

# Chiral 3NFs and elastic scattering in medium mass isotopes

Carlo Barbieri — University of Surrey

Relevant papers:

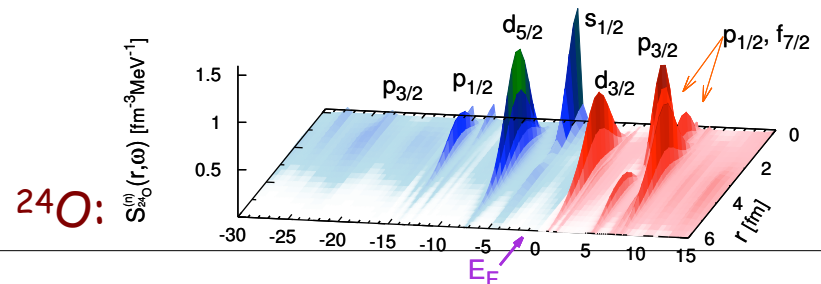
*ab-initio & correlations:*

Phys. Rev. C **89**, 061301R (2014)  
*arXiv:1412.0491 [nucl-th] (2014)*

*optical potential:*

Phys. Rev. C **72**, 014613 (2005)  
Phys. Rev. C **84**, 034616 (2011)

CB, J. Phys.: Conf. Ser. **529**, 012005 (2014)



# Current Status of low-energy nuclear physics

## Composite system of interacting fermions

*Binding and limits of stability*

*Coexistence of individual and collective behaviors*

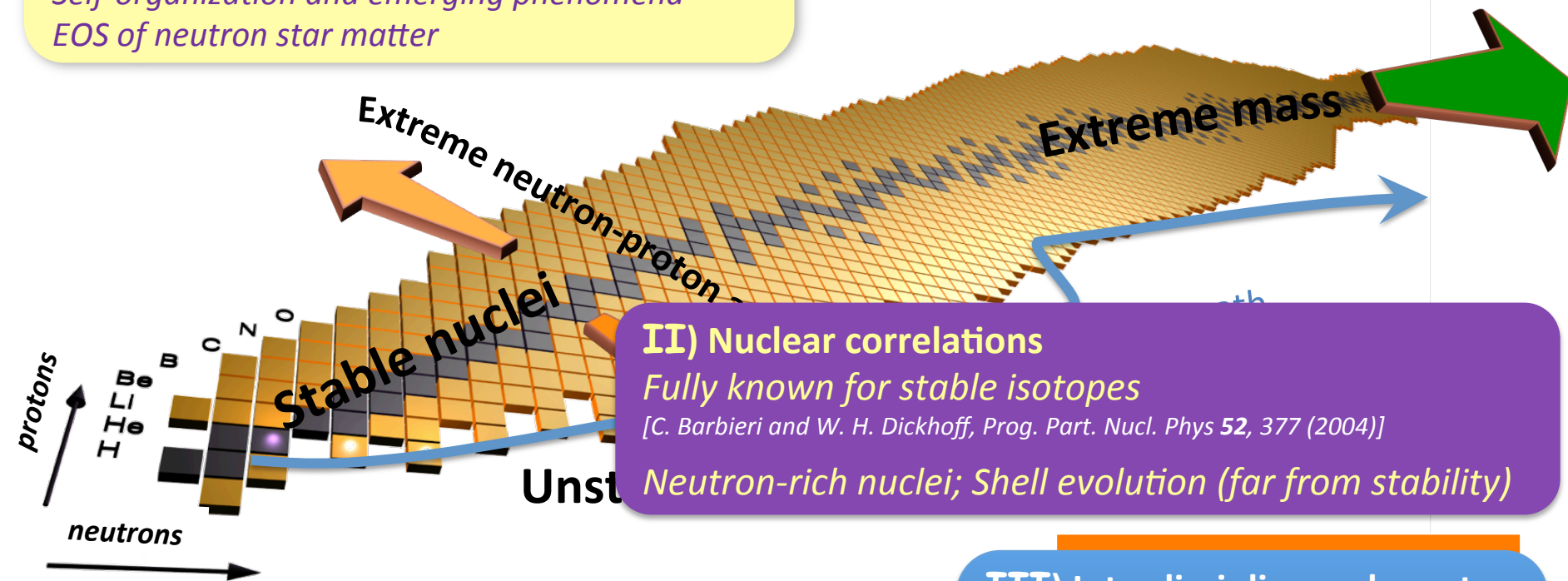
*Self-organization and emerging phenomena*

*EOS of neutron star matter*

Experimental

programs

RIKEN, FAIR, FRIB



## 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;*

# Nuclear forces in exotic nuclei

Nucleon interactions are very complex and difficult to handle

Change of regime from stable to dripline isotopes !

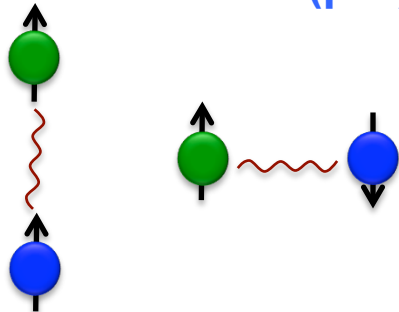
Symmetric matter:  
 $N \approx Z$



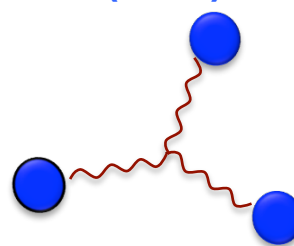
Neutron-rich matter ( $N \gg Z$ ):

- Neutron star matter EoS
- Symmetry energy

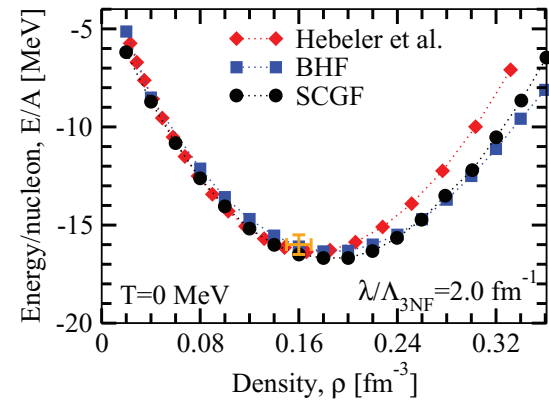
Tensor force (p-n)



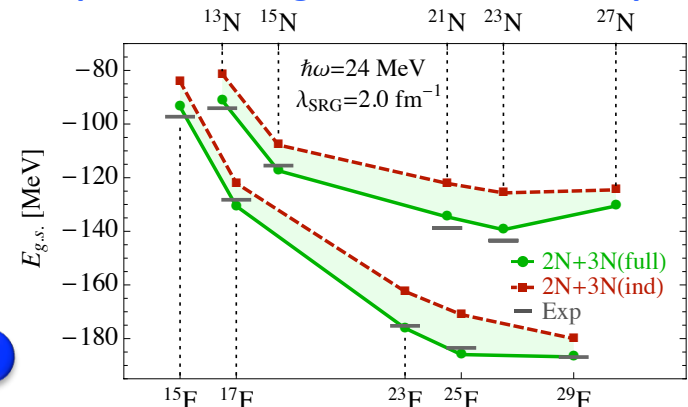
Three-nucleon Force (3NF)



[A. Carbone et al., Phys. Rev. C **88**, 044302 (2013)]



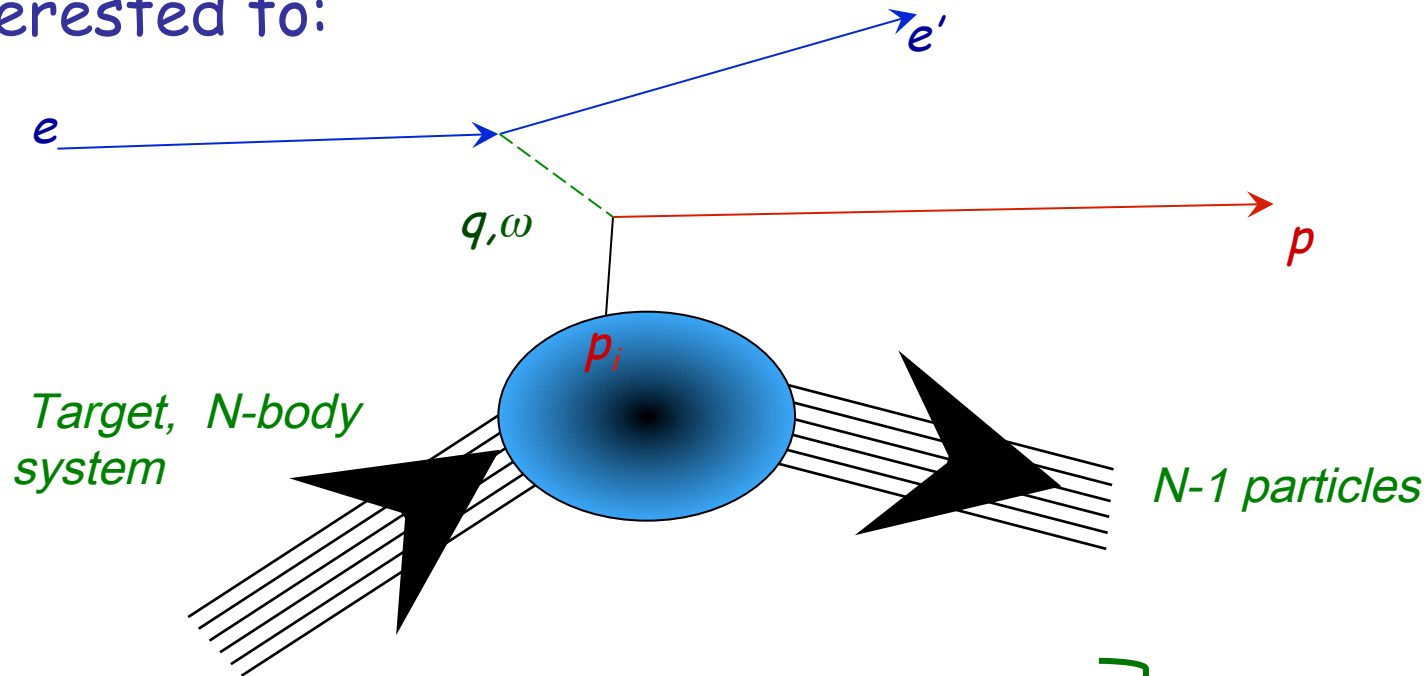
Driplines of nitrogen and fluorine isotopes



[A. Cipollone, CB, P. Navrátil, Phys. Rev. Lett. **111**, 062501 (2013)]

# Spectroscopy via knock out reactions - *basic idea*

Use a probe (ANY probe) to eject the particle we are interested to:



Basic idea:

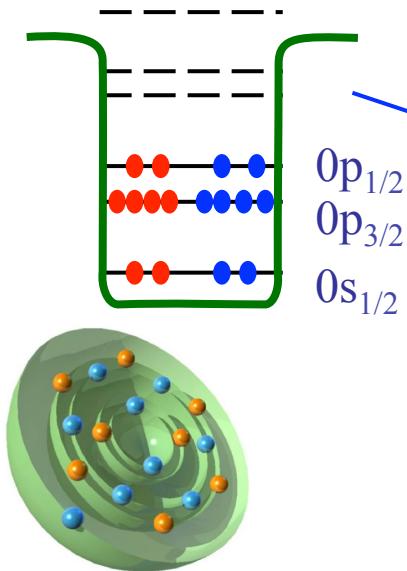
- we know,  $e$ ,  $e'$  and  $p$

- "get" *energy and momentum* of  $p_i$ :  
$$p_i = k_{e'} + k_p - k_e$$
$$E_i = E_{e'} + E_p - E_e$$

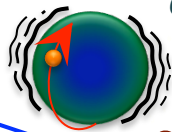
Better to choose  
large transferred  
momentum and weak  
probes!!!

# Concept of correlations

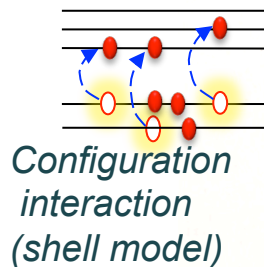
independent particle picture



Particle-vibration coupling (PV)

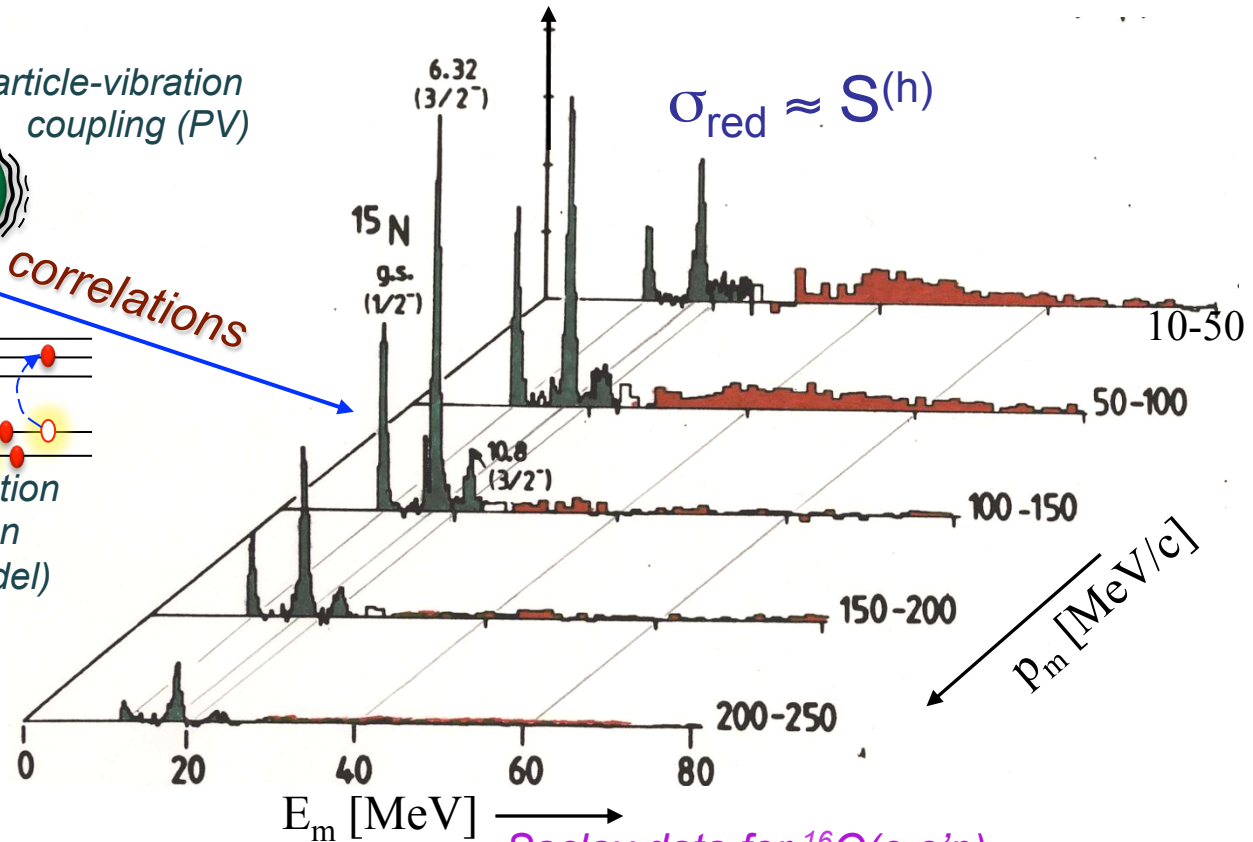


correlations



Configuration interaction (shell model)

Spectral function: distribution of momentum ( $p_m$ ) and energies ( $E_m$ )



Saclay data for  $^{16}O(e, e'p)$

[Mougey et al., Nucl. Phys. A335, 35 (1980)]

[CB and W. H. Dickhoff, Prog. Part. Nucl. Phys 52, 377 (2004)]

# Concept of correlations

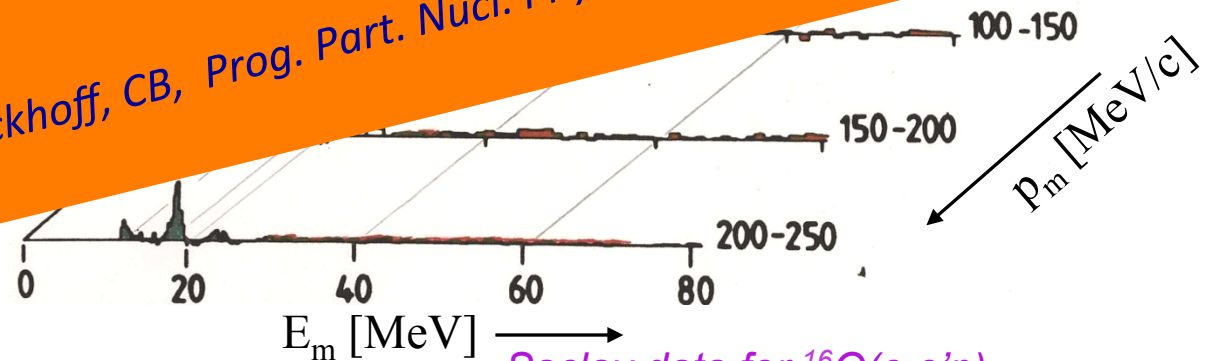
independent  
particle picture

Spectral function: distribution of  
momentum ( $p_m$ ) and energy ( $E_m$ )

Particle-vibration  
coupling

So far, fully characterised only for closed-shell and  
stable isotopes... (!)

[W. Dickhoff, CB, Prog. Part. Nucl. Phys. **52**, 377 (2004)]



Saclay data for  $^{16}\text{O}(e,e'p)$

[Mougey et al., Nucl. Phys. A335, 35 (1980)]

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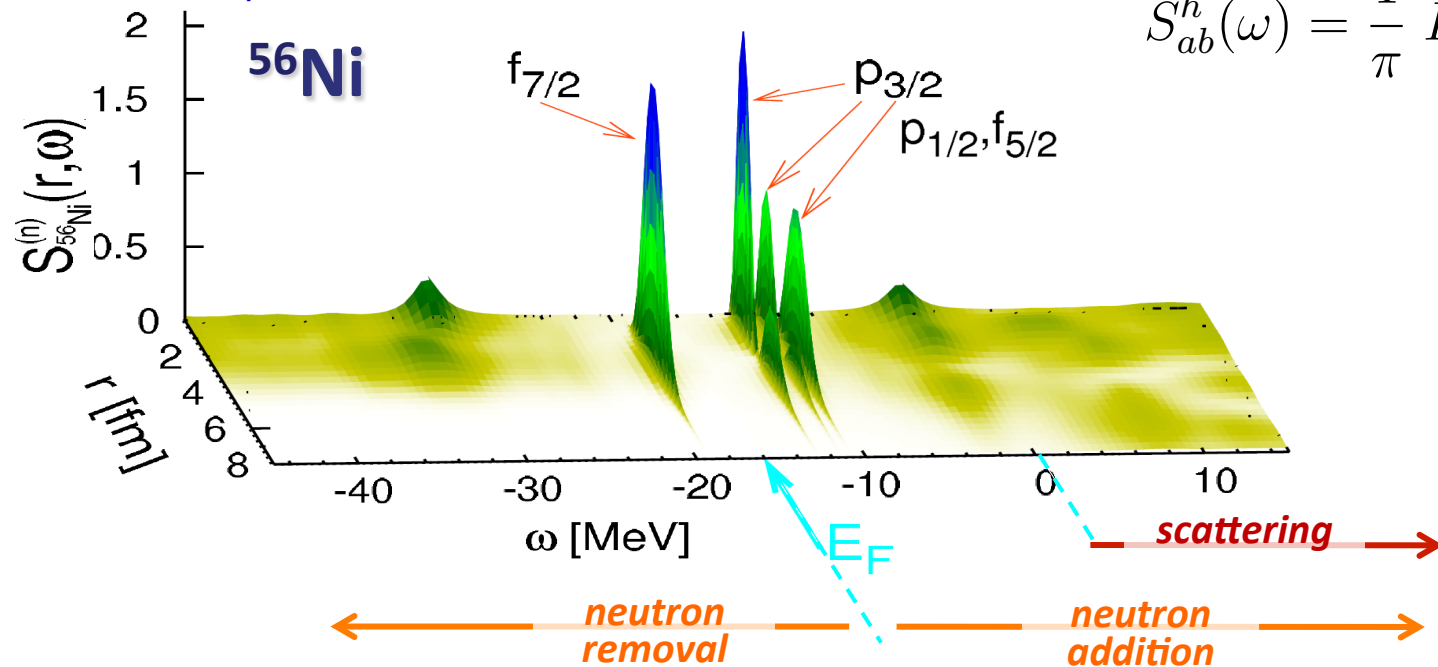
# Example of spectral function $^{56}\text{Ni}$

One-body Green's function (or propagator) describes the motion of quasi-particles and holes:

$$g_{\alpha\beta}(E) = \sum_n \frac{\langle \Psi_0^A | c_\alpha | \Psi_n^{A+1} \rangle \langle \Psi_n^{A+1} | c_\beta^\dagger | \Psi_0^A \rangle}{E - (E_n^{A+1} - E_0^A) + i\eta} + \sum_k \frac{\langle \Psi_0^A | c_\beta^\dagger | \Psi_k^{A-1} \rangle \langle \Psi_k^{A-1} | c_\alpha | \Psi_0^A \rangle}{E - (E_0^A - E_k^{A-1}) - i\eta}$$

...this contains all the structure information probed by nucleon transfer (spectral function):

$$S_{ab}^h(\omega) = \frac{1}{\pi} \text{Im} g_{ab}(\omega)$$

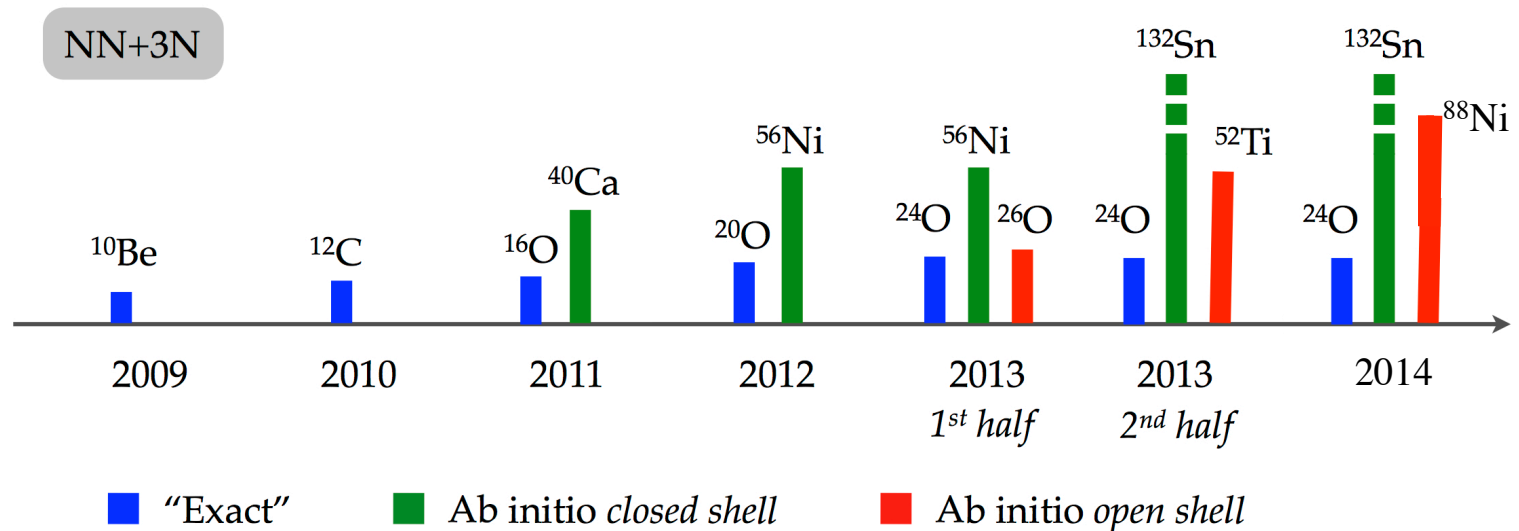


# Ab-Initio SCGF approaches



# Reaching medium mass and neutron rich isotopes

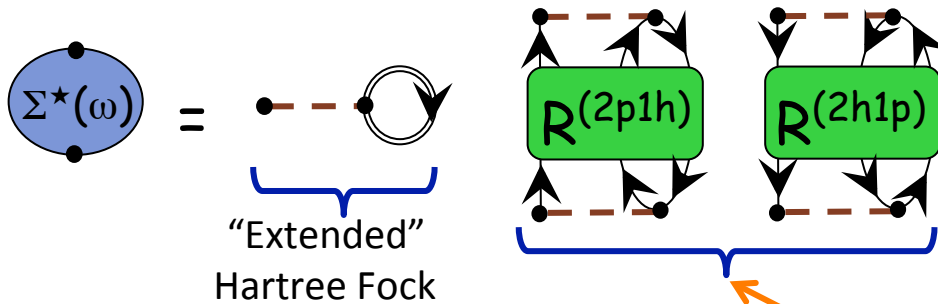
- Degenerate system (open shells, deformations...)
- Hamiltonian, including three nucleon forces



# 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...

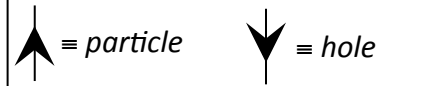
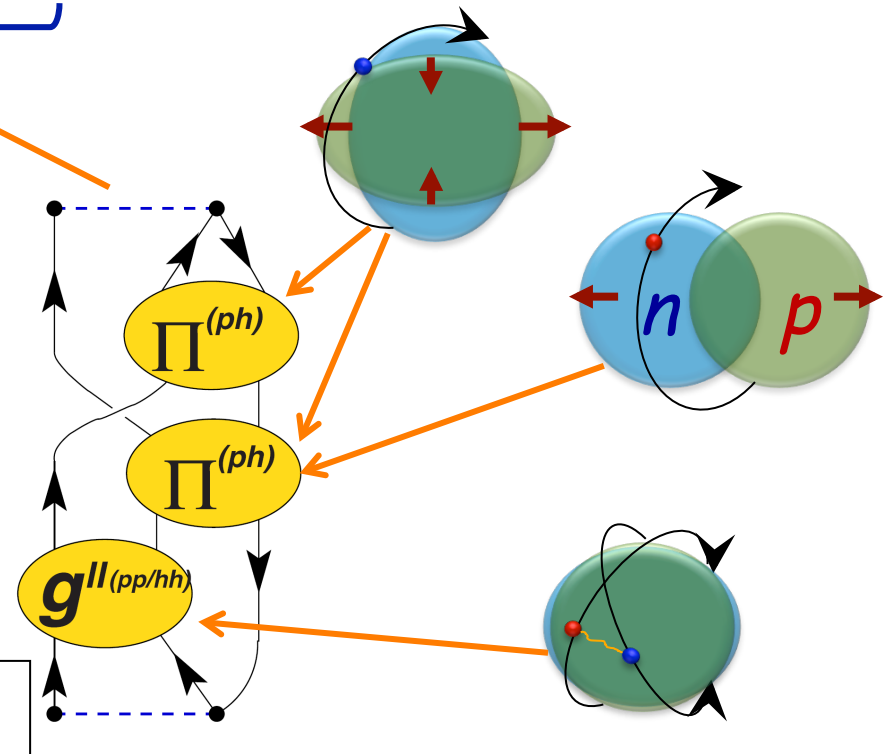
CB et al.,  
 Phys. Rev. C63, 034313 (2001)  
 Phys. Rev. A76, 052503 (2007)  
 Phys. Rev. C79, 064313 (2009)



• 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  $\Sigma^*(\omega)$  yields both single-particle states and scattering



# Gorkov and symmetry breaking approaches

V. Somà, CB, T. Duguet, , Phys. Rev. C **89**, 024323 (2014)

V. Somà, CB, T. Duguet, Phys. Rev. C **87**, 011303R (2013)

V. Somà, T. Duguet, CB, Phys. Rev. C **84**, 064317 (2011)

➤ Ansatz  $\dots \approx E_0^{N+2} - E_0^N \approx E_0^N - E_0^{N-2} \approx \dots \approx 2\mu$

➤ Auxiliary many-body state  $|\Psi_0\rangle \equiv \sum_N^{\text{even}} c_N |\psi_0^N\rangle$

➤ Mixes various particle numbers

➤ Introduce a “grand-canonical” potential  $\Omega = H - \mu N$

➤  $|\Psi_0\rangle$  minimizes  $\Omega_0 = \langle \Psi_0 | \Omega | \Psi_0 \rangle$  under the constraint  $N = \langle \Psi_0 | N | \Psi_0 \rangle$

➤ This approach leads to the following Feynman diagrams:

$$\Sigma_{ab}^{11(1)} = \text{Diagram 1}$$

$$\Sigma_{ab}^{12(1)} = \text{Diagram 2}$$

$$\Sigma_{ab}^{11(2)}(\omega) = \text{Diagram 3} + \text{Diagram 4}$$

$$\Sigma_{ab}^{12(2)}(\omega) = \text{Diagram 5} + \text{Diagram 6}$$

# Approaches in GF theory

Truncation  
scheme:

Dyson formulation  
(closed shells)

Gorkov formulation  
(semi-magic)

1<sup>st</sup> order:

Hartree-Fock

HF-Bogolioubov

2<sup>nd</sup> order:

2<sup>nd</sup> order

2<sup>nd</sup> order (w/ pairing)

...

...

3<sup>rd</sup> and all-orders  
sums,  
P-V coupling:

ADC(3)  
FRPA  
etc...

G-ADC(3)  
...work in progress



# Approaches in GF theory

Truncation scheme:

1<sup>st</sup> order:

2<sup>nd</sup> order:

...

3<sup>rd</sup> and all-order sums,  
P-V coupling

Dyson formulation  
(closed shells)

Hartree-Fock

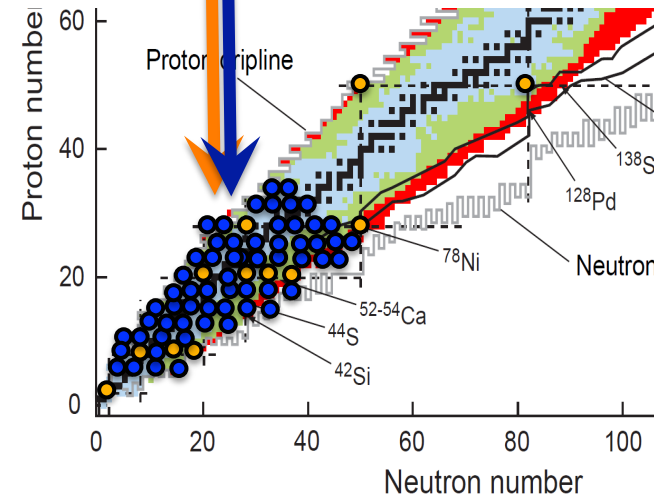
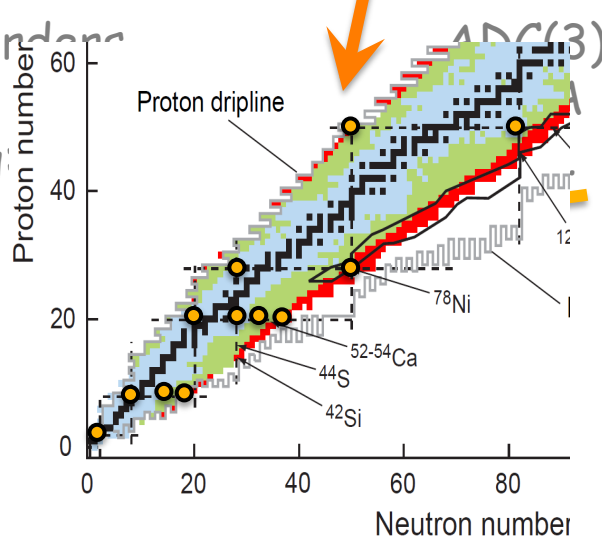
2<sup>nd</sup> order

...

Gorkov formulation  
(semi-magic)

HF-Bogoliubov

2<sup>nd</sup> order (w/ pairing)



# Ab-initio Nuclear Computation & BcDor code

BoccaDorata code:

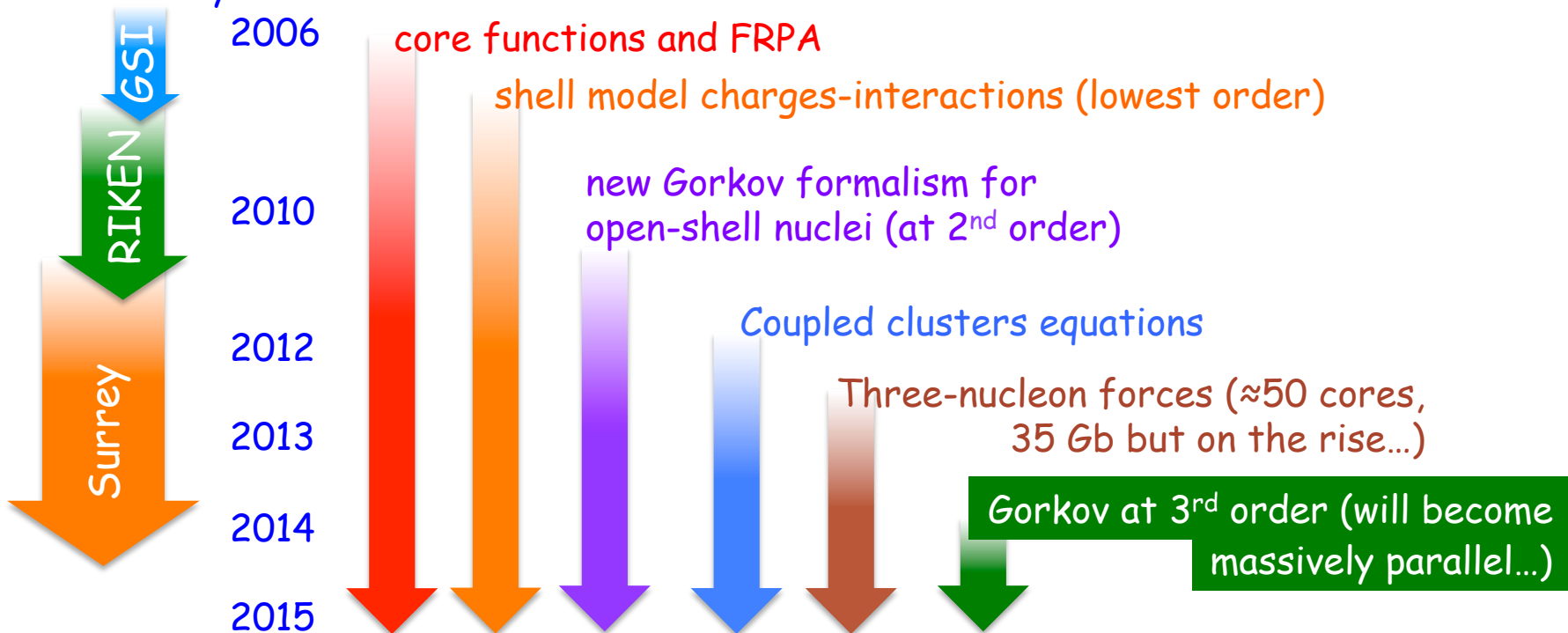
(C. Barbieri 2006-14

V. Somà 2011-14

A. Cipollone 2012-13)

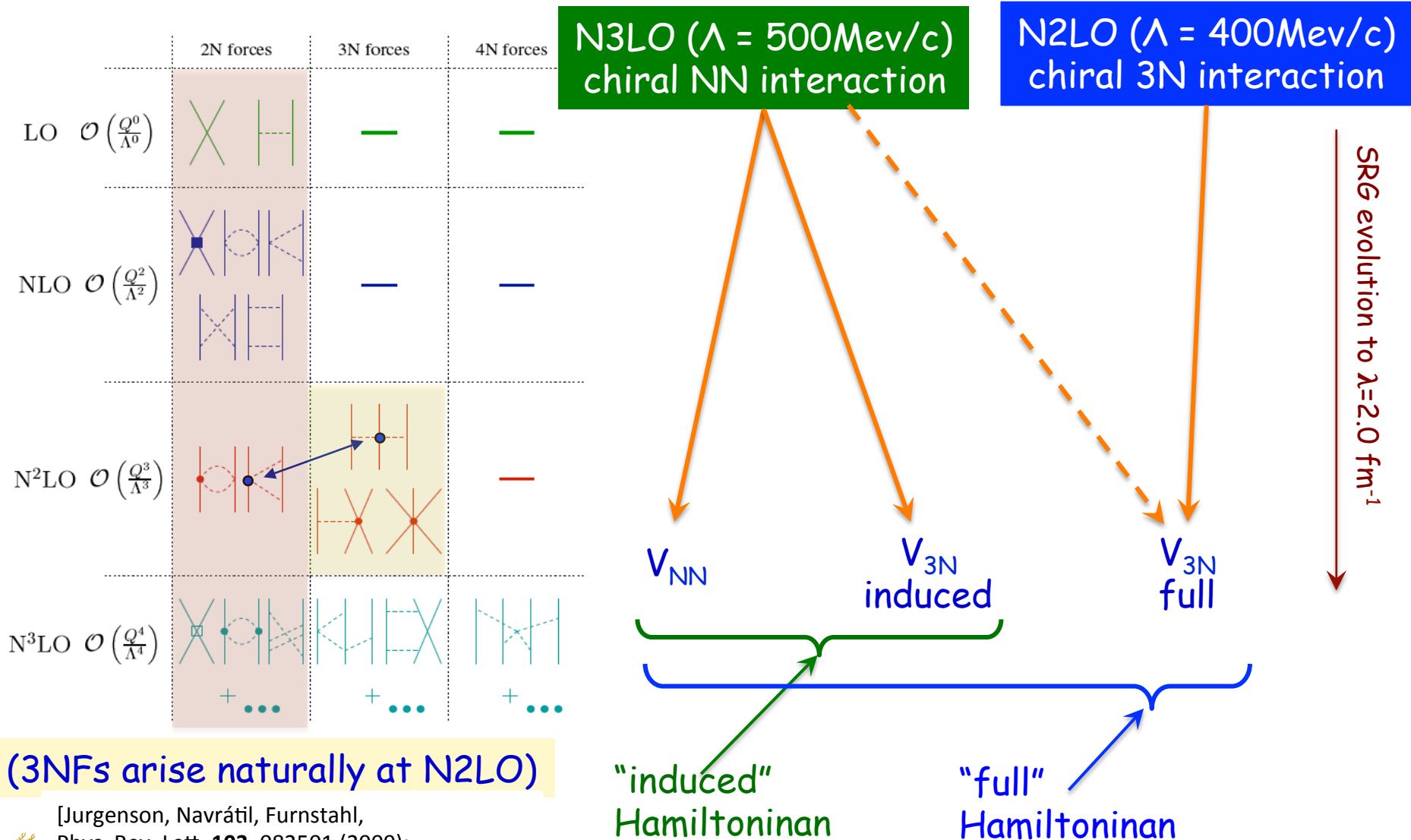
- Provides a *C++ class library* for handling many-body propagators ( $\approx 40,000$  lines, OpenMPI based).
- Allows to solve for nuclear spectral functions, many-body propagators, RPA responses, coupled cluster equations and effective interaction/charges for the shell model.

Code history:



# Results

# Chiral Nuclear forces - SRG evolved



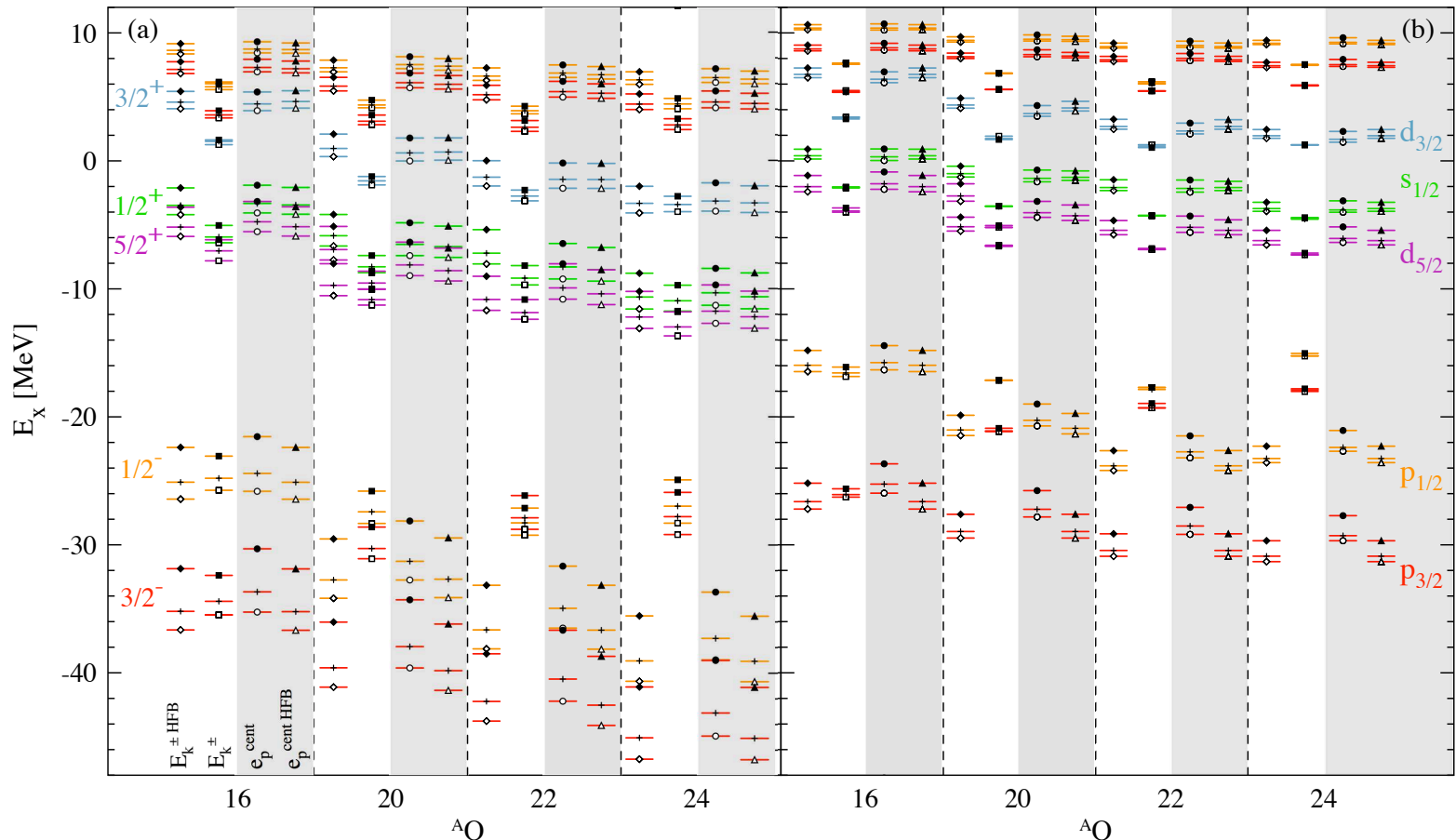


# Convergence of s.p. spectra w.r.t. SRG

Cutoff dependence is reduced, indicating good convergence of many-body truncation and many-body forces

arXiv:1411.1237 (2014)

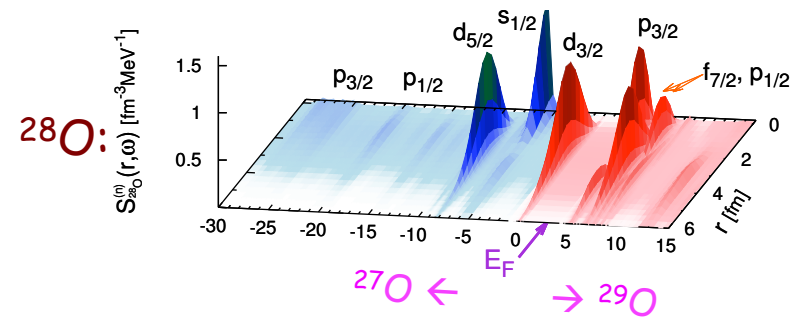
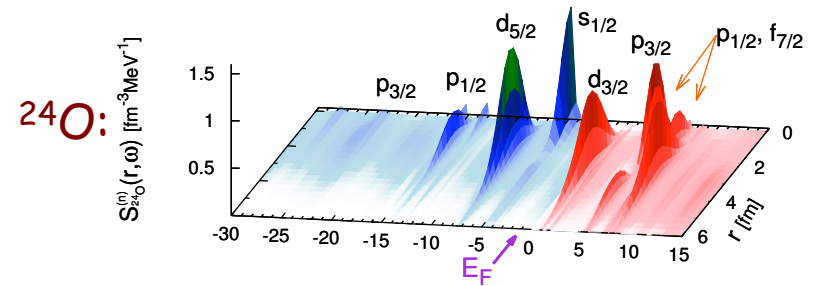
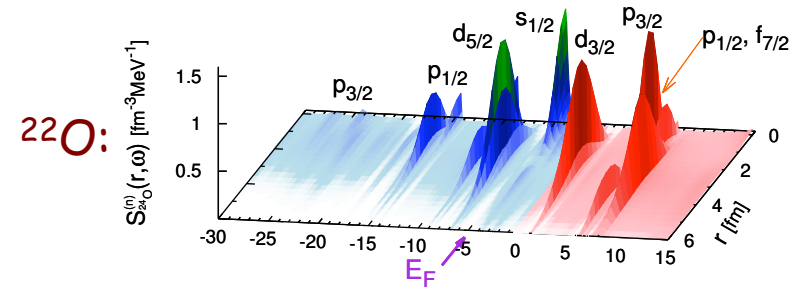
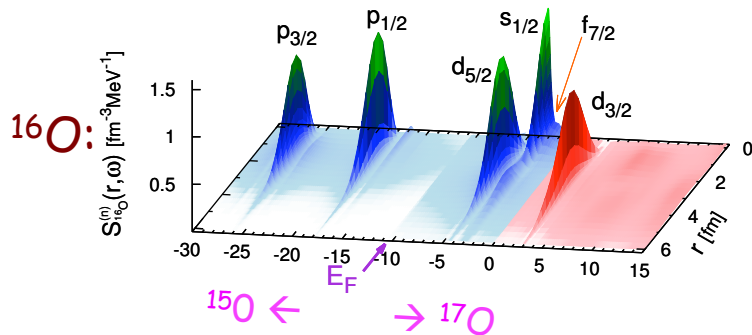
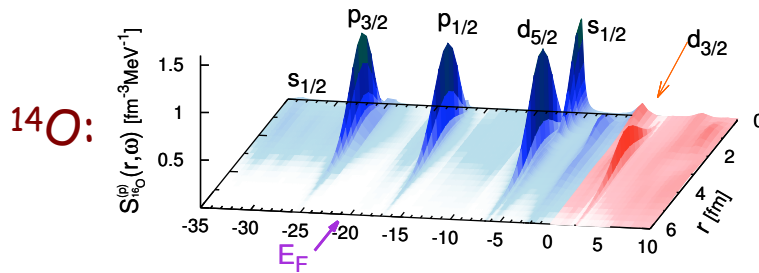
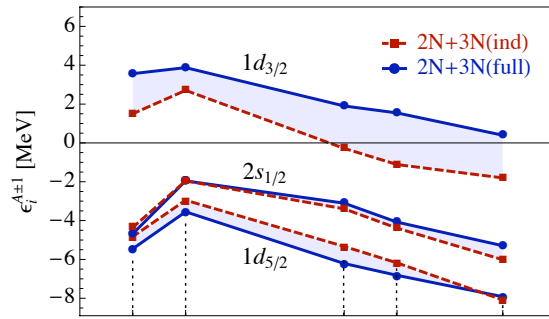
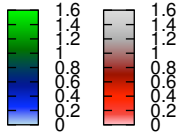
✓ only dominant s.p. states shown



NN terms (no induced 3NF)  $\leftrightarrow$  NN+3NF fully included

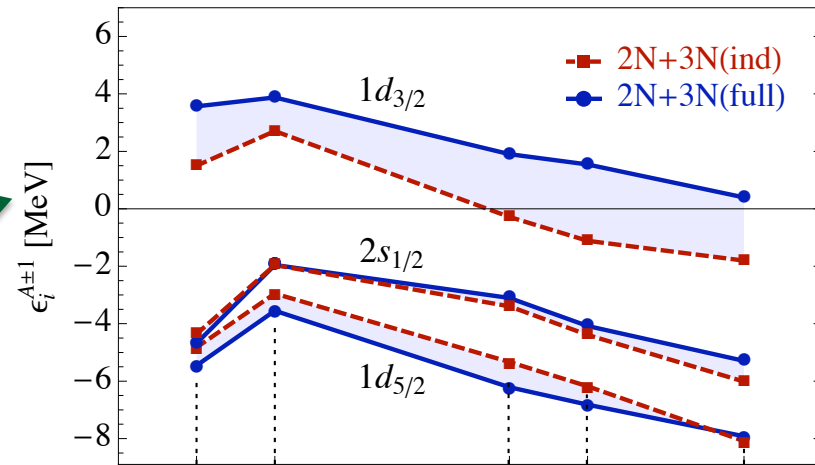
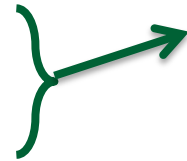
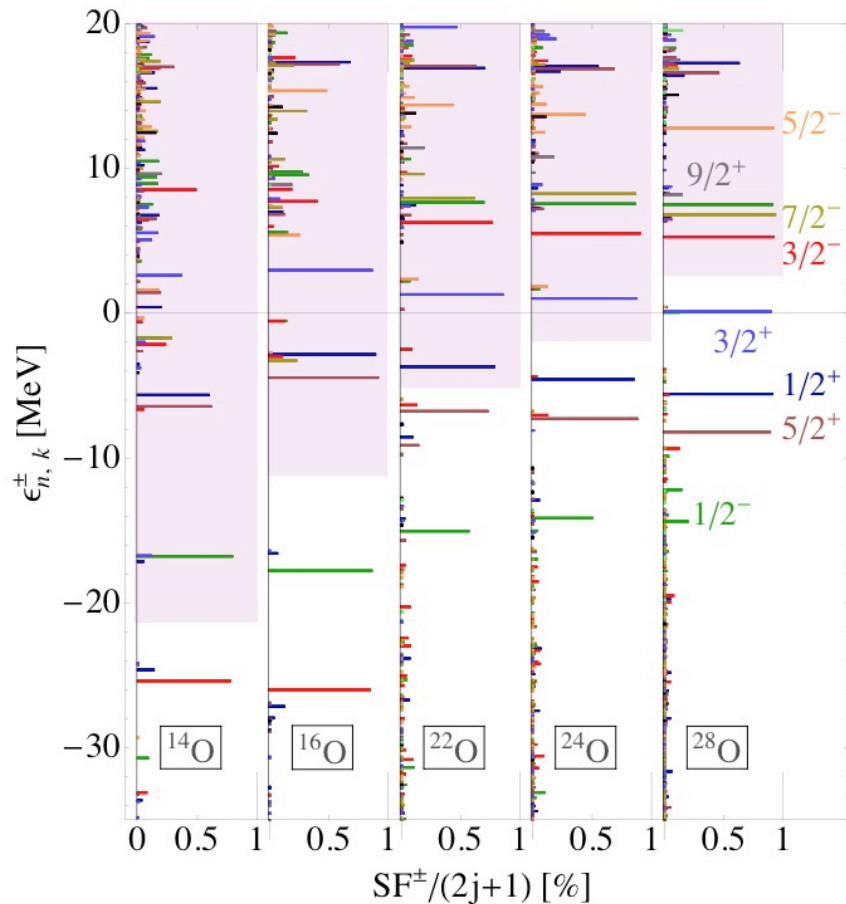
# Neutron spectral function of Oxygens

A. Cipollone, CB P. Navrátil, [arXiv:1412.0491](https://arxiv.org/abs/1412.0491) (2014)



# Results for the N-O-F chains

A. Cipollone, CB, P. Navrátil, Phys. Rev. Lett. **111**, 062501 (2013)  
and arXiv:1412.0491 [nucl-th] (2014)

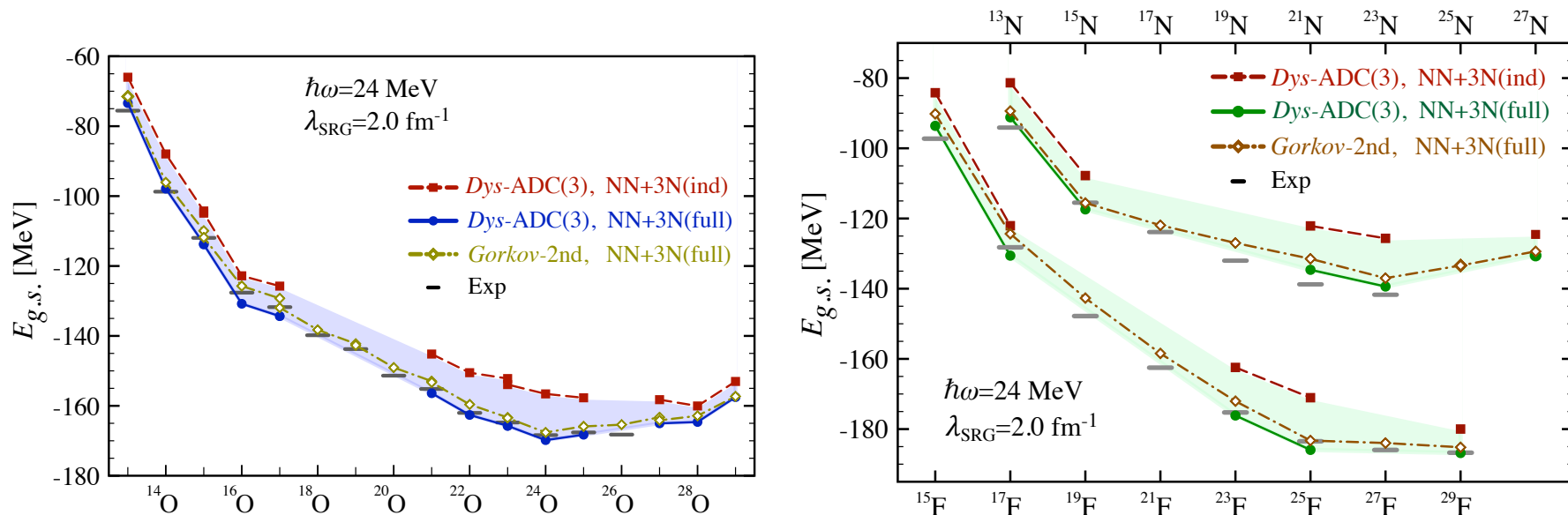


→  $d_{3/2}$  raised by genuine 3NF

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

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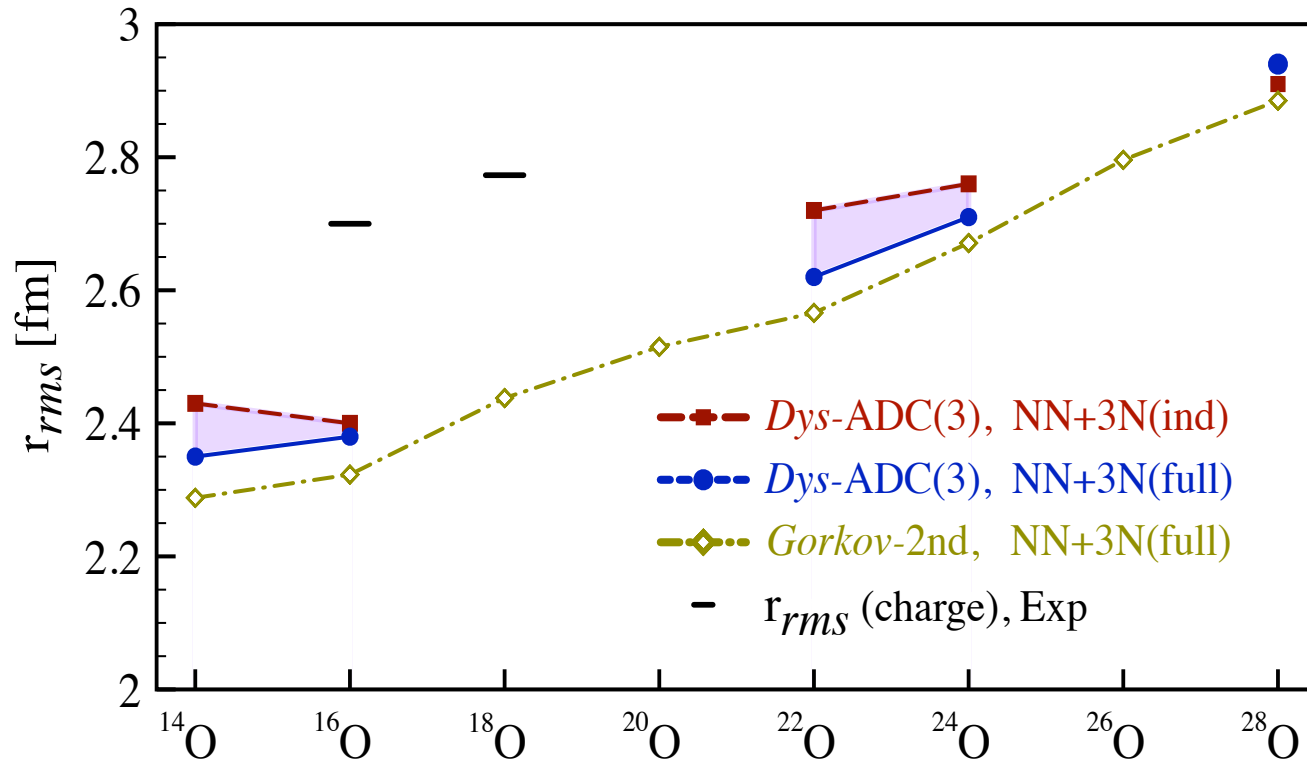


→ 3NF crucial for reproducing binding energies and driplines around oxygen

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

# Results for the oxygen chain

A. Cipollone, CB, P. Navrátil, arXiv:1412.0491 [nucl-th] (2014)

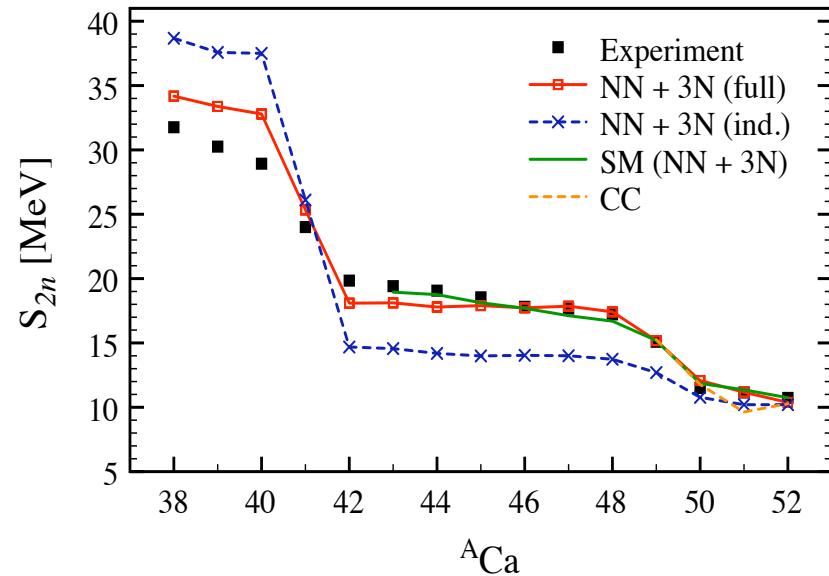
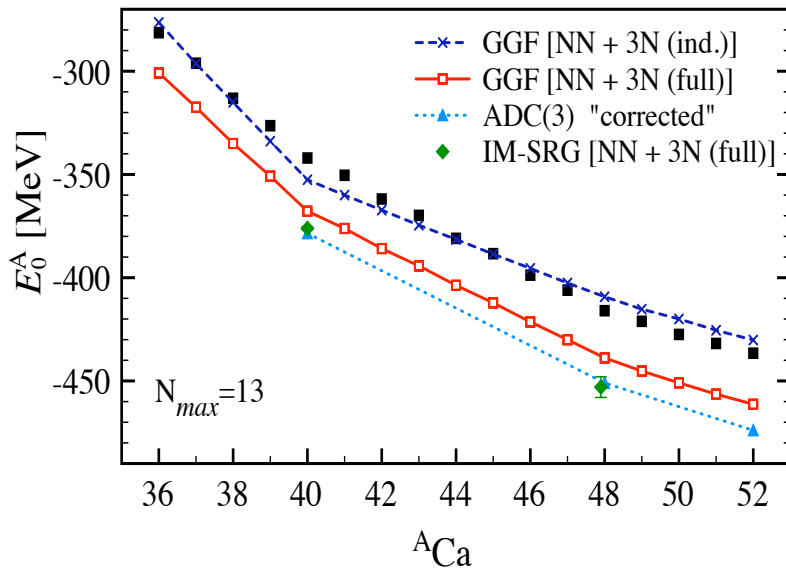


→ Single particle spectra slightly diluted and

→ systematic underestimation of radii

# Calcium isotopic chain

Ab-initio calculation of the whole Ca: *induced* and *full* 3NF investigated



→ *induced* and *full* 3NF investigated

→ *genuine* (N2LO) 3NF needed to reproduce the energy curvature and  $S_{2n}$

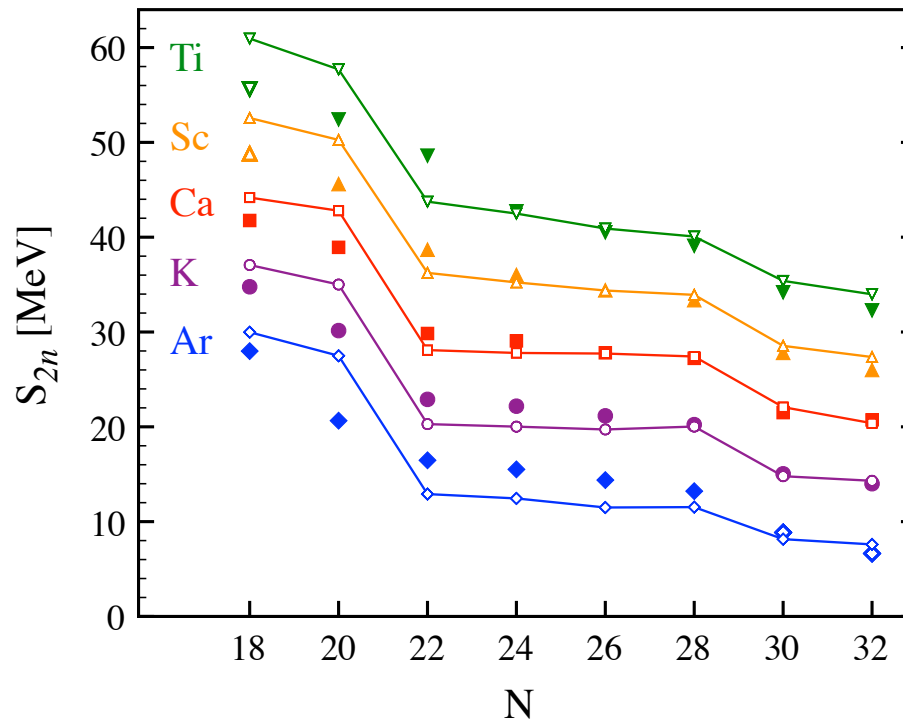
→ N=20 and Z=20 gaps *overestimated!*

→ Full 3NF give a *correct* trend but *over bind!*

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

V. Somà, CB *et al.* Phys. Rev. C89, 061301R (2014)

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

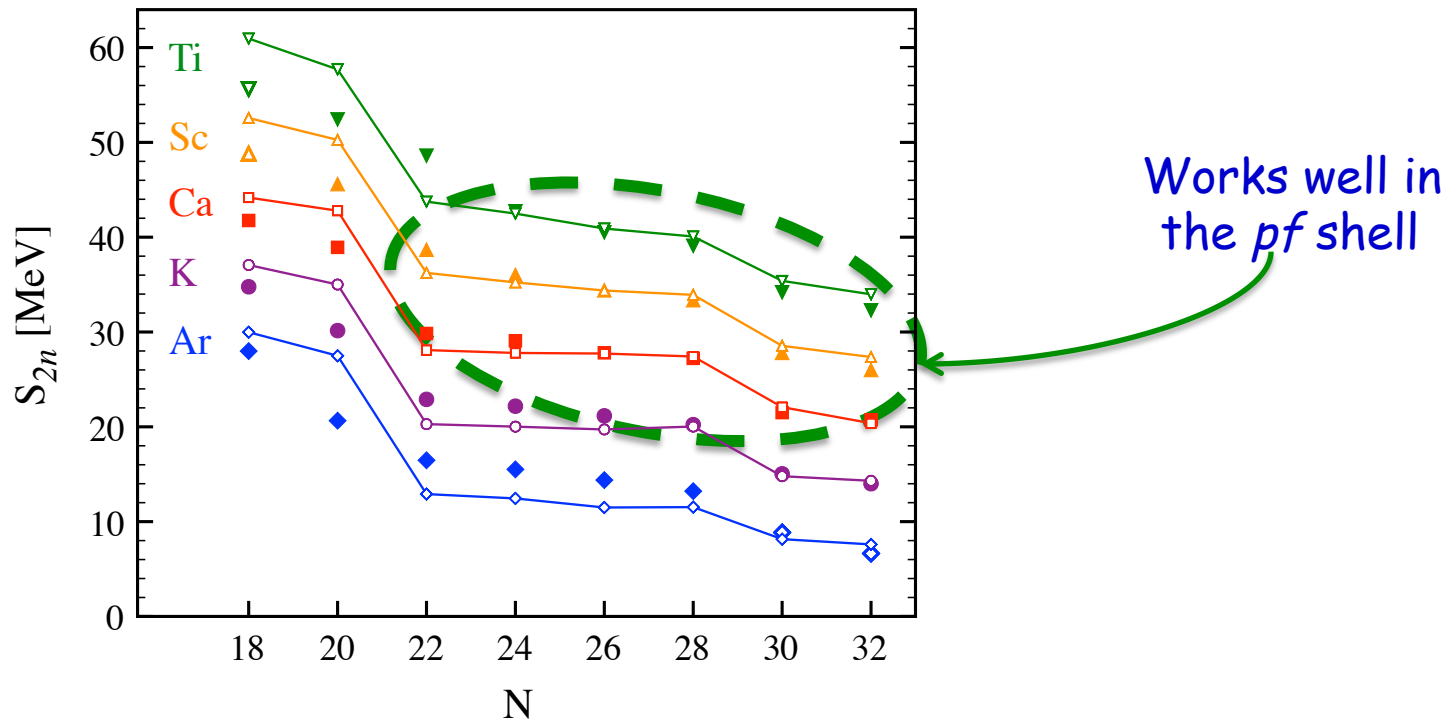


→ First *ab-initio* calculation over a contiguous portion of the nuclear chart—open shells are now possible through the Gorkov-GF formalism

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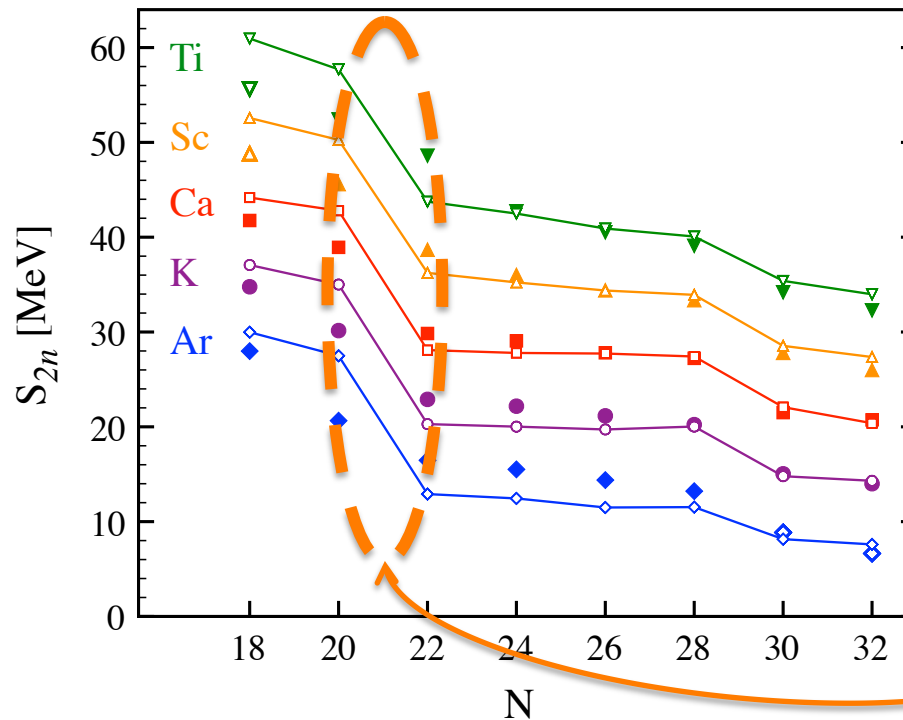
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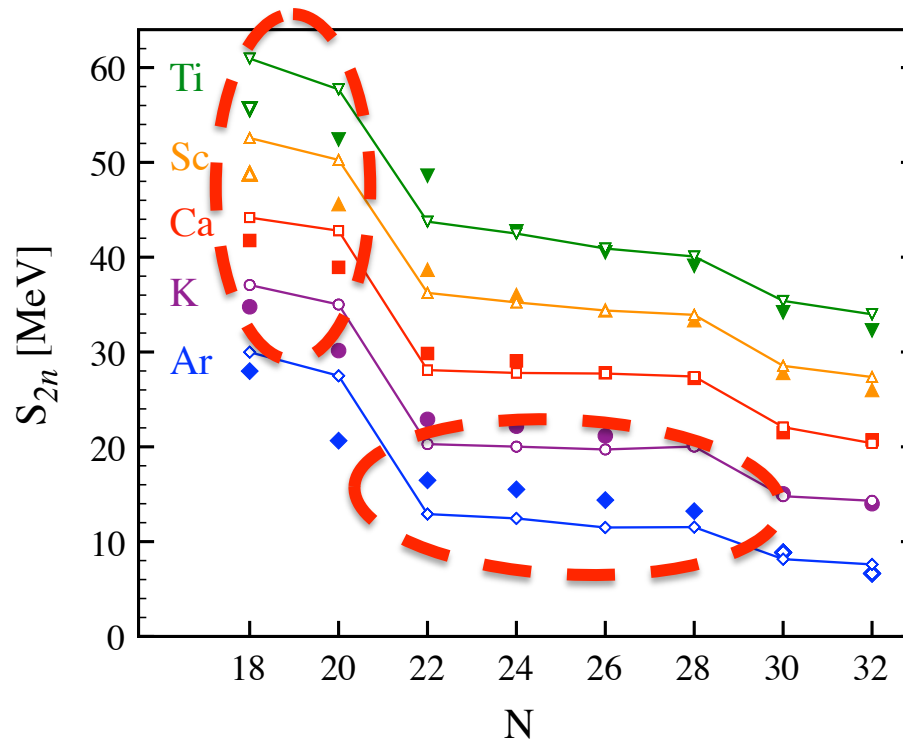
Over estimated  
N=20 and Z=20 gaps

→ 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. C89, 061301R (2014)

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



Lack of deformation due to quenched cross-shell quadrupole excitations

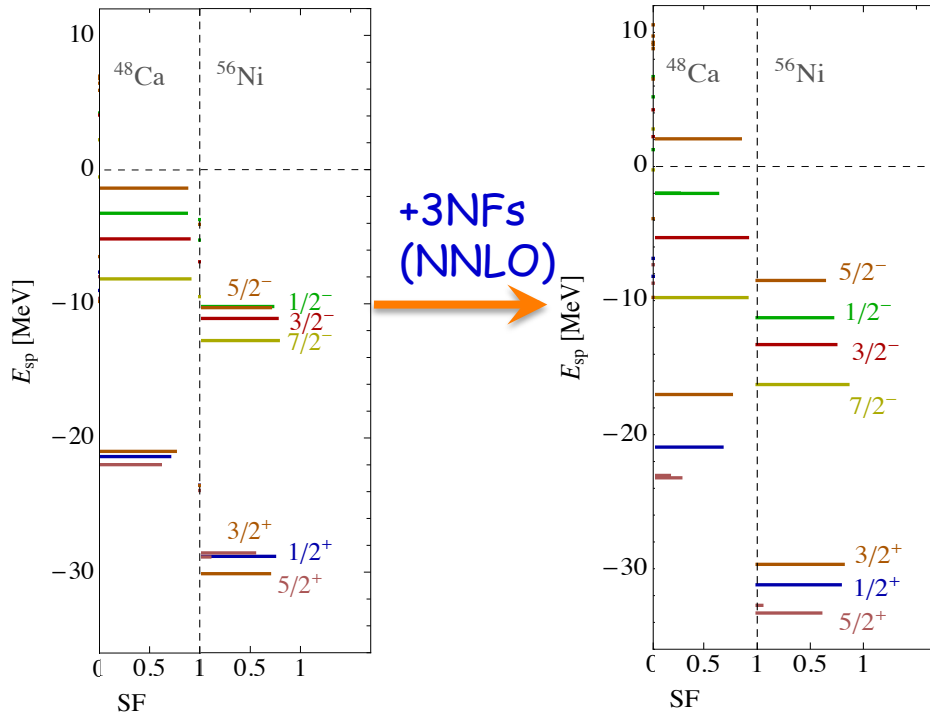
→ First *ab-initio* calculation over a contiguous portion of the nuclear chart—open shells are now possible through the Gorkov-GF formalism

# The *sd*-*pf* shell gap

Neutron spectral distributions for  $^{48}\text{Ca}$  and  $^{56}\text{Ni}$ :

2N + 3NF (induced)

2N + 3NF (FULL)

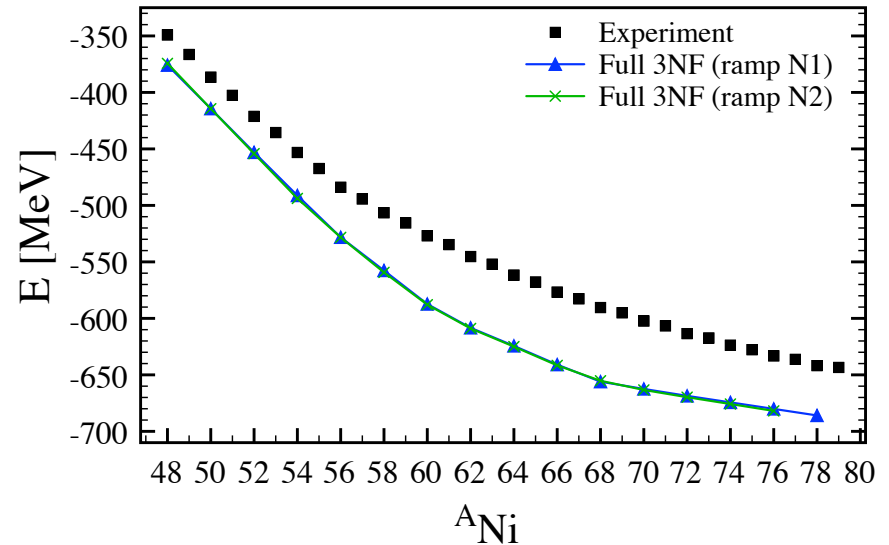
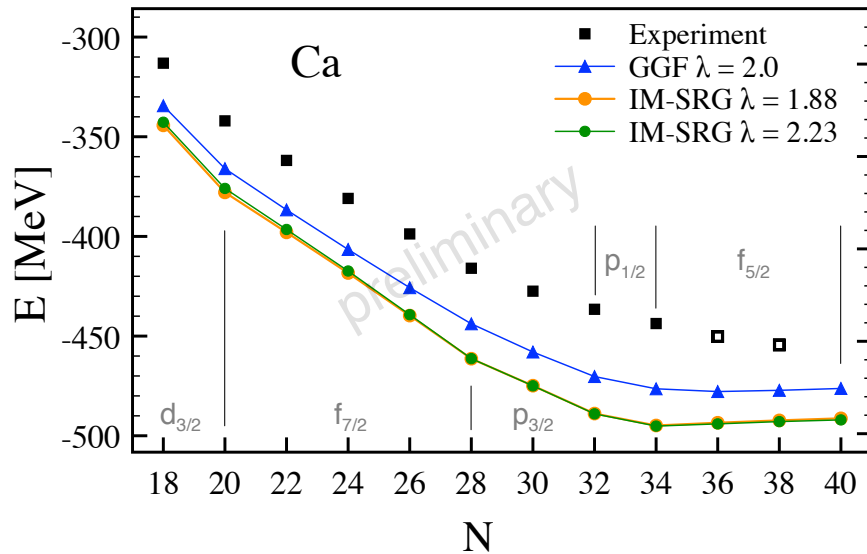


- *sd*-*pf* separation is *overestimated* even with leading order N2LO 3NF
- Correct increase of  $p_{3/2}$ - $f_{7/2}$  splitting (see Zuker 2003)

	2NF only	2+3NF(ind.)	2+3NF(full)	Experiment
$^{16}\text{O}$ :	2.10	2.41	2.38	$2.718 \pm 0.210$ [19]
$^{44}\text{Ca}$ :	2.48	2.93	2.94	$3.520 \pm 0.005$ [20]

CB *et al.*, arXiv:1211.3315 [nucl-th]

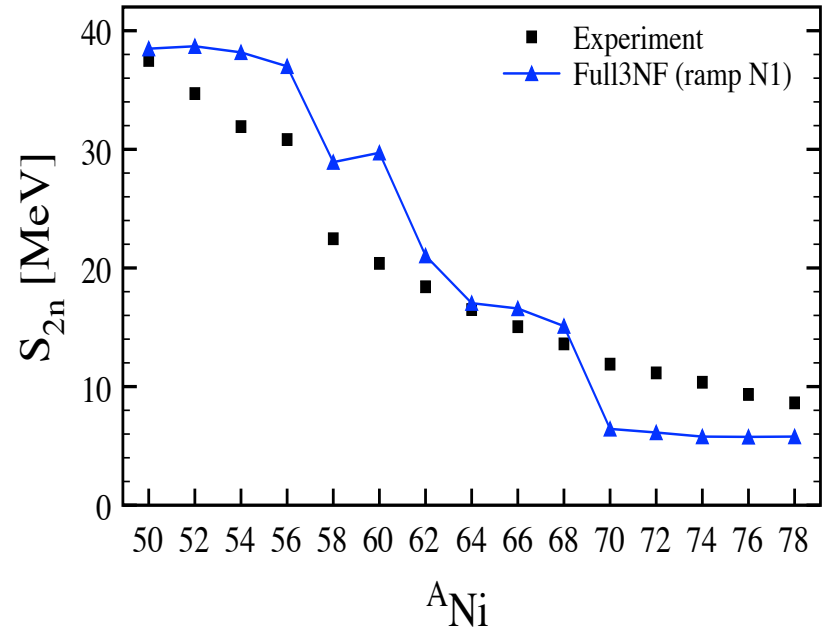
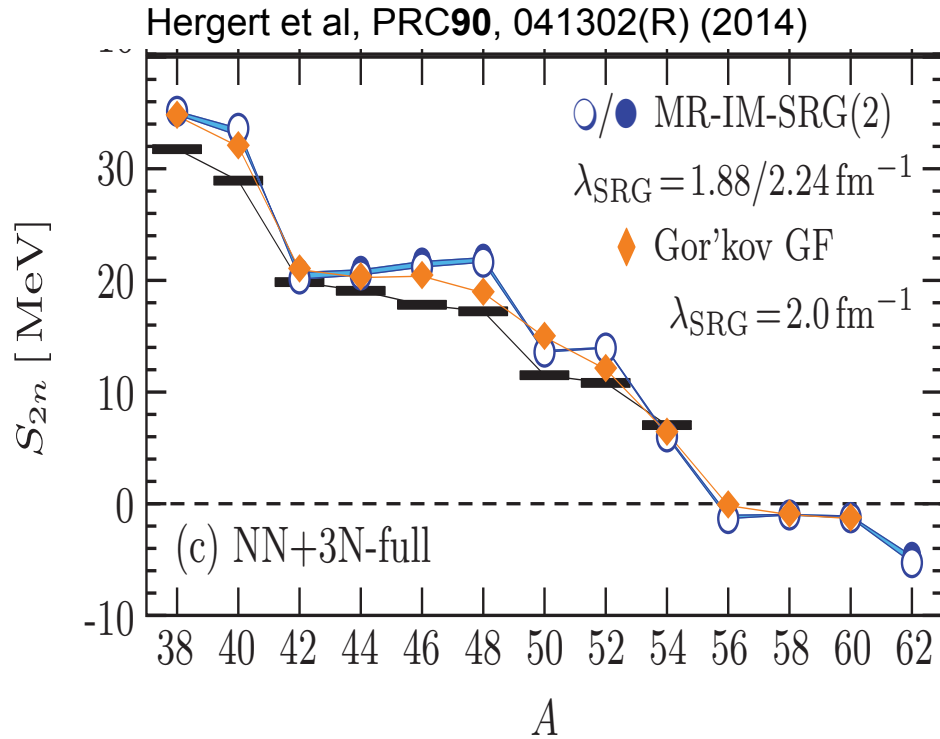
# Ca and Ni isotopic chains



→ Large  $J$  in free space SRG matter (must pay attention to its convergence)

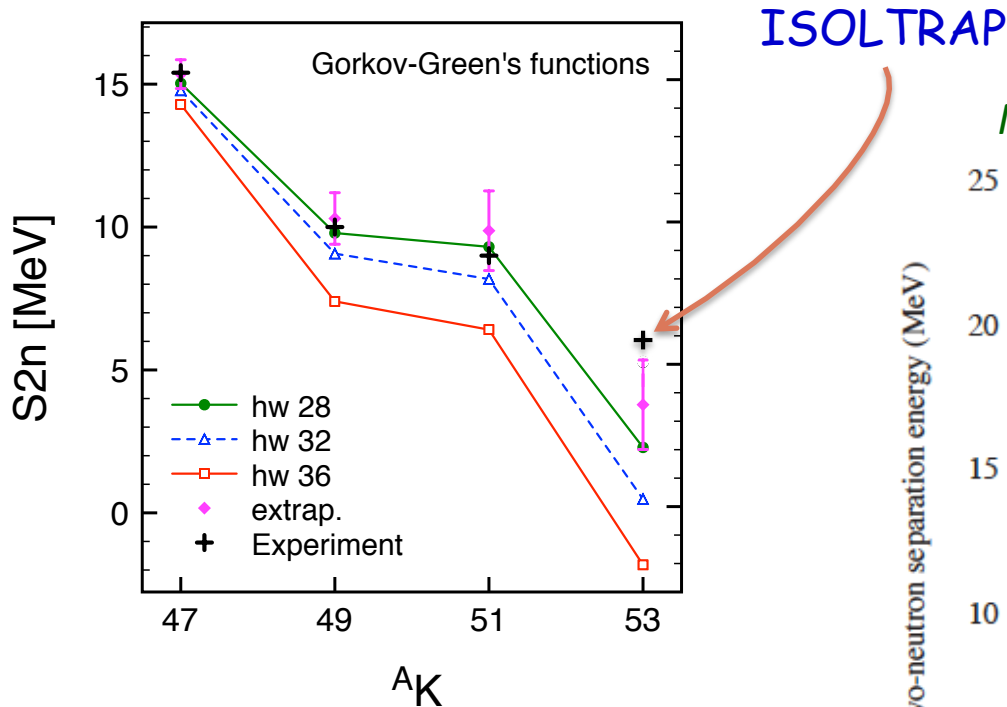
→ Overall conclusions regarding over binding and  $S_{2n}$  remain but details change

# Ca and Ni isotopic chains

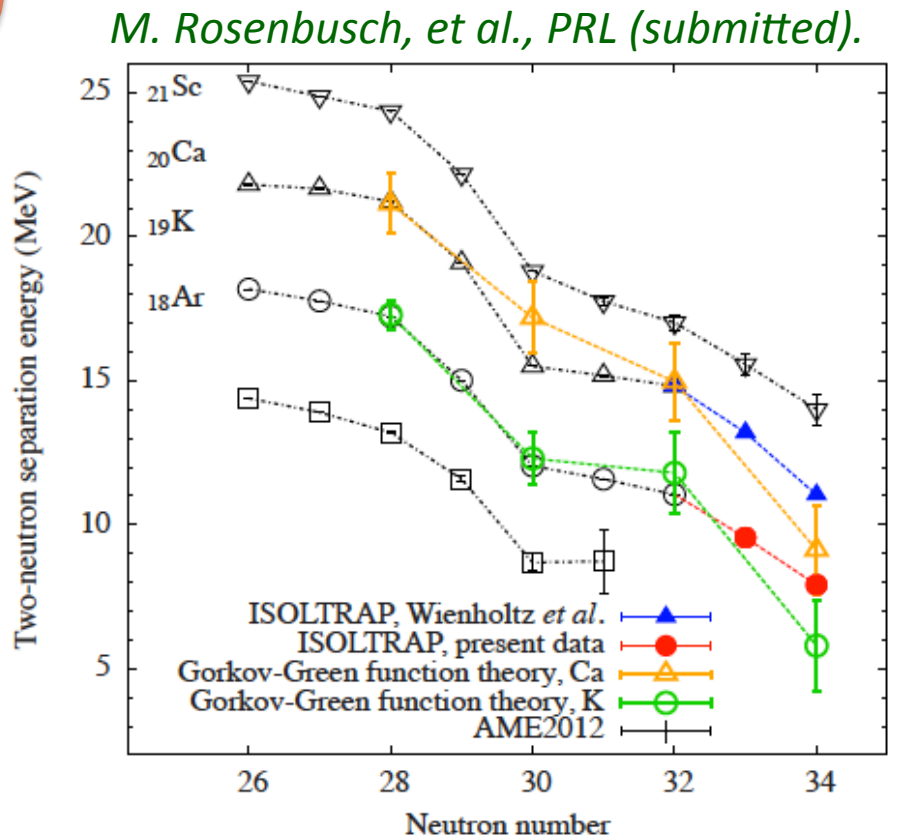


- Large  $J$  in free space SRG matter (must pay attention to its convergence)
- Overall conclusions regarding over binding and  $S_{2n}$  remain but details change

# Two-neutron separation energies for neutron rich K isotopes



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



# Quenching of absolute spectroscopic factors

[CB, Phys. Rev. Lett. **103**, 202520 (2009)]

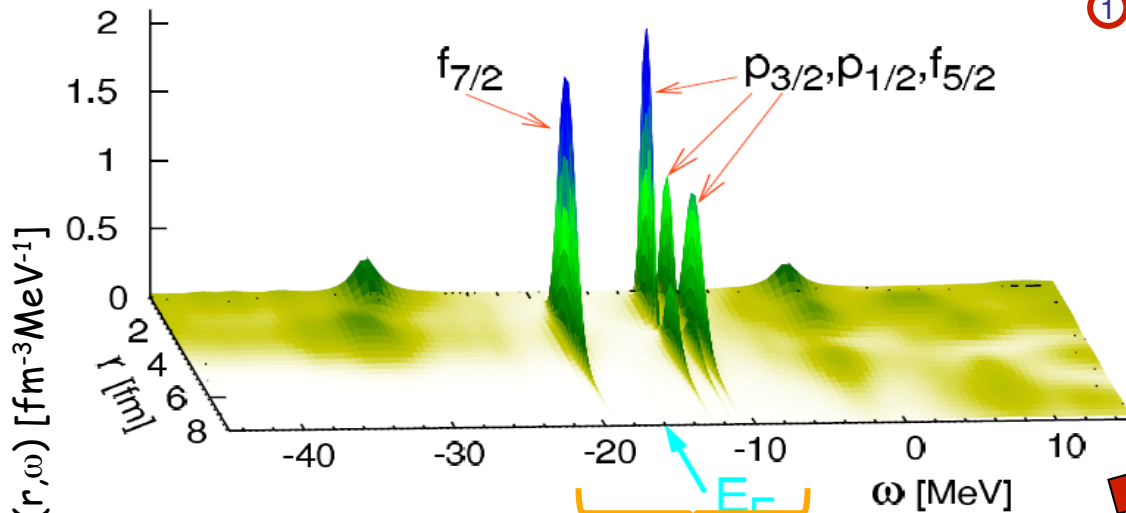
...with analogous conclusions for  $^{48}\text{Ca}$

Overall quenching of *spectroscopic factors* is driven by:

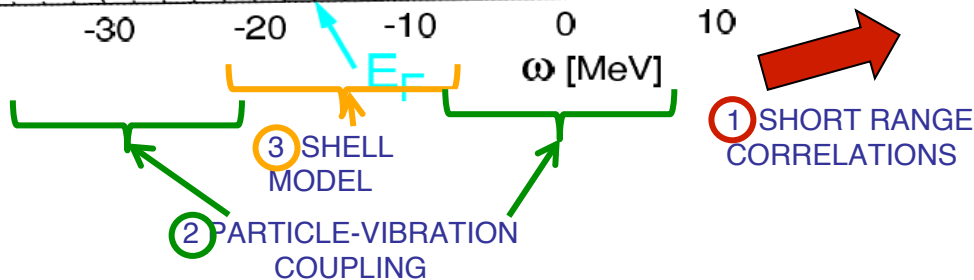
- SRC* → ~10%
- part-vibr. coupling* → dominant
- "shell-model"* → in open shell

	10 osc. shells		Exp. [30]	1p0f space		
	FRPA (SRC)	full FRPA		FRPA	SM	$\Delta Z_\alpha$

$^{57}\text{Ni}$	$\nu 1p_{1/2}$	0.96	0.63	0.61		0.79	0.77	-0.02
	$\nu 0f_{5/2}$	0.95	0.59	0.55		0.79	0.75	-0.04
	$\nu 1p_{3/2}$	0.95	0.65	0.62	0.58(11)	0.82	0.79	-0.03
$^{55}\text{Ni}$	$\nu 0f_{7/2}$	0.95	0.72	0.69		0.89	0.86	-0.03



$$Z_\alpha = \int d^3r |\psi_\alpha^{overlap}(\mathbf{r})|^2 = \frac{1}{1 - \left. \frac{\partial \Sigma_{\hat{\alpha}\hat{\alpha}}(\omega)}{\partial \omega} \right|_{\omega=\epsilon_\alpha}}$$

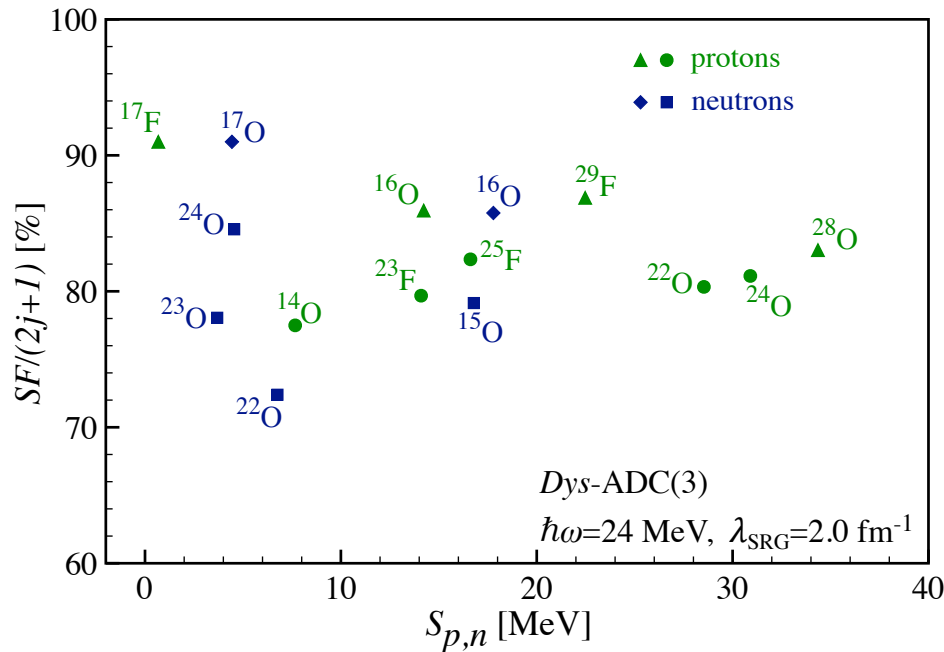


$^{56}\text{Ni}$   
NN-N3LO(500)

# Z/N asymmetry dependence of SFs - Theory

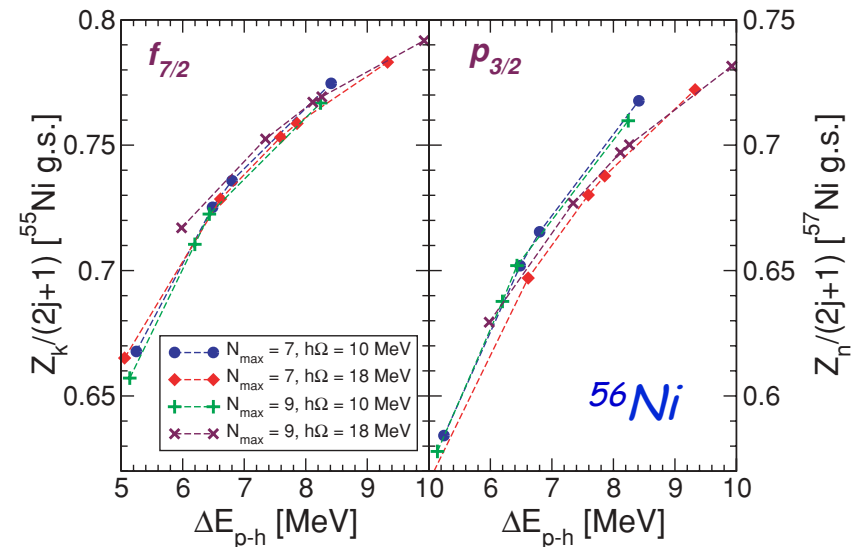
Ab-initio calculations explain the Z/N dependence but the effect is much lower than suggested by direct knockout

Effects of continuum become important at the driplines



arXiv:1412.0491 [nucl-th] (2014)

Spectroscopic factor are strongly correlated to p-h gaps:

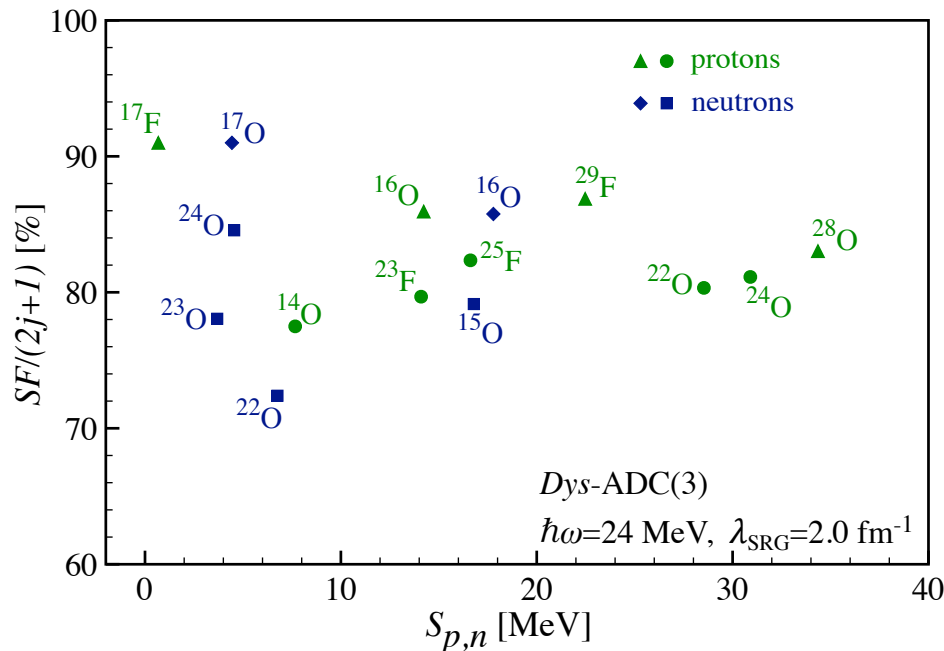




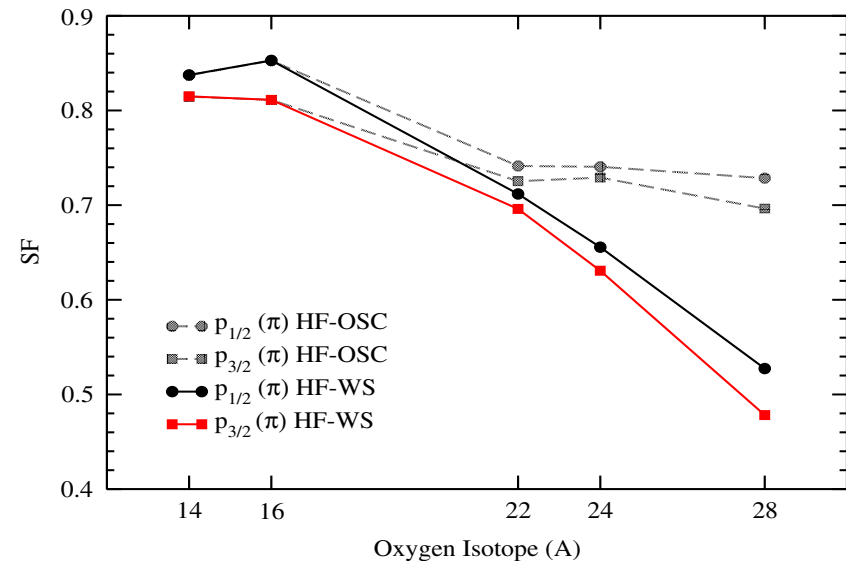
# Z/N asymmetry dependence of SFs - Theory

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arXiv:1412.0491 [nucl-th] (2014)



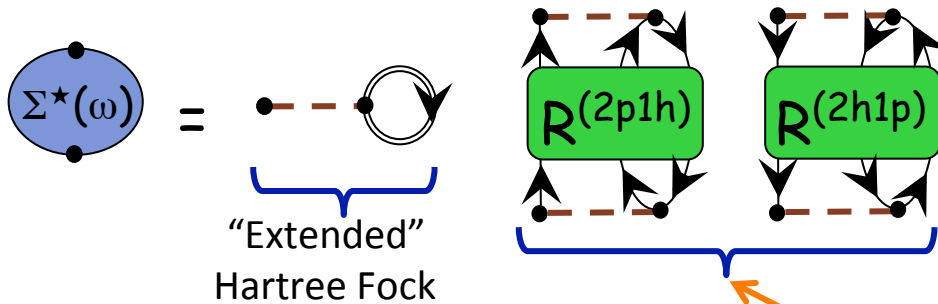
[Hagen et al.  
Phys. Rev. Lett. 107, 032501 (2011)]

# Optical Potentials Based on the Nuclear Self-energy

# 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...

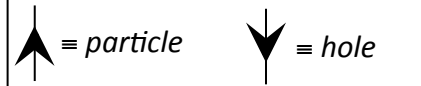
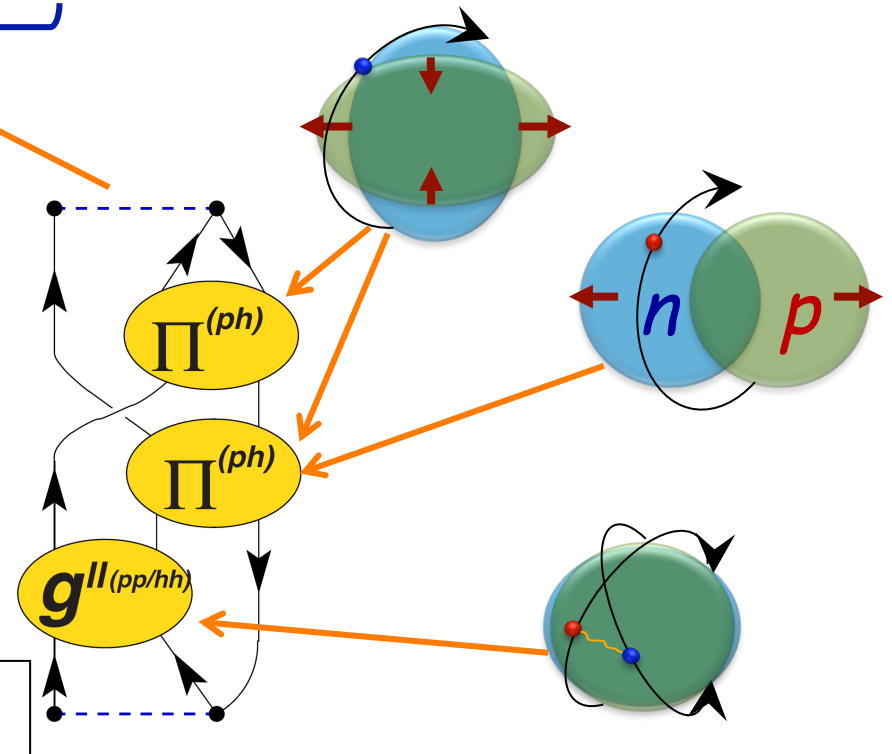
CB et al.,  
 Phys. Rev. C63, 034313 (2001)  
 Phys. Rev. A76, 052503 (2007)  
 Phys. Rev. C79, 064313 (2009)



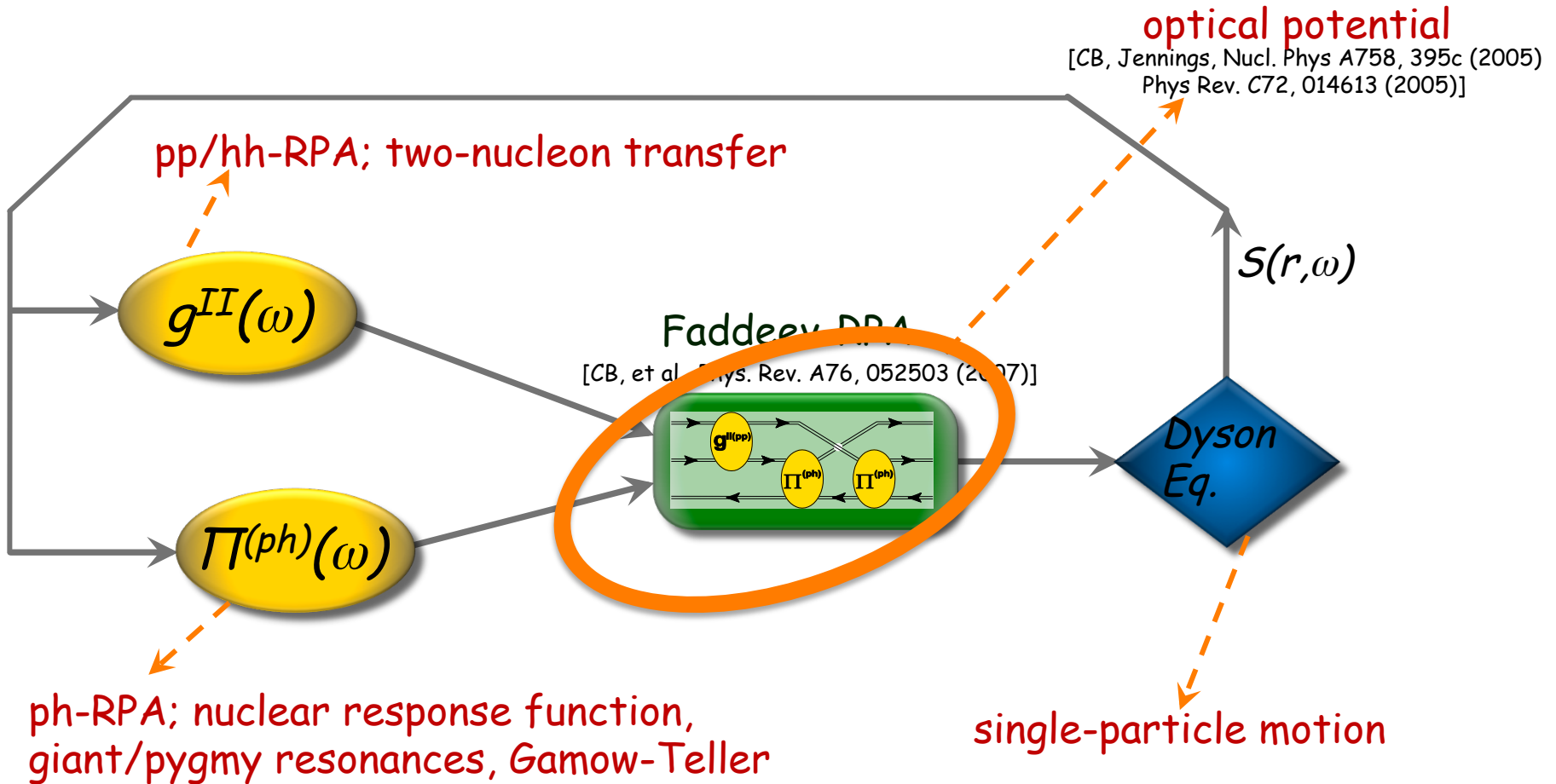
• A complete expansion requires all types of particle-vibration coupling

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

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

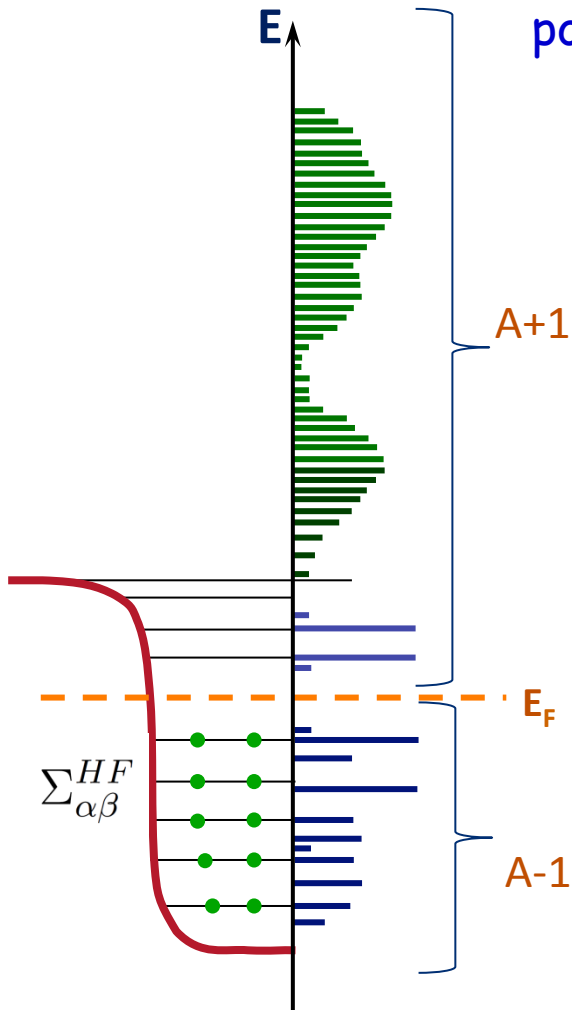


# Self-Consistent Green's Function Approach



# Nucleon-nucleus elastic scattering

The irreducible self-energy is a nucleon-nucleus optical potential [F. Capuzzi and C. Mahaux, Ann. Phys. (NY) **245**, 147 (1996), J. Escher and B. K. Jennings, Phys. Rev. C **66**, 034313 (2002)] :



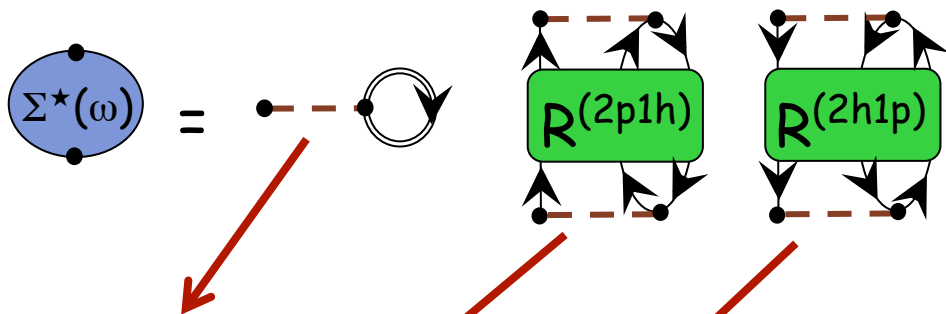
$$\Sigma^*(\mathbf{r}, \mathbf{r}'; \varepsilon) = \Sigma_{\alpha\beta}^{HF} - \frac{1}{\pi} \int_{\varepsilon_T^>}^{\infty} dE' \frac{\text{Im} \Sigma^*(\mathbf{r}, \mathbf{r}'; E')}{\varepsilon - E' + i\eta} + \frac{1}{\pi} \int_{-\infty}^{\varepsilon_T^<} dE' \frac{\text{Im} \Sigma^*(\mathbf{r}, \mathbf{r}'; E')}{\varepsilon - E' - i\eta}$$

mean-field

resonances  
beyond mean-field

→ This provides *consistent* overlaps and scattering wave functions

# Microscopic optical potential

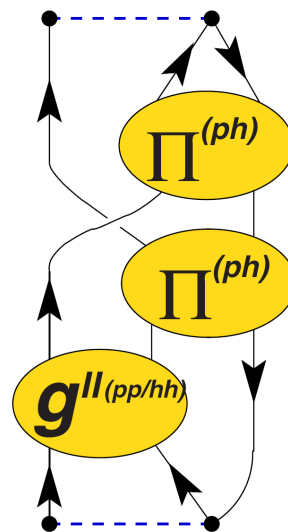


Transform h.o. basis  
to k- or r- space and then  
do scattering  
→ NO NEED CONT. BASIS

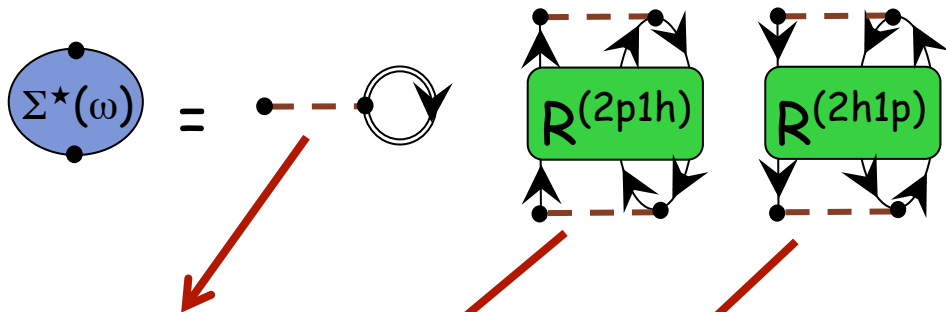
$$\Sigma_{lj}^{\text{MF, Fadd}}(k, k') = \sum_{n_\alpha, n_\beta \in \mathcal{P}} \phi_\alpha(k) \Sigma_{lj, n_\alpha, n_\beta}^{\text{MF, Fadd}} \phi_\beta^*(k')$$

$$\Sigma_{lj}^{(2p1h), \text{Fadd}}(k, k') = \sum_{n_\alpha, n_\beta \in \mathcal{P}} \phi_\alpha(k) \left[ \sum_{n_+} \frac{(m_\alpha^{n_+})^* m_\beta^{n_+}}{\omega - \varepsilon_{lj}^{n_+} + i\eta} \right] \phi_\beta^*(k')$$

$$\Sigma_{lj}^{(2h1p), \text{Fadd}}(k, k') = \sum_{n_\alpha, n_\beta \in \mathcal{P}} \phi_\alpha(k) \left[ \sum_{k_-} \frac{(m_\alpha^{k_-})^* m_\beta^{k_-}}{\omega - \varepsilon_{lj}^{k_-} - i\eta} \right] \phi_\beta^*(k')$$



# Microscopic optical potential



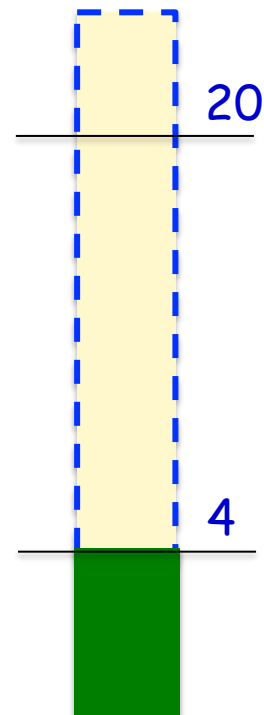
Transform h.o. basis  
to k- or r- space and then  
do scattering  
→ NO NEED CONT. BASIS

$$\Sigma_{lj}^{\text{MF, Fadd}}(k, k') = \sum_{n_\alpha, n_\beta \in \mathcal{P}} \phi_\alpha(k) \Sigma_{lj, n_\alpha, n_\beta}^{\text{MF, Fadd}} \phi_\beta^*(k')$$

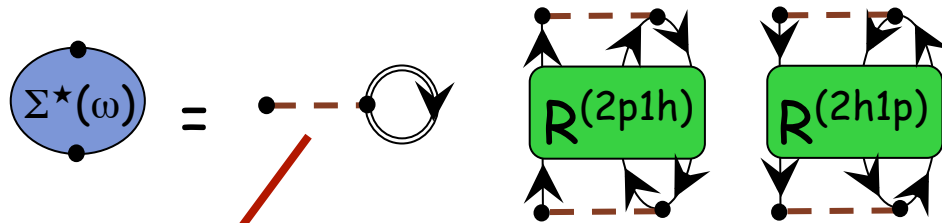
In 2005:  
- 4 h.o. shells  
- Bonn-C

$$\Sigma_{lj}^{(2p1h), \text{Fadd}}(k, k') = \sum_{n_\alpha, n_\beta \in \mathcal{P}} \phi_\alpha(k) \left[ \sum_{n_+} \frac{(m_\alpha^{n_+})^* m_\beta^{n_+}}{\omega - \varepsilon_{lj}^{n_+} + i\eta} \right] \phi_\beta^*(k')$$

$$\Sigma_{lj}^{(2h1p), \text{Fadd}}(k, k') = \sum_{n_\alpha, n_\beta \in \mathcal{P}} \phi_\alpha(k) \left[ \sum_{k_-} \frac{(m_\alpha^{k_-})^* m_\beta^{k_-}}{\omega - \varepsilon_{lj}^{k_-} - i\eta} \right] \phi_\beta^*(k')$$



# Microscopic optical potential



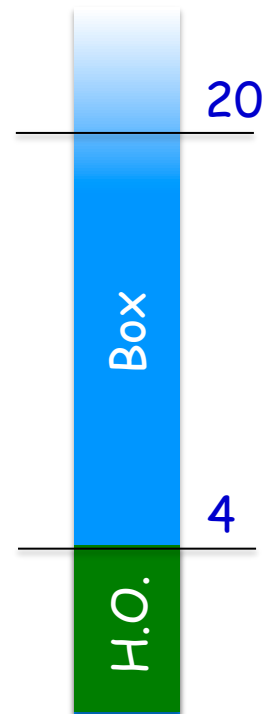
Transform h.o. basis  
to k- or r- space and then  
do scattering  
→ NO NEED CONT. BASIS

In 2005: 4 h.o. shells, Bonn-C  
→ COMPUTE MF IN A SPHERICAL BOX

$$\Sigma_{lj}^{\text{MF},I}(k, k') = N_{lj}^I \Sigma_{lj}^{\text{MF},\text{Fadd}}(k, k') + \Sigma_{1,lj}^{\text{MF},\text{Box}}(k, k')$$

$$\Sigma_{lj}^{\text{MF},II}(k, k') = N_{lj}^{II} \Sigma_{lj}^{\text{MF},\text{Box}}(k, k'),$$

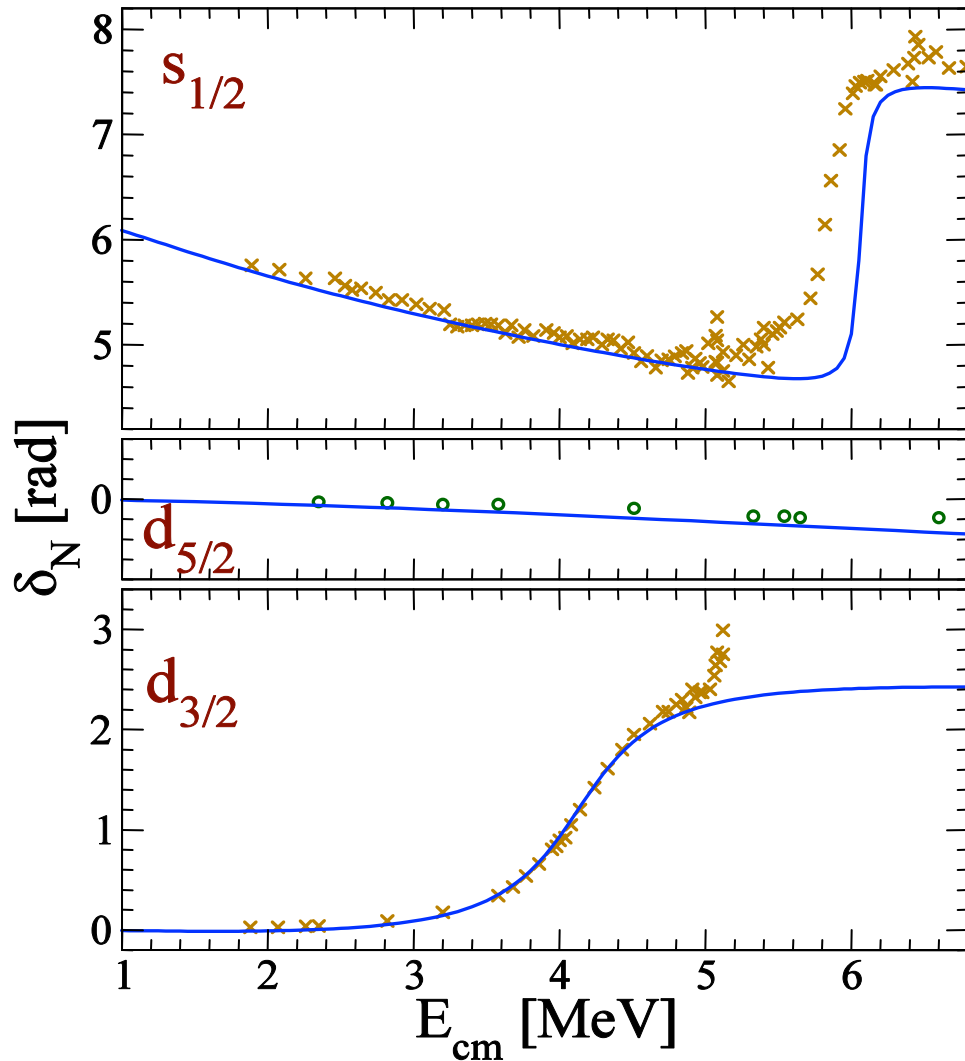
$$\Sigma_{lj}^{\star,I(II)}(k, k'; \omega) = \Sigma_{lj}^{\text{MF},I(II)}(k, k') + \Sigma_{lj}^{(2p1h),\text{Fadd}}(k, k'; \omega) + \Sigma_{lj}^{(2h1p),\text{Fadd}}(k, k'; \omega).$$





# $p$ - $^{16}\text{O}$ phase shifts - positive parity waves

[C.B., B.Jennings,  
Phys. Rev. C72, 014613 (2005)]



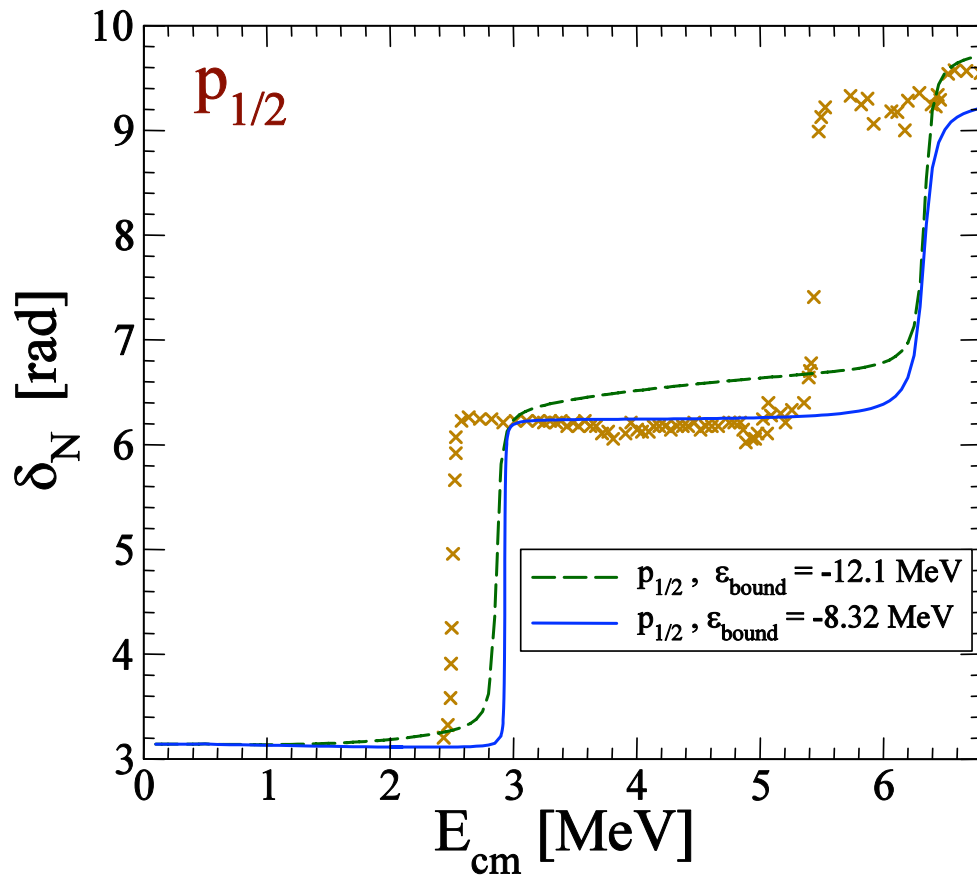
- AV18 interaction

- The phase shifts are in agreement with the experiment!

- BUT does not reproduce phase shifts and bound state energies at the same time  
→ need for improved H / 3NF

- Non-MF resonances "OK"

# $p\text{-}^{16}\text{O}$ phase shifts - $l=1$ waves



- For p waves: cannot describe separation energy and phase shift together...  
→ need for improved H / 3NF (again!)

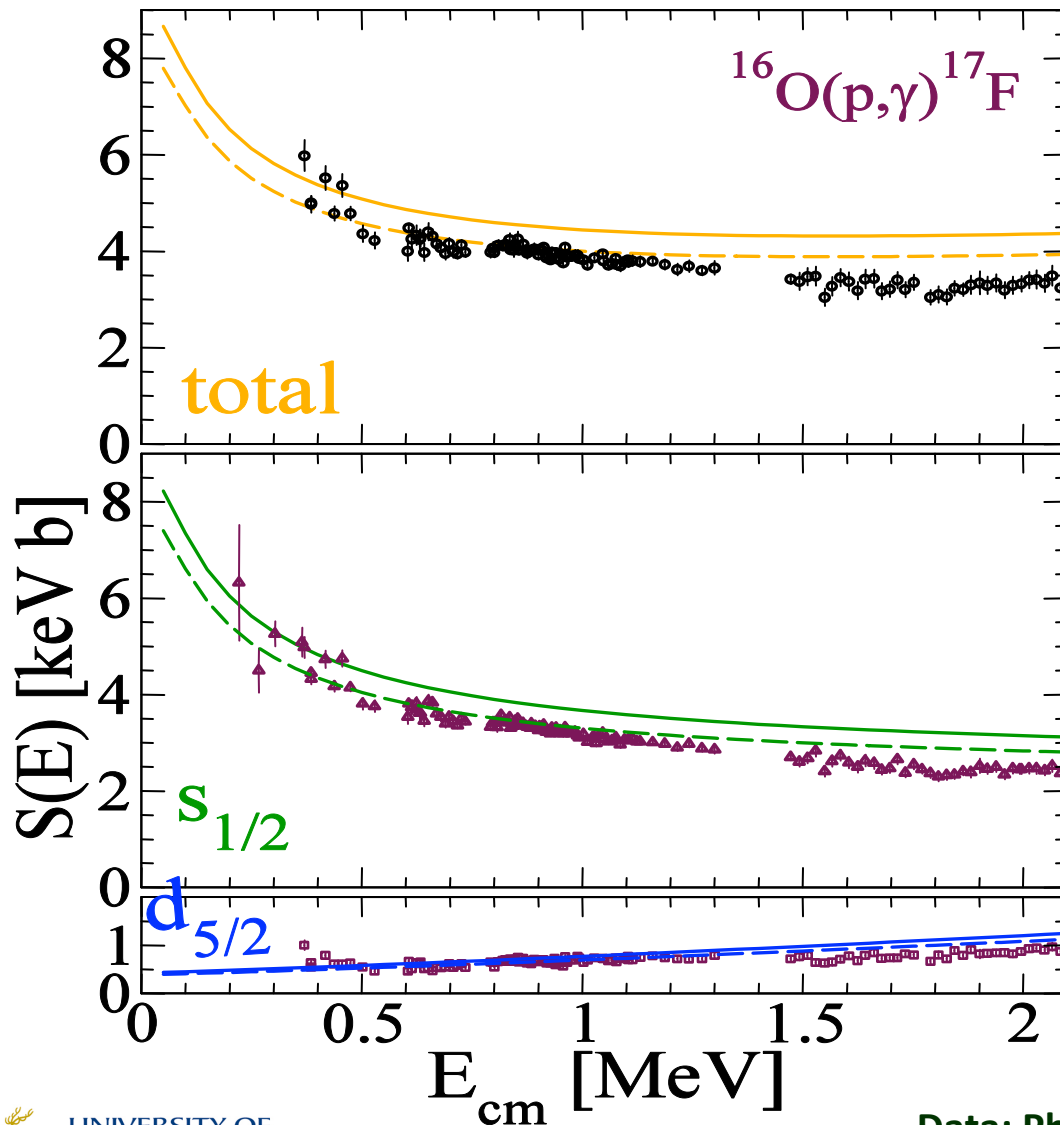
- To obtain the background phase shifts:

$$E_{p_{1/2}} = -8.32 \text{ MeV}$$

$$E_{p_{3/2}} = -15.1 \text{ MeV}$$

- Non-MF resonances

# Radiative capture



- astrophysical factor:

$$S(E) = E e^{2\pi\eta} \sigma(E)$$

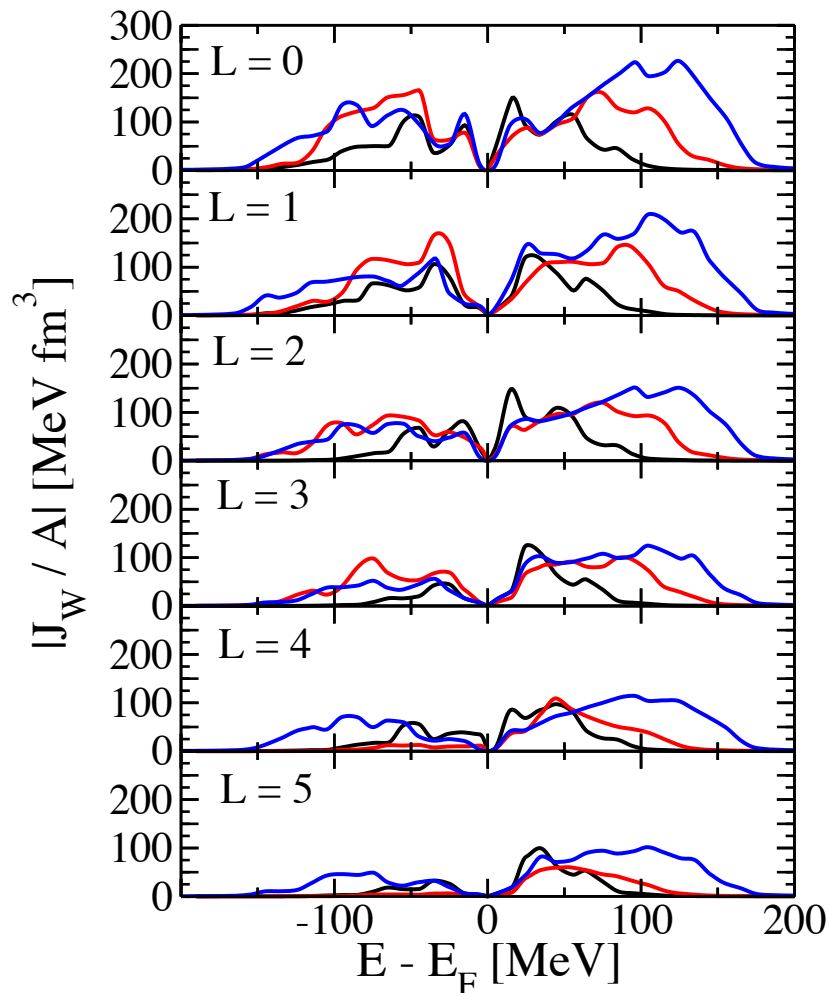
- At zero energy:

$$S(0) \approx 11.5 \text{ keV}\cdot\text{b}$$

CB, Jennings,  
Nucl. Phys A758, 395c (2005)

Data: Phys. Rev. Lett. 79, 3837 ('97)

# Convergence of Ab-Initio Calculated Optical Potentials



←  $J_w$ : volume integral over the imaginary opt. pot. (overall absorption)

$n$ - $^{48}\text{Ca}$  scattering calculated with the NN N3LO chiral interaction

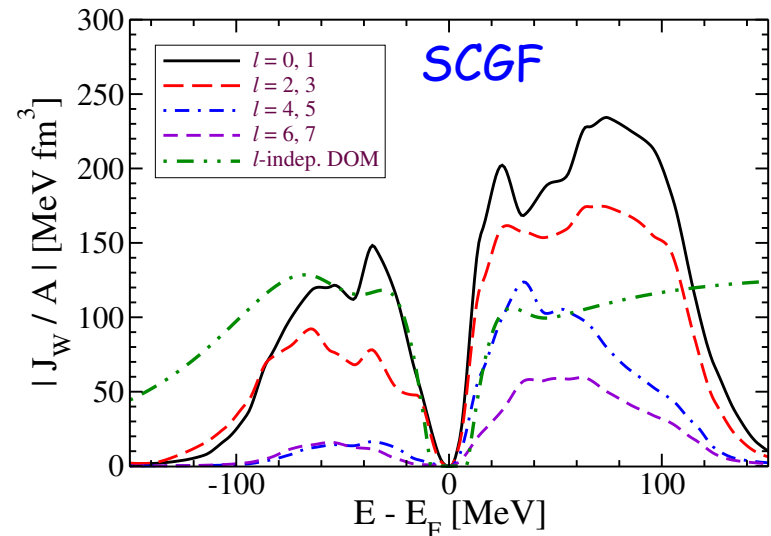
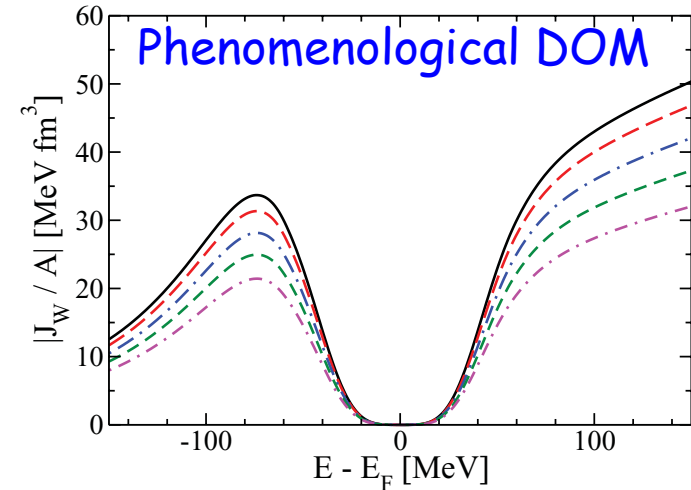
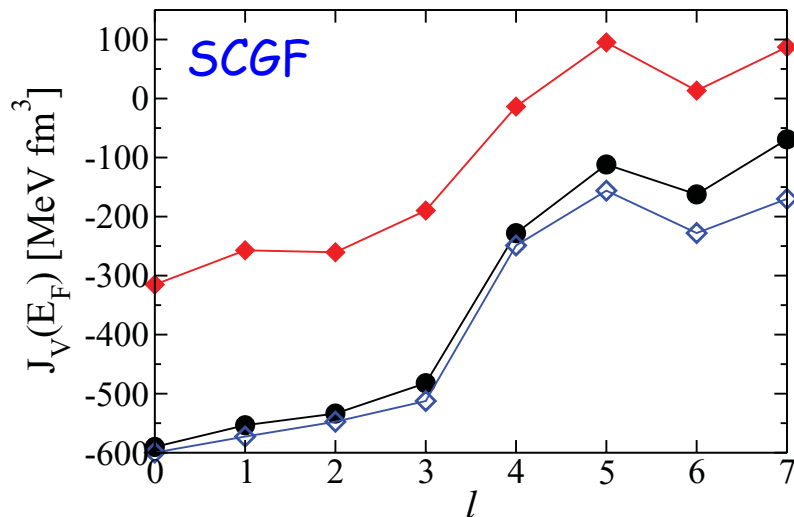
—	6 h.o. shells
—	8 h.o. shells
—	10 h.o. shells

# L-dependence and non locality

Volume integrals of central parts (real and imaginary):

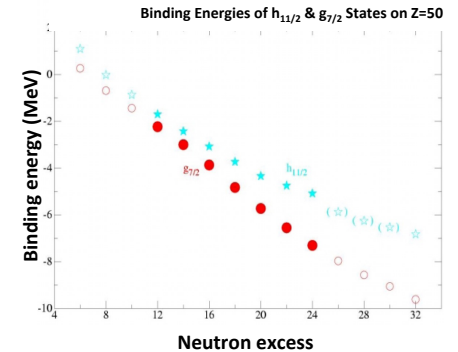
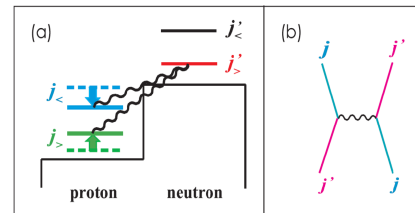
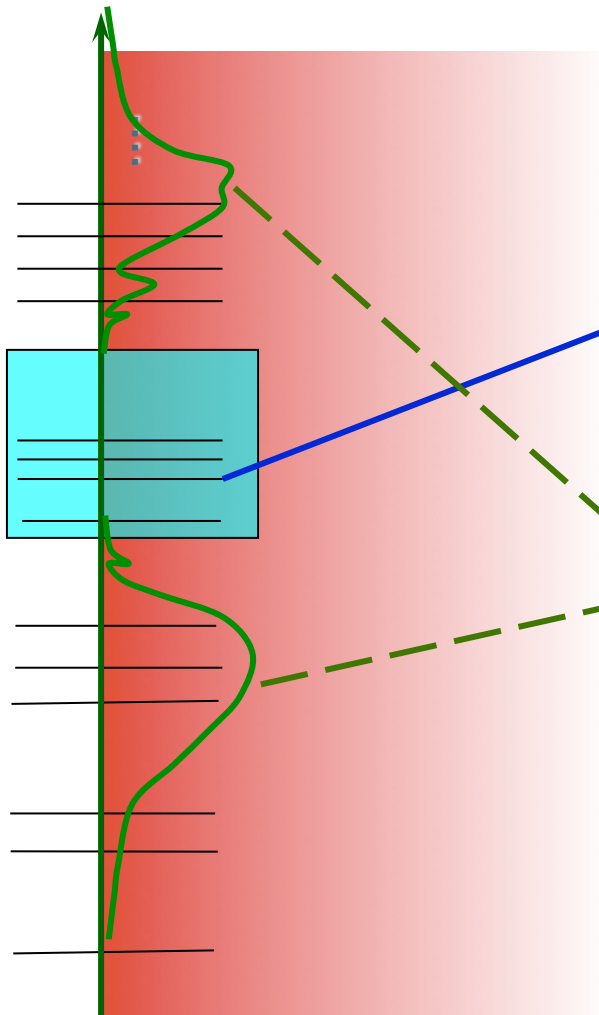
$$J_W^\ell(E) = 4\pi \int dr r^2 \int dr' r'^2 \text{Im} \Sigma_0^\ell(r, r'; E),$$

$$J_V^\ell(E) = 4\pi \int dr r^2 \int dr' r'^2 \text{Re} \Sigma_0^\ell(r, r'; E).$$



# Correlations in sp energies and strengths

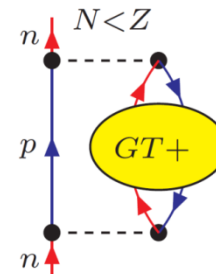
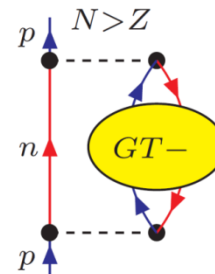
Single particle energies - driven by tensor + 3N force...  
(see works by T. Otsuka PRL2005, 2010)



Quenching of spectral strength (spect. factor) - driven by coupling to collective modes...

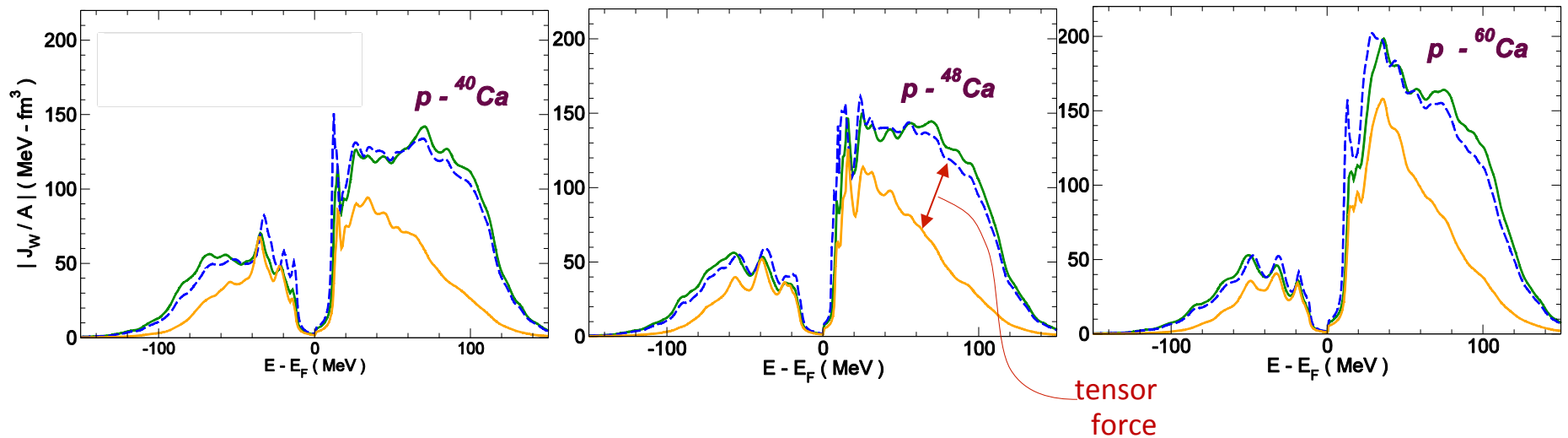
• Role of tensor force??

• Collective, charge exchange effects???



# Microscopic Optical Potential from FRPA

- absorption away from  $E_F$  is enhanced by the tensor force
- little effects from charge exchange (e.g.  $p\text{-}^{48}\text{Ca} \leftrightarrow n\text{-}^{48}\text{Sc}$ )



$J_w$ : integral over the imaginary opt. pot (overall absorption)

- Full FRPA result (w/  $av18$ )
- - Charge-exchange d.o.f. suppressed
- Tensor force suppressed

S. Waldecker, CB, W. Dickhoff – Phys. Rev. C84, 034616 (2011)

# Collaborators



energies atomiques • énergies alternatives



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*P. Navratil*

*A. Polls*

*W.H. Dickhoff, S. Waldecker*

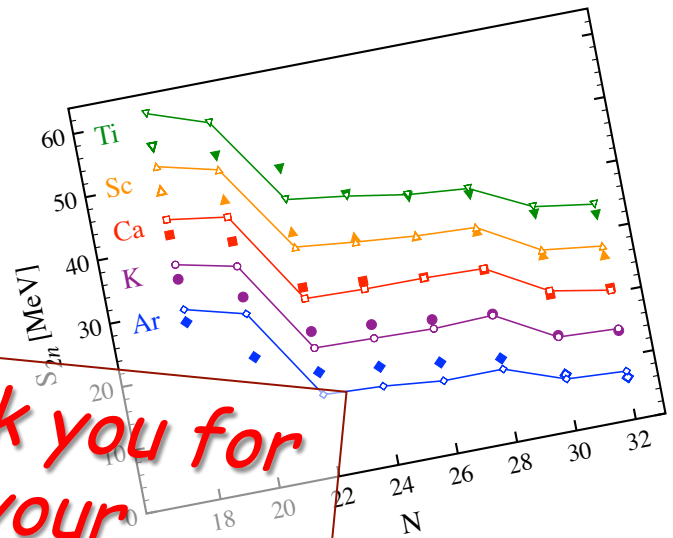
*D. Van Neck, M. Degroote*

*M. Hjorth-Jensen*



# Conclusions

- What to did we learn about realistic chiral forces from ab-initio calculations ?
  - *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 ( $A \approx 30$ ) but deteriorates for medium mass isotopes (Ca and above) with roughly 1 MeV/A over binding.*
  - *more short-range repulsion or fitting to mid masses will help [see NNLOsat talk, etc...].*
  - *Ab-initio optical potentials are a natural 'by-product' of the SCGF method.*
  - *Earlier investigations of SCGF based optical potentials were very promising; it will now be crucial to apply it in modern ab-initio codes.*



**Thank you for  
your  
attention!!!**