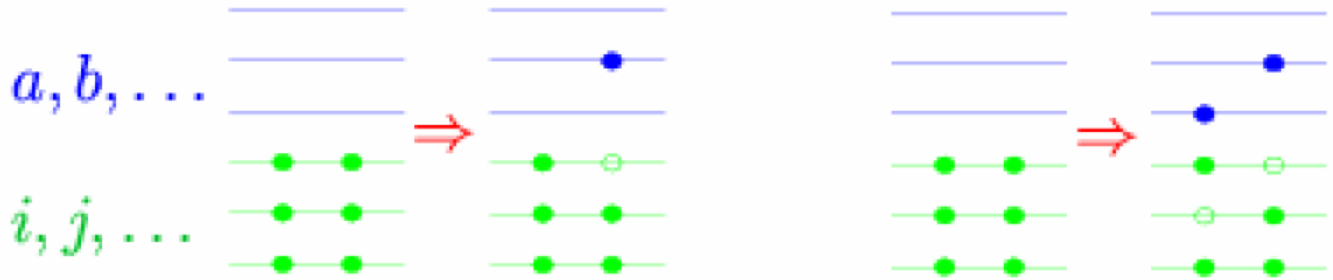
Coupled-cluster method (CCSD approximation)

Ansatz:

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

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

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



Coupled cluster equations

$$
\begin{aligned}
E &= \langle\Phi|\overline{H}|\Phi\rangle \\
0 &= \langle\Phi_i^a|\overline{H}|\Phi\rangle \\
0 &= \langle\Phi_{ij}^{ab}|\overline{H}|\Phi\rangle
\end{aligned}
$$

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

$$
\overline{H} \equiv e^{-T}He^{T} = \left(He^{T}\right)_c = \left(H + HT_1 + HT_2 + \frac{1}{2}HT_1^2 + \dots\right)_c
$$

Coupled-cluster method (CCSD approximation)

$$B_1 = T_1$$

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

$$B_3 = T_3 + T_2T_1 + \frac{1}{6}T_1^3$$

$$B_4 = T_4 + T_3T_1 + \frac{1}{2}T_2^2 + \frac{1}{2}T_2T_1^2 + \frac{1}{24}T_1^4$$

$$\ldots$$

CCSD

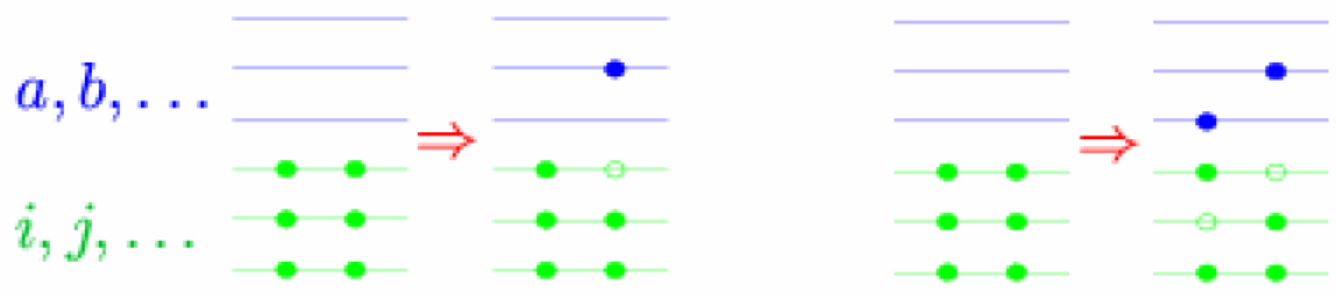
CCSDT

Disconnected quadruples

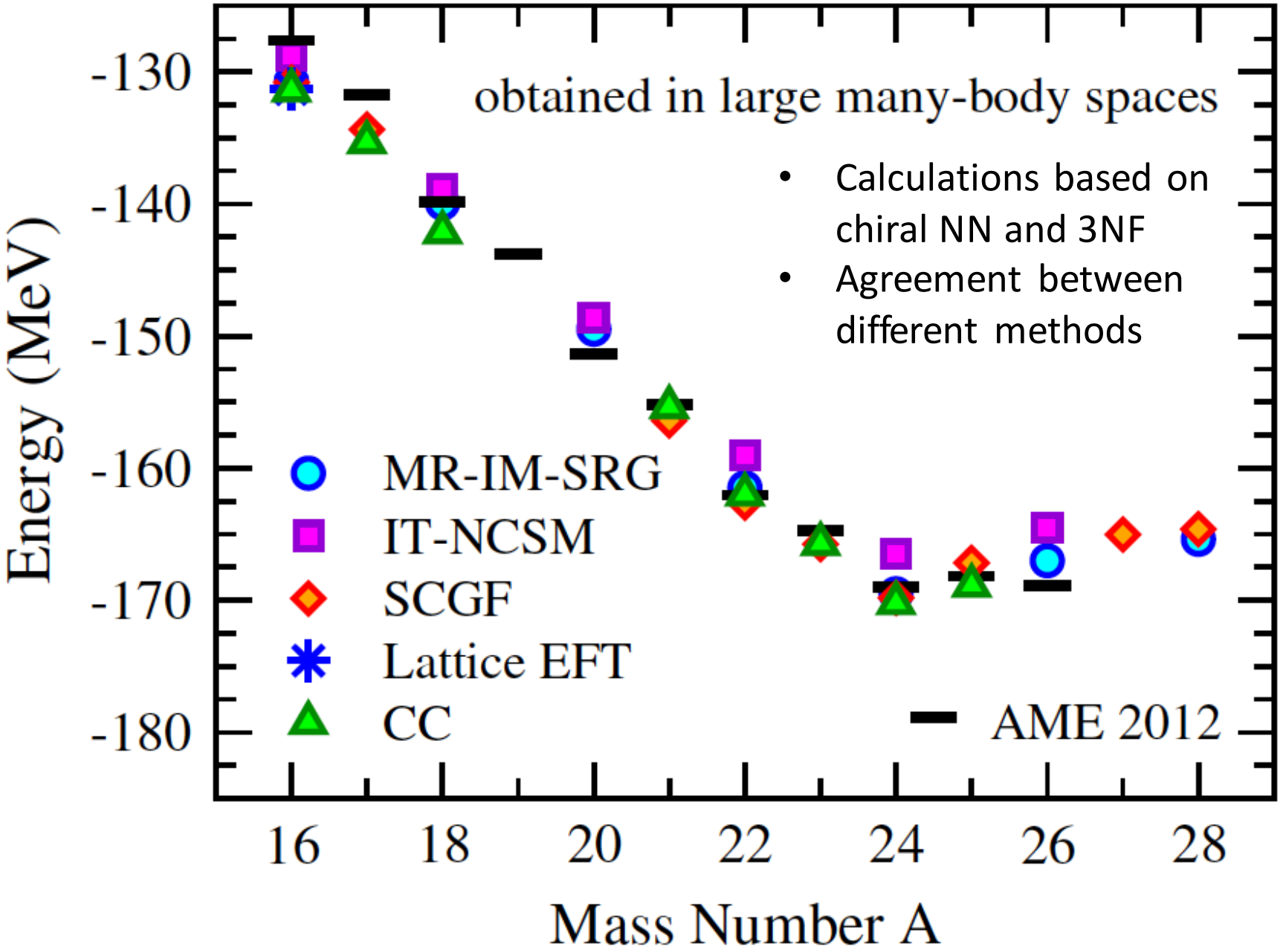
Connected quadruples

- CCSD captures most of the 3p3h and 4p4h excitations (scales as $n_o^2 n_u^4$)
- In order to describe α −cluster states need to include full quadruples (CCSDTQ) (scales $n_o^4 n_u^6$)

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

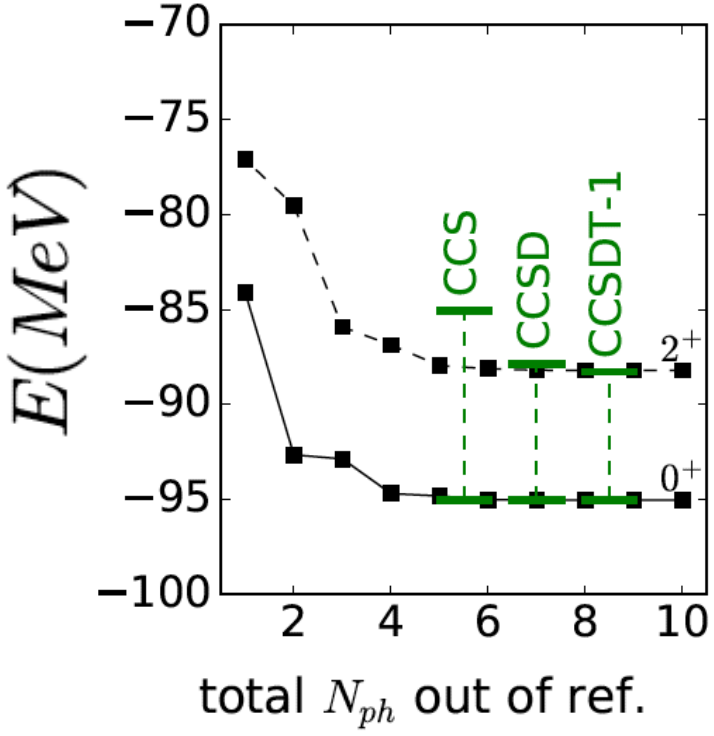


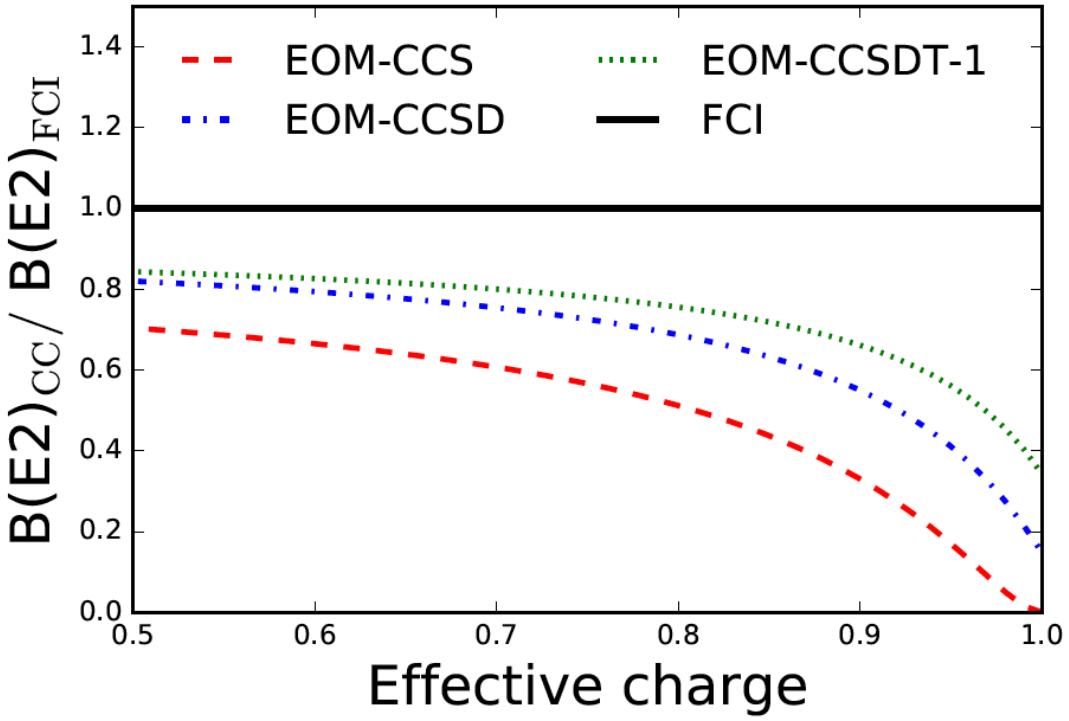
Success: BEs of oxgyen chain

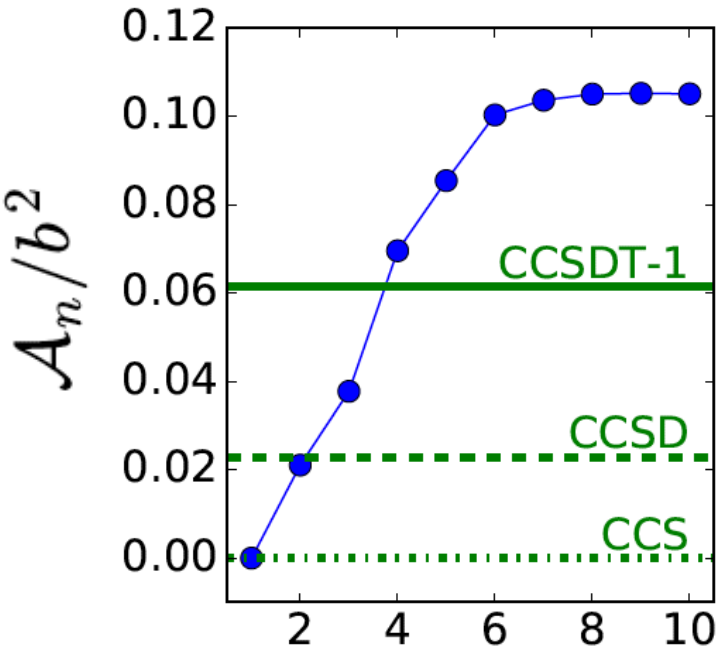


Hebeler, Holt, Menendez, Schwenk, Annu. Rev. Nucl. Part. Sci. 65, 457 (2015)

Challenge: Collectivity and B(E2)

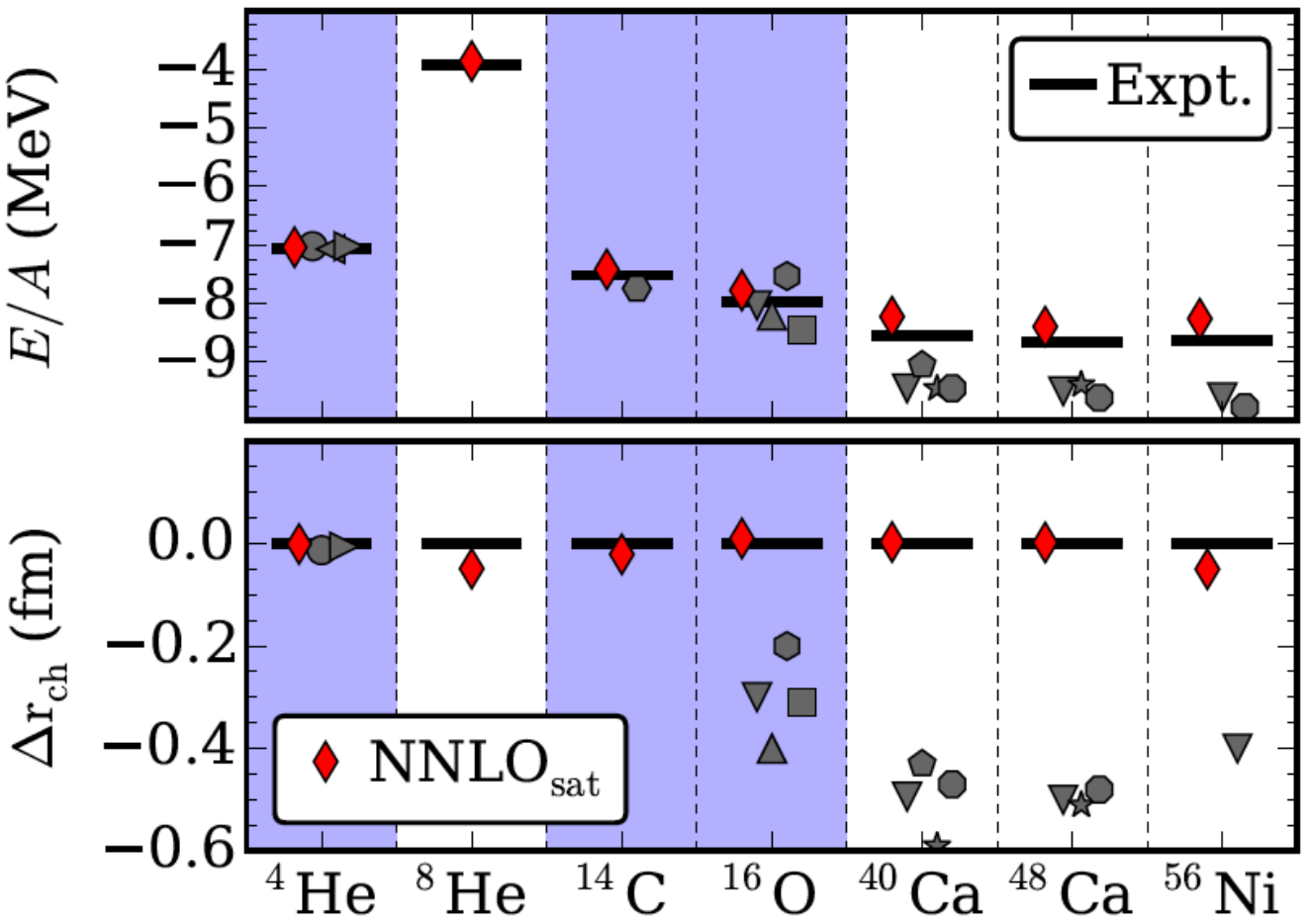






- ^{14}C computed in FCI and CC with psd effective interaction
- As effective charge is varied from 0 to 1 CCSD fails
- Need excitations beyond 4p4h to describe B(E2) even if 2+ energy is reproduced

Accurate nuclear binding energies and radii from a chiral interaction



Navratil et al (2007); Jurgenson et al (2011)

a

b Binder et al (2014)

c Epelbaum et al (2014)

d Epelbaum et al (2012)

e Maris et al (2014)

f Wloch et al (2005)

g Hagen et al (2014)

h Bacca et al (2014)

i Maris et al (2011)

j Hergert et al (2014)

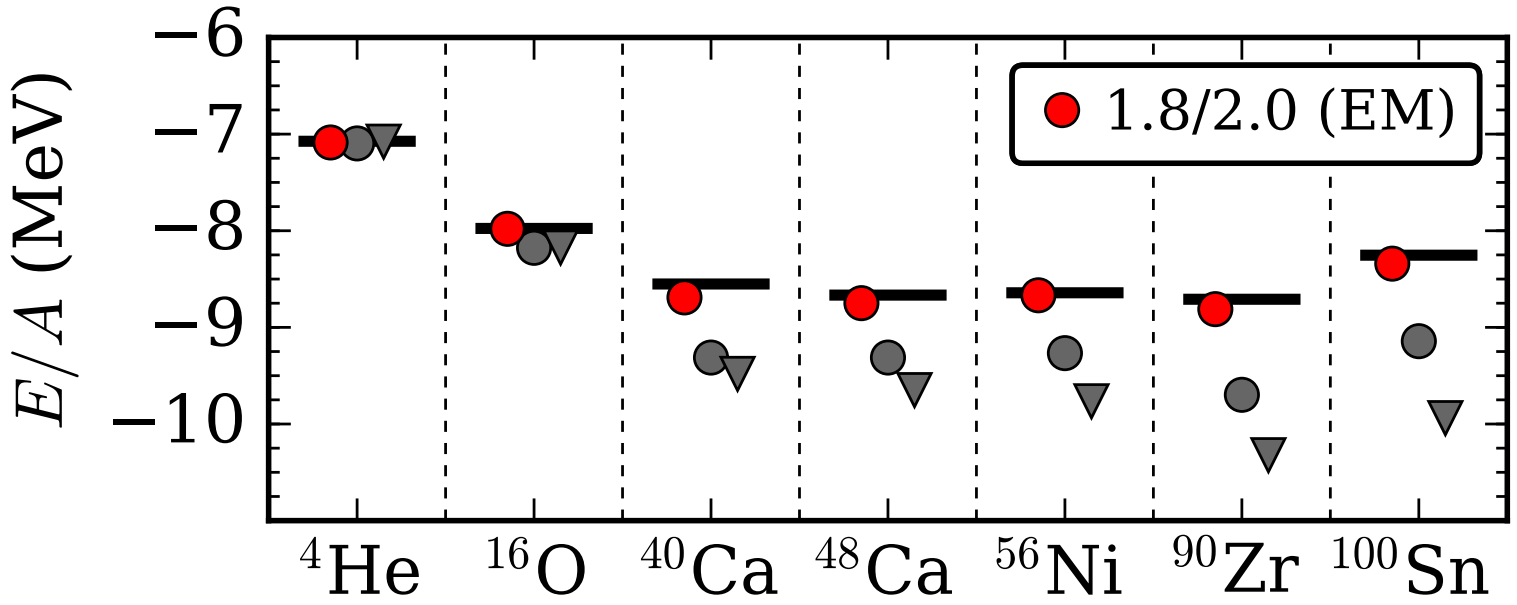
k Soma et al (2014)

Solution: Simultaneous optimization of NN and 3NFs
Include charge radii and binding energies of ^{3}H, ^{3,4}He, ^{14}C, ^{16}O in the optimization ($NNLO_{sat}$)

A. Ekström *et al*, Phys. Rev. C **91**, 051301(R) (2015).
G. Hagen et al, Phys. Scr. **91**, 063006 (2016).

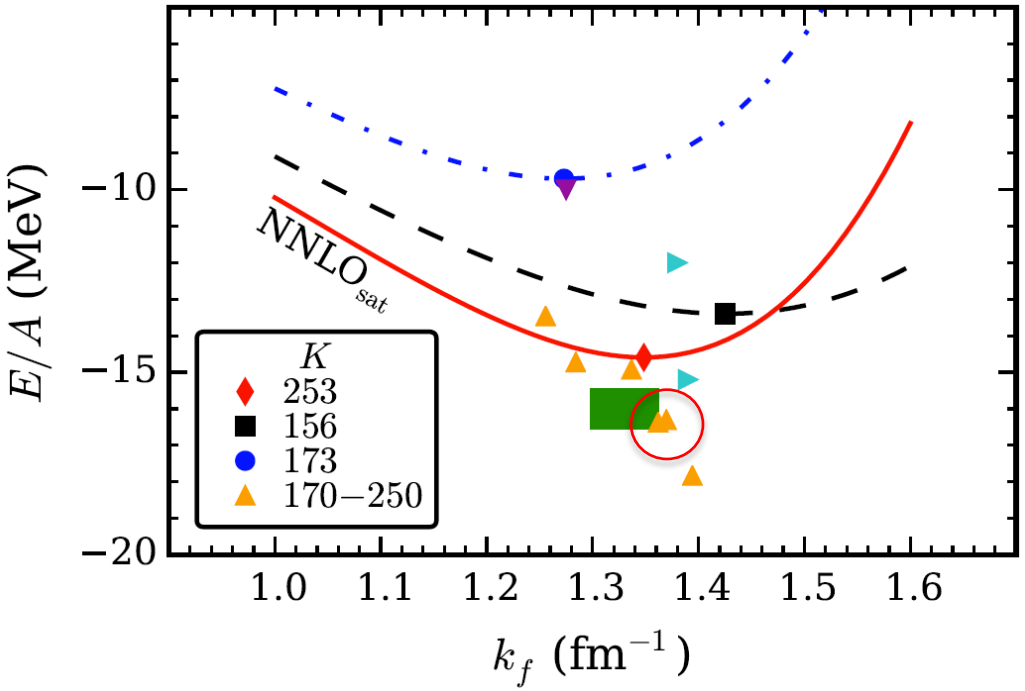
Not new: GFMC with AV18 and Illinois-7 are fit to 23 levels in nuclei with A <10

Accurate BEs from light → heavy → infinite matter from a chiral interaction

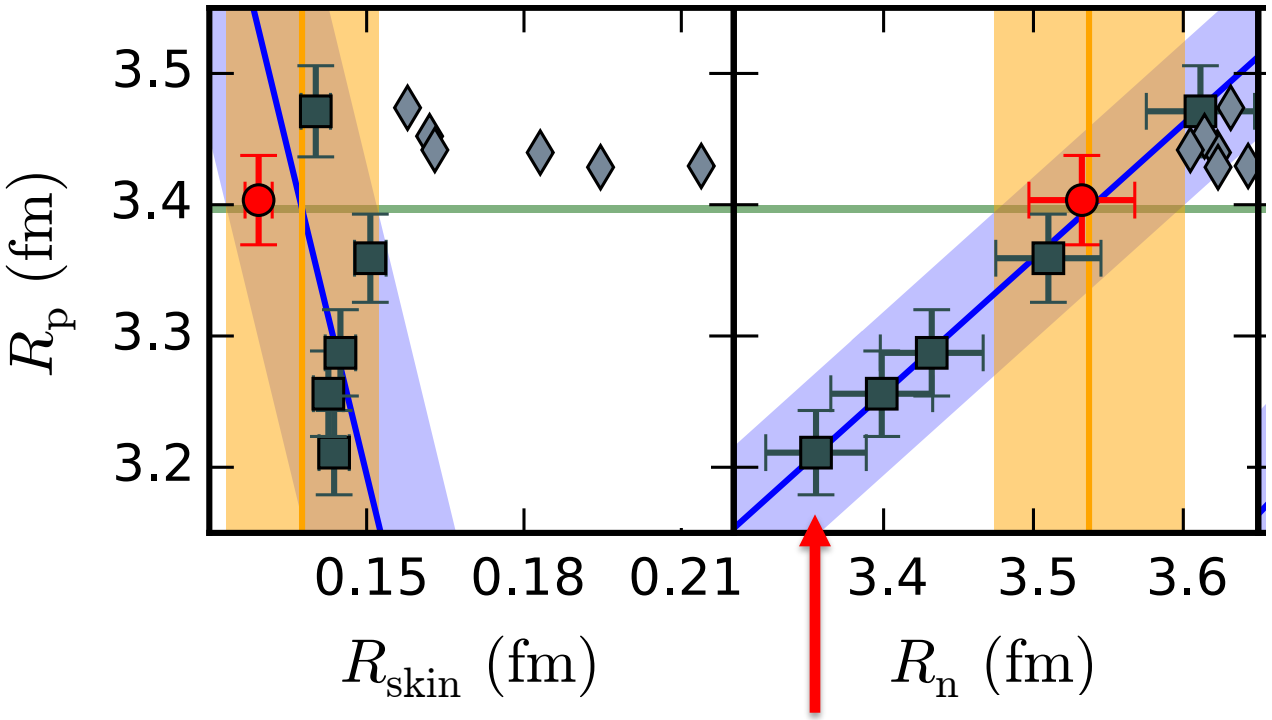


1.8/2.0 (EM) from K. Hebeler *et al* PRC (2011)
The other chiral NN + 3NFs are from Binder et al, PLB (2014)

- Accurate binding energies up to mass 100 from a chiral NN + 3NF
- Fit to nucleon-nucleon scattering and BEs and radii of A=3,4 nuclei
- Reproduces saturation point in nuclear matter within uncertainties
- Deficiencies: Radii are less accurate



Neutron radius and skin of ^{48}Ca

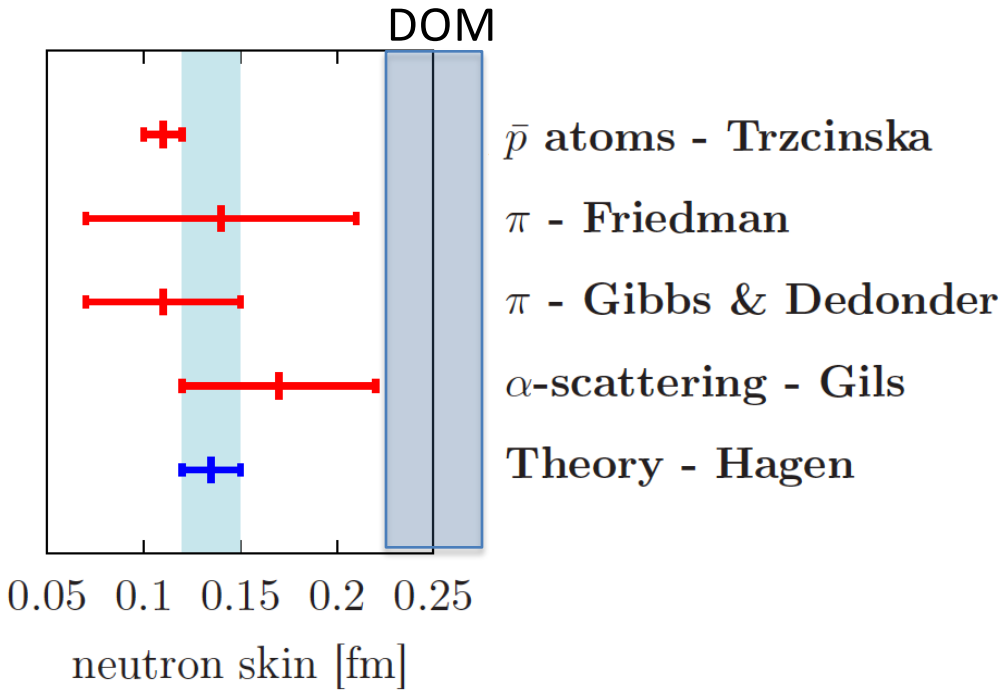


G. Hagen *et al*, Nature Physics **12**, 186–190 (2016)

Uncertainty estimates from family of chiral interactions: K. Hebeler *et al* PRC (2011)

DFT:
SkM*, SkP, Sly4, SV-min, UNEDF0, and UNEDF1

- Neutron skin significantly smaller than in DFT
- Neutron skin almost independent of the employed Hamiltonian
- Our predictions for ^{48}Ca are consistent with existing data



Optical potentials from coupled-cluster theory

J. Rotureau et al, Phys. Rev. C 95, 024315 (2017)

Coupled-cluster Green's function:

$$G^{CC}(\alpha,\beta,E) \equiv$$
$$\langle\Phi_{0,L}|\overline{a_\alpha}\frac{1}{E-(\overline{H}-E^A_{gs})+i\eta}\overline{a^\dagger_\beta}|\Phi_0\rangle$$
$$+\langle\Phi_{0,L}|\overline{a^\dagger_\beta}\frac{1}{E-(E^A_{gs}-\overline{H})-i\eta}\overline{a_\alpha}|\Phi_0\rangle$$

Solve for A$\pm$1 systems with PA/PR-EOMCCSD truncated at 2p1h and 1p2h

$$\left[E-(\bar{H}-E^A_{gs})\right]|\Psi^{A+1}_{R,\beta}(E)\rangle = \bar{a^\dagger_\beta}|\Phi_{0,R}\rangle$$

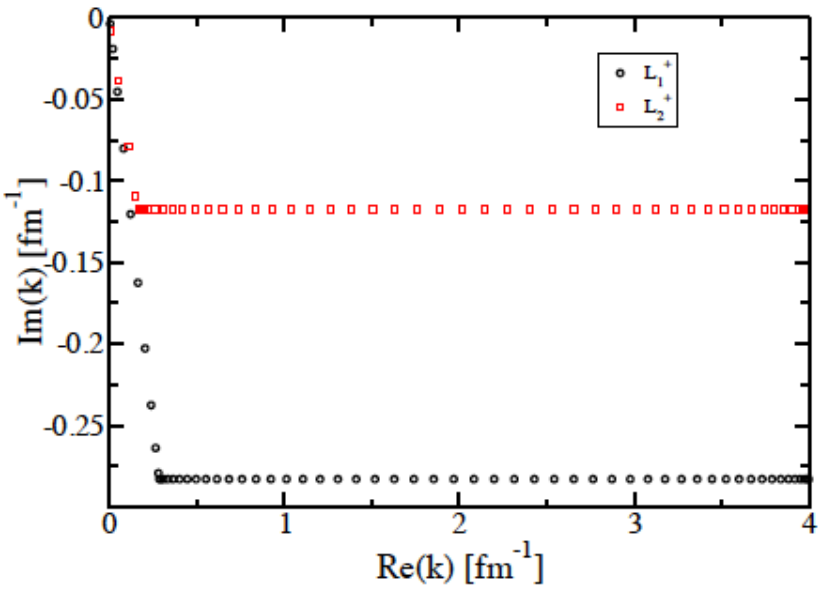
$$\left[E-(E^A_{gs}-\bar{H})\right]|\Psi^{A-1}_{R,\alpha}(E)\rangle = \bar{a_\alpha}|\Phi_{0,R}\rangle$$

The coupled-cluster Green's function can then be written:

$$G(\alpha,\beta,E) = \langle\phi_{0,L}|\bar{a_\alpha}|\Psi^{A+1}_{R,\beta}(E)\rangle + \langle\phi_{0,L}|\bar{a^\dagger_\beta}|\Psi^{A-1}_{R,\alpha}(E)\rangle$$

See also talk by Andrea Idini, and C. Barbieri and B. K Jennings Phys.Rev. C72 (2005) 014613

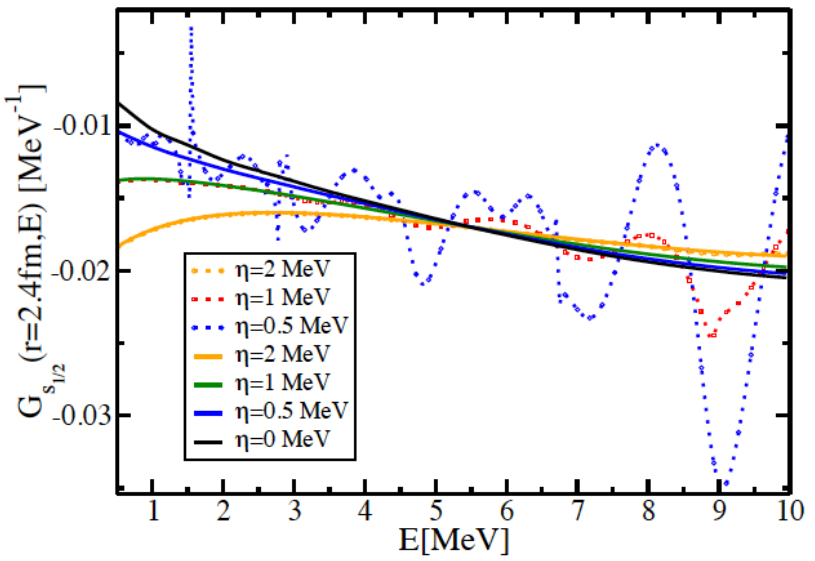
Optical potentials from coupled-cluster theory



Using a Berggren basis allows stable results for eta –> 0

$$\sum_i |u_i\rangle\langle\tilde{u}_i| + \int_{L^+} dk|u(k)\rangle\langle u(\tilde{k})| = \hat{1}$$

See also Hagen 04, Kruppa 07, Carbonell 2014, Papadimitriou 2015 for few-body applicatiobs



Imaginary part of the neutron s-wave Green's function

Inverting the Dyson equation we obtain the self-energy:

$$\Sigma^*(E) = [G^{(0)}(E)]^{-1} - G^{-1}(E)$$

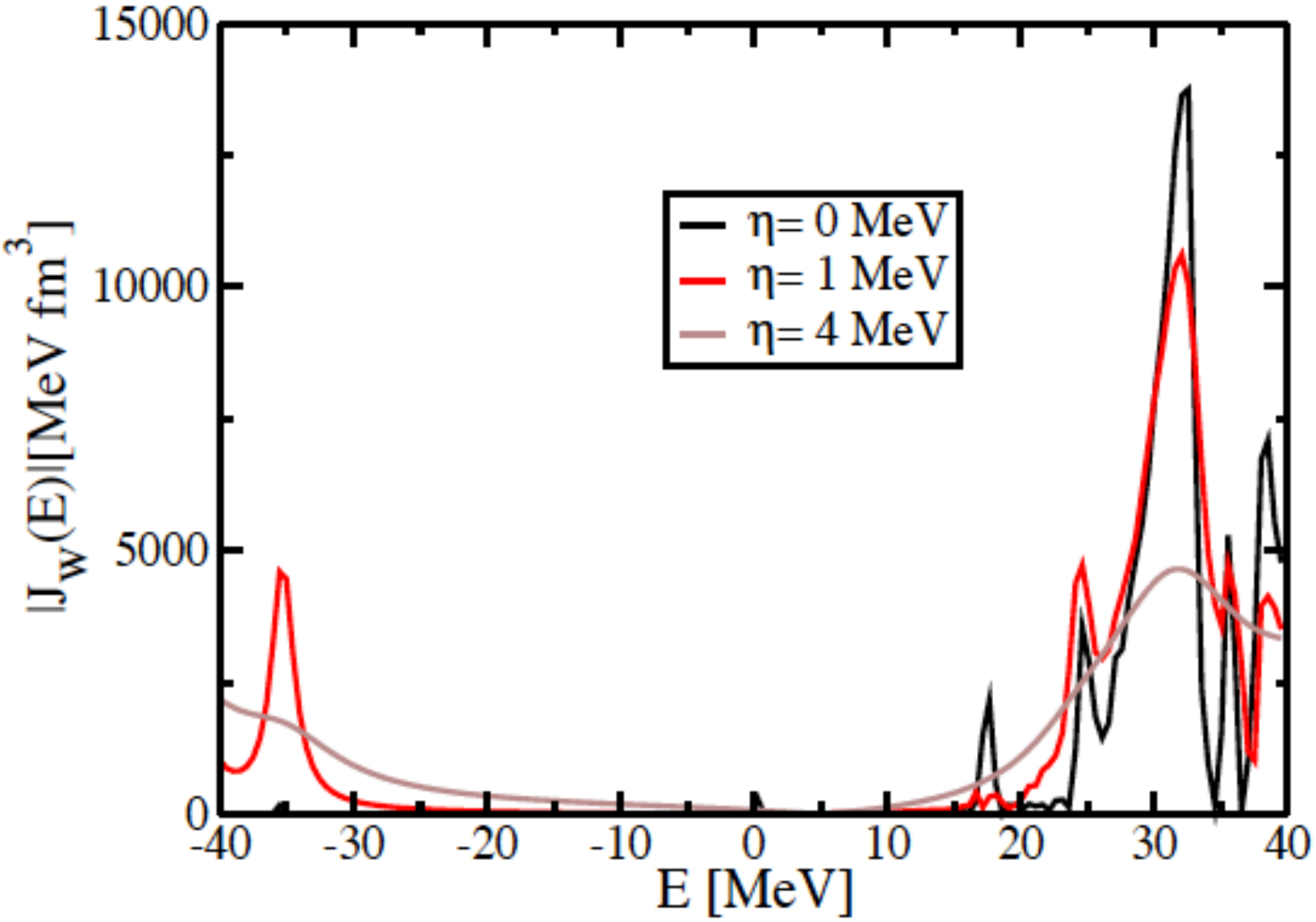
Scattering phase shifts are obtained by the solving the equation:

$$-\frac{\hbar^2}{2\mu}\nabla^2\xi(\mathbf{r}) + \int d\mathbf{r}'\Sigma'(\mathbf{r},\mathbf{r}',E^+)\xi(\mathbf{r}') = E^+\xi(\mathbf{r})$$

Optical potentials from coupled-cluster theory

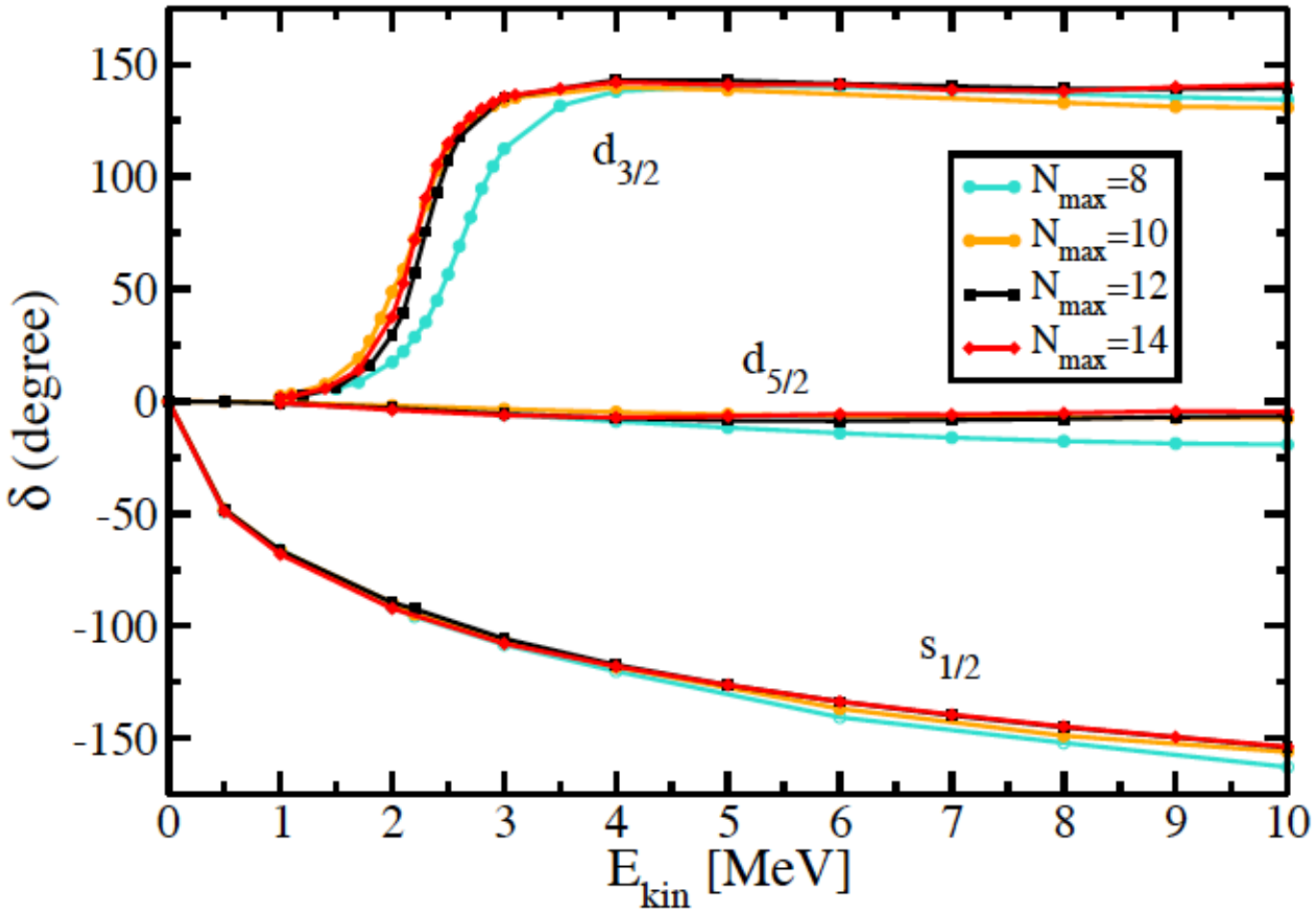
J. Rotureau et al, Phys. Rev. C 95, 024315 (2017)

Neutron s-wave imaginary volume integral



Neutron elastic scattering on ^{16}O with NNLO$_{opt}$

J. Rotureau et al, Phys. Rev. C 95, 024315 (2017)



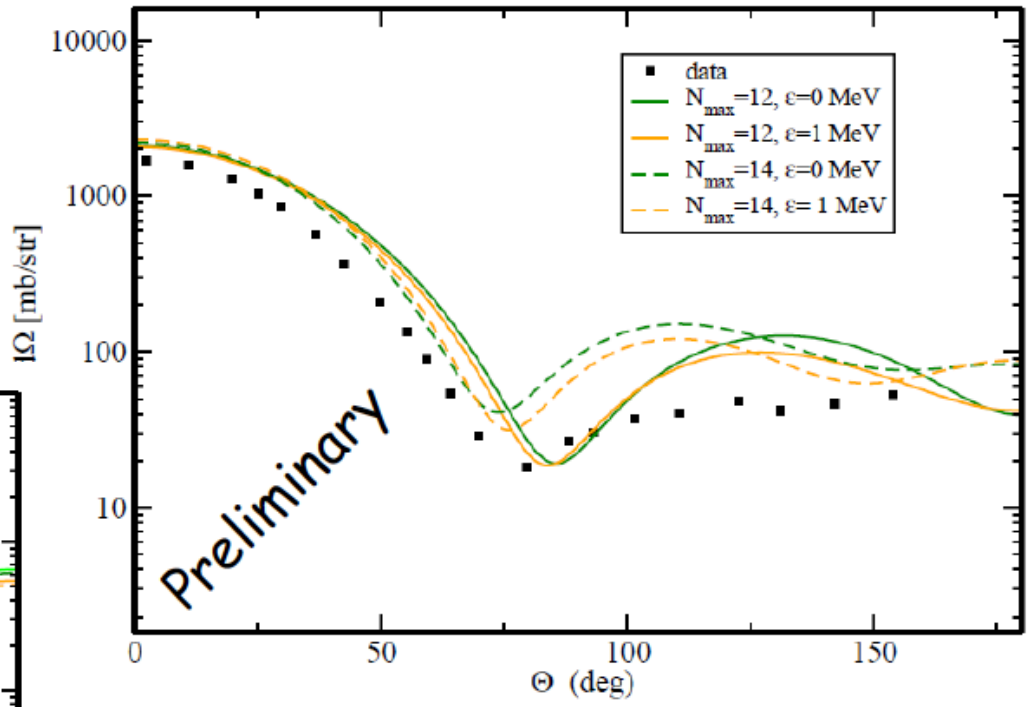
Consistent results between computed phase shifts and resonances computed directly in the Berggren basis via PA-EOMCCSD

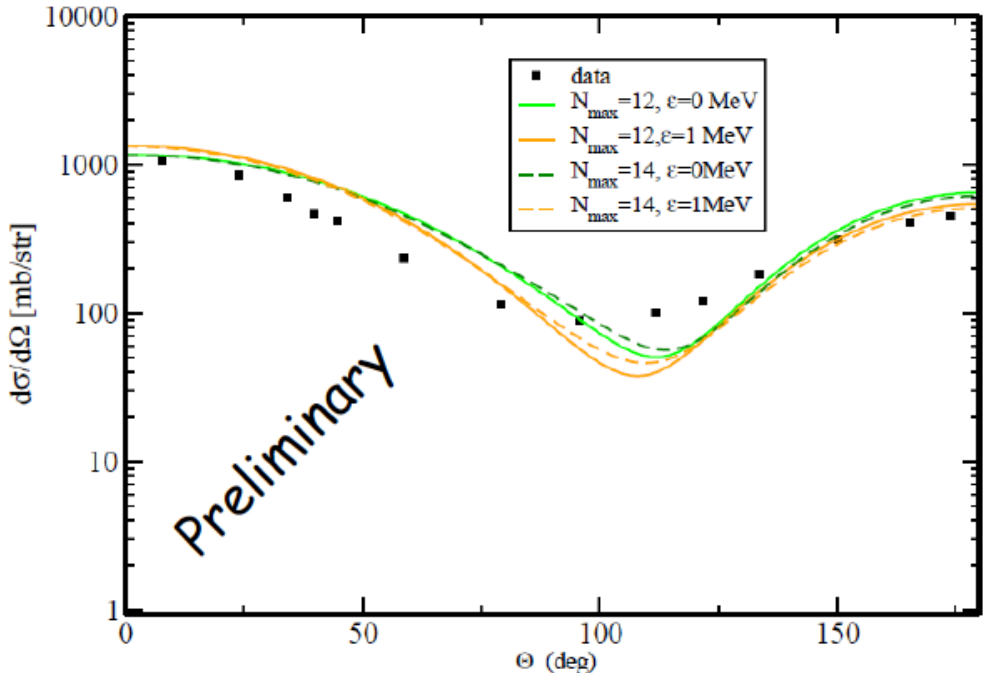
$N_{\max}$	$E(5/2^+)$	$E(1/2^+)$	$E(3/2^+)$
8	-4.35	-2.62	2.68-i0.32
10	-4.49	-2.73	2.24-i0.25
12	-4.56	-2.76	2.34-i0.21
14	-4.57	-2.80	2.26-i0.12

Neutron elastic scattering on ^{40}Ca

- Diffraction minima in good agreement with data
- Cross section overestimated due to lack of absorption (e.g. 0^+ state in ^{40}Ca too high)
- Using a Berggren basis allows for stable results as ε –> 0.

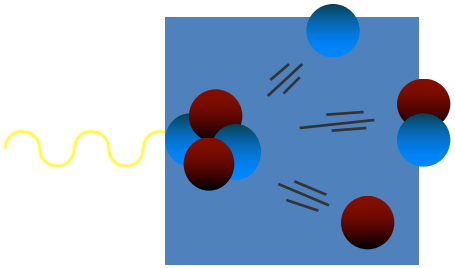
$^{40}Ca(n,n)^{40}Ca$, E_{lab} =5.3 MeV





$^{40}Ca(n,n)^{40}Ca$, E_{lab} =2.1 MeV

Response function from coupled-cluster theory



Cross section is related to the Response Function in the continuum

$$S(\omega) = \sum_f \left| \left\langle \psi_f \left| \hat{O} \right| \psi_0 \right\rangle \right|^2 \delta(E_f - E_0 - \omega)$$

Cannot be calculated beyond 3-body break-up even for A=4

Solution: Lorentz Integral Transform method (Efros, Leidemann,Orlandini, Barnea, Bacca)

Efros *et al.*,J. Phys. G: Nucl. Part. Phys. 34 (2007)

$$\mathcal{L}(\sigma,\Gamma) = \int d\omega \frac{S(\omega)}{(\omega-\sigma)^2+\Gamma^2} = \langle \tilde{\Psi} | \tilde{\Psi} \rangle$$

$$(H - E_0 - \sigma + i\Gamma) |\tilde{\Psi}\rangle = O|\Psi_0\rangle$$

Bound-state-like object. Need bound state technique to calculate it

Inclusive electron scattering and the Coulomb sum rule

The CSR is the total integerated strength of inelastic longitudinal response function

$$CSR(q) = \int d\omega \; R_L^{in}(\omega, \mathbf{q}) / G_p^2(Q^2)$$

$$R_L^{in}(\omega, \mathbf{q}) = \sum_f |\langle f|\rho(\mathbf{q})|\mathbf{0}\rangle|^2 \delta(\omega - \mathbf{E_f} + \mathbf{E_0})$$

Here $\rho(q)$ is the nuclear charge operator
Final state different from g.s. since we want the inelastic response

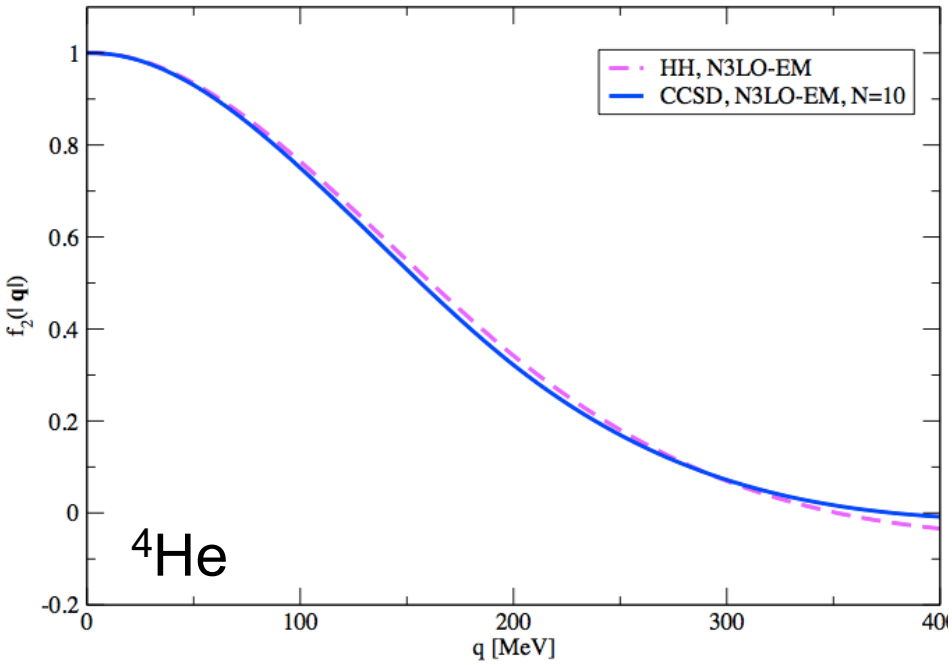
We approached the problem as we do for the calculation of the total strength of the dipole response function in PRL **111**, 122502 (2013).

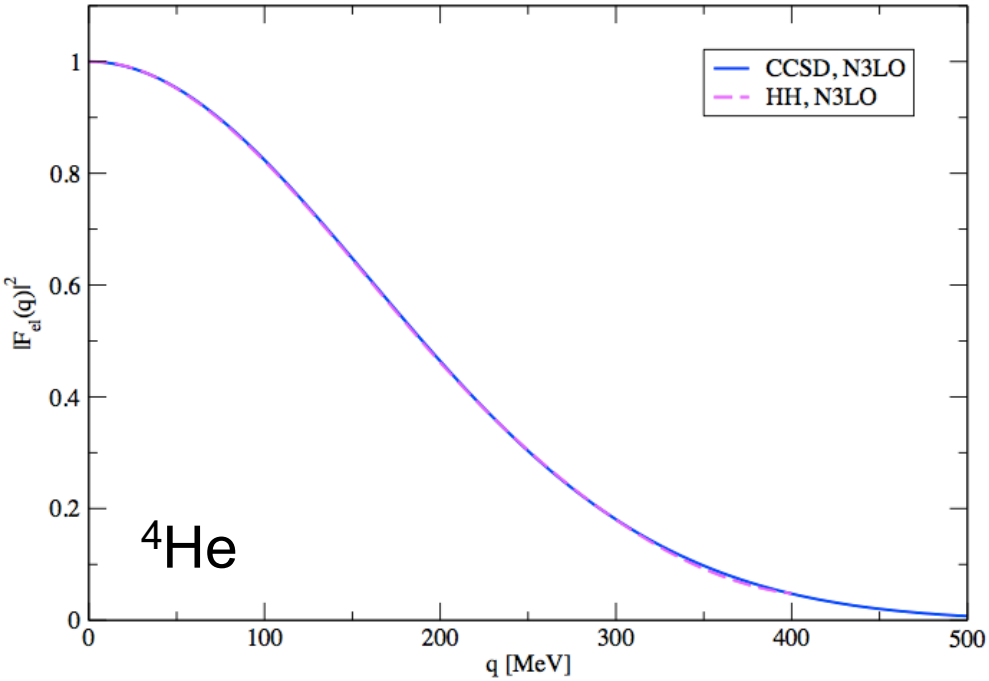
Inclusive electron scattering and the Coulomb sum rule

$$\mathrm{CSR}(q) = Z + \langle 0| \sum_{i \neq j} e^{i\mathbf{q}\cdot(\mathbf{r}_i - \mathbf{r}_j)} |0\rangle - |F(\mathbf{q})|^2 Z^2$$

$$\| \quad Z(Z-1) f_2(|\mathbf{q}|)$$

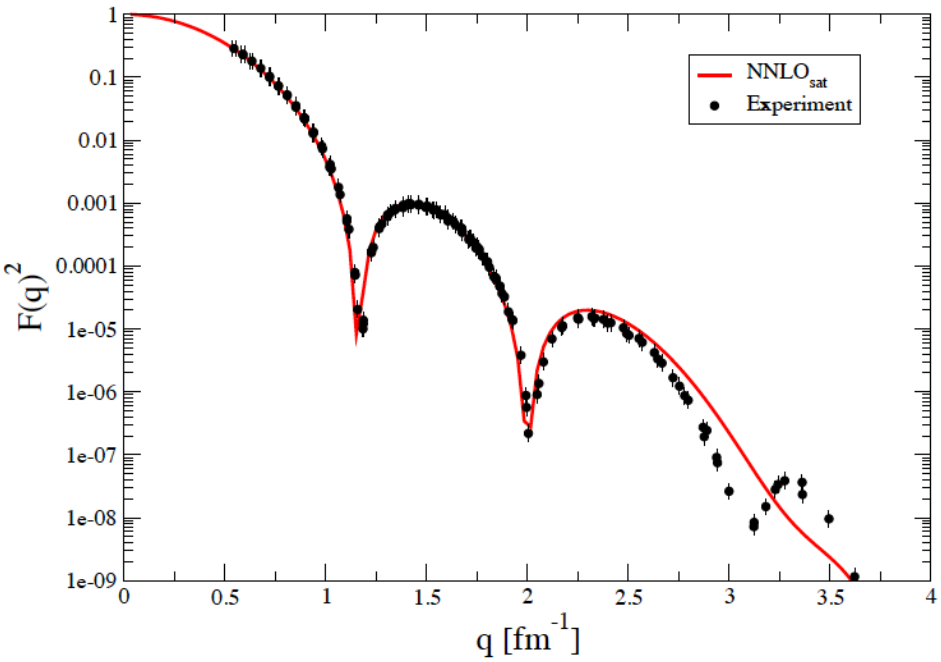
Benchmark with Exact Hyperspherical Harmonics for ^{4}He

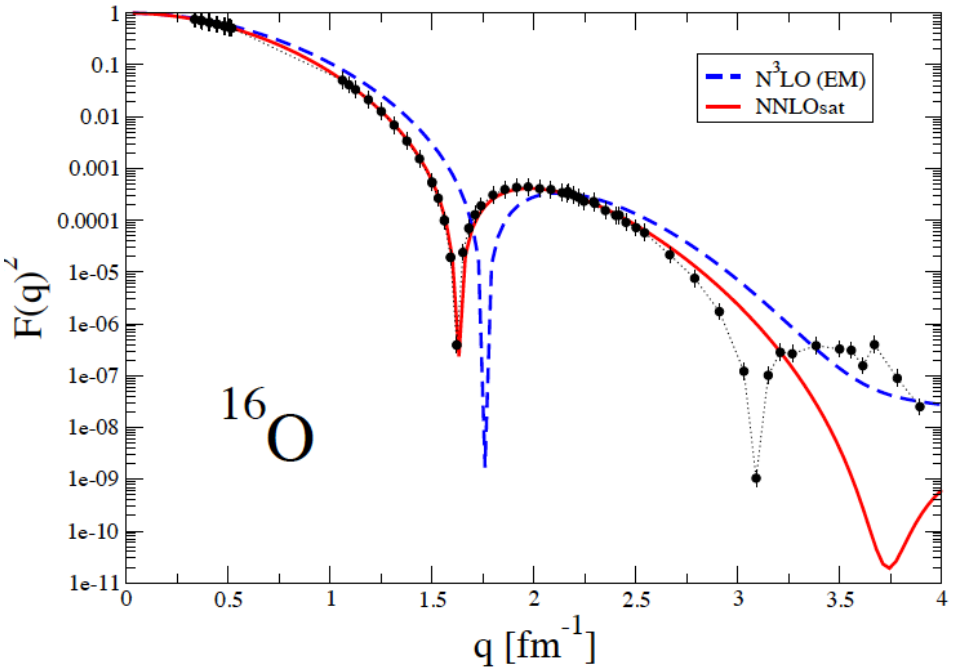




Very nice agreement!

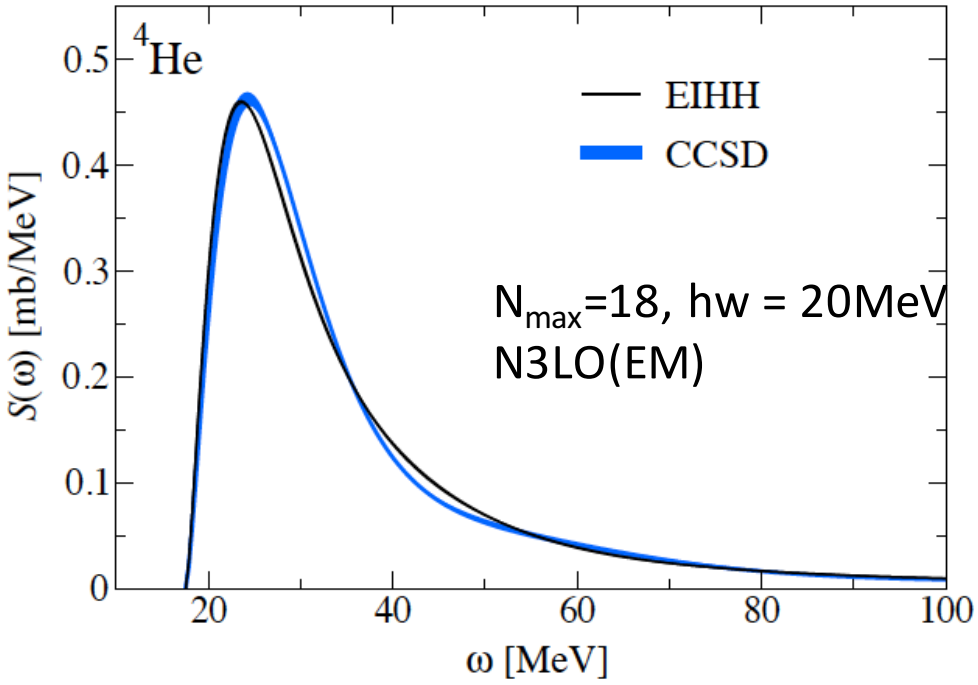
Comparison to data in ^{16}O and ^{40}Ca for elastic charge formfactor





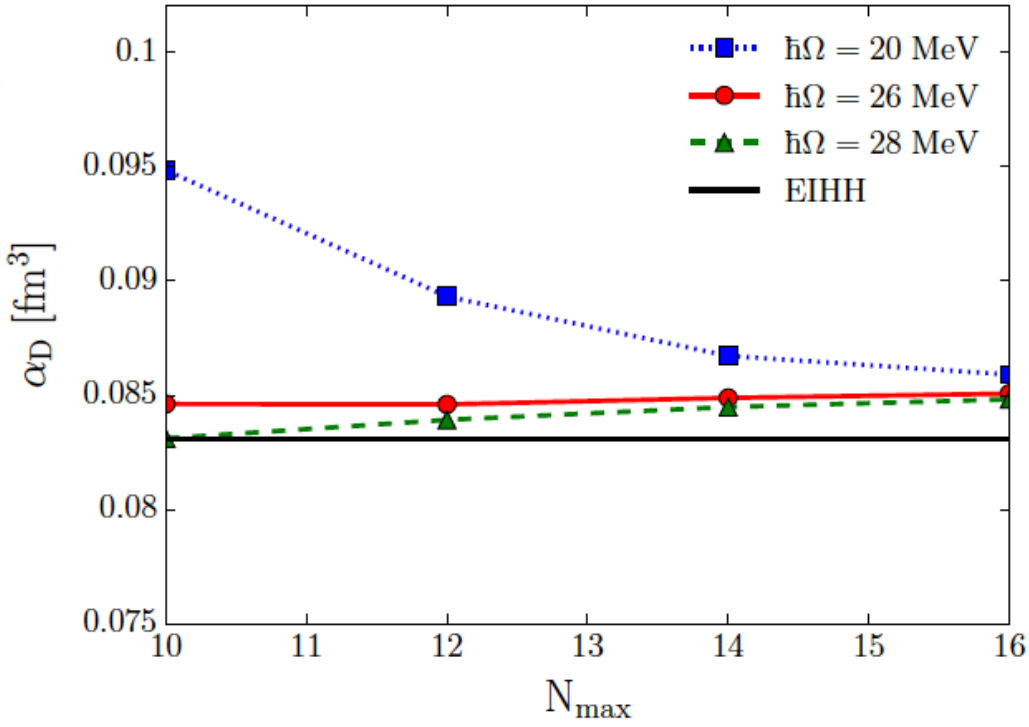
Dipole response from coupled-cluster

S. Bacca, N. Barnea, G. Hagen, G. Orlandini, T. Papenbrock, PRL 111, 143402 (2013).
S. Bacca, N. Barnea, G. Hagen, M. Miorelli, G. Orlandini, T. Papenbrock, PRC 90, 064610 (2014)



Lorentz Integral transform from coupled-cluster benchmarked with "exact" hyper-spherical harmonics for ^{4}He

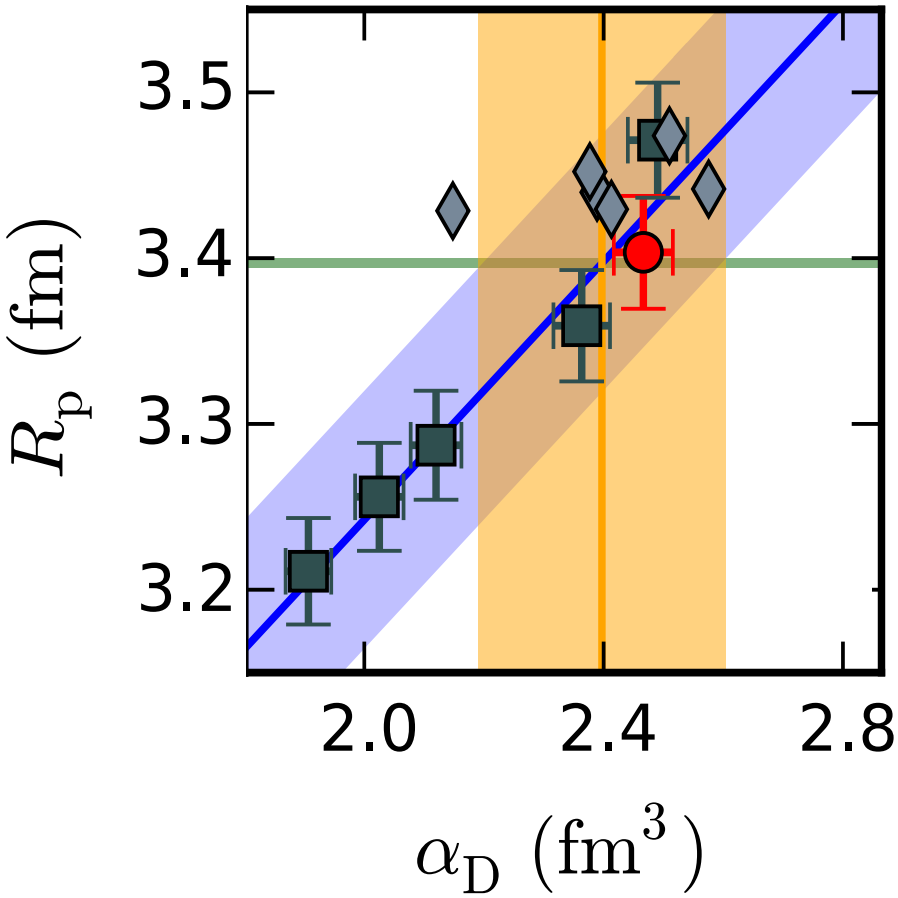
M. Miorelli *et al*, Phys. Rev. C 94, 034317 (2016)



Dipole polarizability in ^{4}He from CCSD within 1% of exact Hyper-spherical harmonics

$$\alpha_D = 2\alpha \int_{\omega_{\rm th}}^{\infty} d\omega \frac{S(\omega)}{\omega}$$

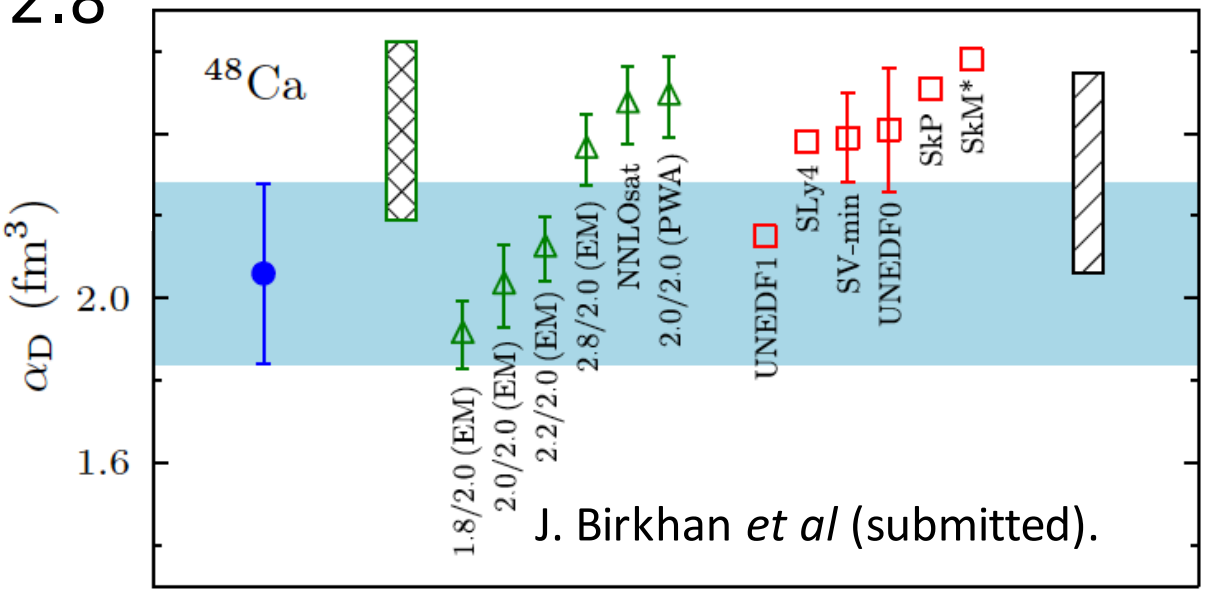
Dipole polarizability of ^{48}Ca



G. Hagen *et al*, Nature Physics **12**, 186–190 (2016)

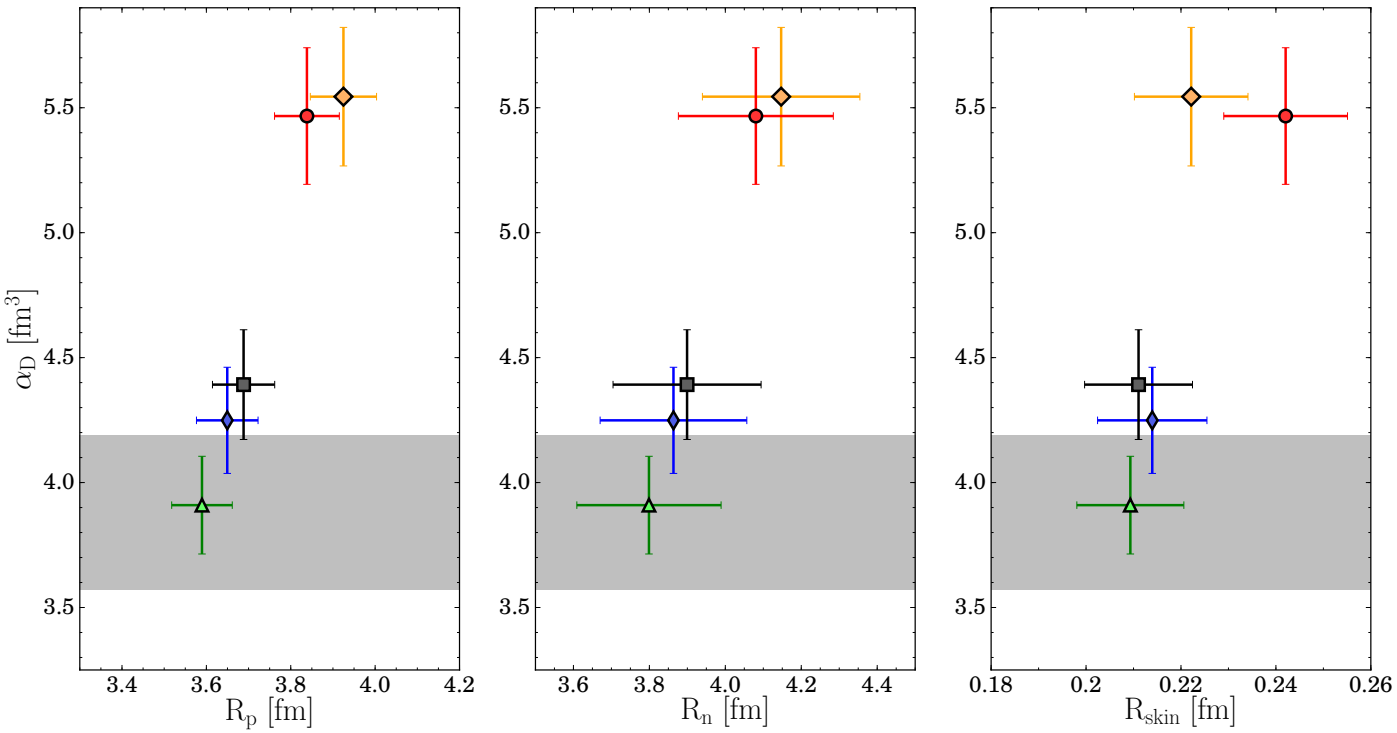
Ab-initio prediction from correlation with R_p:
$2.19 \lesssim \alpha_D \lesssim 2.60$ fm^3

- DFT results are consistent and within band of ab-initio results
- Data has been analyzed by Osaka-Darmstadt collaboration
- Ab-initio prediction overlaps with experimental uncertainty



J. Birkhan *et al* (submitted).

Neutron skin/dipole polarizability of ^{68}Ni

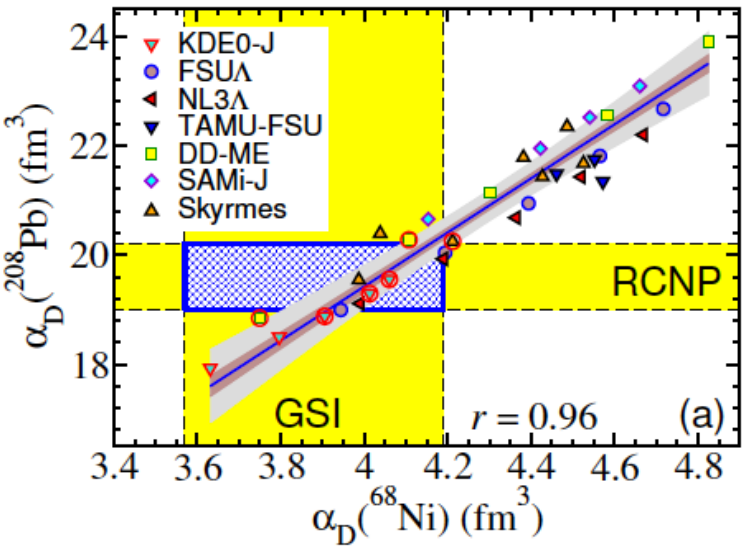


- Charge radii have been measured by the the COLLAPS collaboration at ISOLDE, CERN
- Neutron skin significantly larger than RPA results

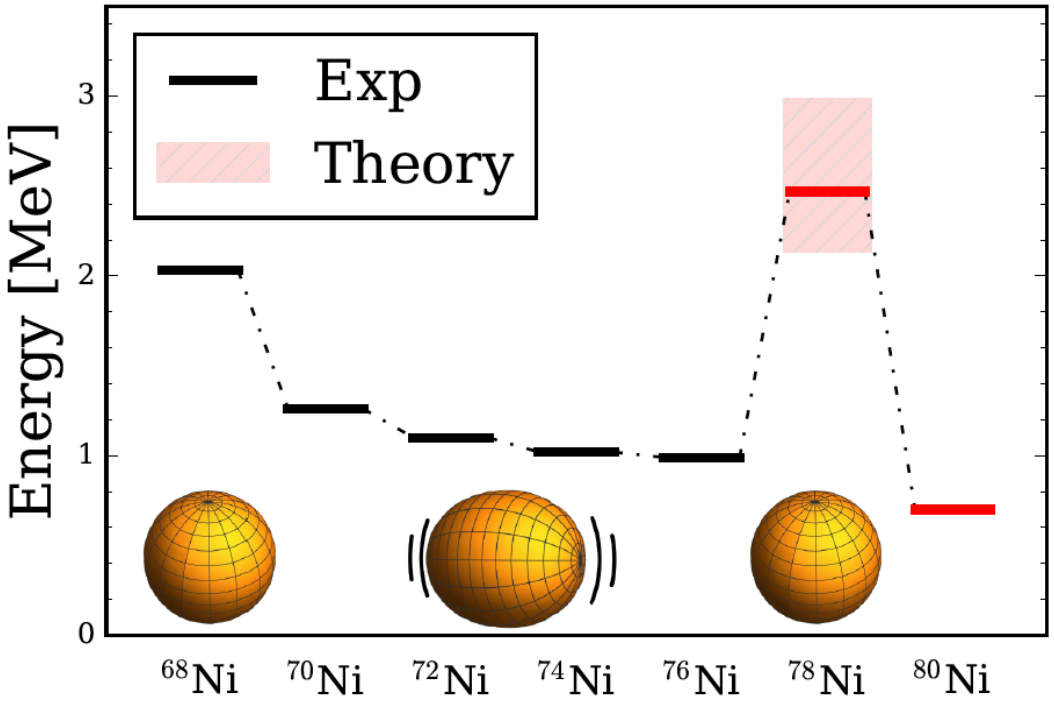
Self consistent RPA results based on large set of EDFs from X. Roca-Maza Phys. Rev. C 92, 064304 (2015)

Measuremet of dipole strength in ^{68}Ni:
D. Rossi et al, PRL 111 242503 (2013)

Nucleus	Δr_{np} (a)	Δr_{np} (b)	Δr_{np} (c)
^{68}Ni	0.15–0.19	0.18 ± 0.01	0.16 ± 0.04
^{120}Sn	0.12–0.16	0.14 ± 0.02	0.12 ± 0.04
^{208}Pb	0.13–0.19	0.16 ± 0.02	0.16 ± 0.03



Structure of ^{78}Ni from first principles

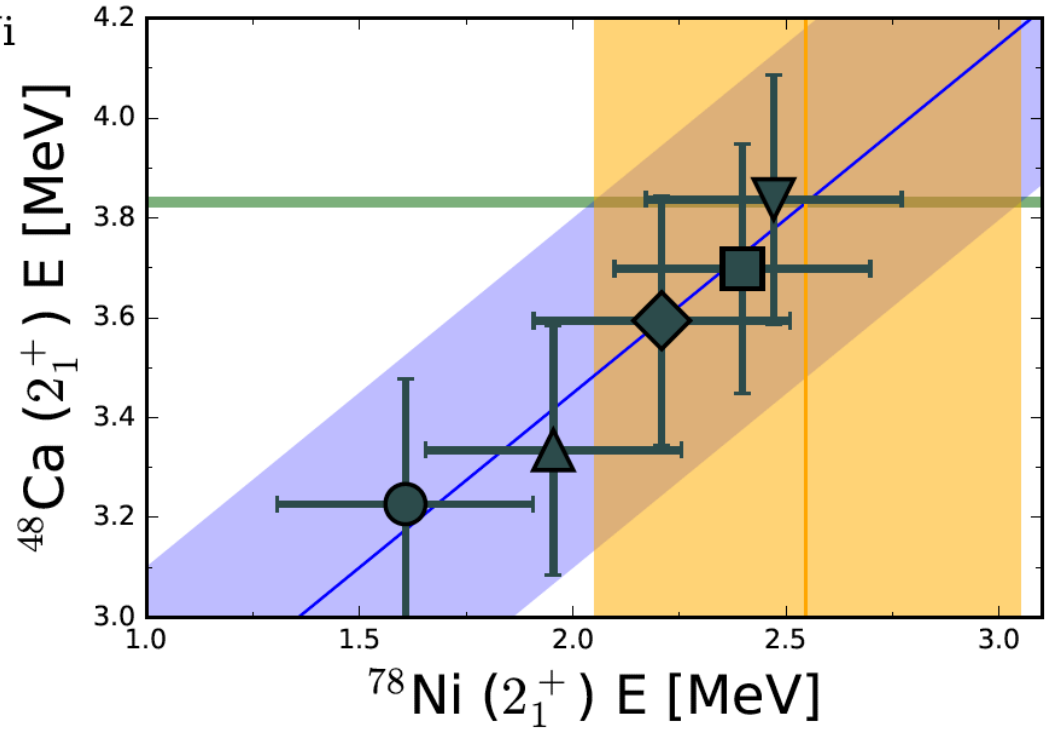


A high 2^+ energy in ^{78}Ni indicates that this nucleus is doubly magic

A measurement of this state has been made at RIBF, RIKEN
R. Taniuchi *et al.*, in preparation

Consistent with recent shell-model studies
F. Nowacki *et al.*, PRL 117, 272501 (2016)

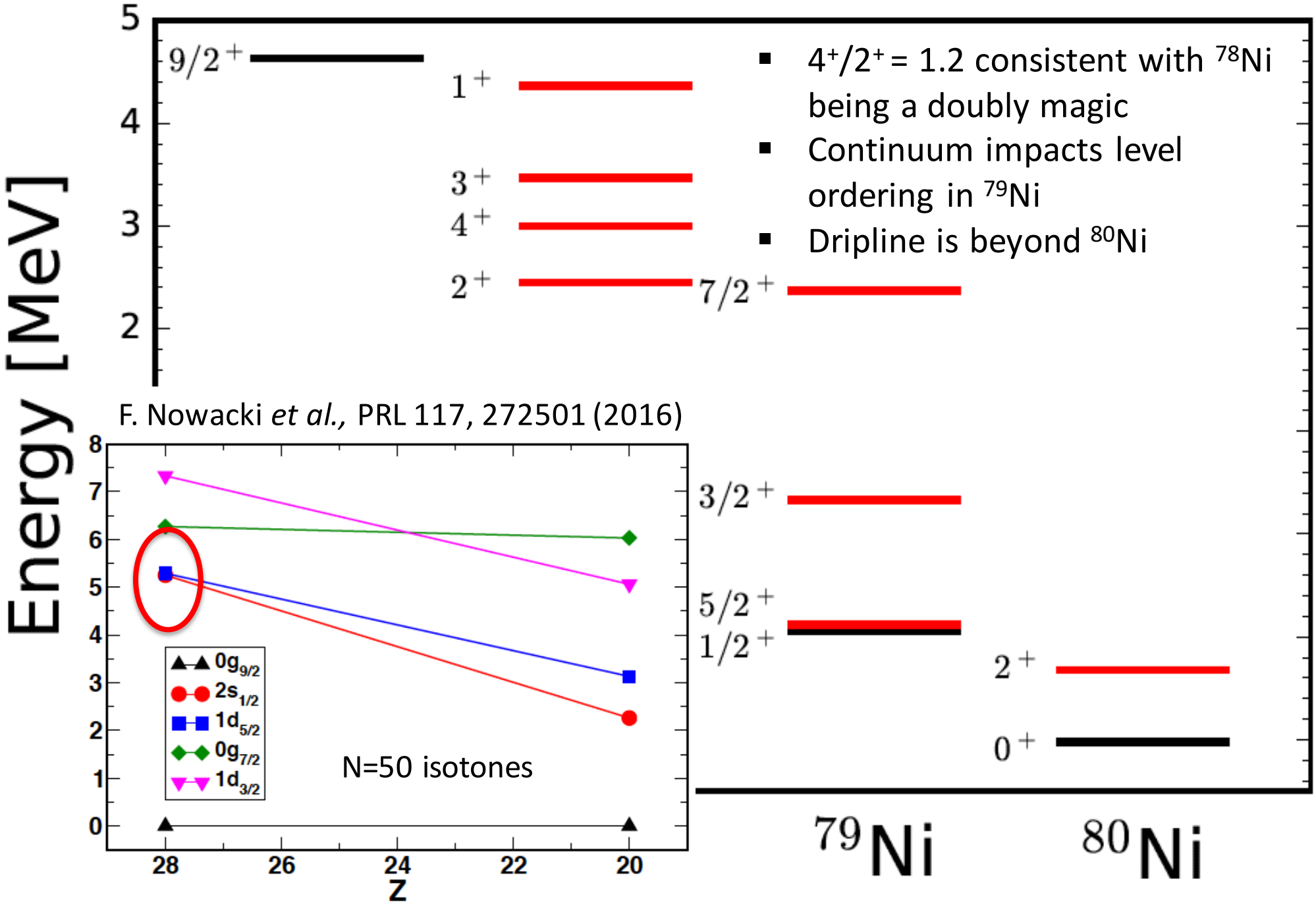
- From an observed correlation we predict the 2^+ excited state in ^{78}Ni using the experimental data for the 2^+ state in ^{48}Ca
- Similar correlations have been observed in other nuclei, e.g. Tjon line in light nuclei



G. Hagen, G. R. Jansen, and T. Papenbrock
Phys. Rev. Lett. **117**, 172501 (2016)

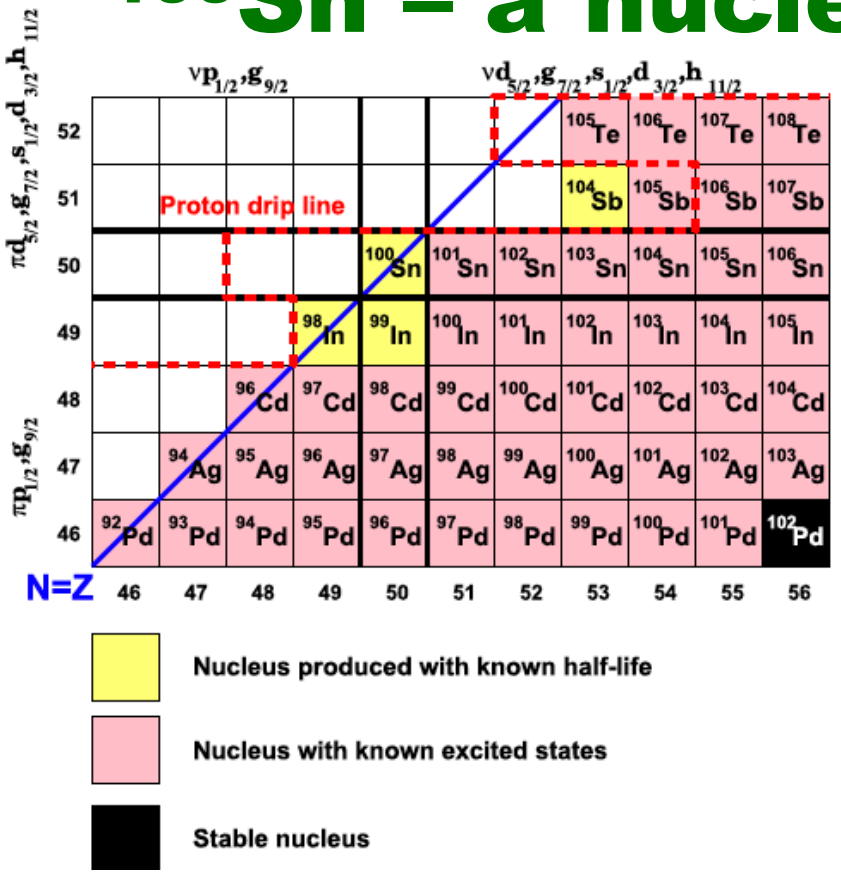
Excited states in ^{78}Ni and its neighbors

- $4^+/2^+$ = 1.2 consistent with ^{78}Ni being a doubly magic
- Continuum impacts level ordering in ^{79}Ni
- Dripline is beyond ^{80}Ni

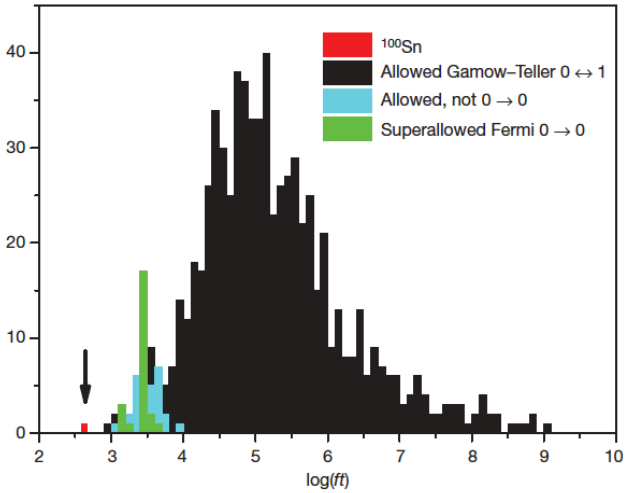


F. Nowacki *et al.,* PRL 117, 272501 (2016)

^{100}Sn – a nucleus of superlatives



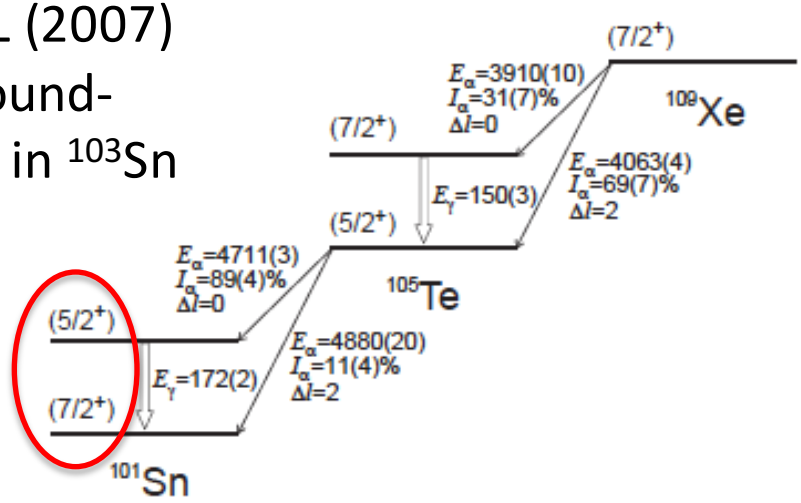
- Heaviest self-conjugate doubly magic nucleus
- Largest known strength in allowed nuclear β-decay
- In the closest proximity to the proton dripline
- At the endpoint of the rapid proton capture process (Sn-Sb-Te cycle)
- Unresolved controversy regarding s.p. structure of ^{101}Sn



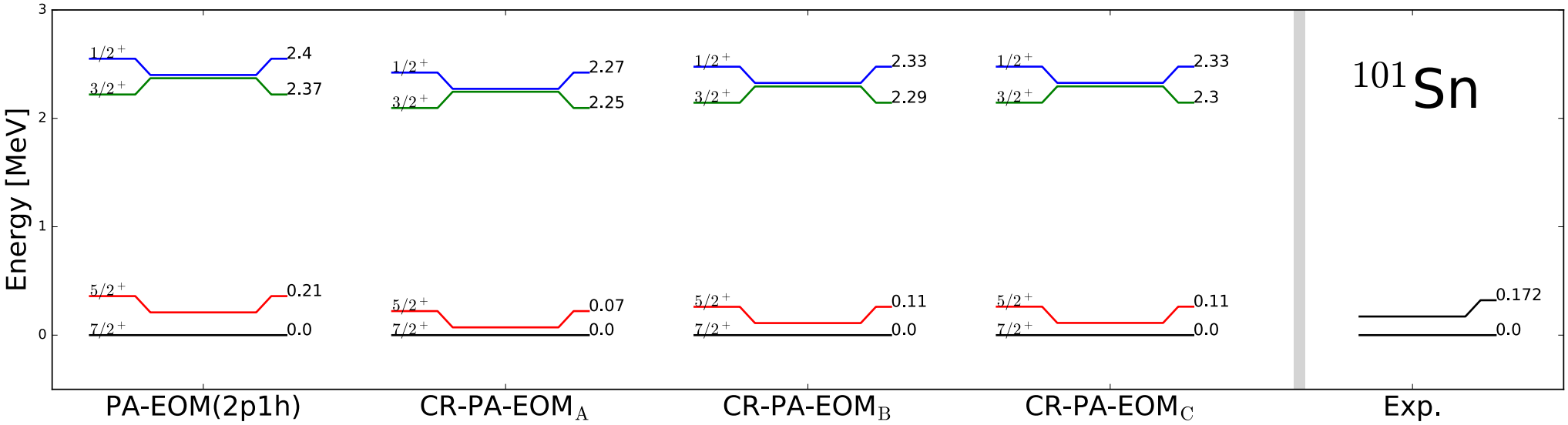
Hinke et al, Nature (2012)

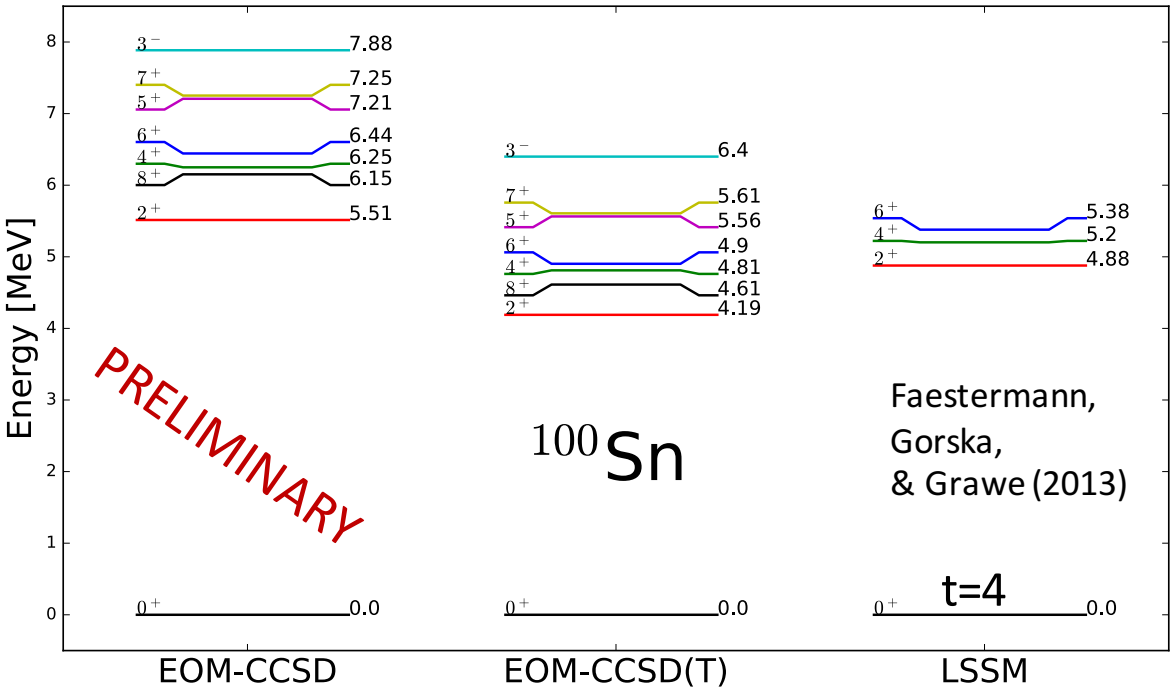
Sewernyiak et al PRL (2007) predicted a 5/2+ ground-state as presumably in ^{103}Sn

Darby et al, PRL (2010)



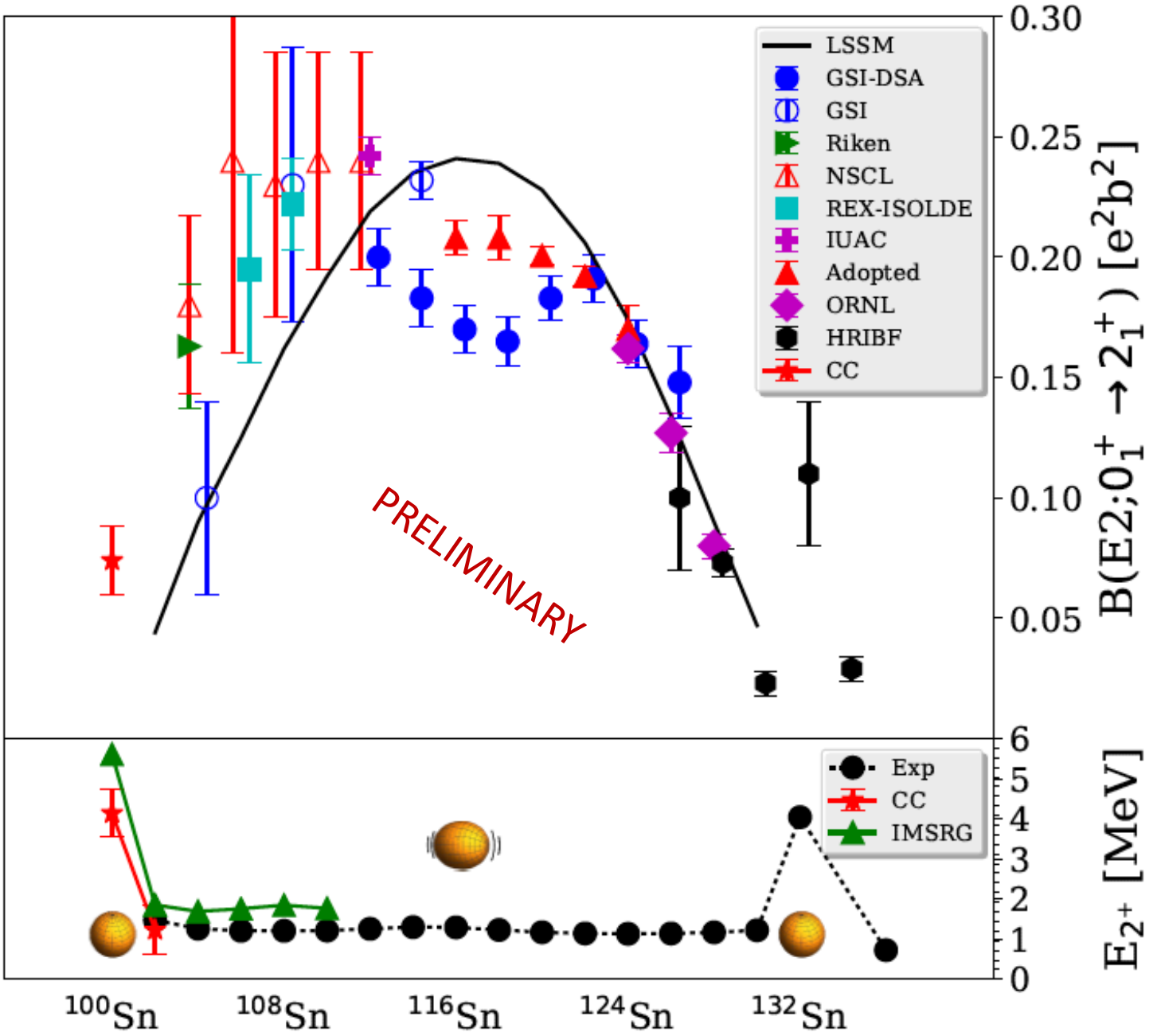
Structure of the ligthest tin isotopes



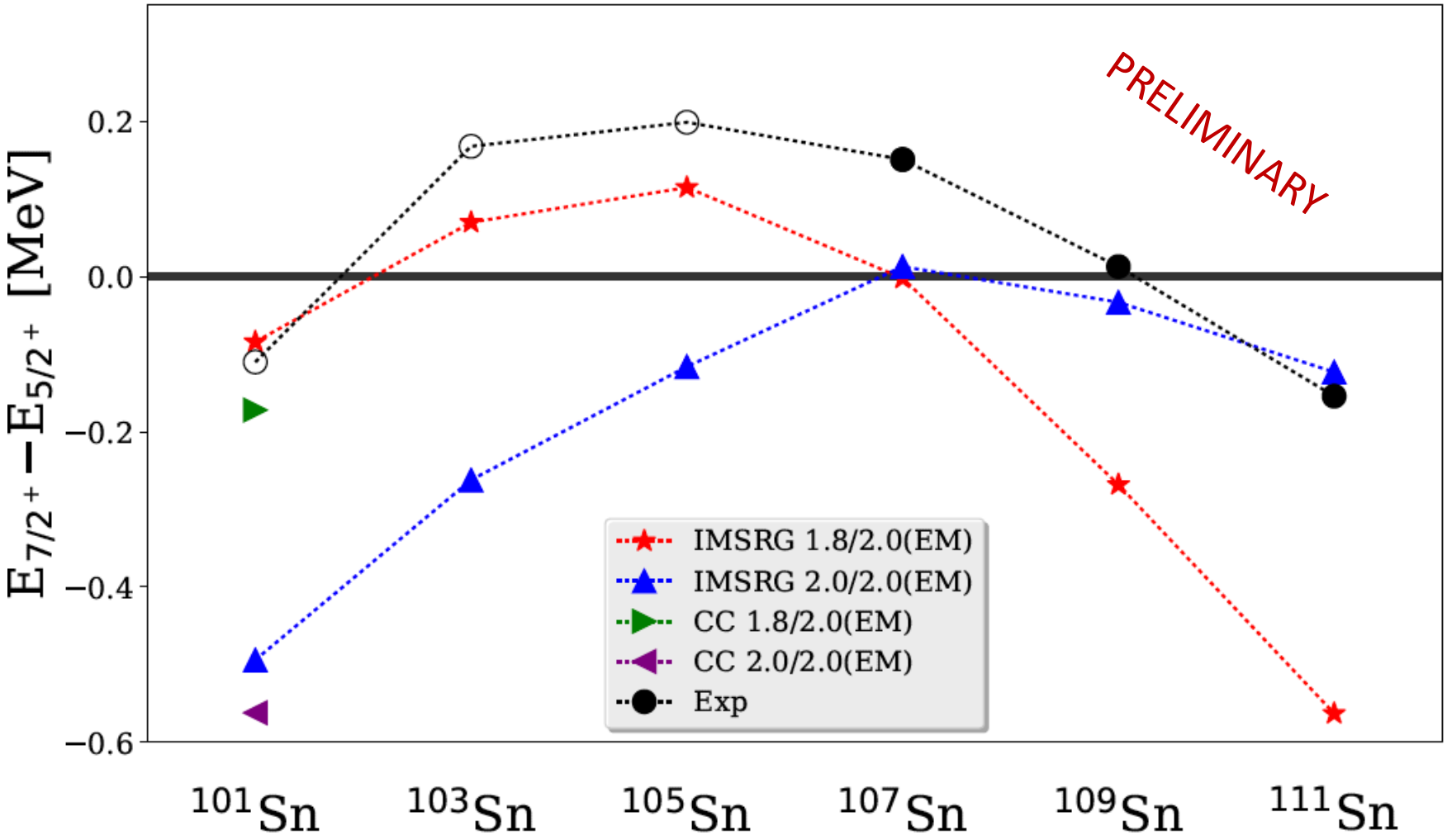


- High 2^+ energy in ^{100}Sn
- Predict $7/2^+$ ground-state in ^{101}Sn
- Experimental splitting between $7/2^+$ and $5/2^+$ reproduced
- Ground-state spins of $^{101\text{-}121}$Sn will be measured at CERN (CRIS collaboration)

Structure of the ligthest tin isotopes



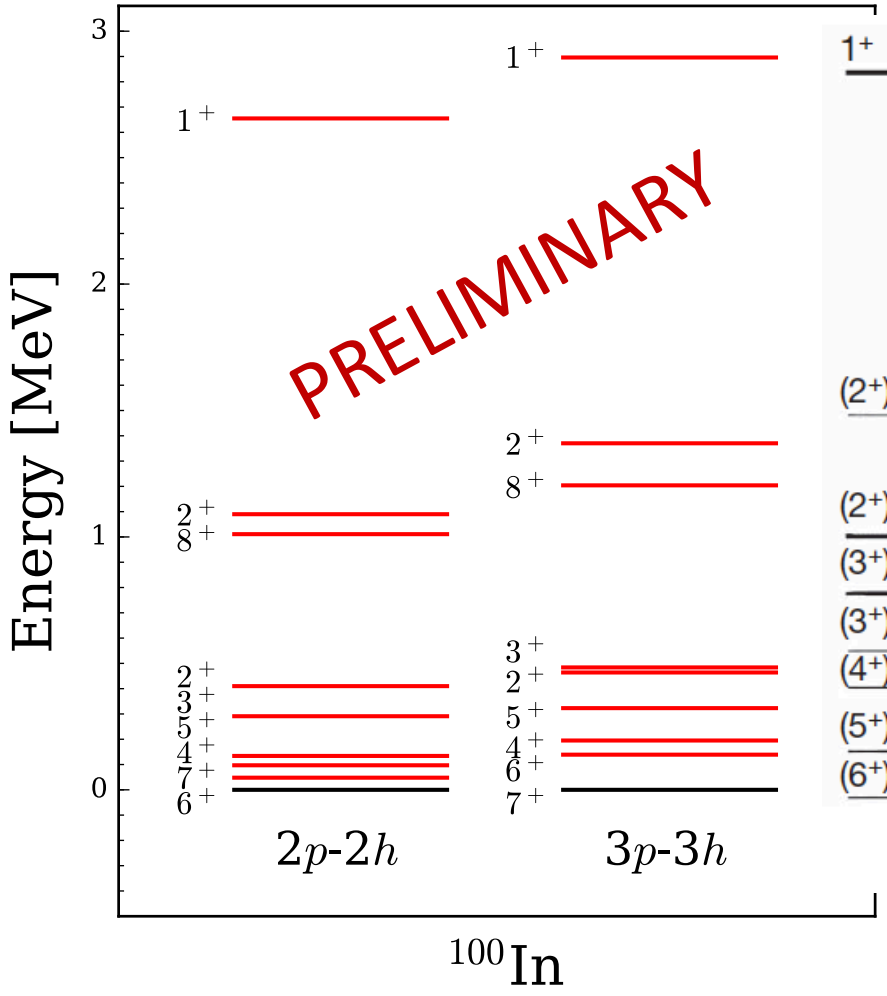
Structure of the ligthest tin isotopes

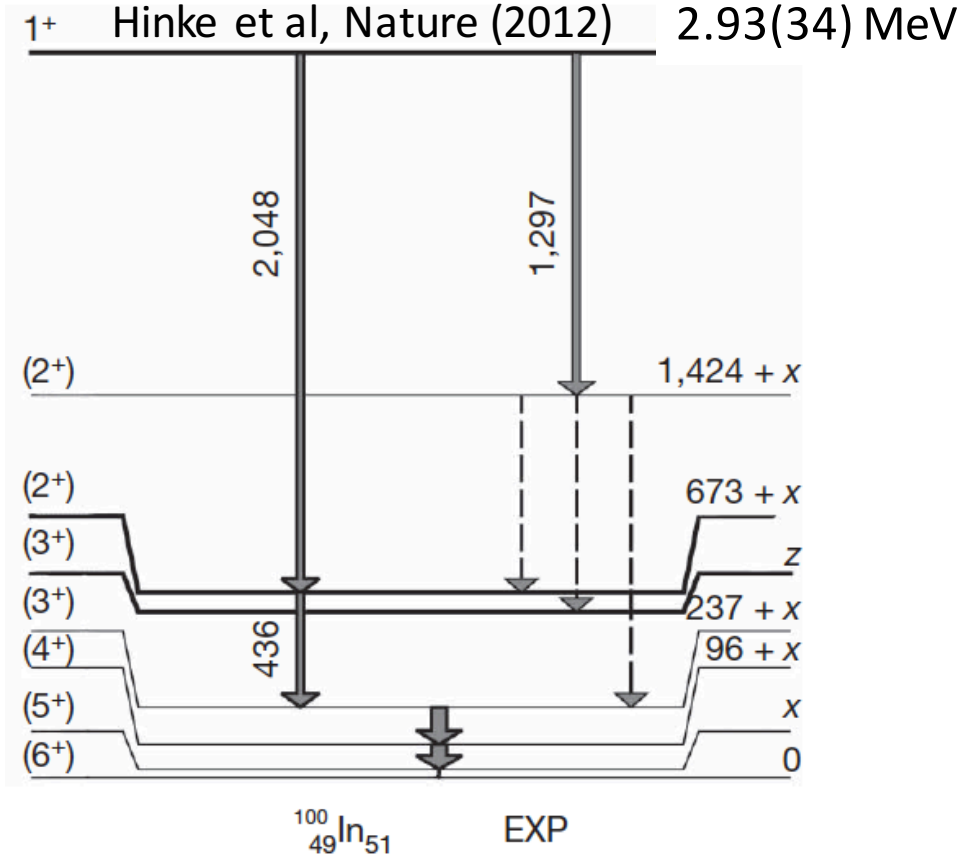


G.s. spin of ^{107}Sn correctly predicted to be 5/2+
[G. Cerizza et al Phys. Rev. C **93**, 021601 (2016)]

Importance truncated CI results from **C. Stumpf** and R. Roth, valence space effective interactions from **S. R. Stroberg** and J. Holt.

^{100}In from a novel charge exchange coupled-cluster equation-of-motion method





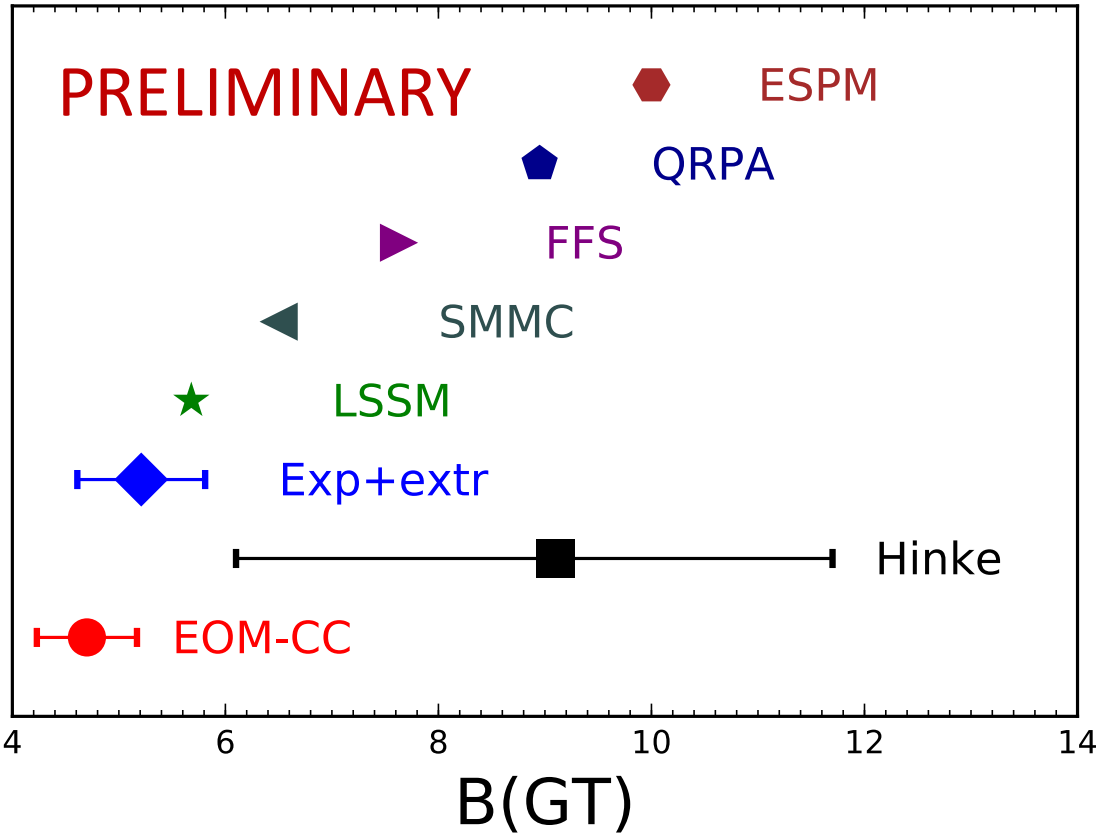
New method: 3p-3h charge-exchange EOM

$$\overline{H}_N R_\mu |\Phi_0\rangle = E_\mu R_\mu |\Phi_0\rangle$$

- Reproduce known 1^+ state at 2.93(34) MeV
- Predict a 7^+ ground-state for ^{100}In
- Ground-state spin of ^{100}In can be measured by CRIS collab. at CERN

Superallowed Gamow-Teller transition

- Prediction for the Gamow-Teller transition consistent with data
- Towards understanding the quenching of g_A
- Important implications for computations of $0\nu\beta\beta$ decay



Hinke et al, Nature (2012)

Model	Ref	unquenched	quenched
ESPM	[30]	17.78	10.00
MCSM	[8]	10.3	6.5
QRPA	[9]	8.95	
FFS	[9]	7.63	
extrapol.	[10]	9.8	5.2
SM+corr.	[7]	14.2	
LSSM	this work	~ 13.90	~ 7.82
LSSM (only 1_1^+)	this work	10.10	5.68

- Coupled-cluster computations predict a B(GT) of **4.7(5)**
- B(GT) is currently targeted by upcoming precision measurements

Summary

- Optical potentials from coupled-cluster theory – promising first results for ^{40}Ca+*n* with NNLO$_{sat}$
- Prediction of dipole polarizability of ^{48}Ca consistent with data
- ^{78}Ni is predicted to be doubly magic
- Structure and decay of ^{100}Sn