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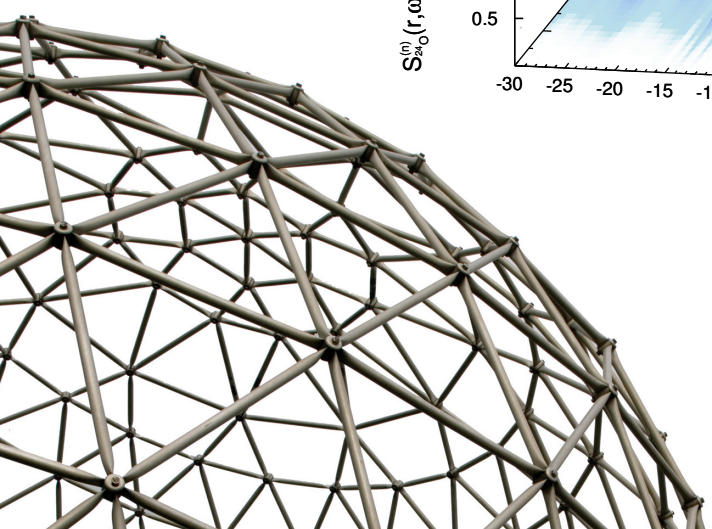
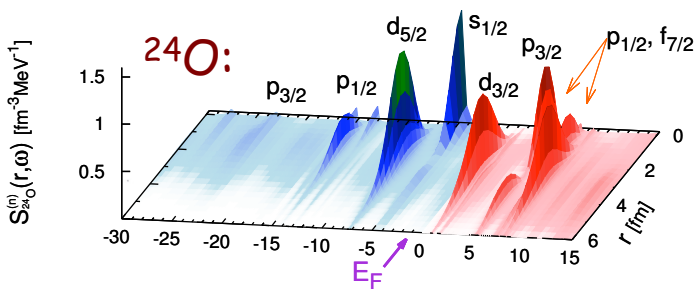
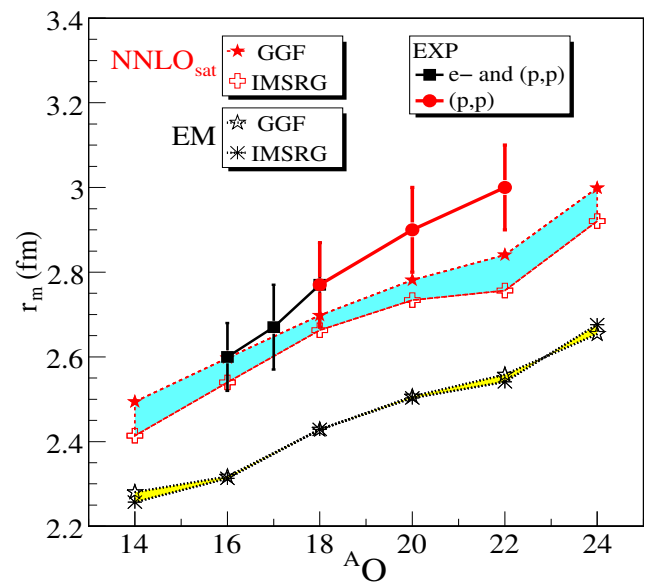
Self-Consistent Green's Function Calculations of Medium Mass Isotopes

Carlo Barbieri — University of Surrey

July 26th, 2016







Current Status of low-energy nuclear physics

Composite system of interacting fermions

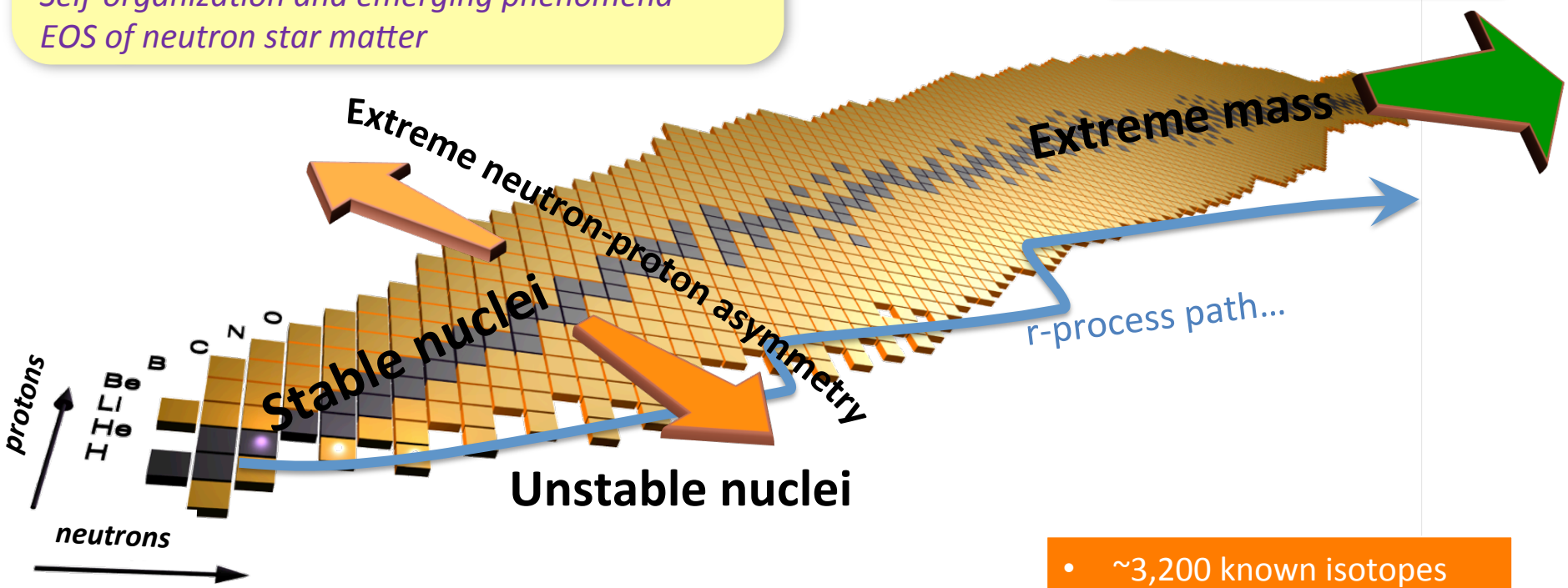
Binding and limits of stability

Coexistence of individual and collective behaviors

Self-organization and emerging phenomena

EOS of neutron star matter

Experimental programs
RIKEN, FAIR, FRIB



- ~3,200 known isotopes
- ~7,000 predicted to exist
- Correlation characterised in full for ~283 stable

Nature **473**, 25 (2011); **486**, 509 (2012)

Current Status of low-energy nuclear physics

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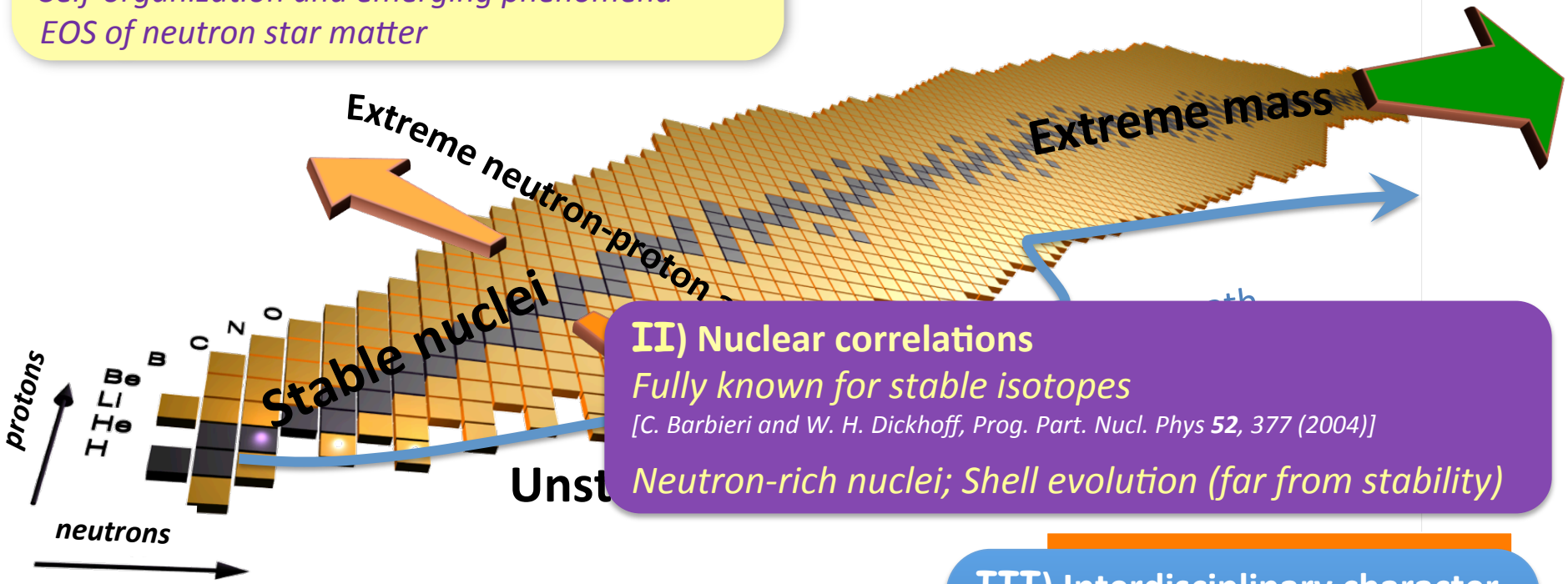


II) Nuclear correlations
Fully known for stable isotopes
*[C. Barbieri and W. H. Dickhoff, Prog. Part. Nucl. Phys **52**, 377 (2004)]*
Neutron-rich nuclei; Shell evolution (far from stability)

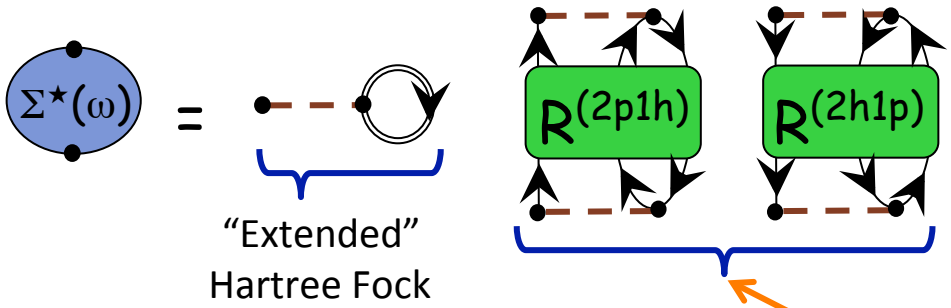
I) Understanding the nuclear force
QCD-derived; 3-nucleon forces (3NFs)
First principle (ab-initio) predictions

III) Interdisciplinary character
Astrophysics
Tests of the standard model
Other fermionic systems:
ultracold gasses; molecules;

The FRPA Method in Two Words

Particle vibration coupling is the main cause driving the distribution of particle strength—on both sides of the Fermi surface…

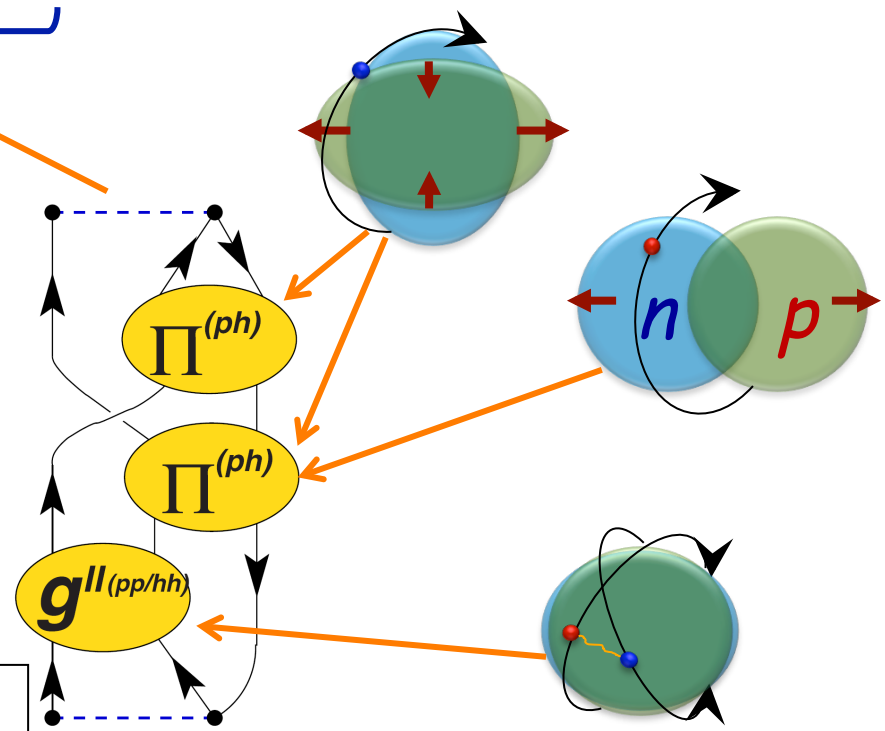
CB et al.,
*Phys. Rev. C**63**, 034313 (2001)*
*Phys. Rev. A**76**, 052503 (2007)*
*Phys. Rev. C**79**, 064313 (2009)*



- A complete expansion requires *all types* of particle-vibration coupling

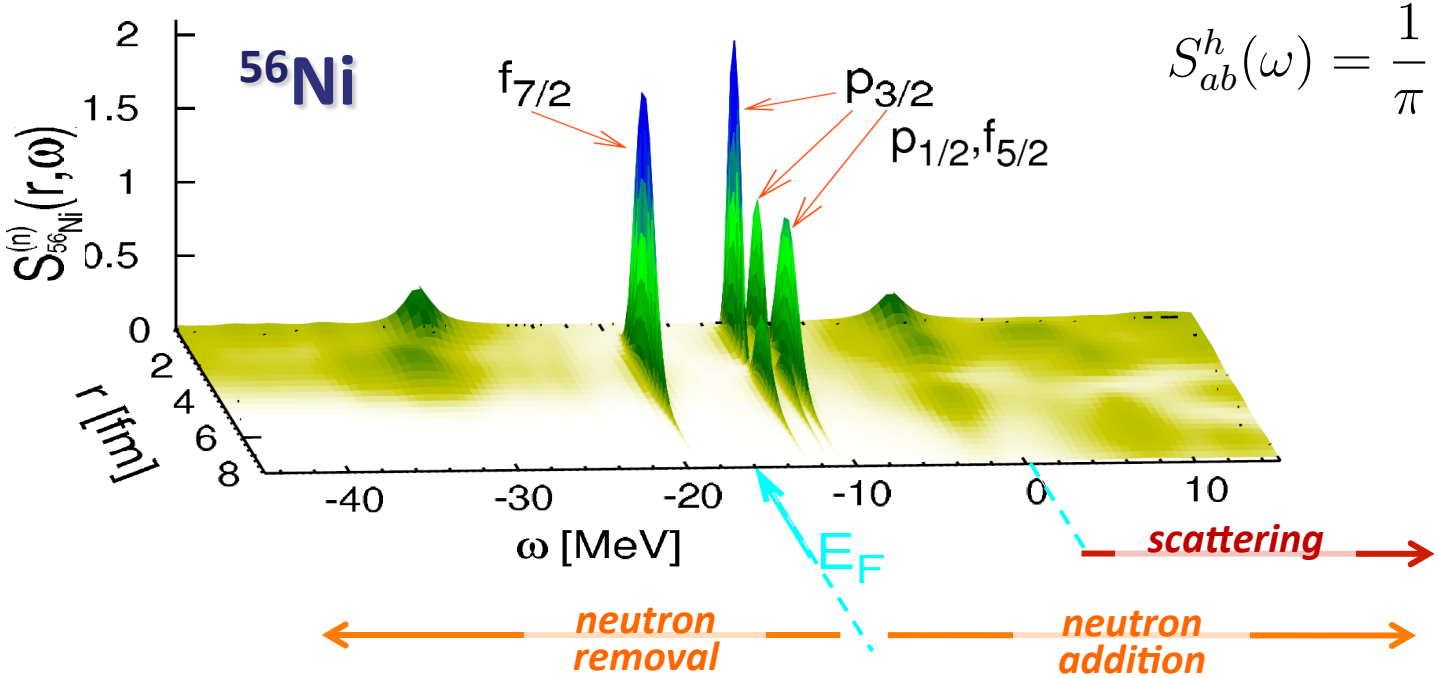
  …these modes are all resummed exactly and to all orders in a *ab-initio* many-body expansion.

- The Self-energy $\Sigma^{\star}(\omega)$ yields *both* single-particle states and scattering



≡ particle ≡ hole

^{56}Ni neutron spectral function



$$S^h_{ab}(\omega) = \frac{1}{\pi}\, Im\, g_{ab}(\omega)$$

W. Dickhoff, CB, Prog. Part. Nucl. Phys. 53, 377 (2004)
CB, M.Hjorth-Jensen, Pys. Rev. C**79**, 064313 (2009)

Approaches in GF theory

Truncation scheme:	Dyson formulation (closed shells)	Gorkov formulation (semi-/doubly-magic)
1st order:	Hartree-Fock	HF-Bogolioubov
2nd order:	2nd order	2nd order (w/ pairing)
. . .	. . .	
3rd and all-orders sums, P-V coupling:	ADC(3) FRPA etc…	G-ADC(3) …work in progress

Approaches in GF theory

Truncation scheme:

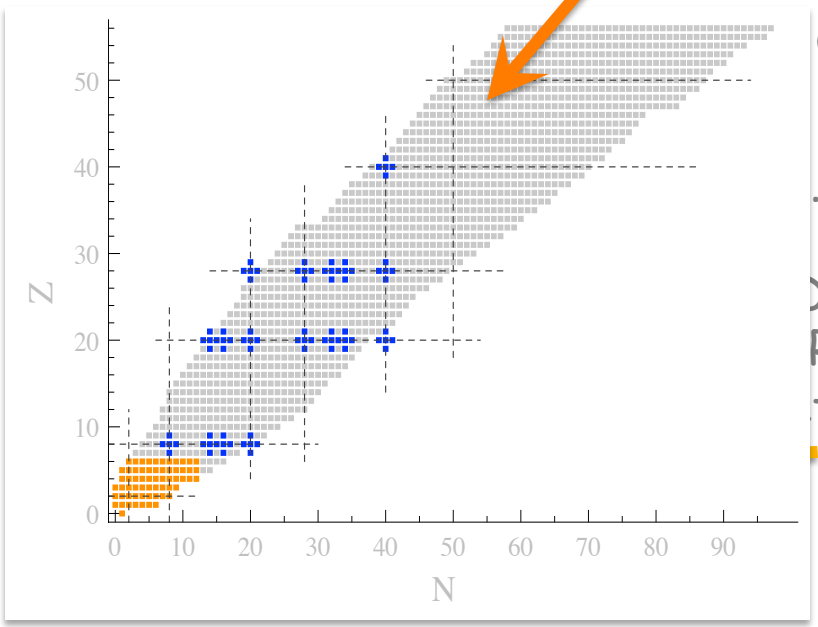
Dyson formulation (closed shells)

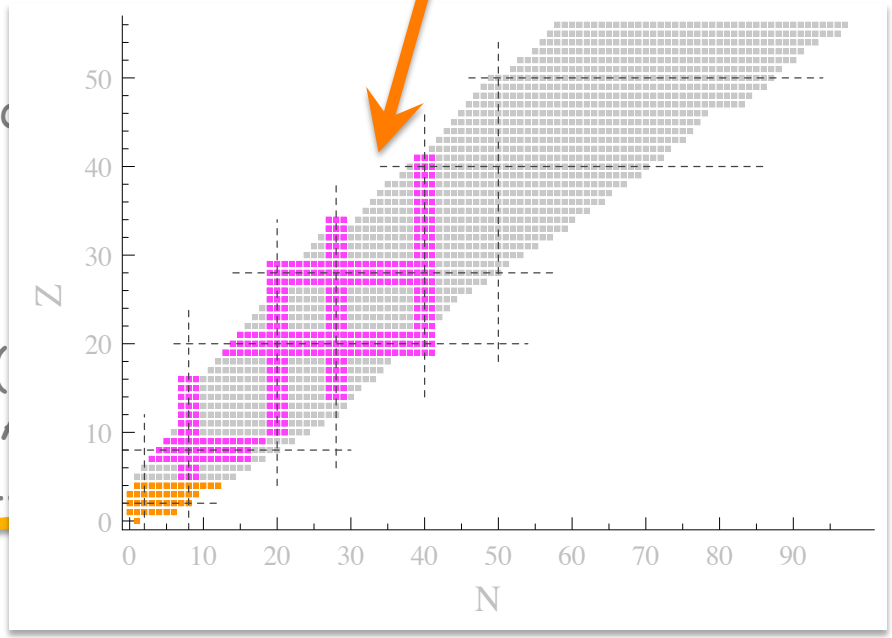
Gorkov formulation (semi-/doubly-magic)

1st order:

Hartree-Fock

HF-Bogolioubov

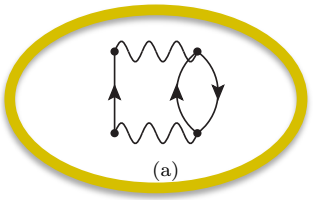


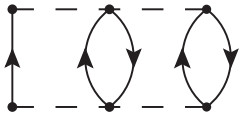


pics. credits: V. Somà

Inclusion of NNN forces

- *Second order* PT diagrams with 3BFs:





*A. Carbone, CB, et al., Phys. Rev. C**88**, 054326 (2013) and F. Raimondi, CB, in preparation (2016).*

- *Third order* PT diagrams with 3BFs:

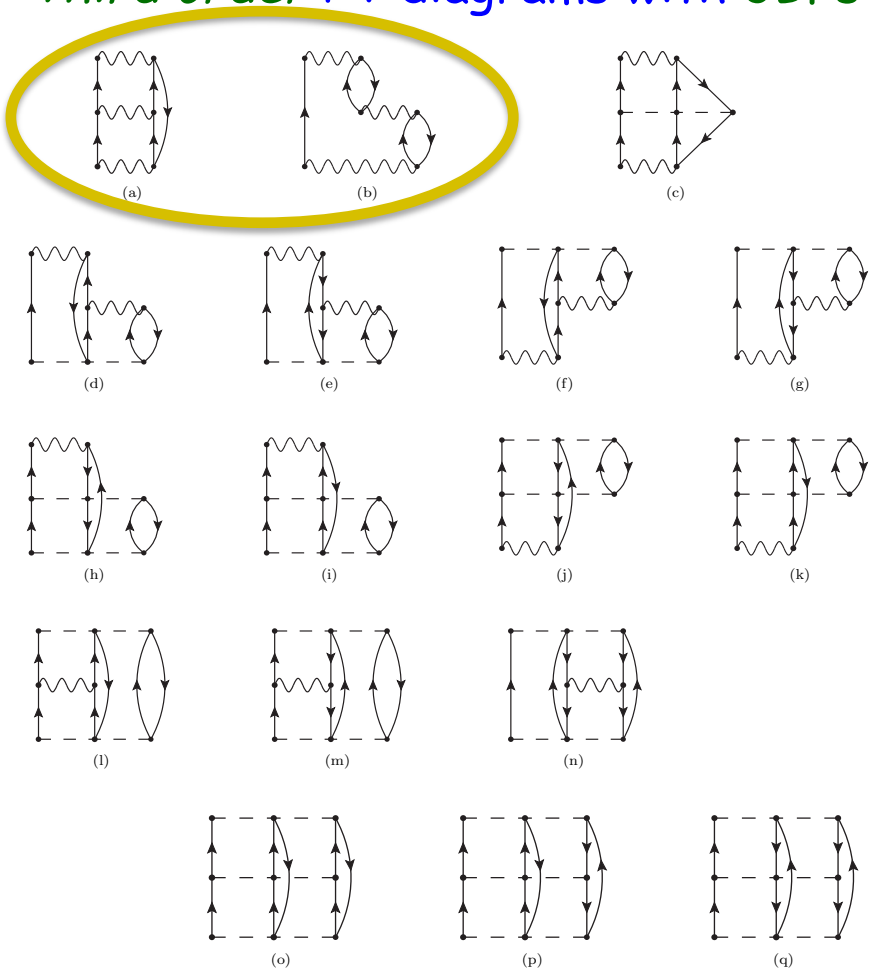


FIG. 5. 1PI, *skeleton* and *interaction irreducible* self-energy diagrams appearing at 3rd-order in perturbative expansion (7), making use of the effective hamiltonian of Eq. (9).

➔ Use of irreducible 2-body interactions

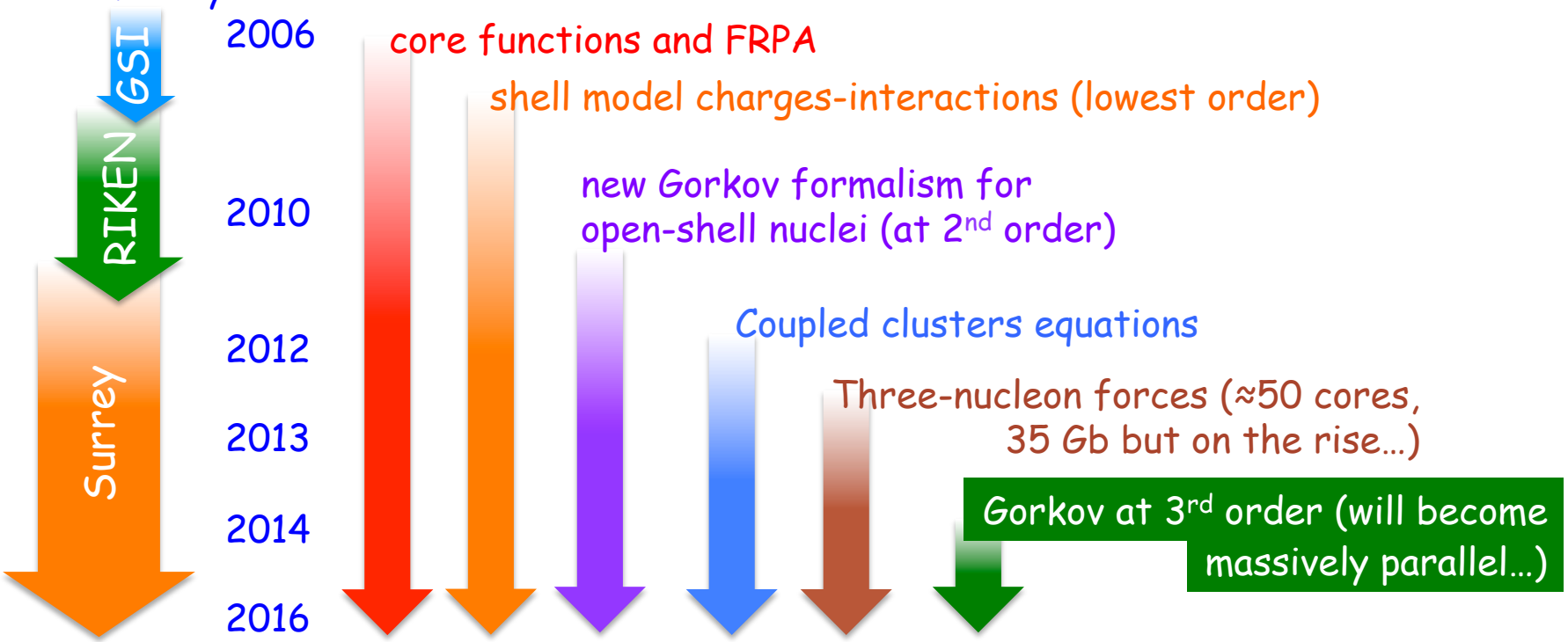
➔ Need to correct the Koltun sum rule (for energy)

Ab-initio Nuclear Computation & BcDor code

BoccaDorata code:
(C. Barbieri 2006-16
V. Somà 2011-14
A. Cipollone 2012-13)

- Provides a *C++ class library* for handling many-body propagators (≈40,000 lines, MPI&OpenMP based).
- Allows to solve for nuclear spectral functions, many-body propagators, RPA responses, coupled cluster equations and effective interaction/charges for the shell model.

Code history:

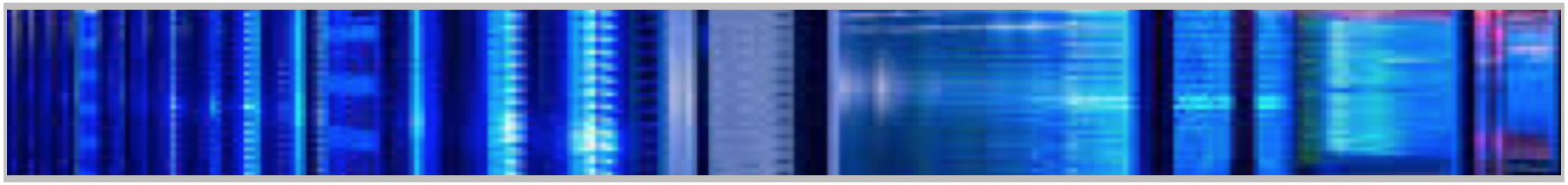


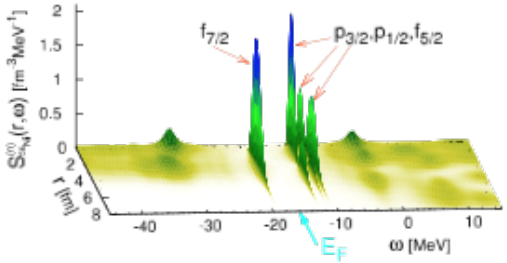
… applications …

Ab-initio Nuclear Computation & BcDor code

http://personal.ph.surrey.ac.uk/~cb0023/bcdor/

Computational Many-Body Physics





Download

Documentation

Welcome

From here you can download a public version of my self-consistent Green's function (SCGF) code for nuclear physics. This is a code in J-coupled scheme that allows the calculation of the single particle propagators (a.k.a. one-body Green's functions) and other many-body properties of spherical nuclei.

This version allows to:

- Perform Hartree-Fock calculations.
- Calculate the the correlation energy at second order in perturbation theory (MBPT2).
- Solve the Dyson equation for propagators (self consistently) up to second order in the self-energy.
- Solve coupled cluster CCD (doubles only!) equations.

When using this code you are kindly invited to follow the creative commons license agreement, as detailed at the weblinks below. In particular, we kindly ask you to refer to the publications that led the development of this software.

Relevant references (which can also help in using this code) are:

Prog. Part. Nucl. Phys. 52, p. 377 (2004),
Phys. Rev. A76, 052503 (2007),
Phys. Rev. C79, 064313 (2009),
Phys. Rev. C89, 024323 (2014)

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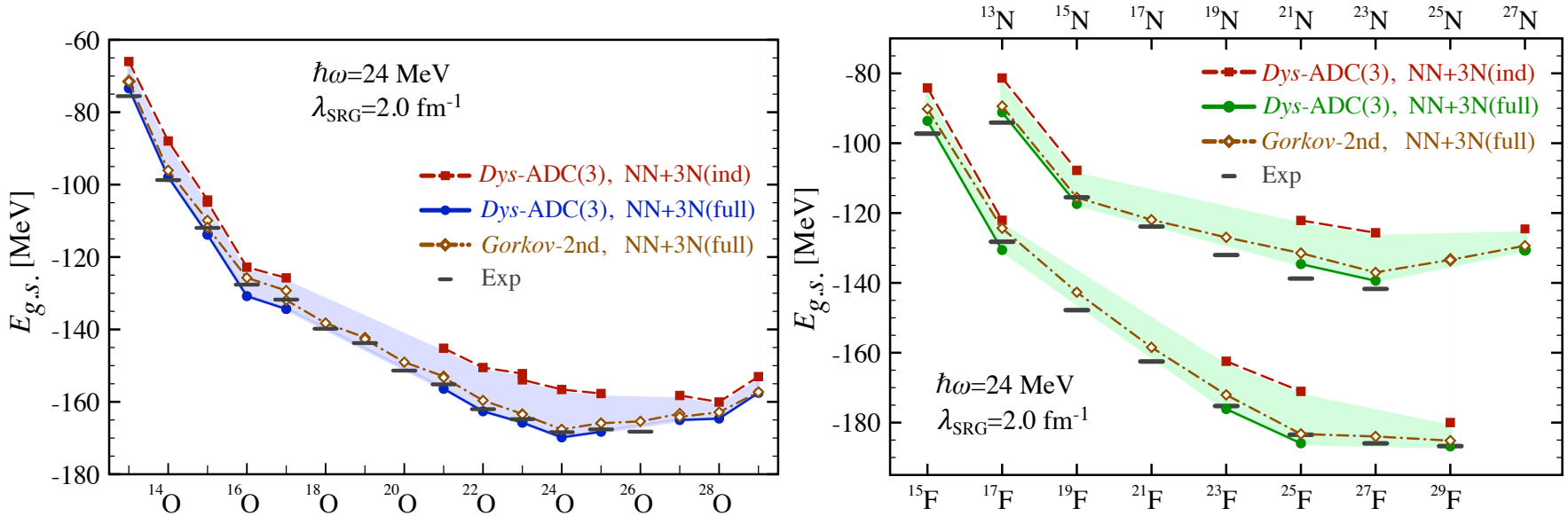
Results for the N-O-F chains

A. Cipollone, CB, P. Navrátil, Phys. Rev. Lett. **111**, 062501 (2013)
and Phys. Rev. C **92**, 014306 (2015)



→ 3NF crucial for reproducing binding energies and driplines around oxygen

→ cf. microscopic shell model [Otsuka et al, PRL**105**, 032501 (2010).]

N3LO (Λ = 500Mev/c) chiral NN interaction evolved to 2N + 3N forces (2.0fm^{-1})
N2LO (Λ = 400Mev/c) chiral 3N interaction evolved (2.0fm^{-1})

Inversion of $d_{3/2}$—$s_{1/2}$ at N=28

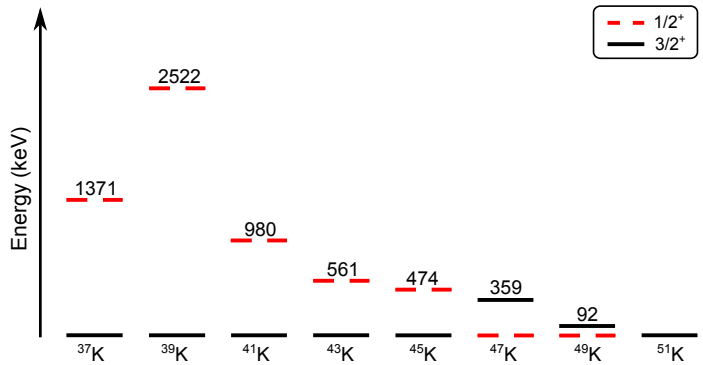


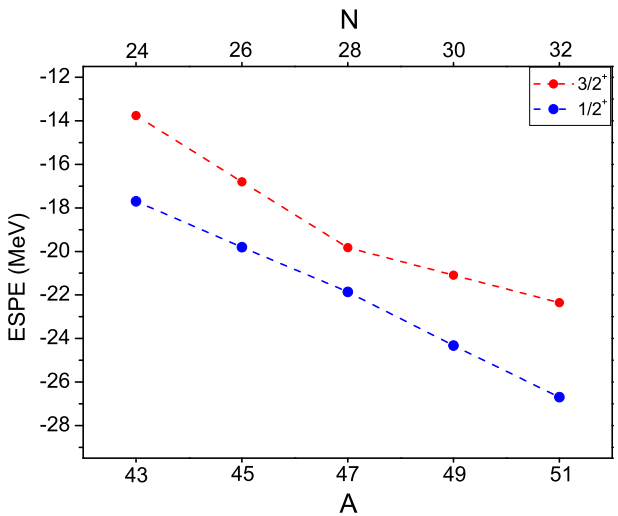
FIG. 1. (color online) Experimental energies for $1/2^+$ and $3/2^+$ states in odd-A K isotopes. Inversion of the nuclear spin is obtained in ^{47,49}K and reinversion back in ^{51}K. Results are

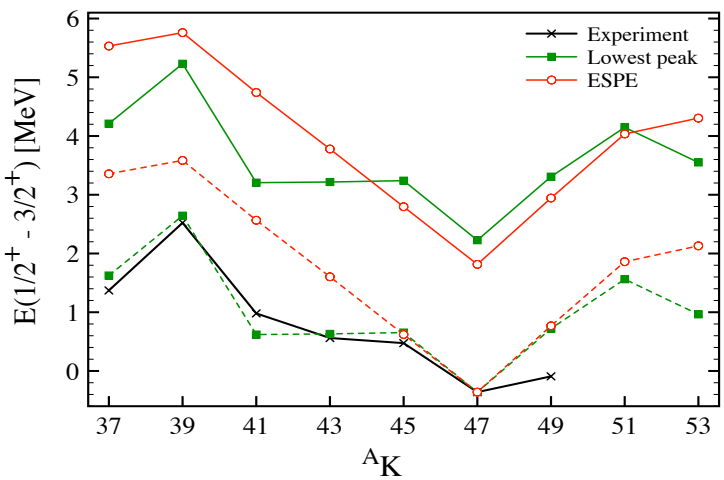
J. Papuga, et al., Phys. Rev. Lett. **110**, 172503 (2013);
J. Papuga, CB, et al., Phys. Rev. C **90**, 034321 (2014)

^{A}K isotopes

Laser spectroscopy @ ISOLDE

Change in separation described by chiral NN+3NF:



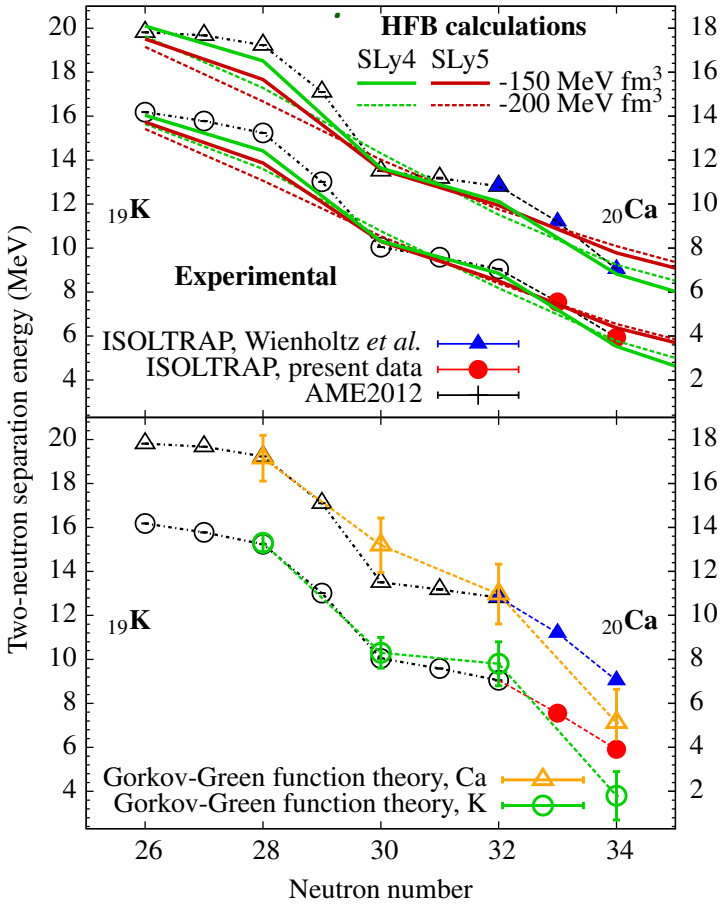


ESPE: "centroid" energies

(Gorkov calculations at 2nd order)

Two-neutron separation energies for neutron rich K isotopes

*M. Rosenbusch, CB, et al., PRL**114**, 202501 (2015)*



Measurements @ ISOLTRAP

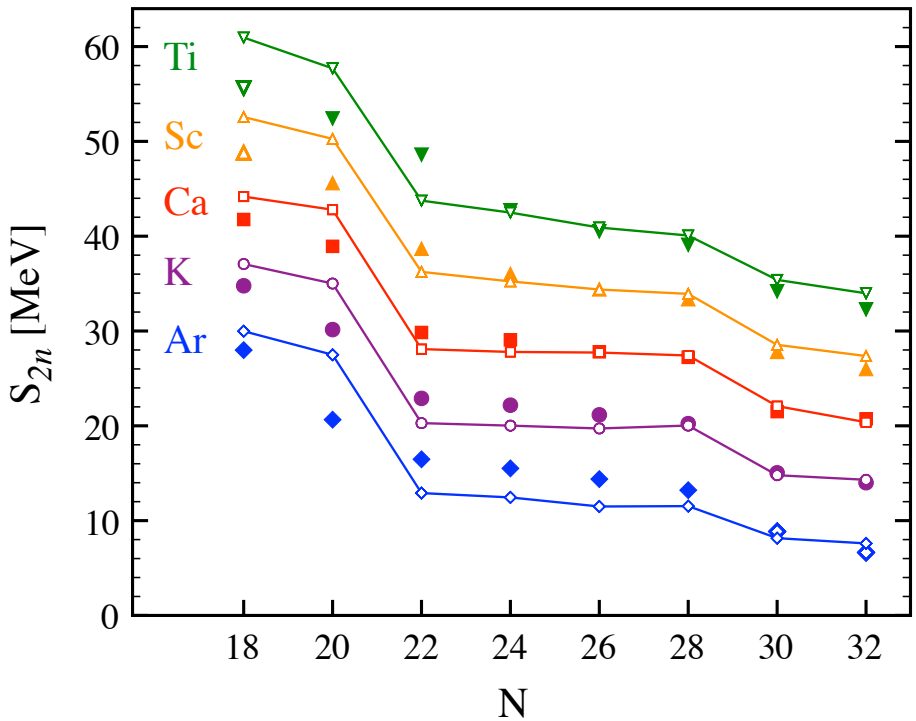
Theory tend to overestimate the gap at N=34, but overall good

→ *Error bar in predictions* are from extrapolating the many-body expansion to convergence of the model space.

Neighbouring Ar, K, Ca, Sc, and Ti chains

V. Somà, CB *et al.* Phys. Rev. C**89**, 061301R (2014)

Two-neutron separation energies predicted by chiral NN+3NF forces:



→ First *ab-initio* calculation over a contiguous portion of the nuclear chart—open shells are now possible through the Gorkov-GF formalism

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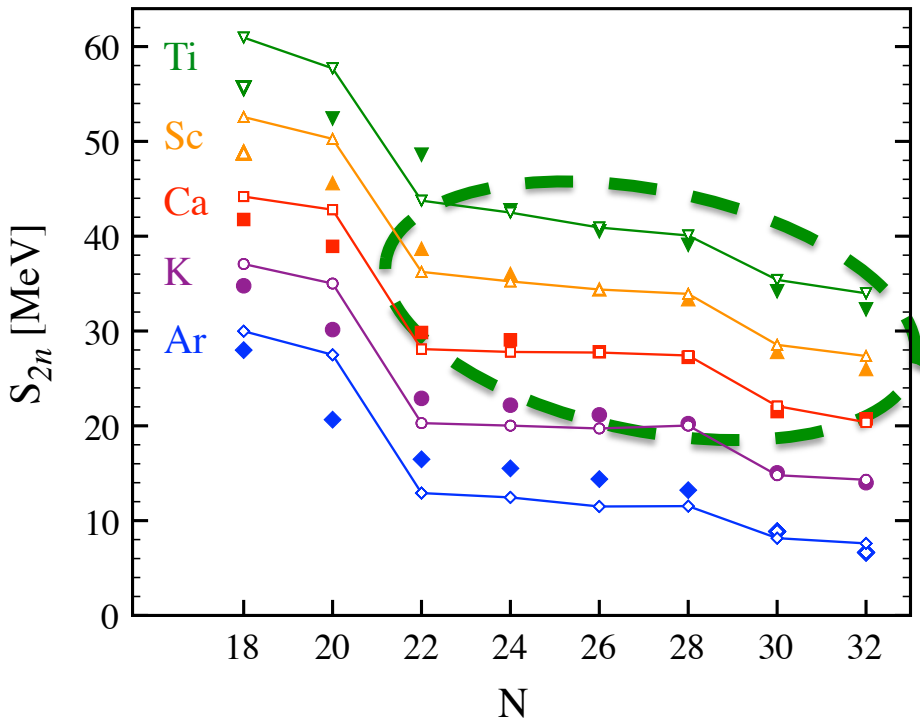

Works well in the *pf* shell

→ First *ab-initio* calculation over a contiguous portion of the nuclear chart—open shells are now possible through the Gorkov-GF formalism

Neighbouring Ar, K, Ca, Sc, and Ti chains

V. Somà, CB *et al.* Phys. Rev. C**89**, 061301R (2014)

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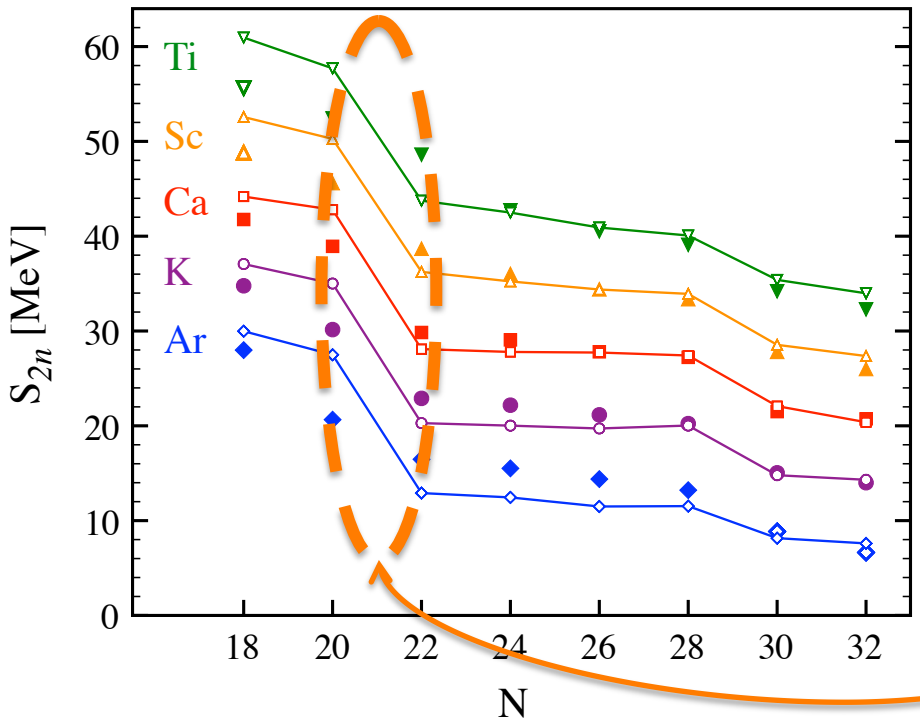


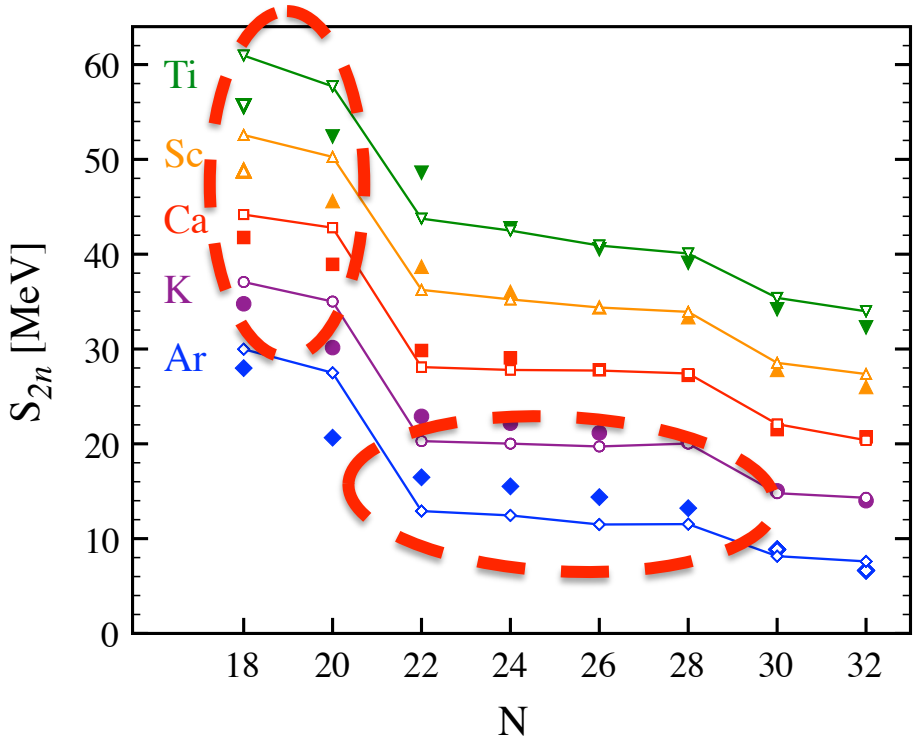
Over estimated
N=20 and Z=20 gaps

→ First *ab-initio* calculation over a contiguous portion of the nuclear chart—open shells are now possible through the Gorkov-GF formalism

Neighbouring Ar, K, Ca, Sc, and Ti chains

V. Somà, CB *et al.* Phys. Rev. C**89**, 061301R (2014)

Two-neutron separation energies predicted by chiral NN+3NF forces:

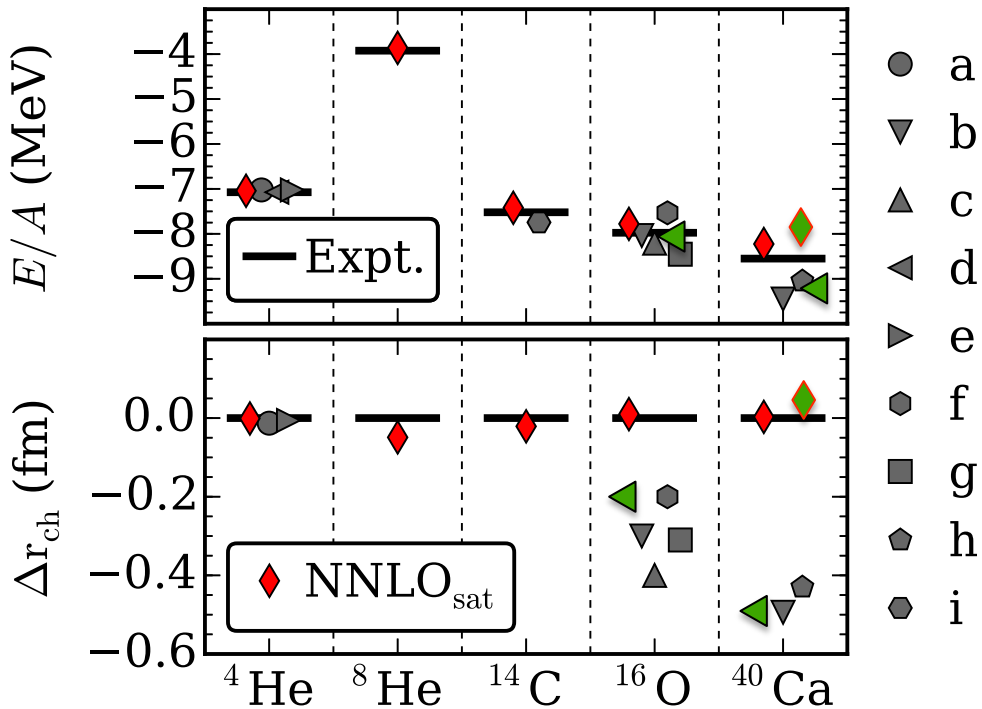


Lack of deformation due to quenched cross-shell quadrupole excitations

→ First *ab-initio* calculation over a contiguous portion of the nuclear chart—open shells are now possible through the Gorkov-GF formalism

NNLO-sat : a global fit up to A≈24

A. Ekström *et al.* Phys. Rev. C**91**, 051301(R) (2015)



- Constrain NN phase shifts

- Constrain radii and energies up to A≲24

➔ Provides saturation up to large masses!

NNLOsat (V2 + W3) -- *Grkv 2nd ord.*

From **SCGF:**

V2-N3LO(500) + W3-NNLO(400MeV/c) w/ SRG at 2.0 fm^{-1}
A. Cipollone, CB, P. Navrátil, Phys. Rev. Lett. **111**, 062501 (2013)
V. Somà, CB *et al.* Phys. Rev. C**89**, 061301R (2014)

BE and radii for Oxygens

- New fits of chiral interactions (NNLOsat) highly improve comparison to data

- Deficiencies remain for neutron rich isotopes

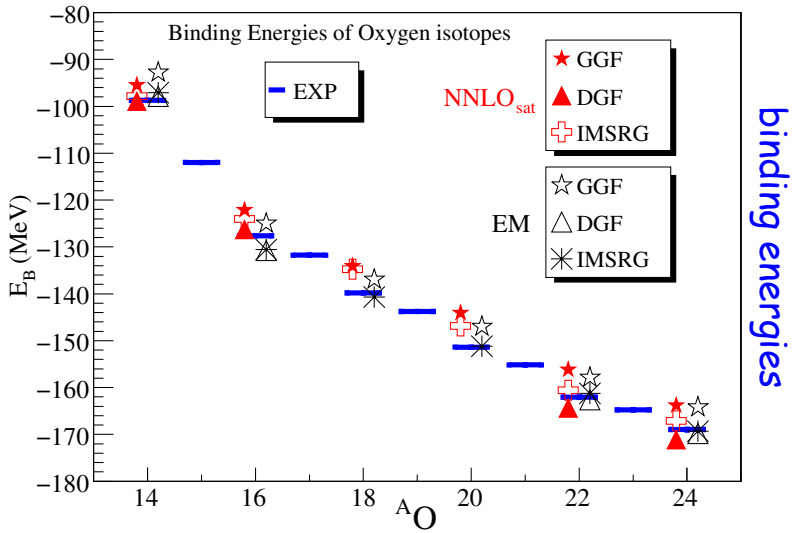
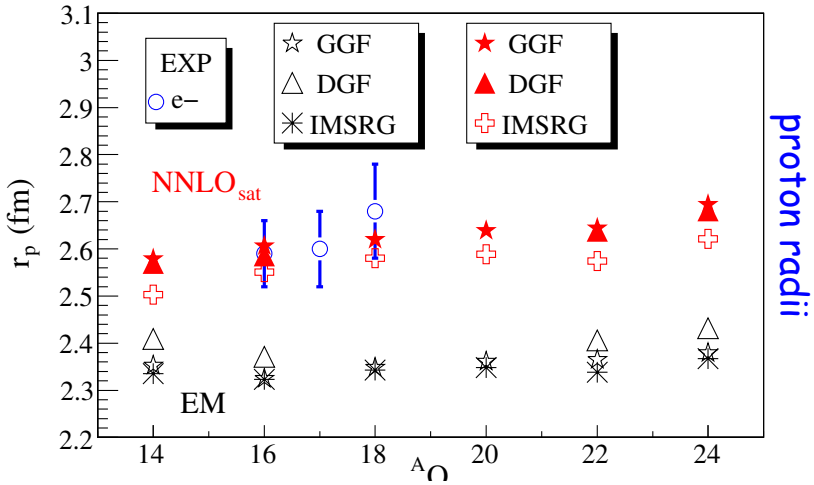
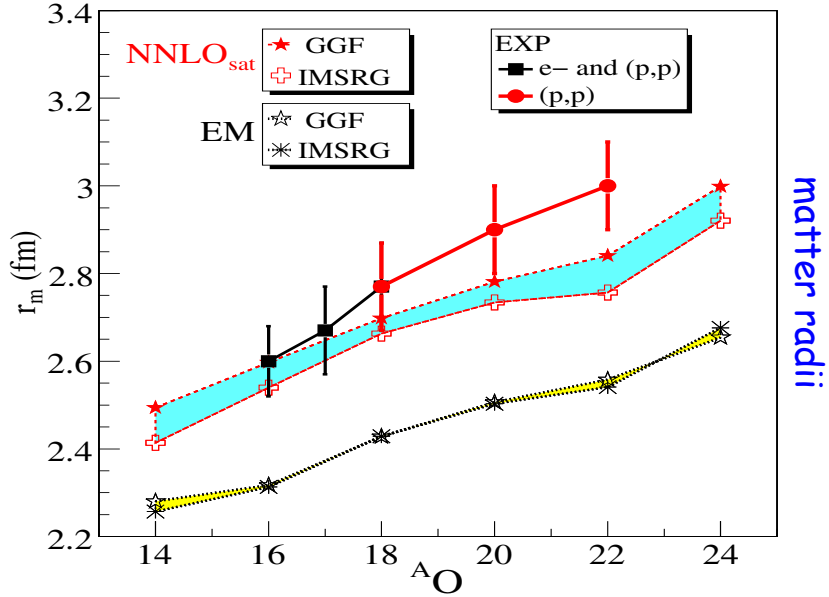


FIG. 1. Oxygen binding energies. Results from SCGF and IMSRG calculations performed with EM [20–22] and NNLO$_{sat}$ [26] interactions are displayed along with available experimental data.





V. Somà, V. Lapuox, CB, et al., Phys. Rev. Lett. (2016) -- *in press*

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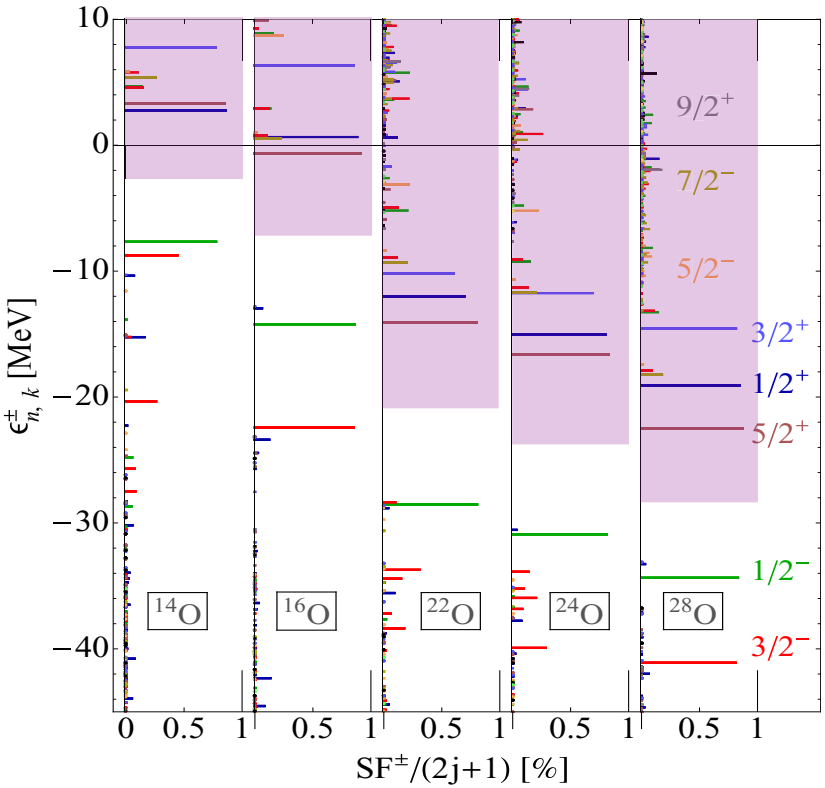
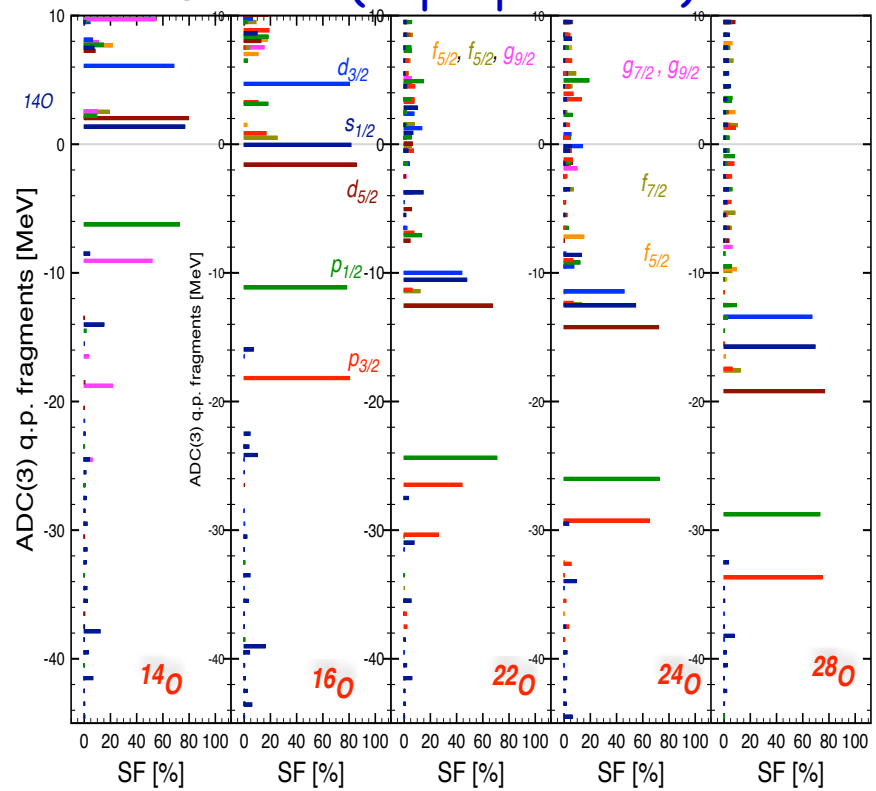
Proton spectral strength in Oxygen

A. Cipollone, CB, P. Navrátil, Phys. Rev. Lett. **111**, 062501 (2013)
and Phys. Rev. C **92**, 014306 (2015)
and ***in preparation***

EM-N3LO(500)/3NF-NNLO(400)



NNLO-sat (in preparation)

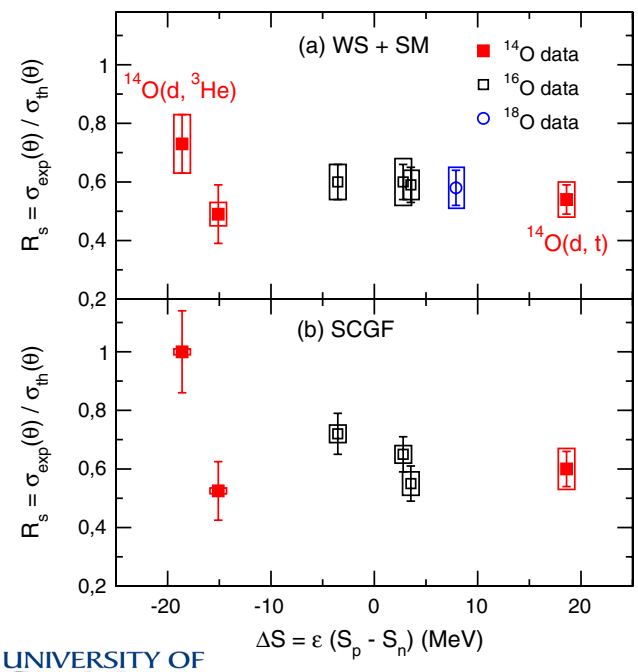


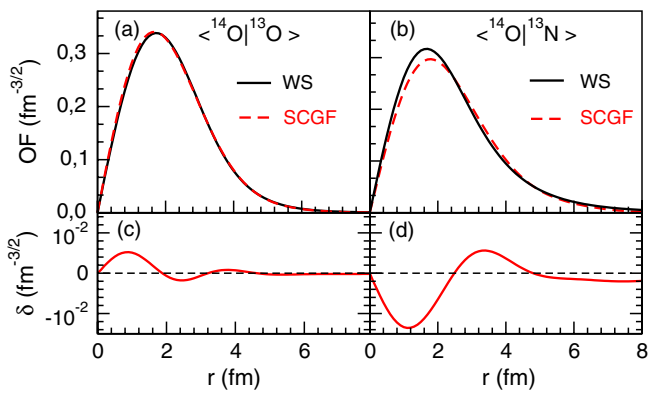
Single nucleon transfer in the oxygen chain

[F. Flavigny et al, PRL**110**, 122503 (2013)]

→ Analysis of $^{14}O(d,t)^{13}O$ and $^{14}O(d,^{3}He)^{13}N$ transfer reactions @ SPIRAL

Reaction	E^* (MeV)	J^π	R_{rms}^{HFB} (fm)	r_0 (fm)	C^2S_{exp} (WS)	C^2S_{th} $0p+2\hbar\omega$	R_s (WS)	C^2S_{exp} (SCGF)	C^2S_{th} (SCGF)	R_s (SCGF)
^{14}O (d, t) ^{13}O	0.00	$3/2^-$	2.69	1.40	1.69 (17)(20)	3.15	0.54(5)(6)	1.89(19)(22)	3.17	0.60(6)(7)
^{14}O $(d, {}^3He)$ ^{13}N	0.00	$1/2^-$	3.03	1.23	1.14(16)(15)	1.55	0.73(10)(10)	1.58(22)(2)	1.58	1.00(14)(1)
	3.50	$3/2^-$	2.77	1.12	0.94(19)(7)	1.90	0.49(10)(4)	1.00(20)(1)	1.90	0.53(10)(1)
^{16}O (d, t) ^{15}O	0.00	$1/2^-$	2.91	1.46	0.91(9)(8)	1.54	0.59(6)(5)	0.96(10)(7)	1.73	0.55(6)(4)
^{16}O $(d, {}^3He)$ ^{15}N [19,20]	0.00	$1/2^-$	2.95	1.46	0.93(9)(9)	1.54	0.60(6)(6)	1.25(12)(5)	1.74	0.72(7)(3)
	6.32	$3/2^-$	2.80	1.31	1.83(18)(24)	3.07	0.60(6)(8)	2.24(22)(10)	3.45	0.65(6)(3)
^{18}O $(d, {}^3He)$ ^{17}N [21]	0.00	$1/2^-$	2.91	1.46	0.92(9)(12)	1.58	0.58(6)(10)			

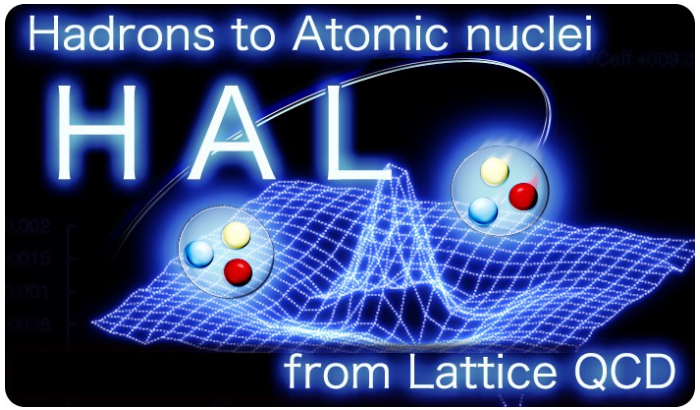




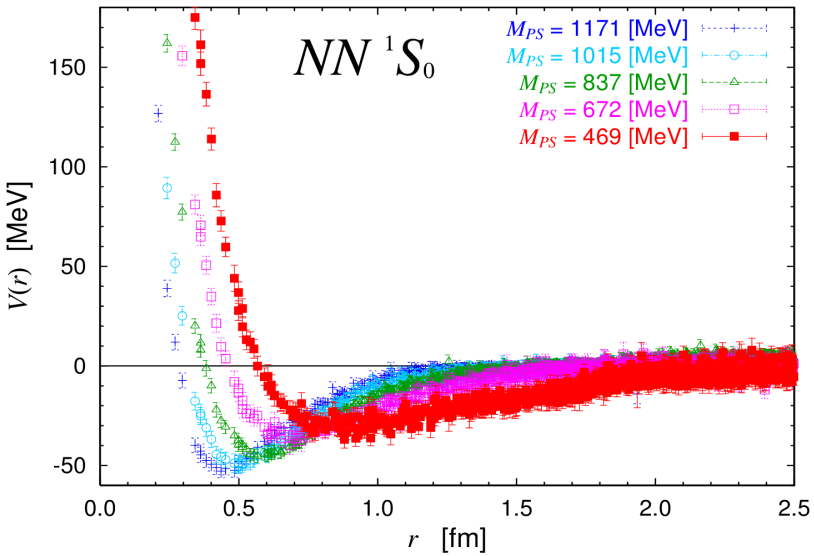
- Overlap functions and strengths from GF
- Rs independent of asymmetry

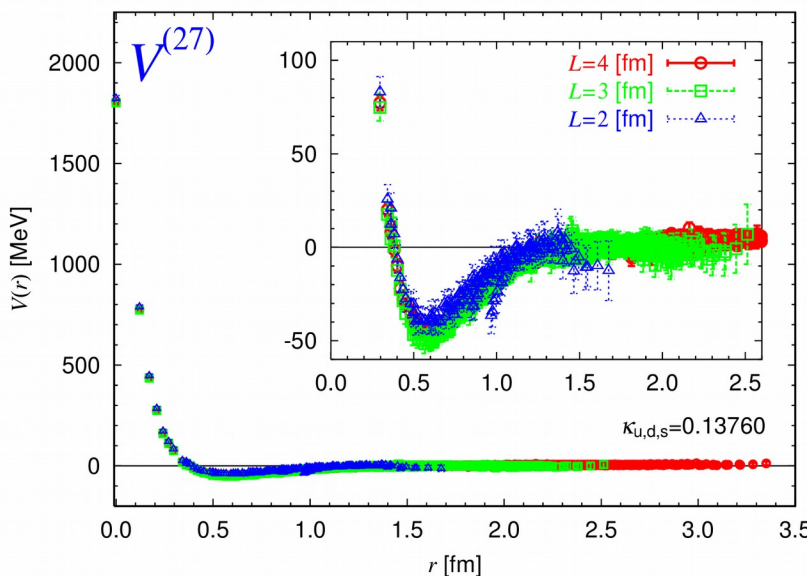
Study of nuclear interactions from Lattice QCD

In collaboration with:



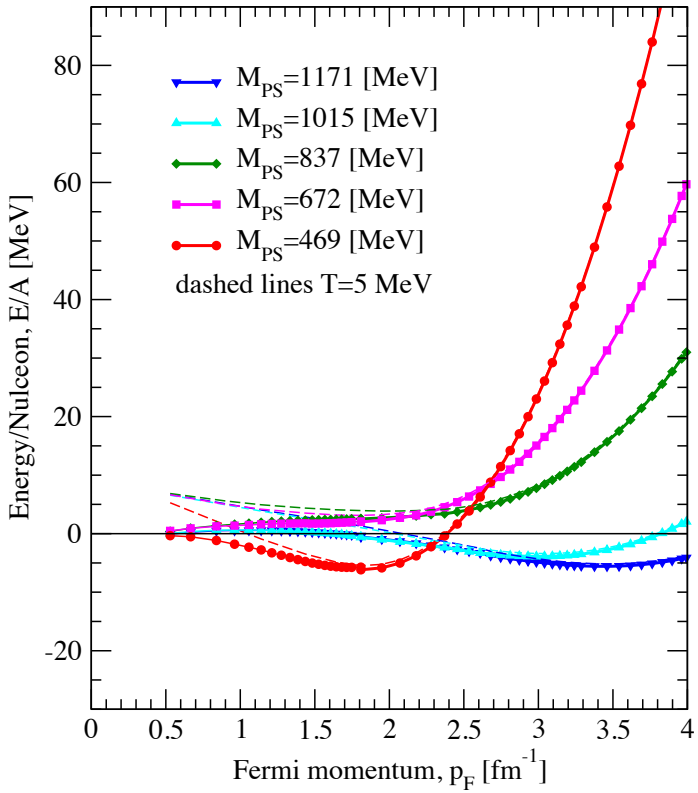
Two-Nucleon HAL potentials





Quark mass dependence of *V(r)* for NN partial wave ($^1S_0$, $^3S_1$, $^3S_1$-$^3D_1$)

➔ Potentials become stronger m_π as decreases.



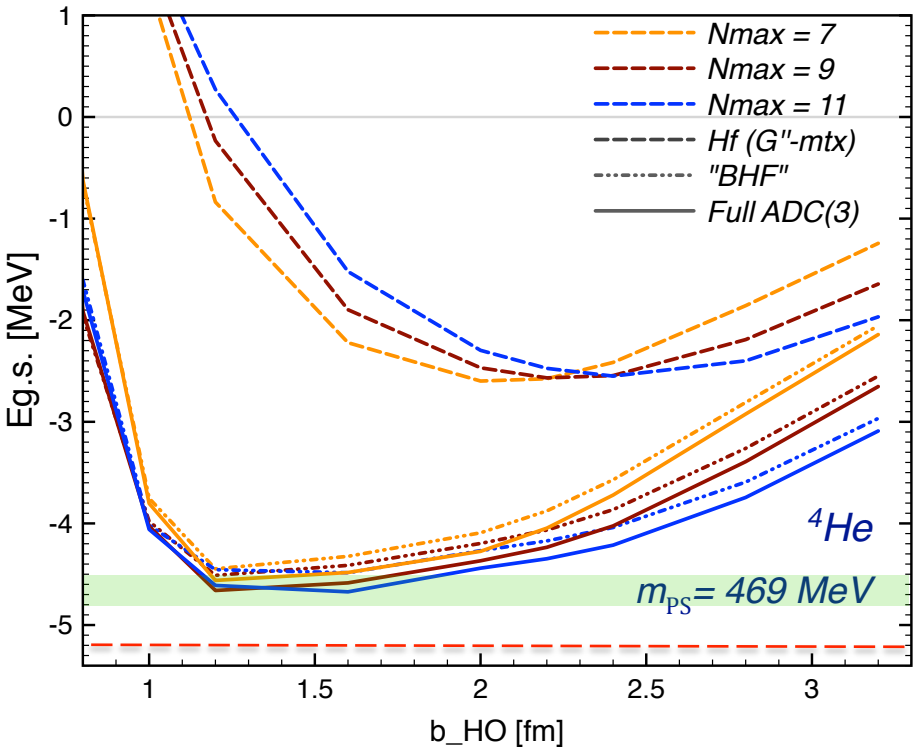
T. Inoue *et al.*,
Phys. Rev. Lett. **111** 112503 (2013).

UNIVERSITY OF SURREY

Prog. Theor. Exp. Phys. 01A105 (2012)

(Finite-T results by A. Carbone, priv. comm.)

Benchmark on ^{4}He

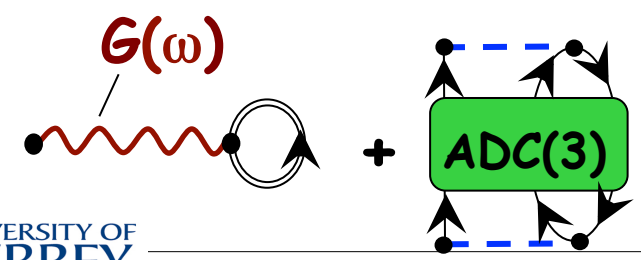


Can benchmark the Gmtx+ADC(3) method on light ^{4}He, where exact solutions are possible:

	G(ω) + ADC(3)	Exact
HALQCD @ m_π=469MeV	4.7(2) MeV	5.09 MeV[1]

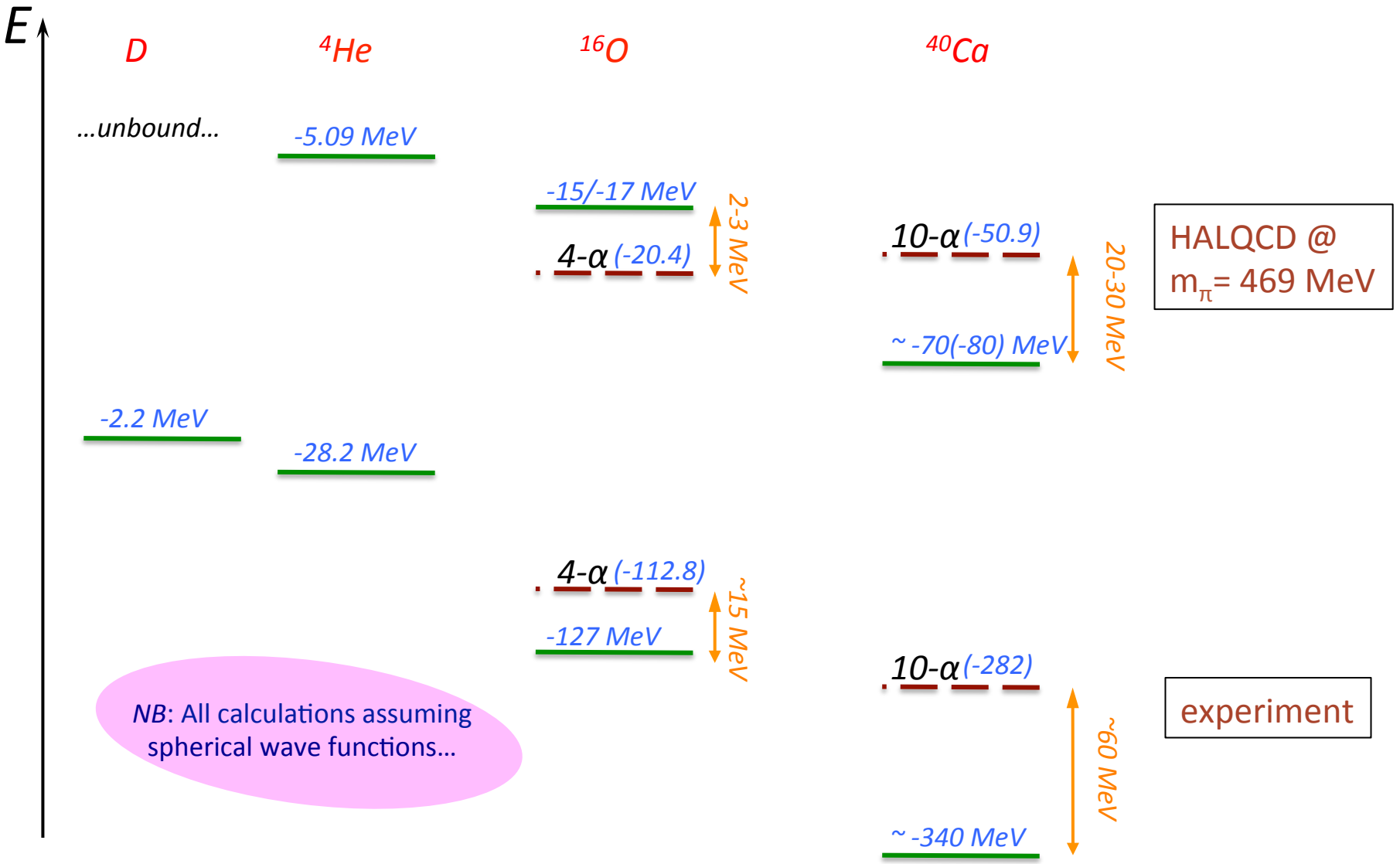
[1]H. Nemura *et al.*, Int. J. Mod. Phys. E **23**, 1461006 (2014)

➔ *Can expect accuracy on binding energies at about 10%*



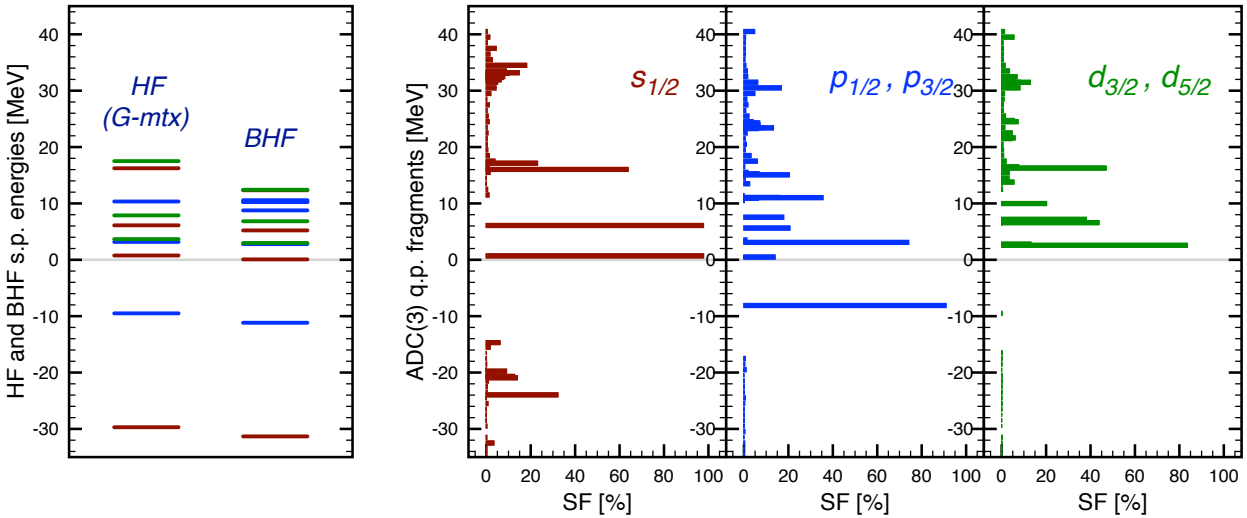
$$G''(\omega) = V + \int dk_a dk_b V \frac{\hat{Q}''}{\omega - \varepsilon(k_a) - \varepsilon(k_b) + i\eta} G''(\omega)$$

Results for binding



C. McIlroy, CB, et al., *in preparation*

Spectral strength in ^{16}O and ^{40}Ca:



Particle-hole gaps

^{16}O

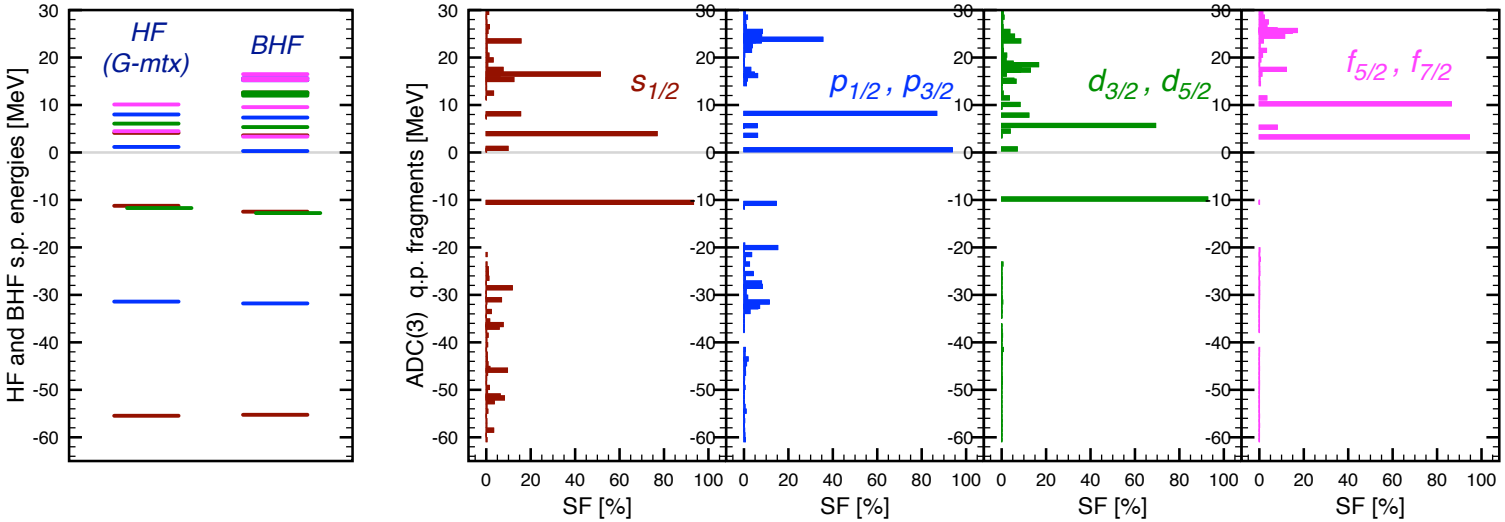
m_π= 469 MeV: ~8 MeV

Expt (phys m_π): 11.5 MeV

^{40}Ca

m_π= 469 MeV: ~10 MeV

Expt (phys m_π): 7.5 MeV

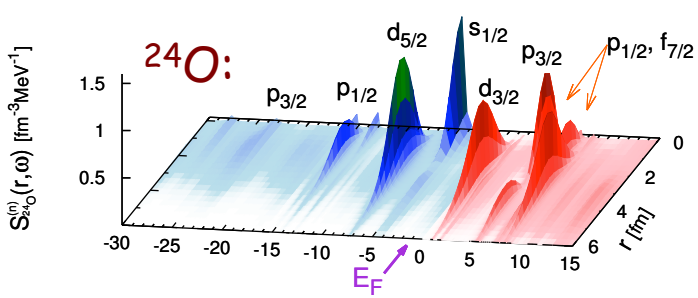


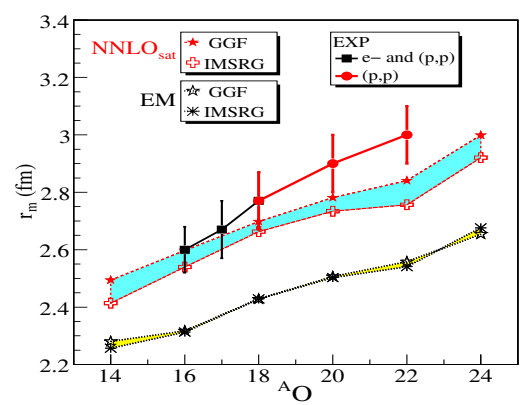
Summary

Thank you for your attention!!!

Mid-masses and chiral interactions:

- → *Leading order 3NF are crucial to predict many important features that are observed experimentally (drip lines, saturation, orbit evolution, etc…)*
- → *Experimental binding is predicted accurately up to the lower sd shell (A≈30) but deteriorates for medium mass isotopes (Ca and above) with roughly 1 MeV/A over binding.*
- → *New fits of chiral interaction are promising for low-energy observables*
- → *Comparison of spectroscopic strength with experiment is much improved…*
- → *Nuclear forces from Lattice-QCD approaching physical pion mass*





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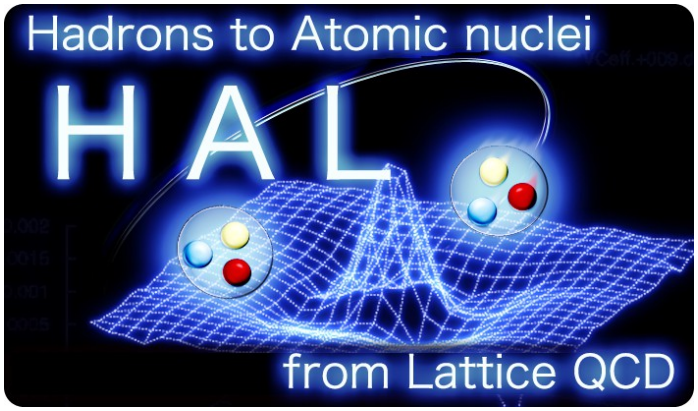

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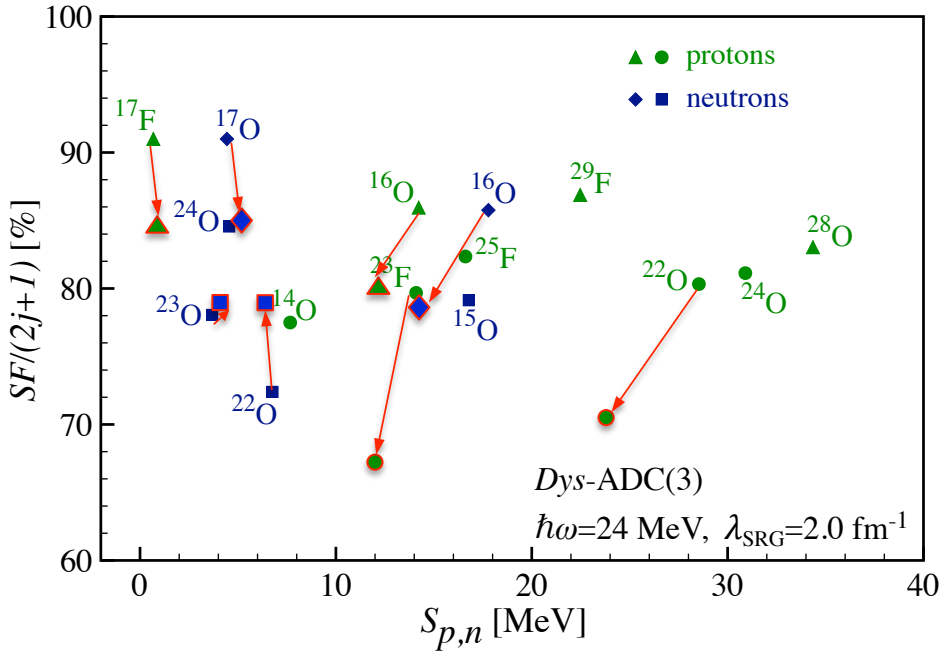
Z/N asymmetry dependence of SFs - Theory

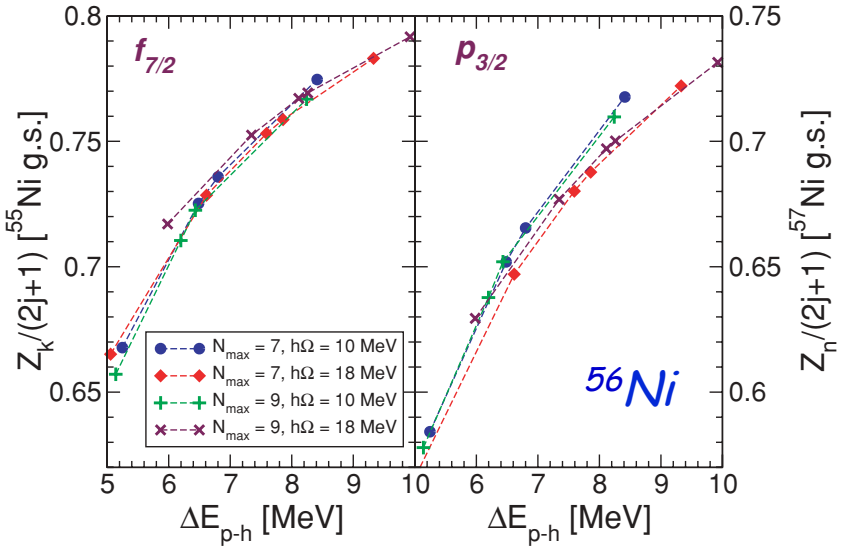
Ab-initio calculations explain (a very weak) the Z/N dependence but the effect is much lower than suggested by direct knockout

Rather the quenching is high correlated to the gap at the Femi surface.



A. Cipollone, CB, P Navrátil
Phys. Rev. C**92**, 014306 (2015)

Spectroscopic factor are strongly correlated to p-h gaps:



CB, M. Hjorth-Jensen,
Phys. Rev. C **79**, 064313 (2009)