

# Ab initio Self-Consistent Green's function computations of nuclei

59<sup>th</sup> Zakopane Conference on Nuclear Physics  
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**Carlo Barbieri**

Università degli Studi di Milano & INFN

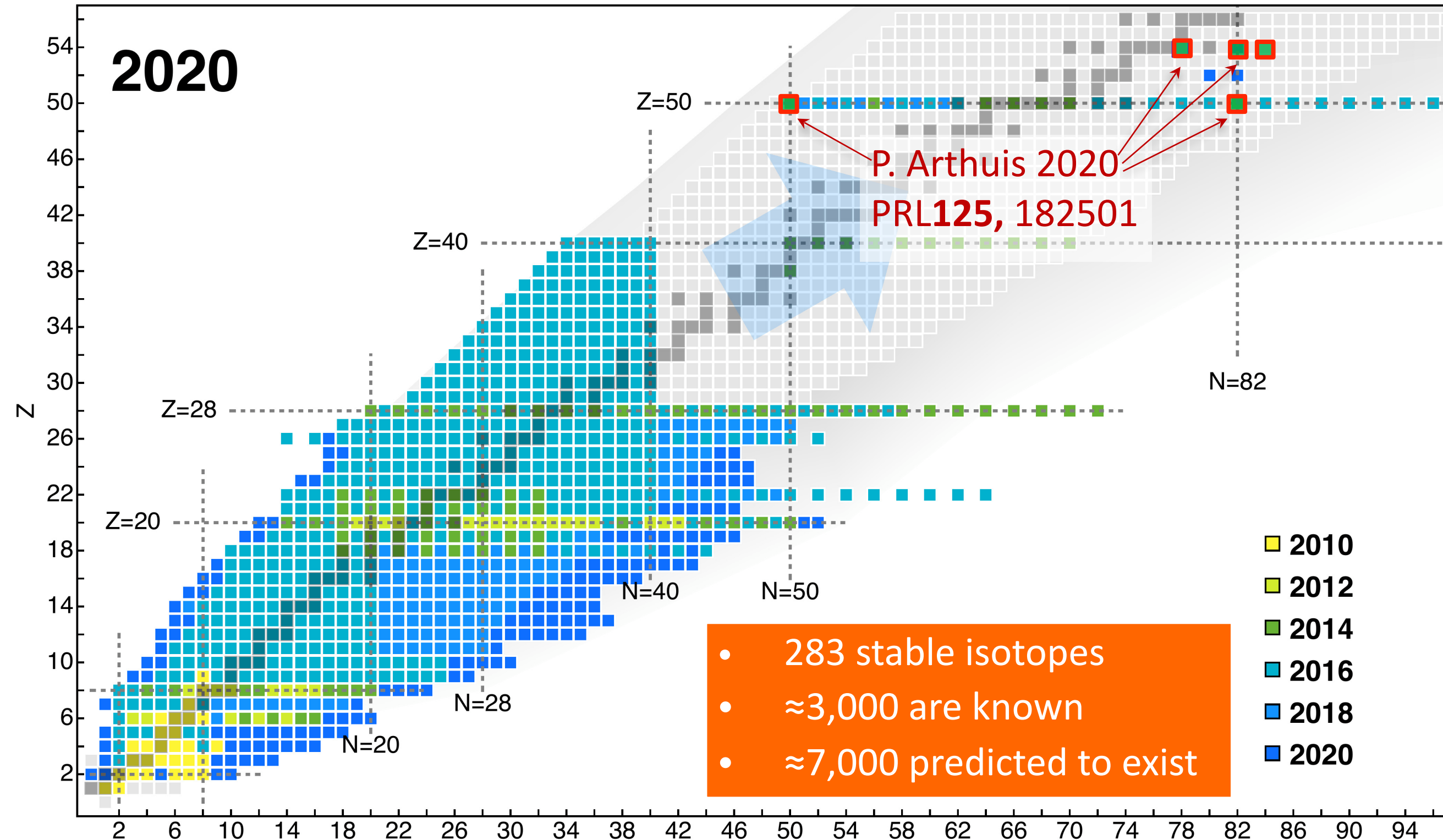




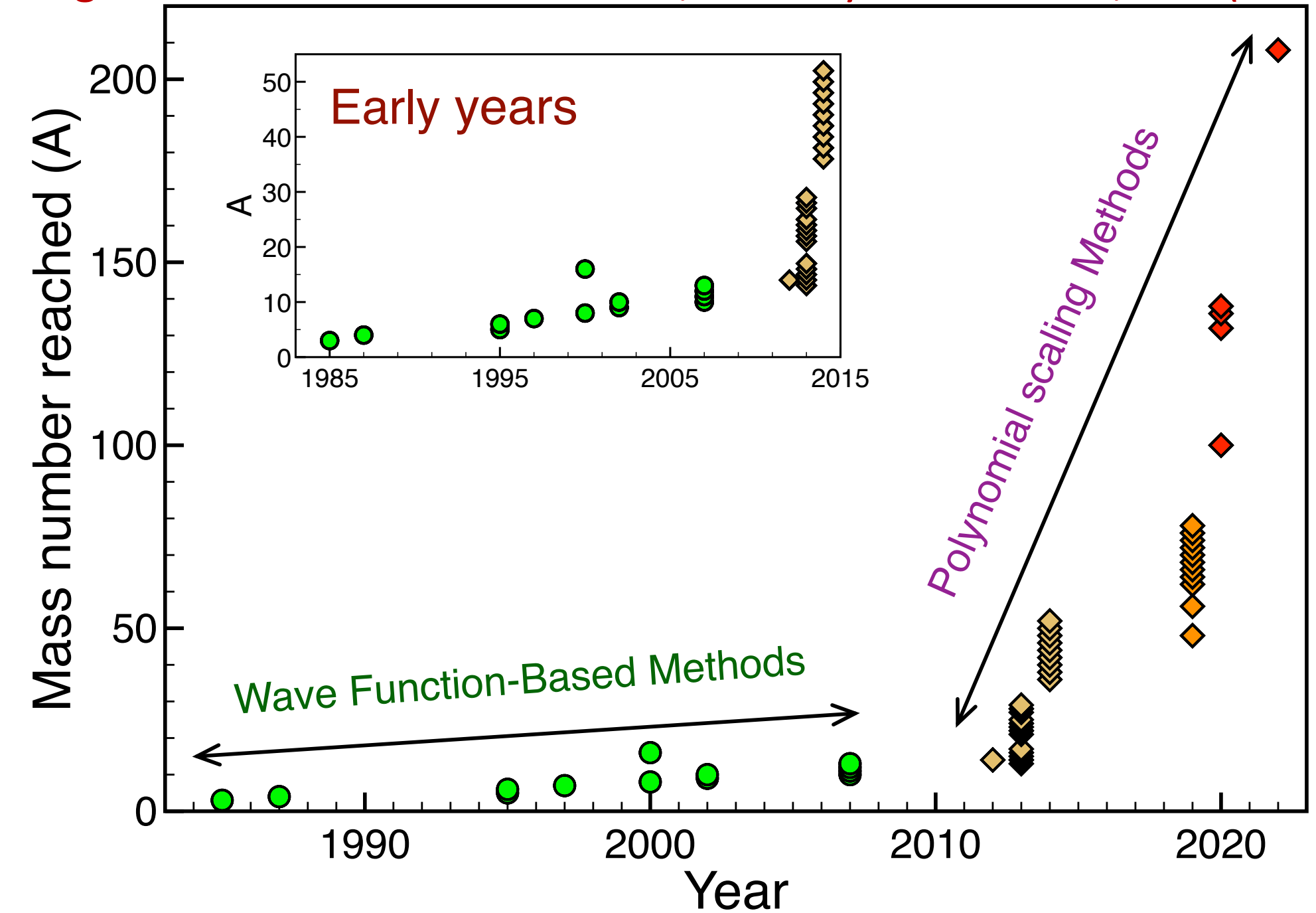
# Reach of ab initio methods across the nuclear chart

Extension beyond few-nucleons thanks to:

- Soft (nearly perturbative) effective nuclear forces
- Diagrammatic many-body approaches



Legnaro Natl' Lab Mid Term Plan; Eur. Phys. J. Plus **138**, 709 (2023)



Open challenges:

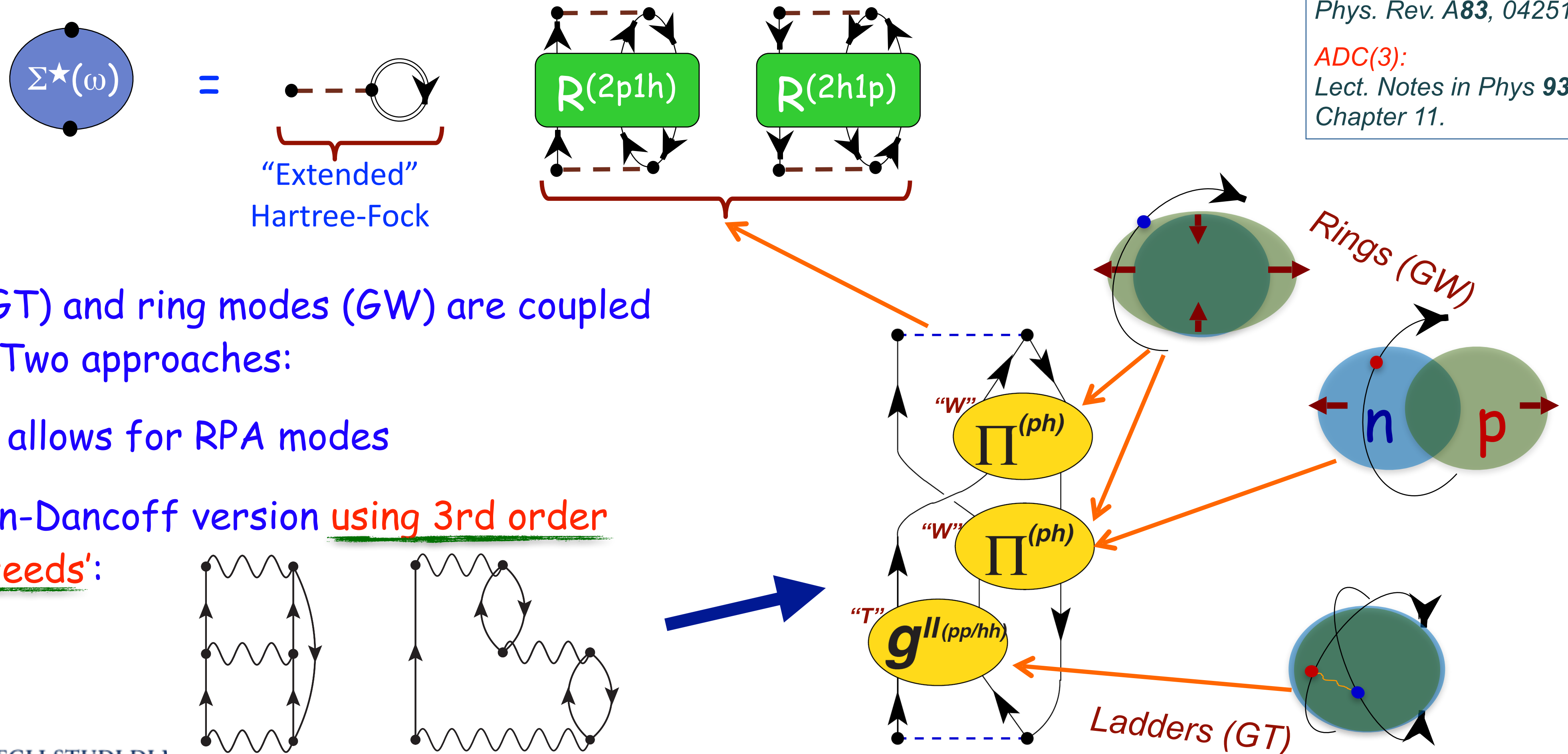
- Accuracy (better theory of nuclear forces)
- Mass number limit (optimised model spaces)
- Precision & scattering (high-order diag. resummations)



# The Faddev-RPA and ADC(3) methods in a few words

Compute the nuclear self energy to extract both scattering (optical potential) and spectroscopy.

Both ladders and rings are needed for atomi nuclei:



**F-RPA:**

Phys. Rev. C **63**, 034313 (2001)

Phys. Rev. A **76**, 052503 (2007)

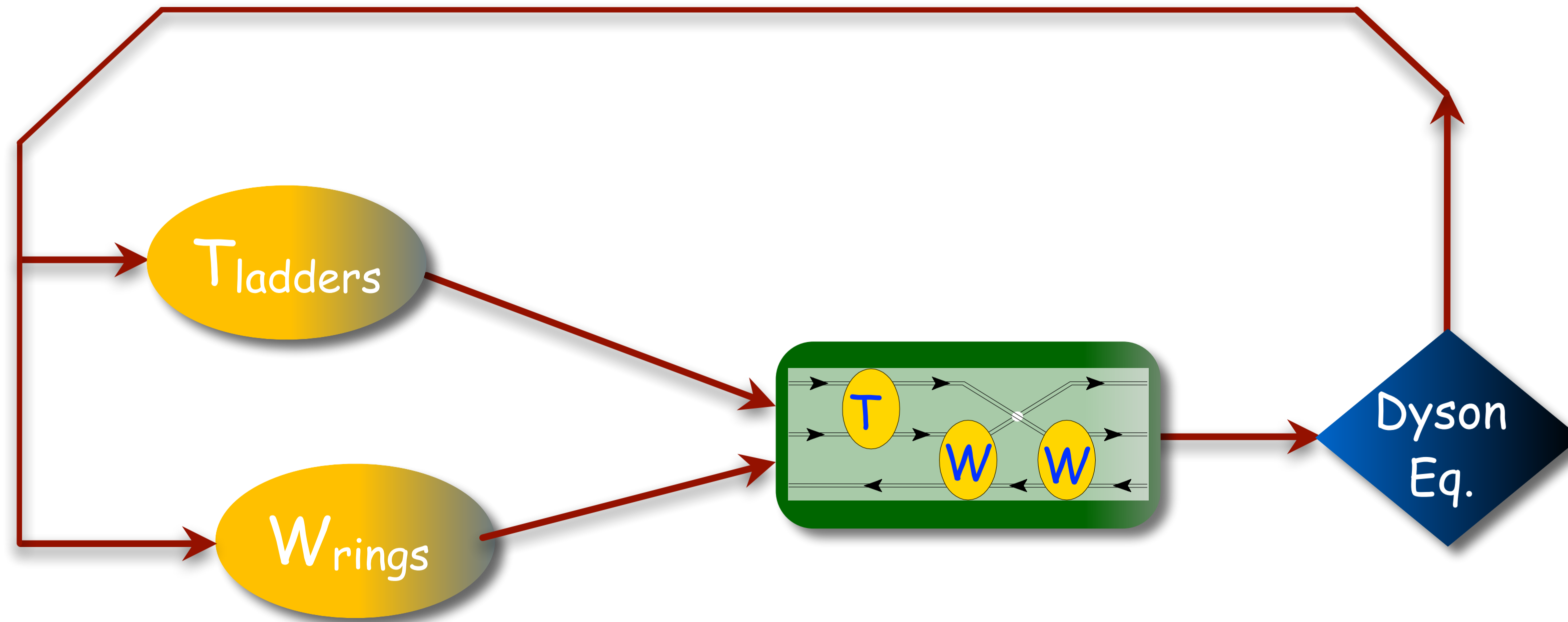
Phys. Rev. A **83**, 042517 (2011)

**ADC(3):**

Lect. Notes in Phys **936** (2017)-  
Chapter 11.



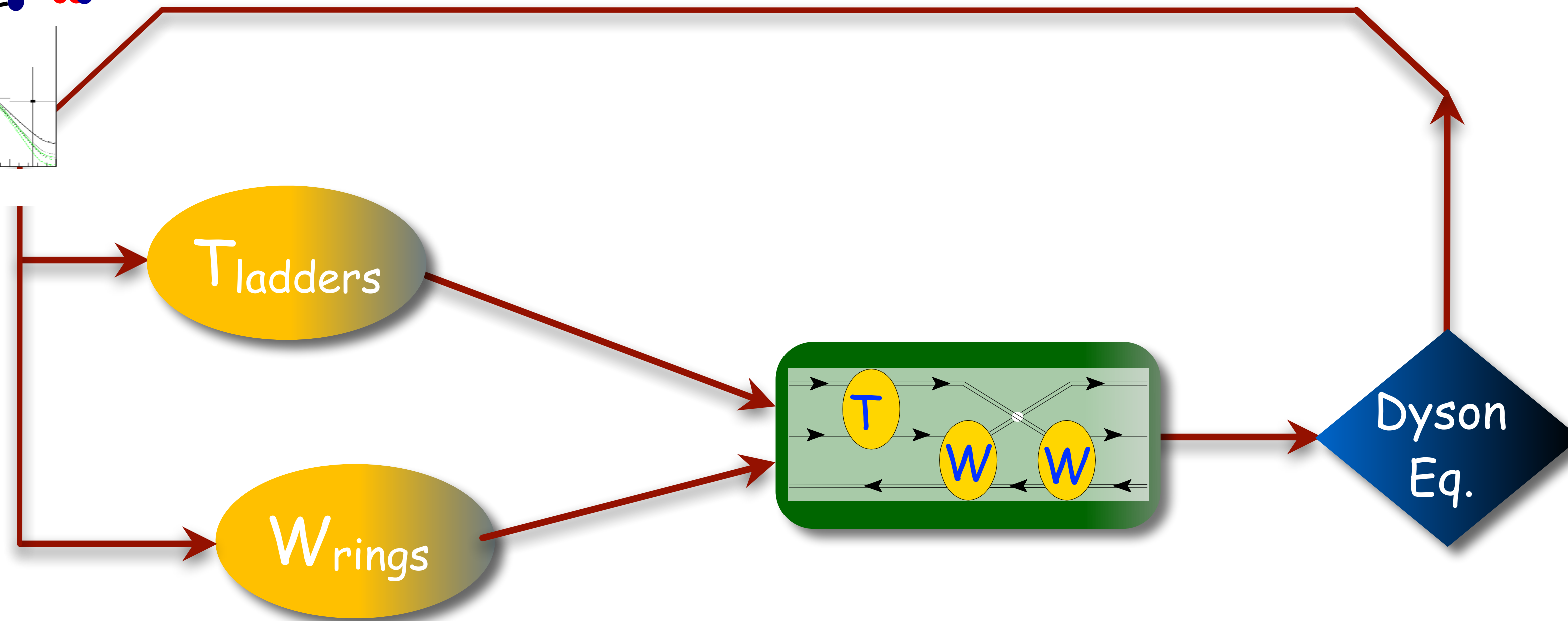
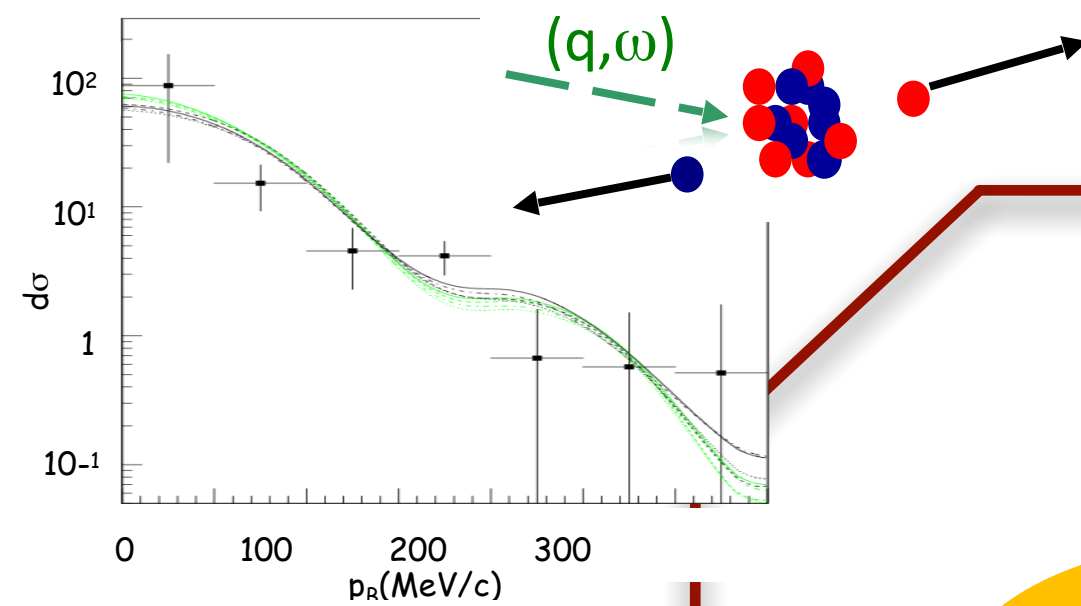
# The Self-Consistent Green's Function with Faddeev-RPA





# The Self-Consistent Green's Function with Faddeev-RPA

Two-nucleon emission:  $^{16}\text{O}(e,e'pn)^{14}\text{N}$   
[Eur. Phys. J. A43, 137 (2010)]

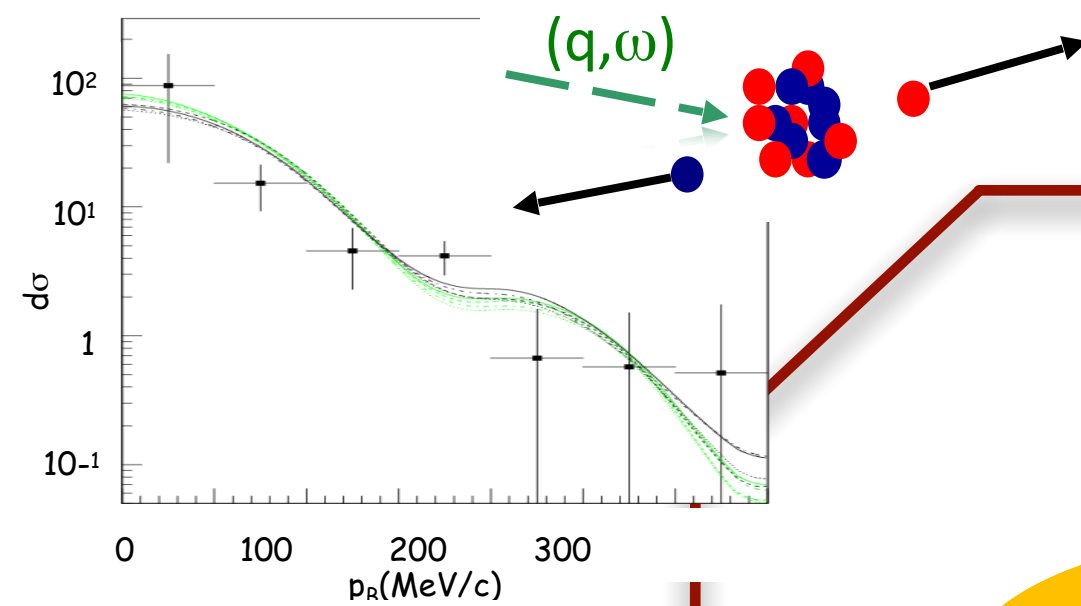




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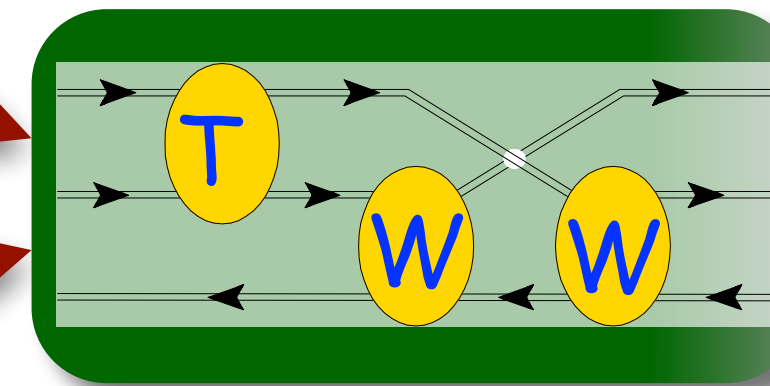
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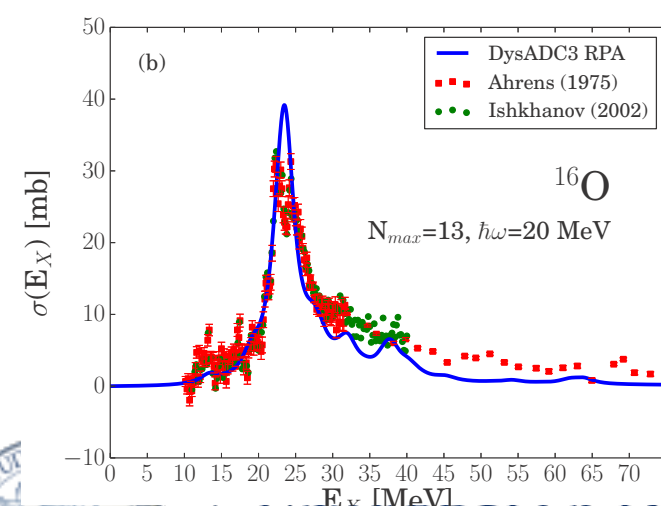
$W_{\text{rings}}$



Dyson Eq.

Nuclear ELM response and dipole polarisability,  $\alpha_D$

[Phys Rev. C77, 024304 (2008)]



$^{68}\text{Ni}$ :

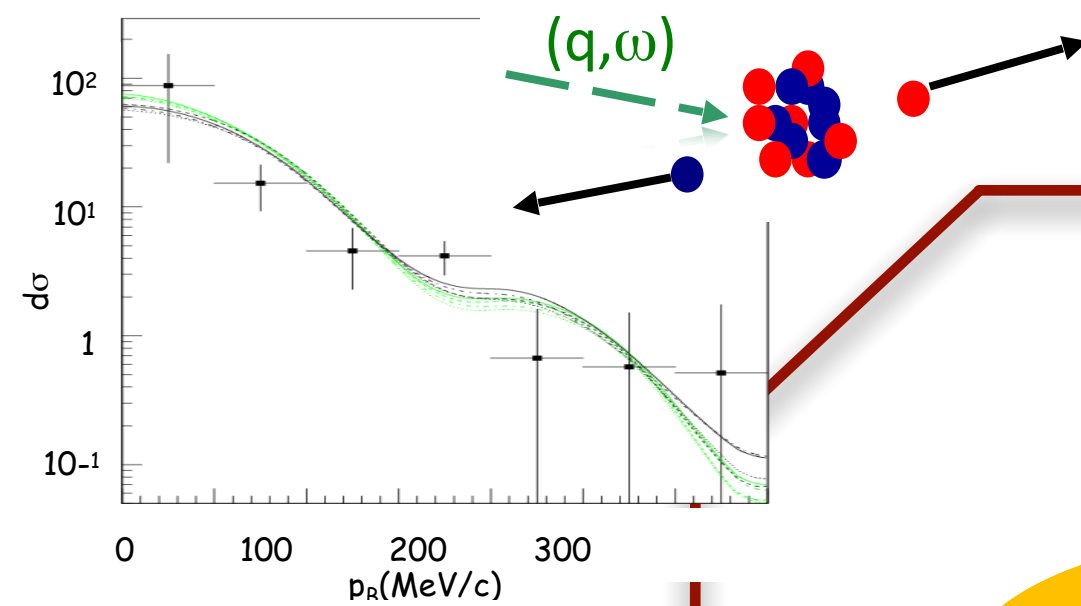
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| $E_{\text{GDR}} \text{ (MeV)}$   | 18.1           | 17.1(2)              |
| $\alpha_D \text{ (fm}^3\text{)}$ | 3.60           | 3.40(23)<br>3.88(31) |



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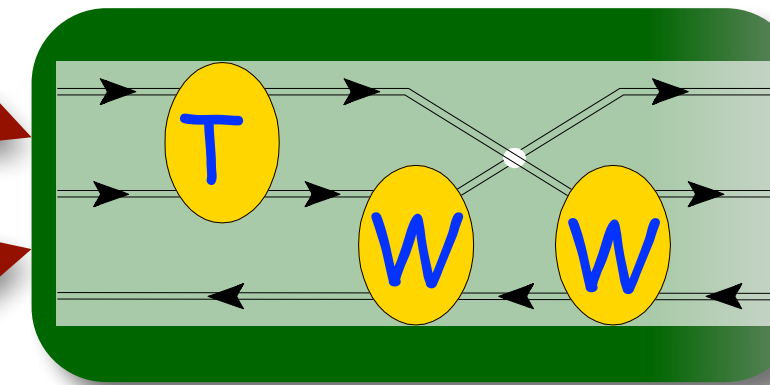
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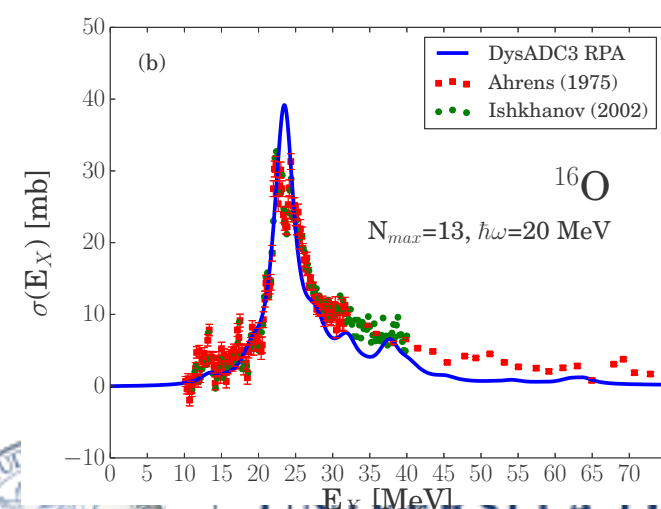
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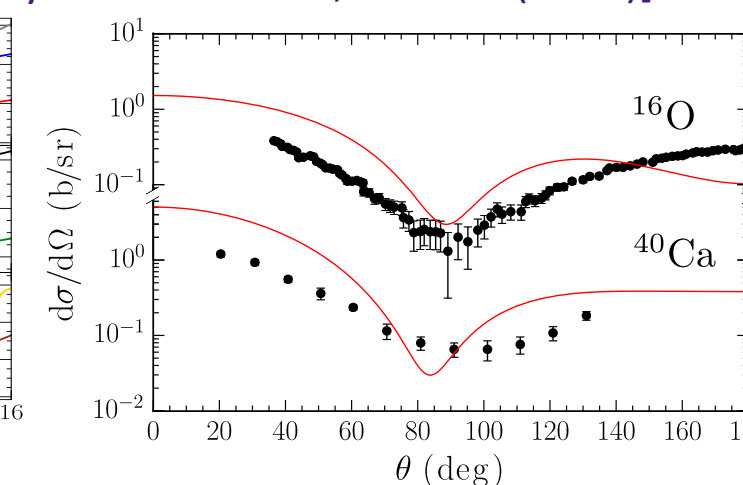
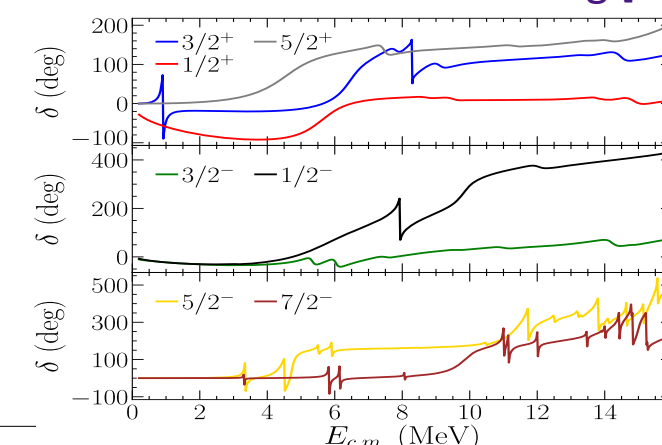


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## Optical potential

Elastic neutron scattering [Phys. Rev. Lett. 123, 092501 (2013)]

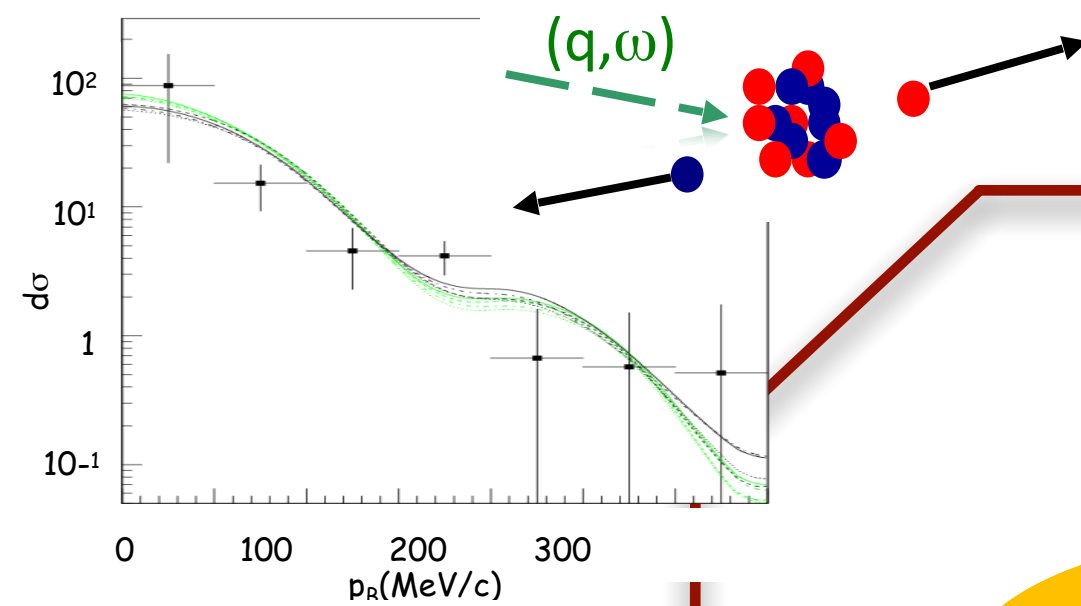




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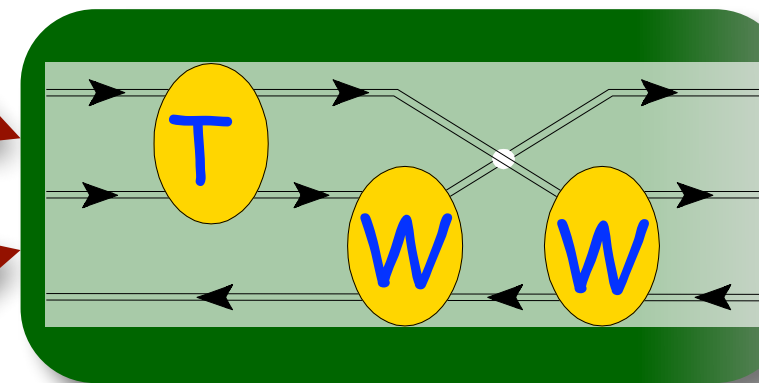
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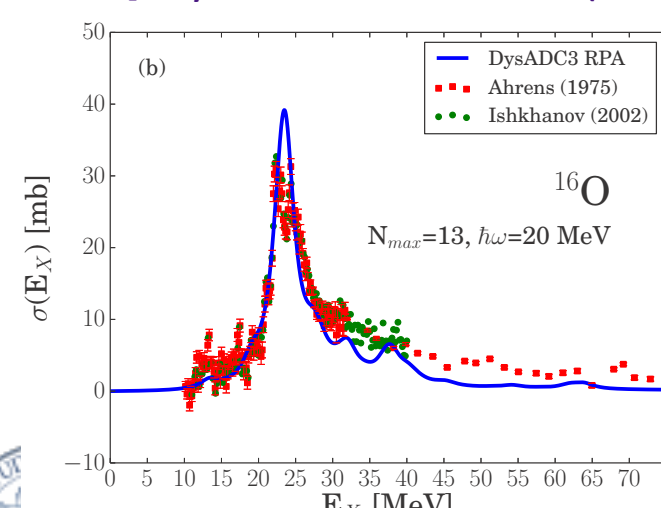
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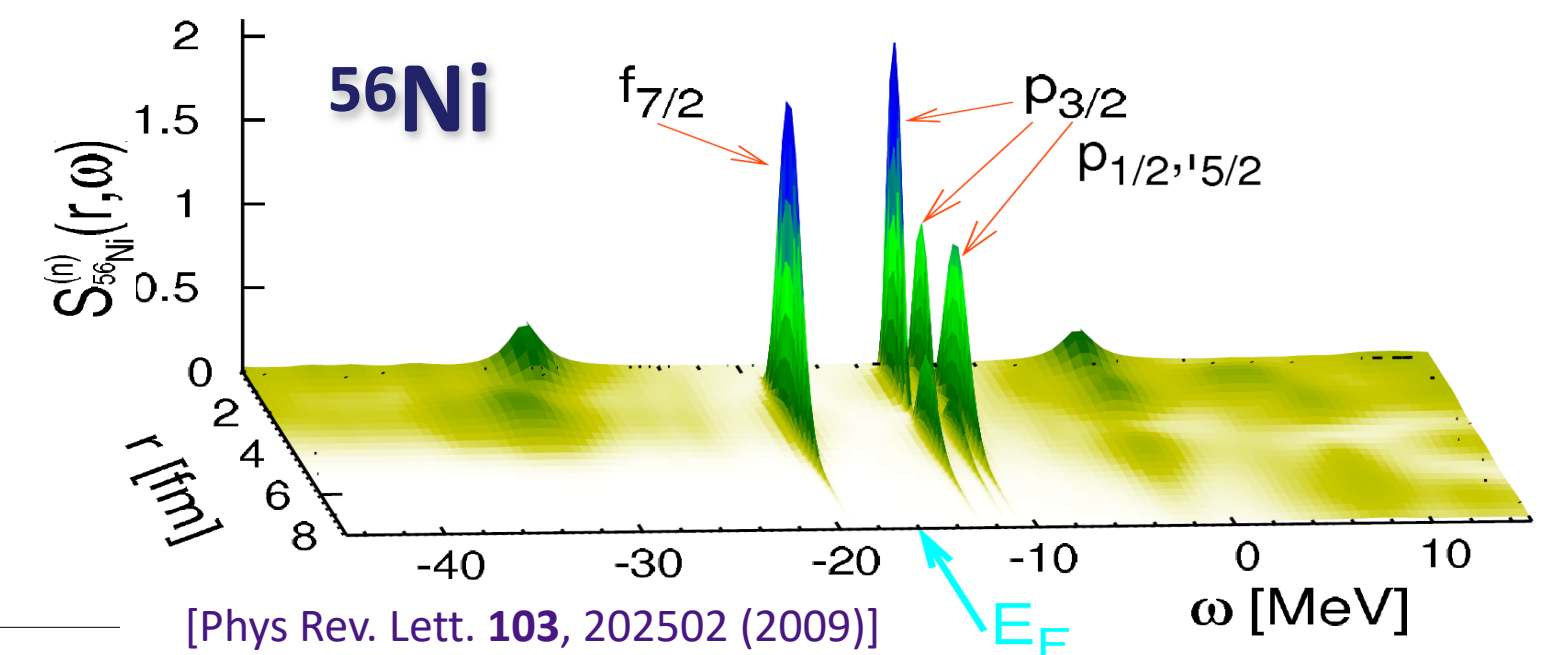
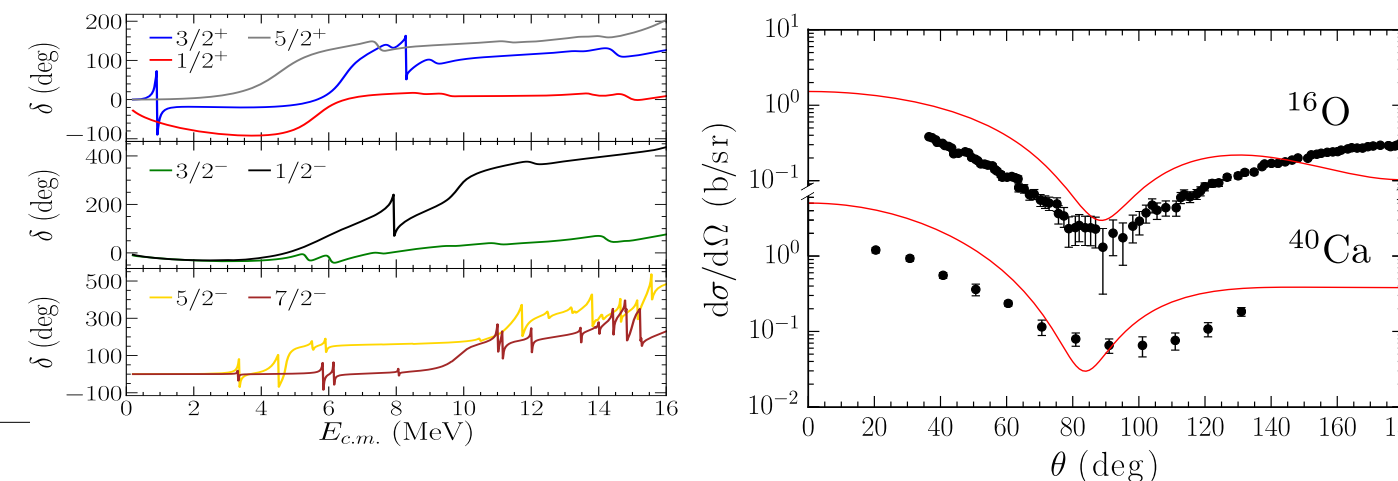


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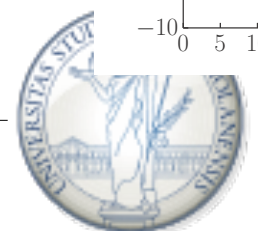
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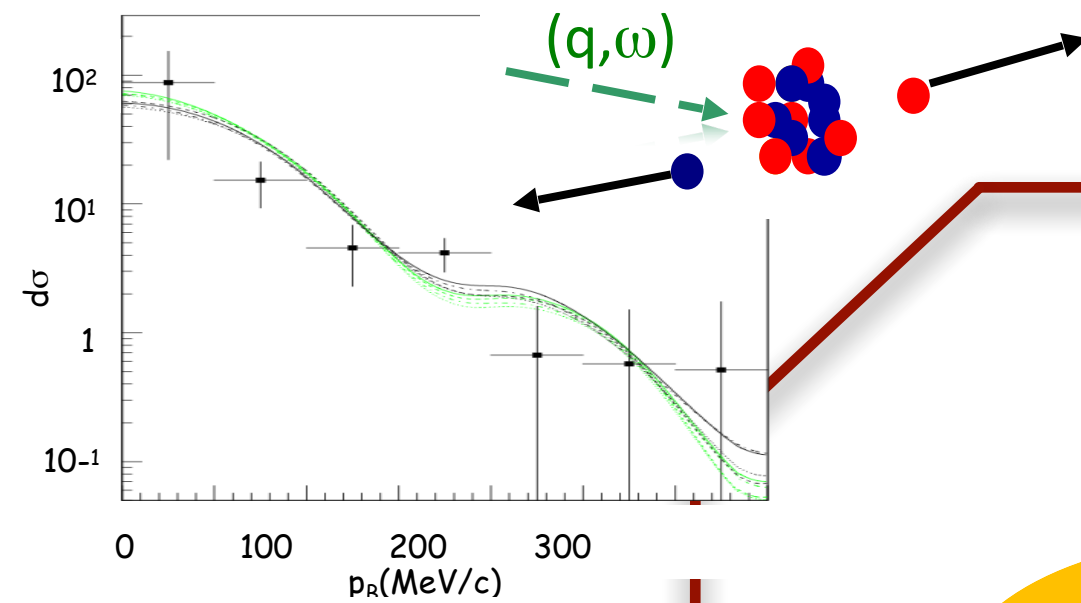
[Phys. Rev. Lett. 103, 202502 (2009)]



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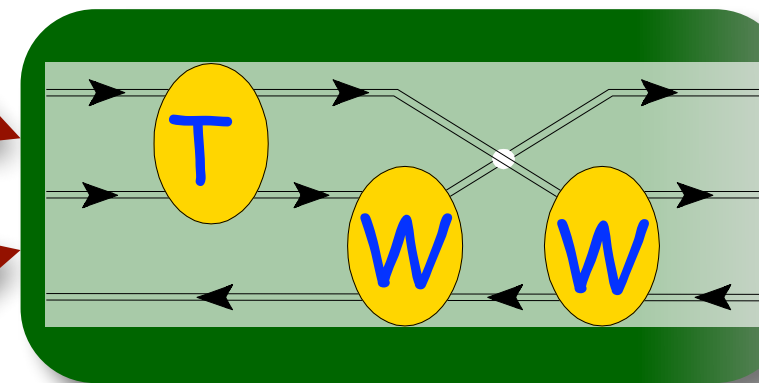
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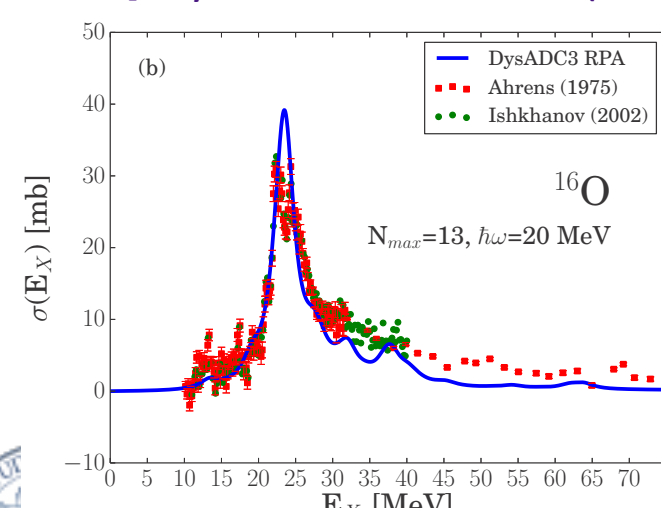
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[Phys. Rev. A. 83, 042517 (2011); 85, 012501 (2012)]

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| HF                   | $1\pi$                     | 16.48      | 16.05      | 16.35      | 16.05 |
|                      | $3\sigma$                  | 20.36      | 20.03      | 20.24      | 20.0  |
| CO                   | $5\sigma$                  | 13.94      | 14.37      | 13.69      | 14.01 |
|                      | $1\pi$                     | 16.98      | 16.95      | 16.84      | 16.91 |
|                      | $4\sigma$                  | 20.19      | 19.46      | 19.59      | 19.72 |
| $\text{H}_2\text{O}$ | $1b_1$                     | 12.86      | 12.62      | 12.67      | 12.62 |
|                      | $3a_1$                     | 15.15      | 14.91      | 14.98      | 14.74 |
|                      | $1b_2$                     | 19.21      | 19.06      | 19.13      | 18.51 |
|                      | $\bar{\Delta}$ (eV)        | 0.30(0.30) | 0.25(0.23) | 0.31(0.26) |       |
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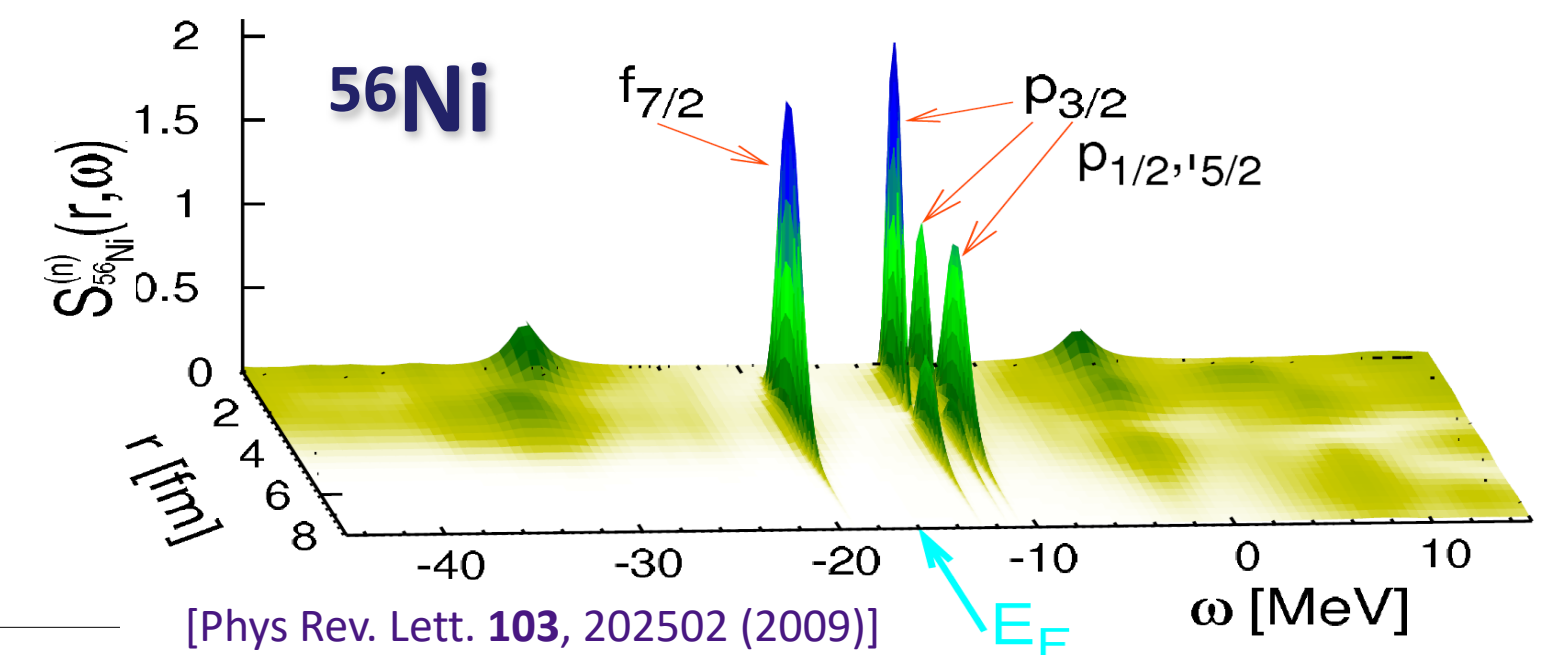
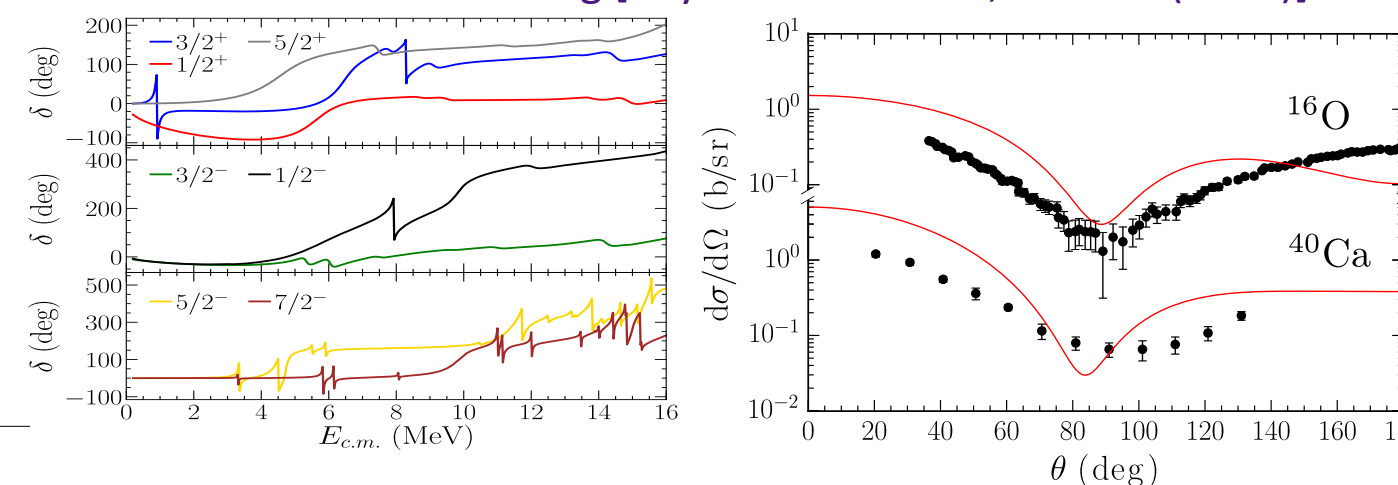


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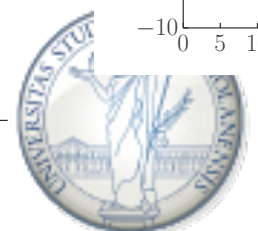
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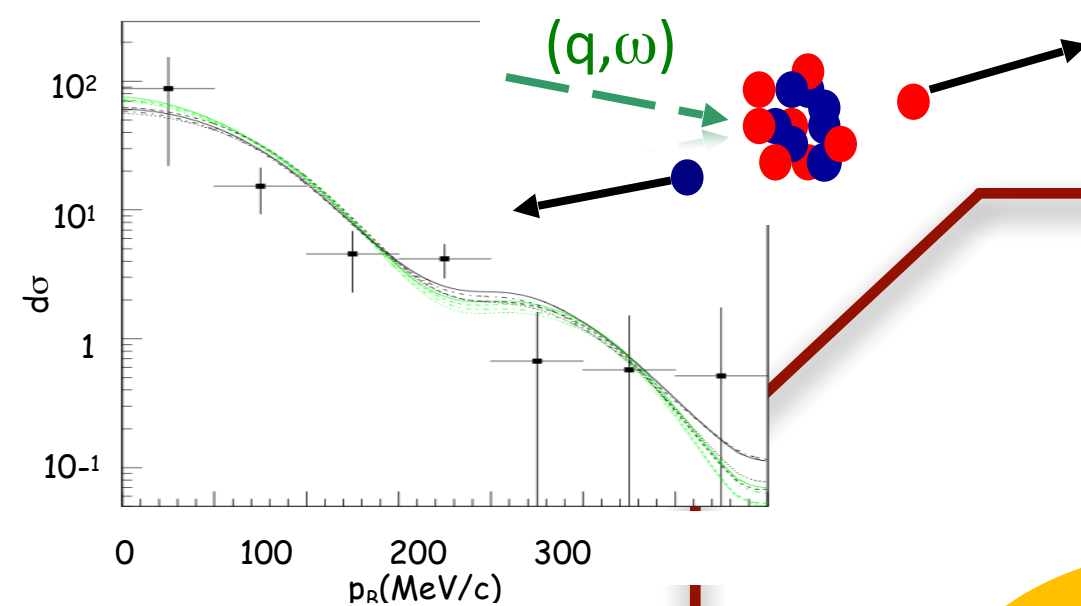




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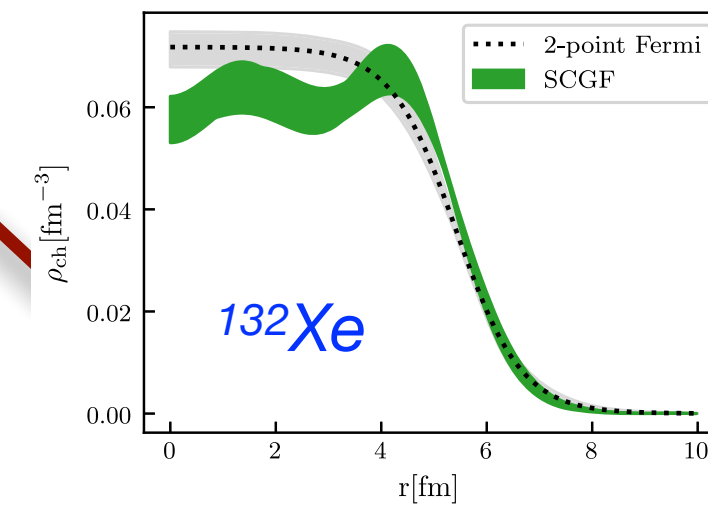
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|                   | SCGF          | Exp.   |
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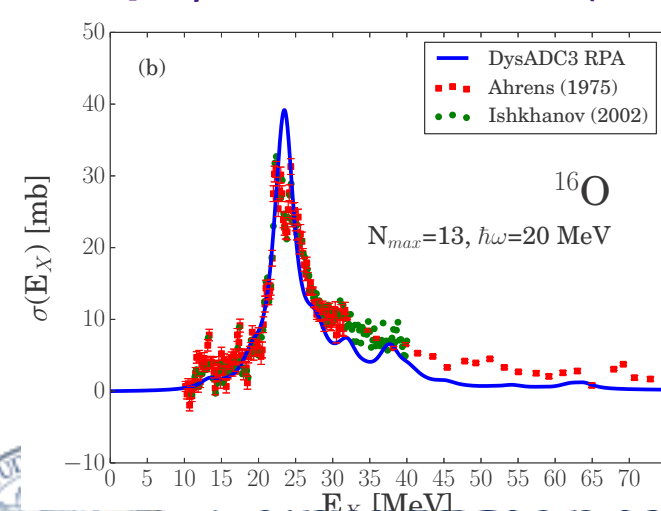
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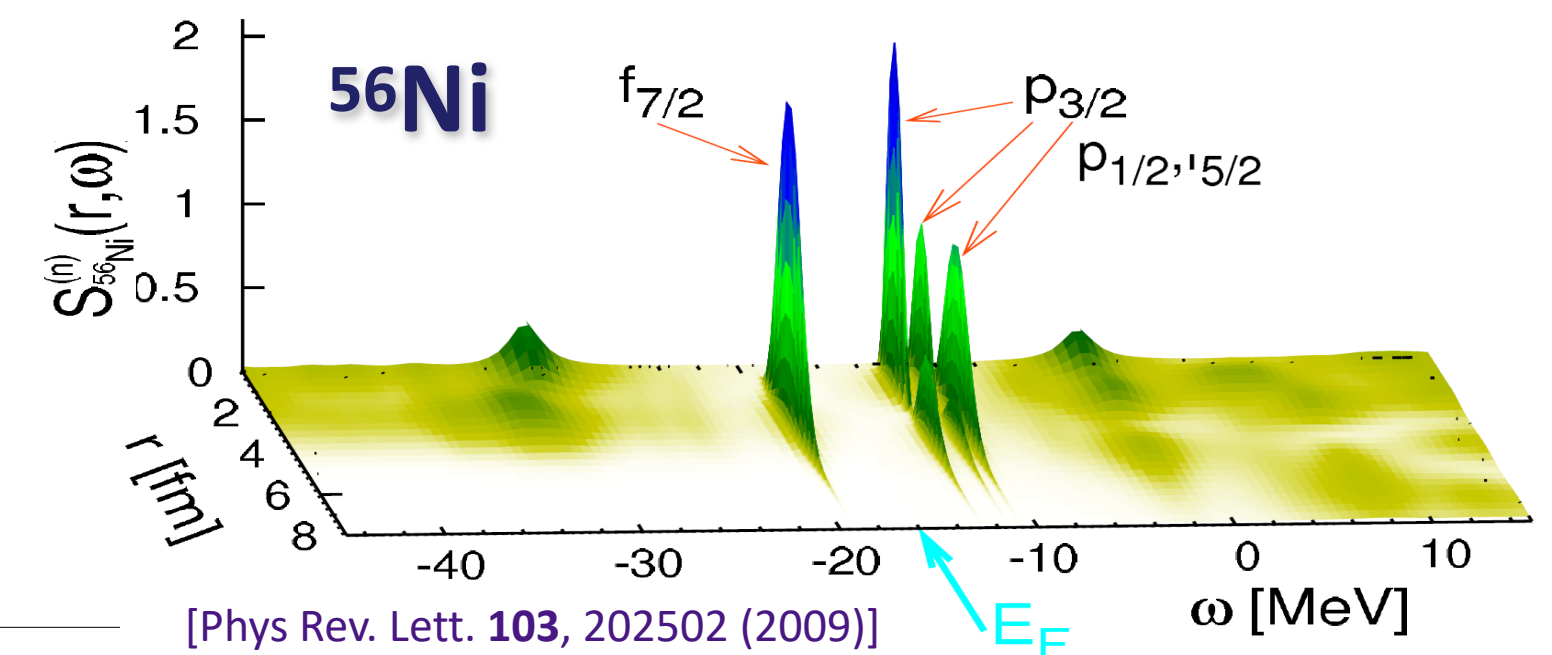
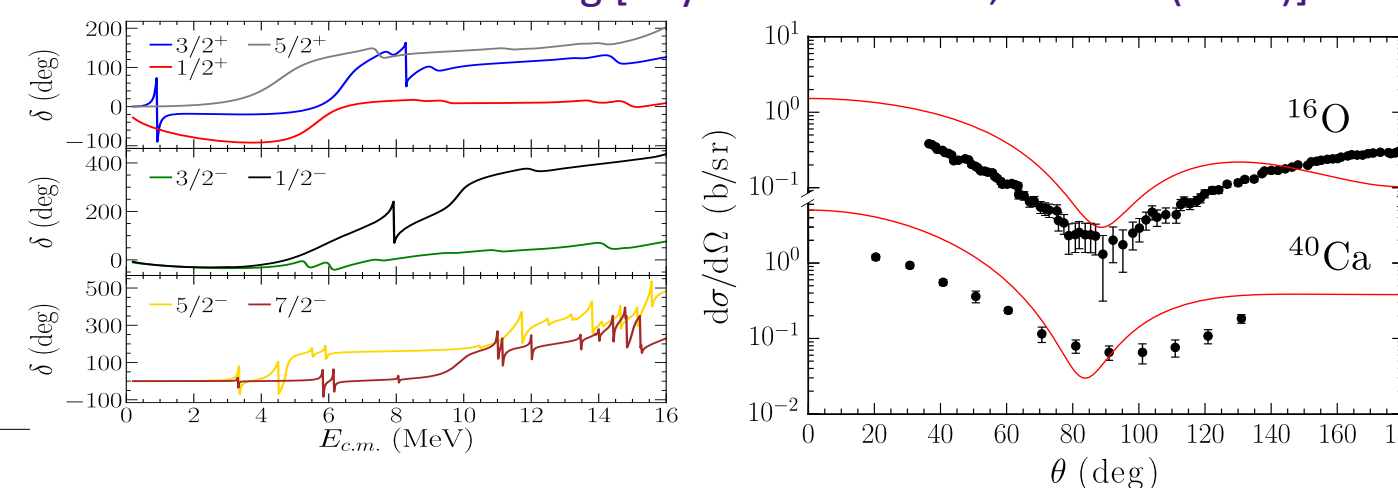


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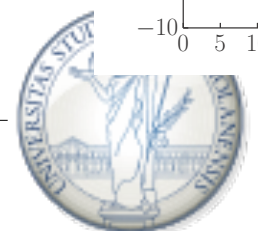
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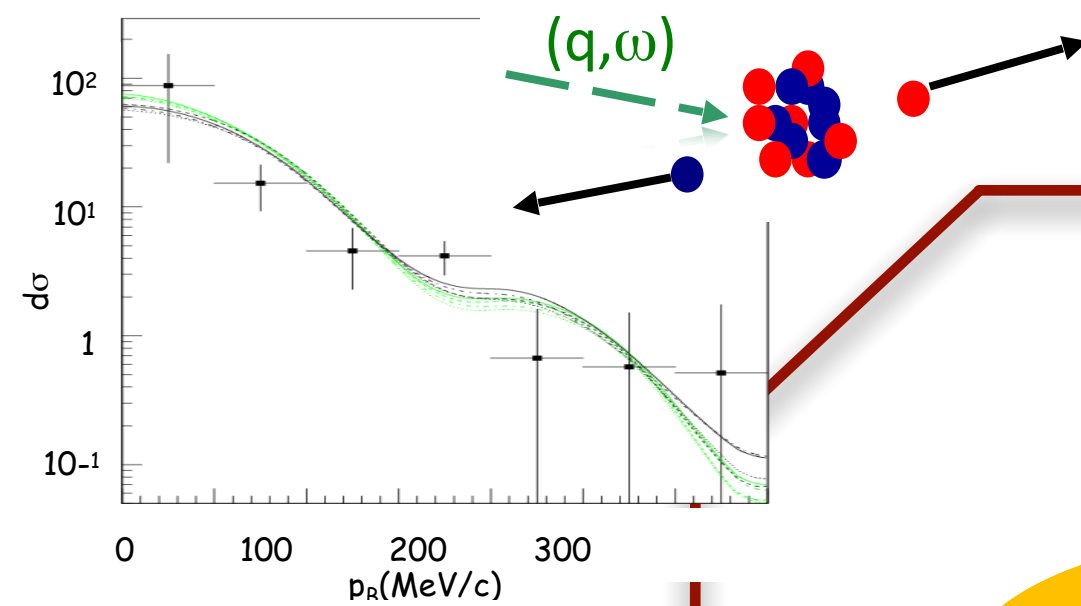




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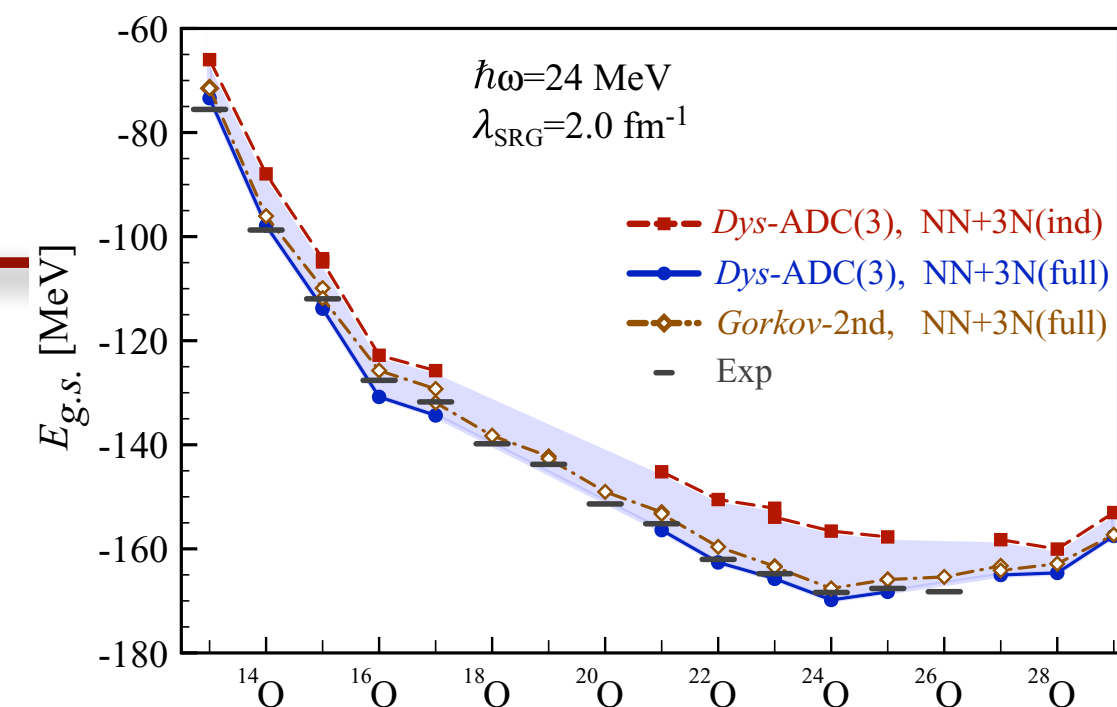
[Eur. Phys. J. A43, 137 (2010)]



## Binding energies

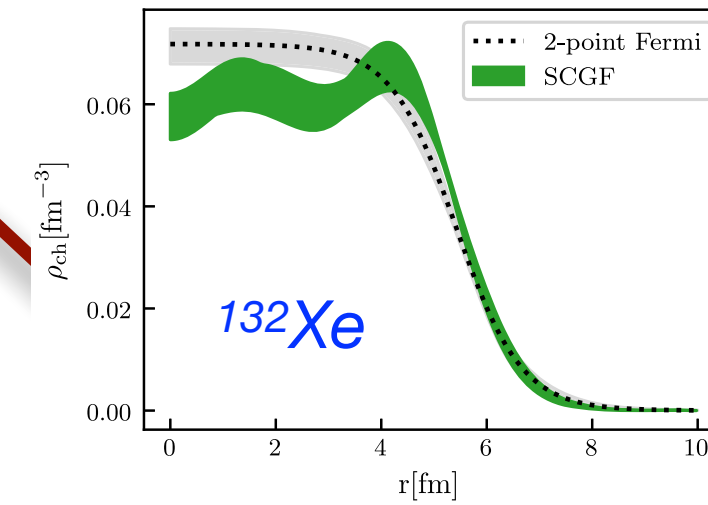
Oxygen drip line

[Phys. Rev. Lett. 111, 062501 (2013)]



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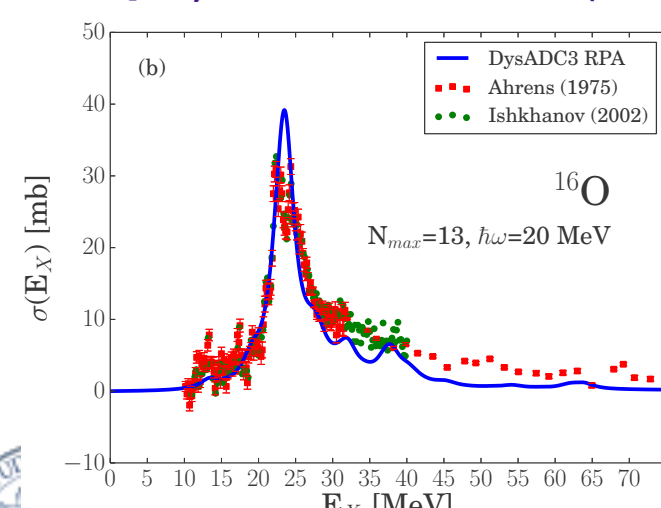
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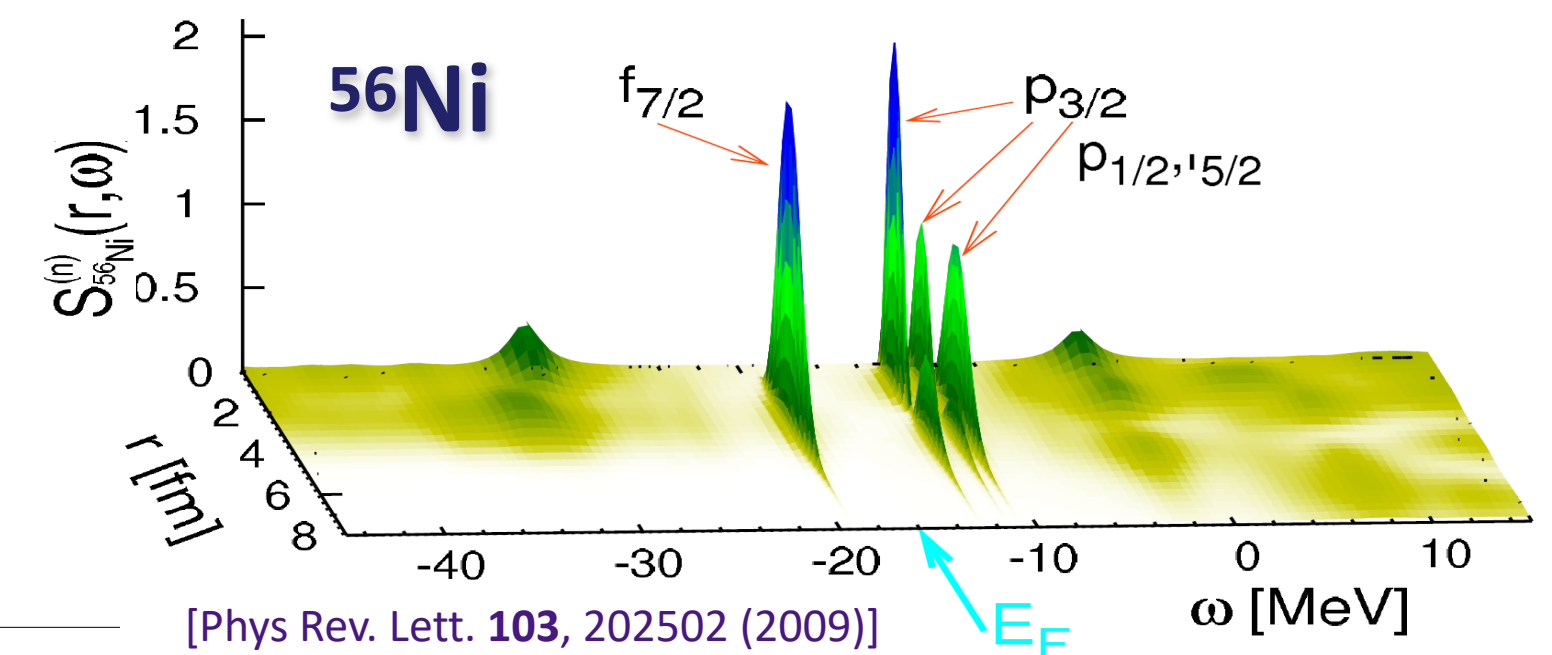
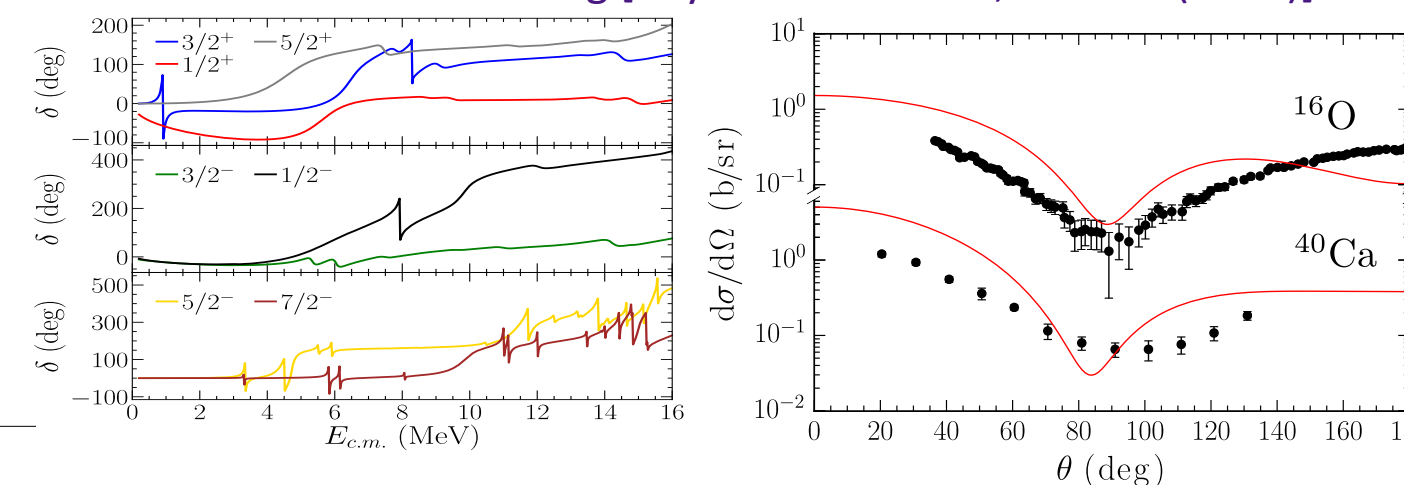


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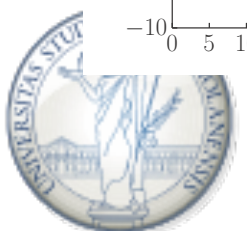
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## Optical potential

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# The physics contained in the **one-body** Green's function

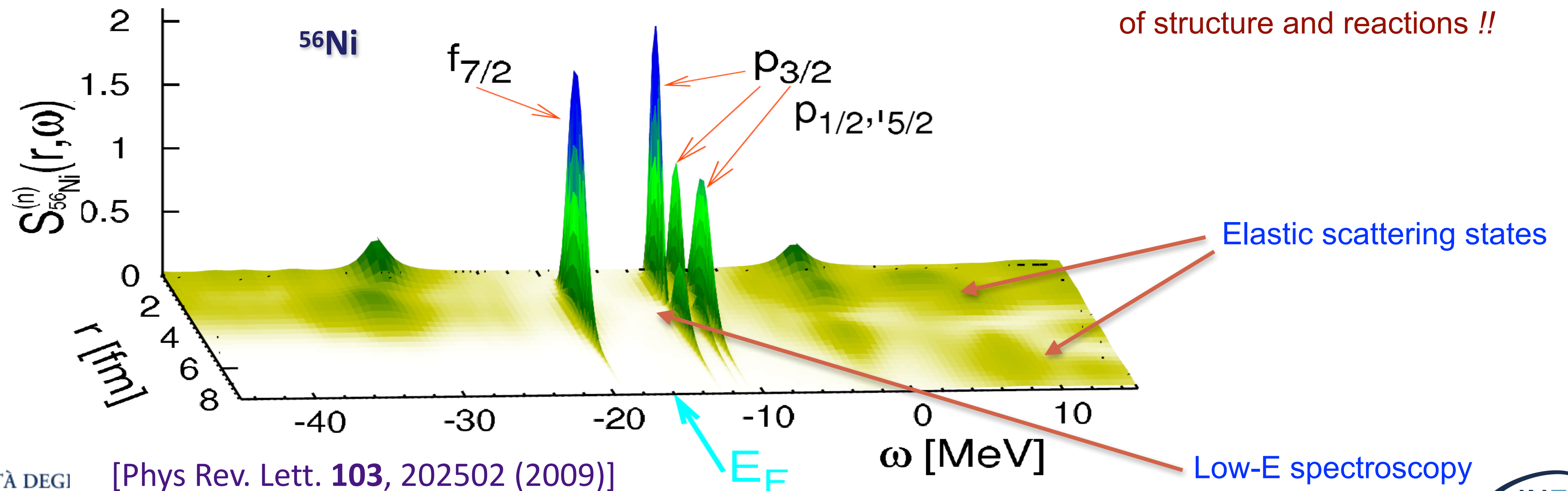
One-body propagator:  $g_{\alpha\beta}(t - t') = -i/\hbar \langle \Psi_0^A | T[c_\alpha(t) c_\beta^\dagger(t')] | \Psi_0^A \rangle$

Dyson Equation:  $g_{\alpha\beta}(\omega) = g_{\alpha\beta}^{(0)}(\omega) + \sum_{\gamma\delta} g_{\alpha\gamma}^{(0)}(\omega) \Sigma_{\gamma\delta}^*(\omega) g_{\delta\beta}(\omega)$

(One-body) spectral function:  $S(\alpha, \omega) := \pm \frac{1}{2\pi} \Im m \{ g_{\alpha\alpha}(\omega) \}$

The self-energy  $\Sigma_{\alpha\beta}^*(\omega)$  'decides' both ground state observables and elastic scattering.

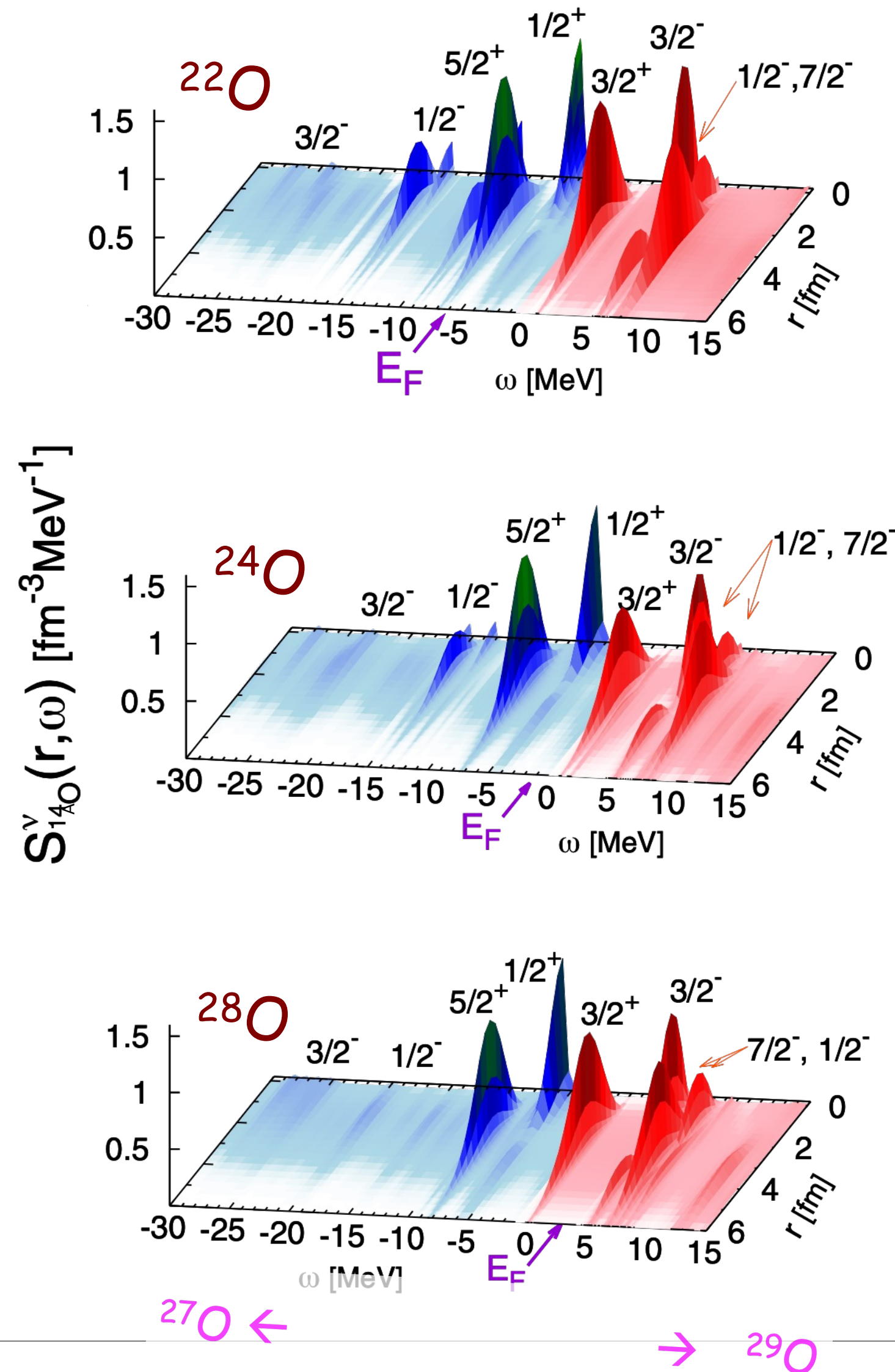
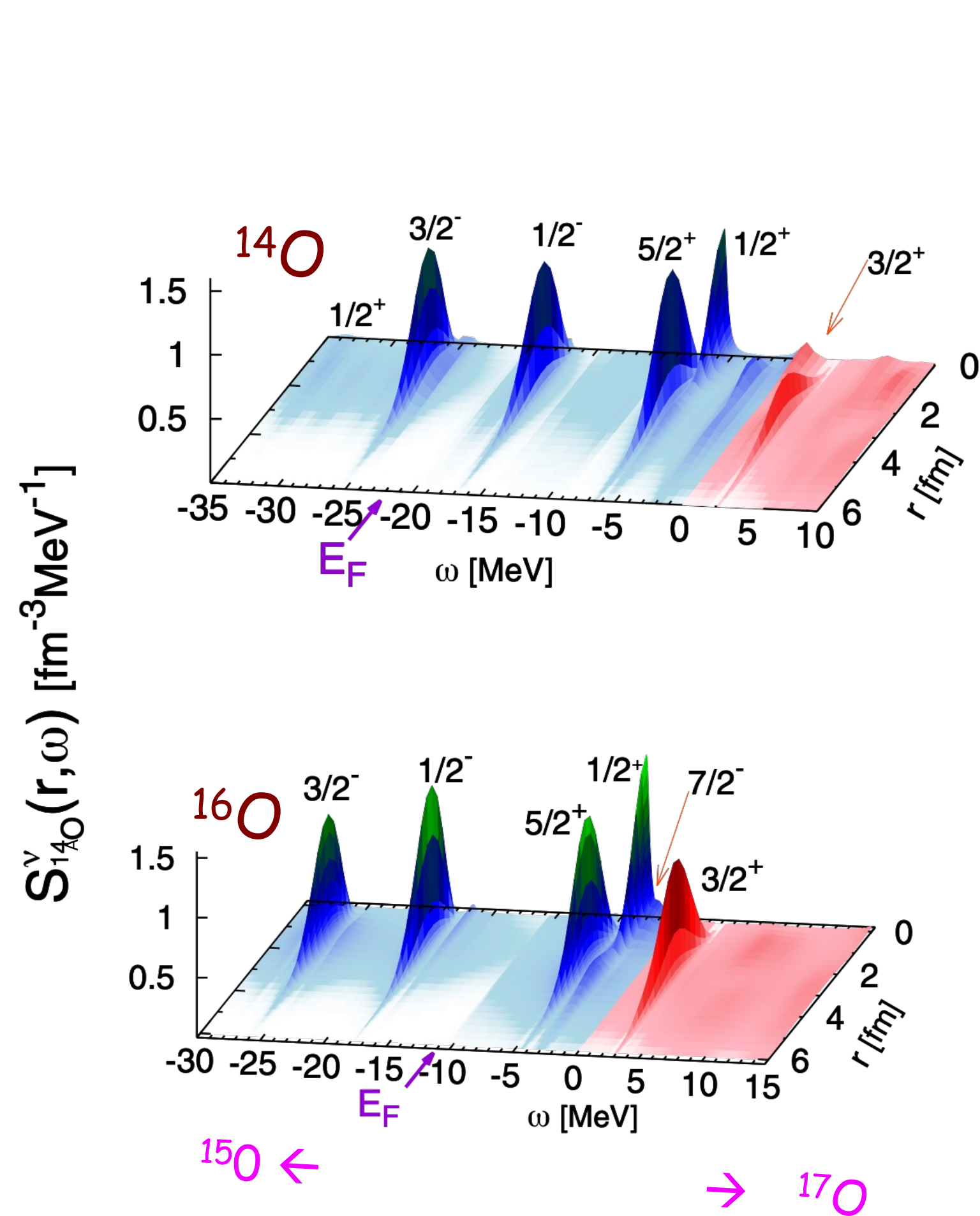
==> Consistent computation of structure and reactions !!



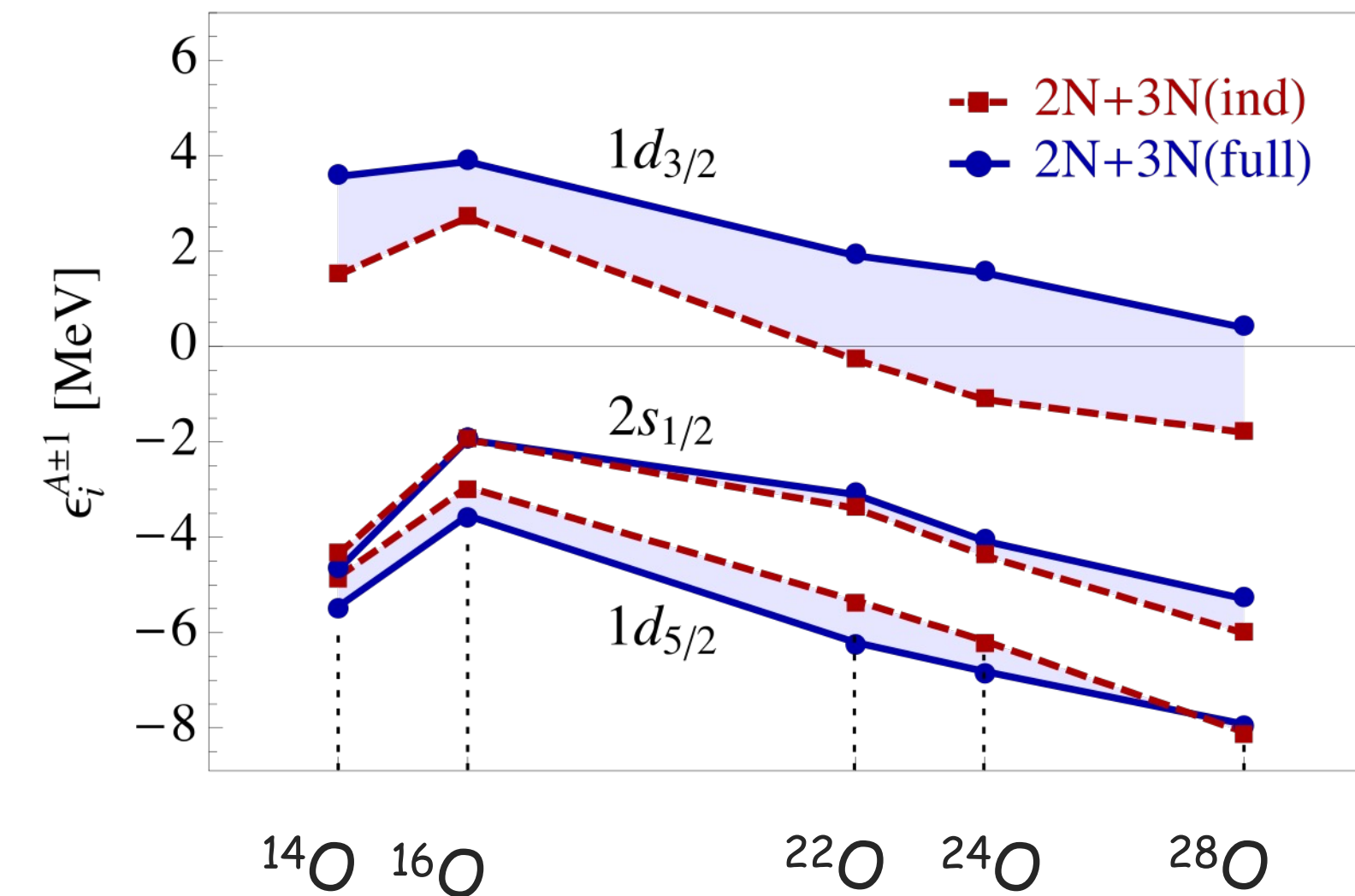


# Neutron spectral function for oxygen isotopes

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



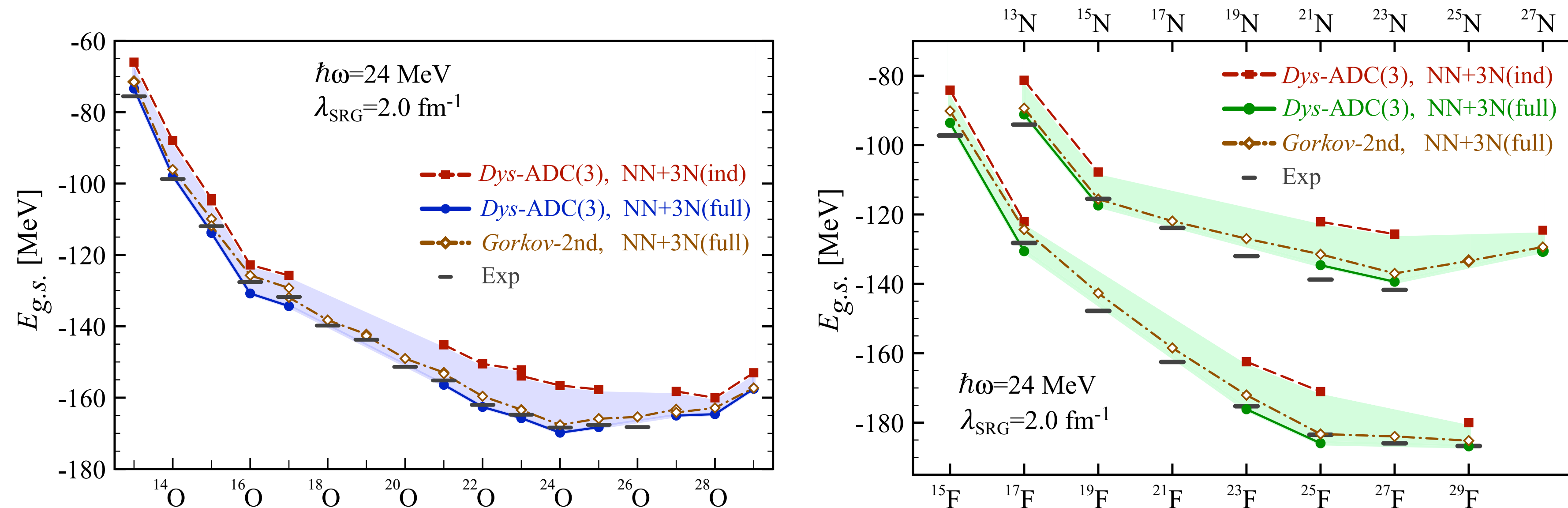
## Neutron quasiparticle energies





# 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)



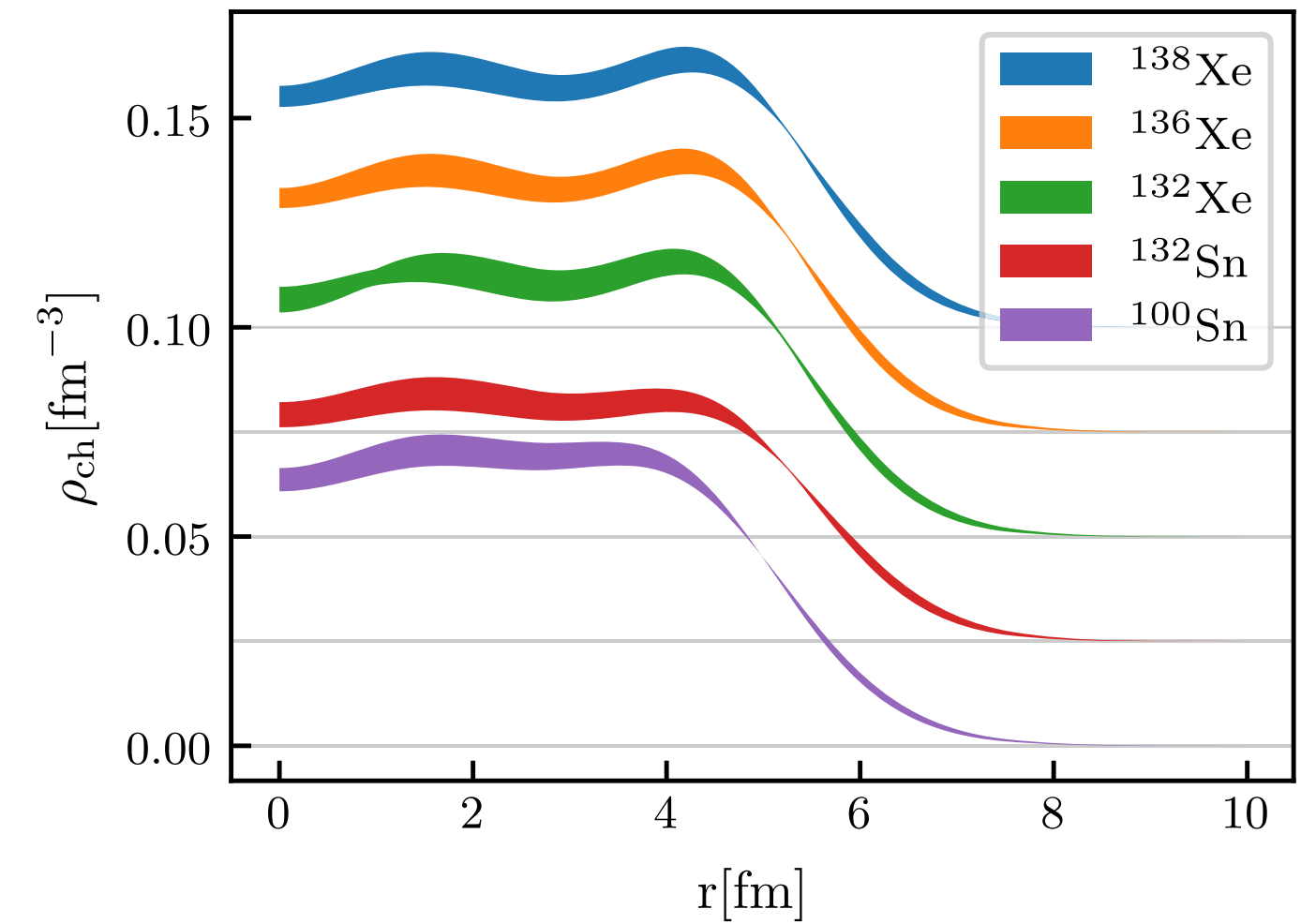
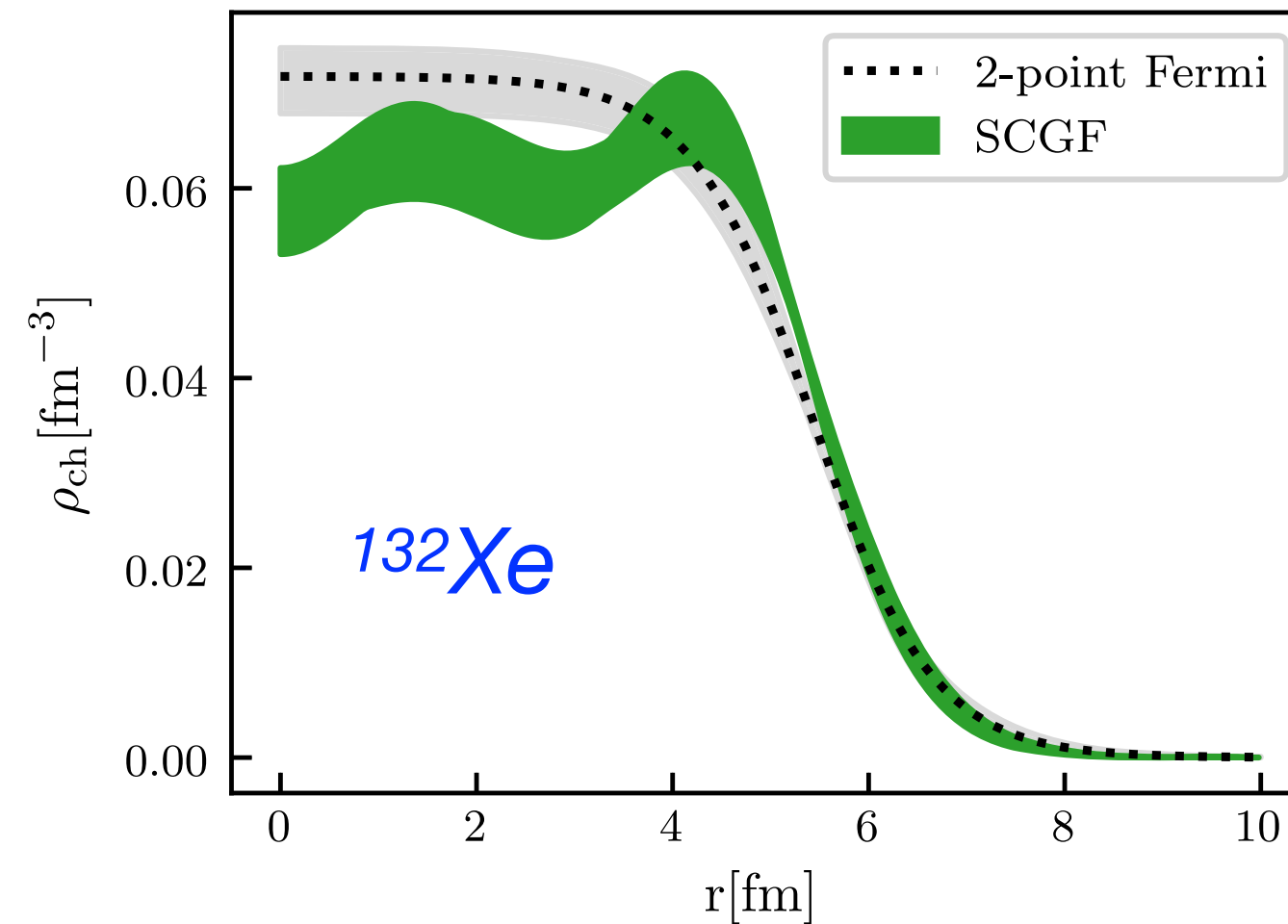
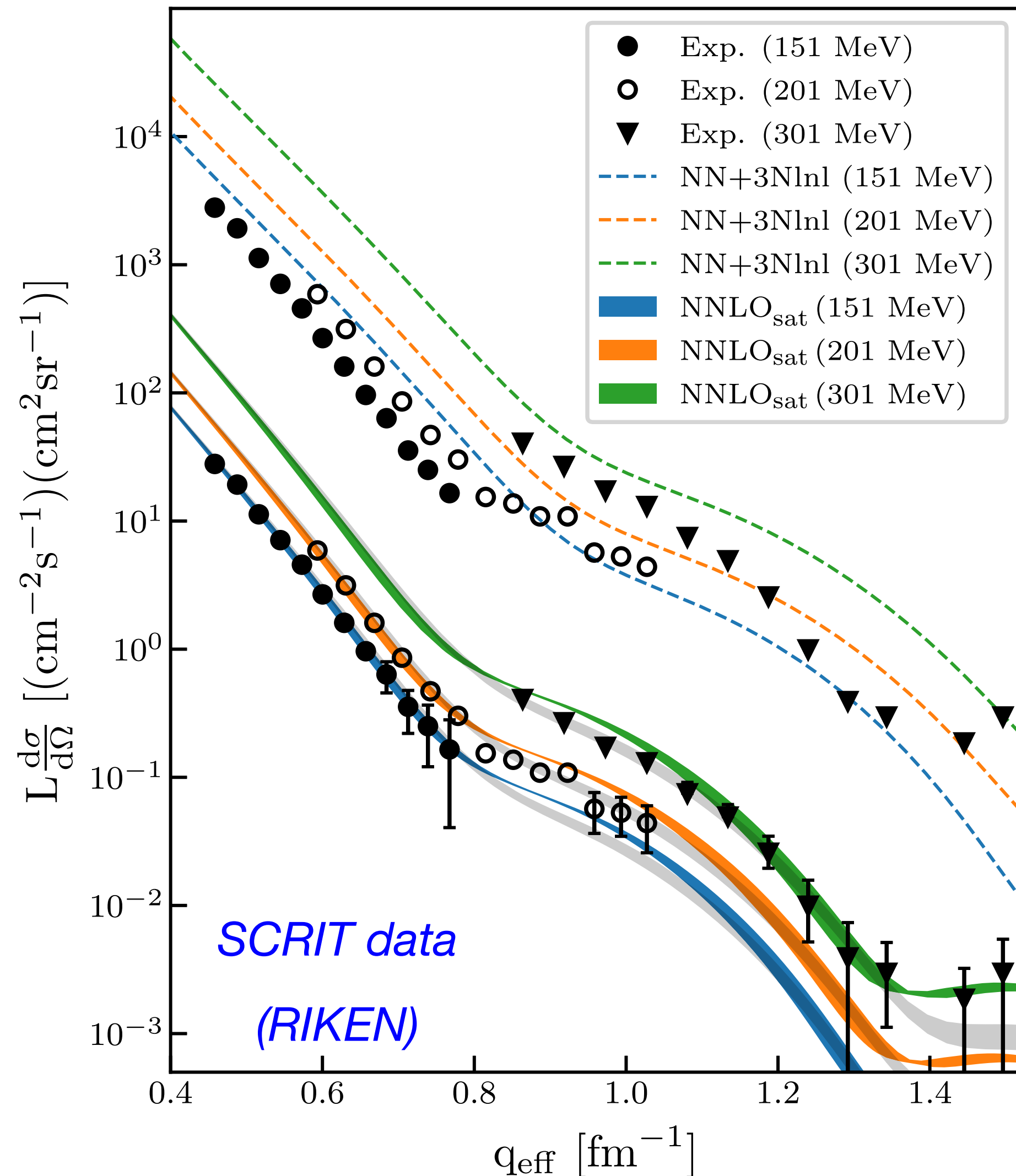
→ 3NF crucial for reproducing binding energies and driplines around oxygen

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





# Charge density for Sn and Xe isotopes



Charge radii (NNLOsat):

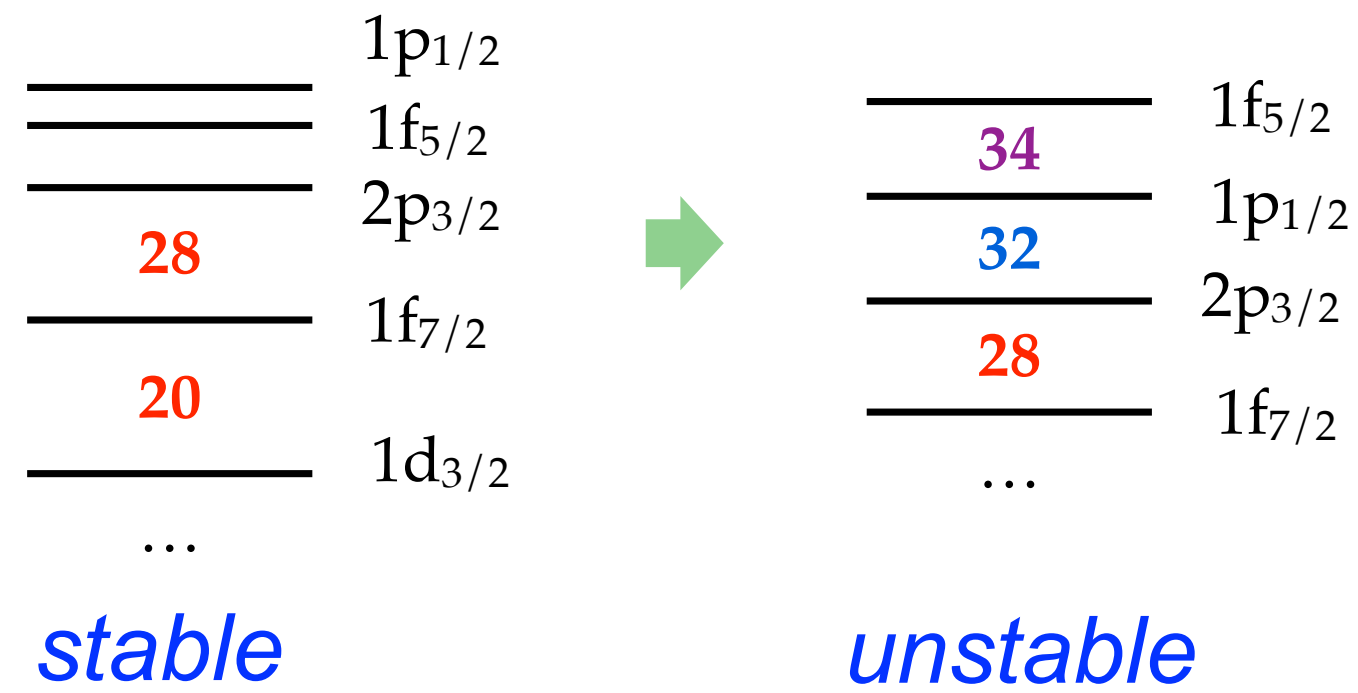
|                   | SCGF          | Exp.   |
|-------------------|---------------|--------|
| $^{100}\text{Sn}$ | 4.525 – 4.707 |        |
| $^{132}\text{Sn}$ | 4.725 – 4.956 | 4.7093 |
| $^{132}\text{Xe}$ | 4.700 – 4.948 | 4.7859 |
| $^{136}\text{Xe}$ | 4.715 – 4.928 | 4.7964 |
| $^{138}\text{Xe}$ | 4.724 – 4.941 | 4.8279 |

...and accompanying predictions for neutron skins (see paper).

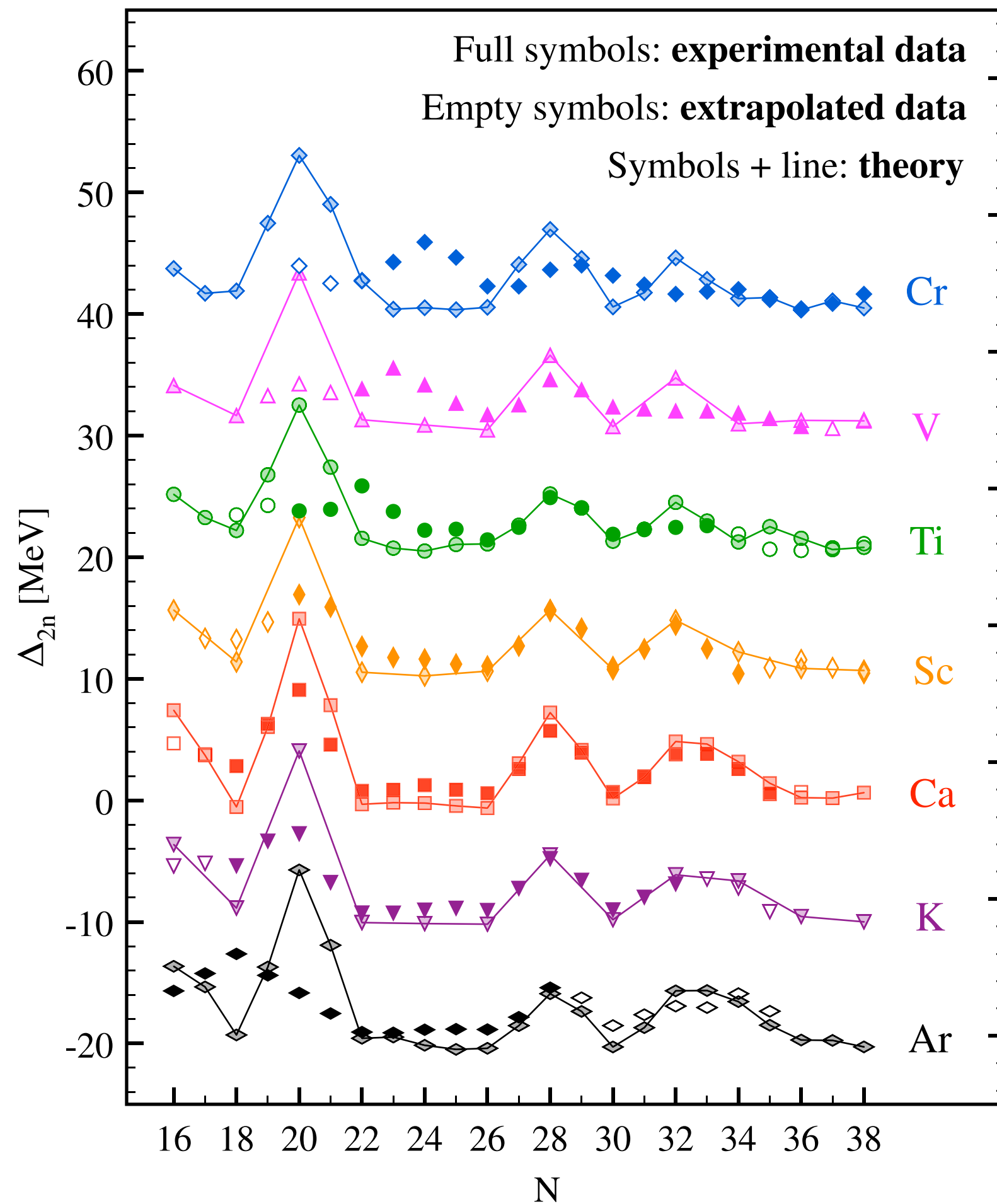


# Magic numbers

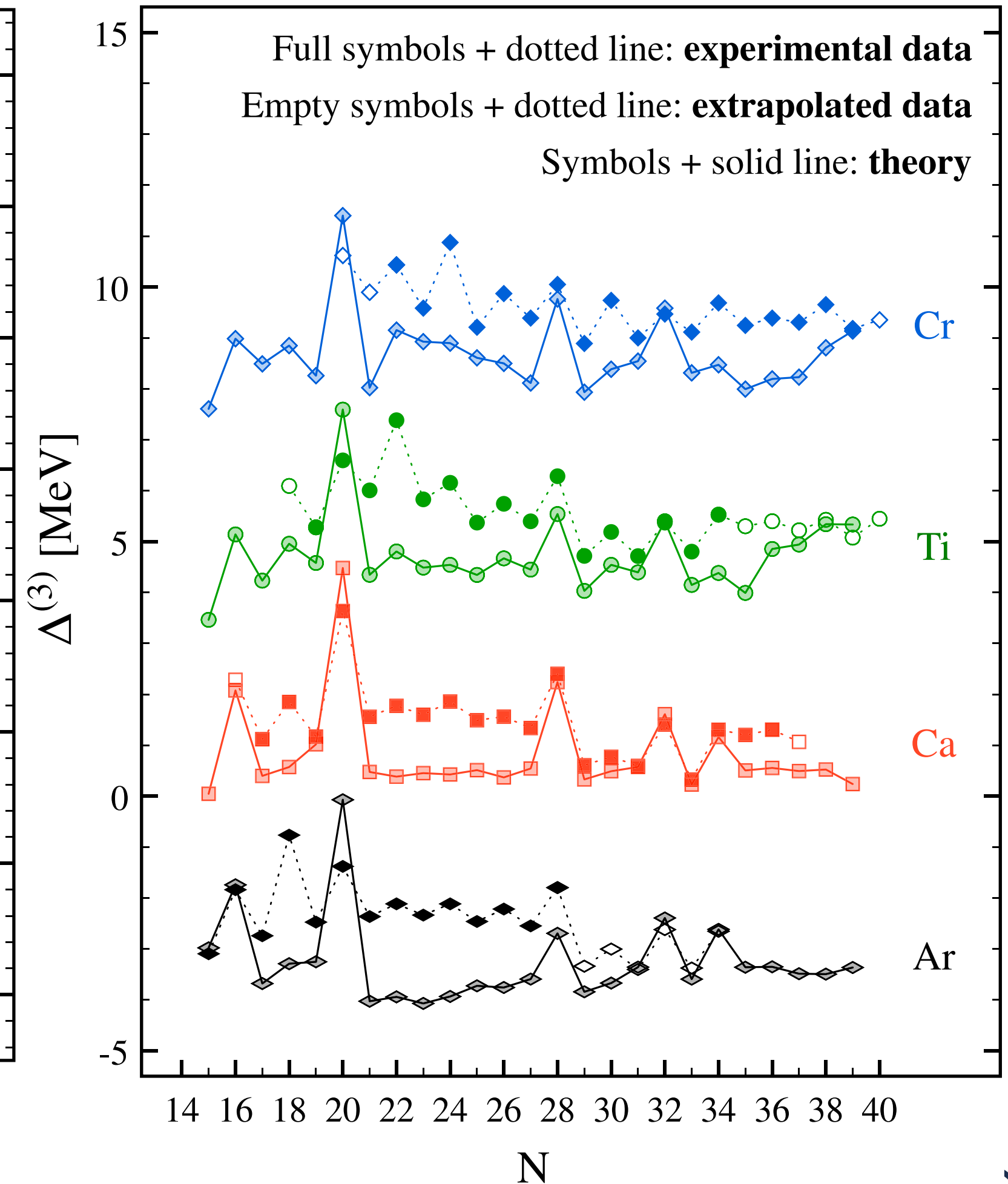
- Magic numbers: extra-stable combinations of N & Z



$$\Delta_{2n}(N, Z) \equiv S_{2n}(N, Z) - S_{2n}(N + 2, Z)$$



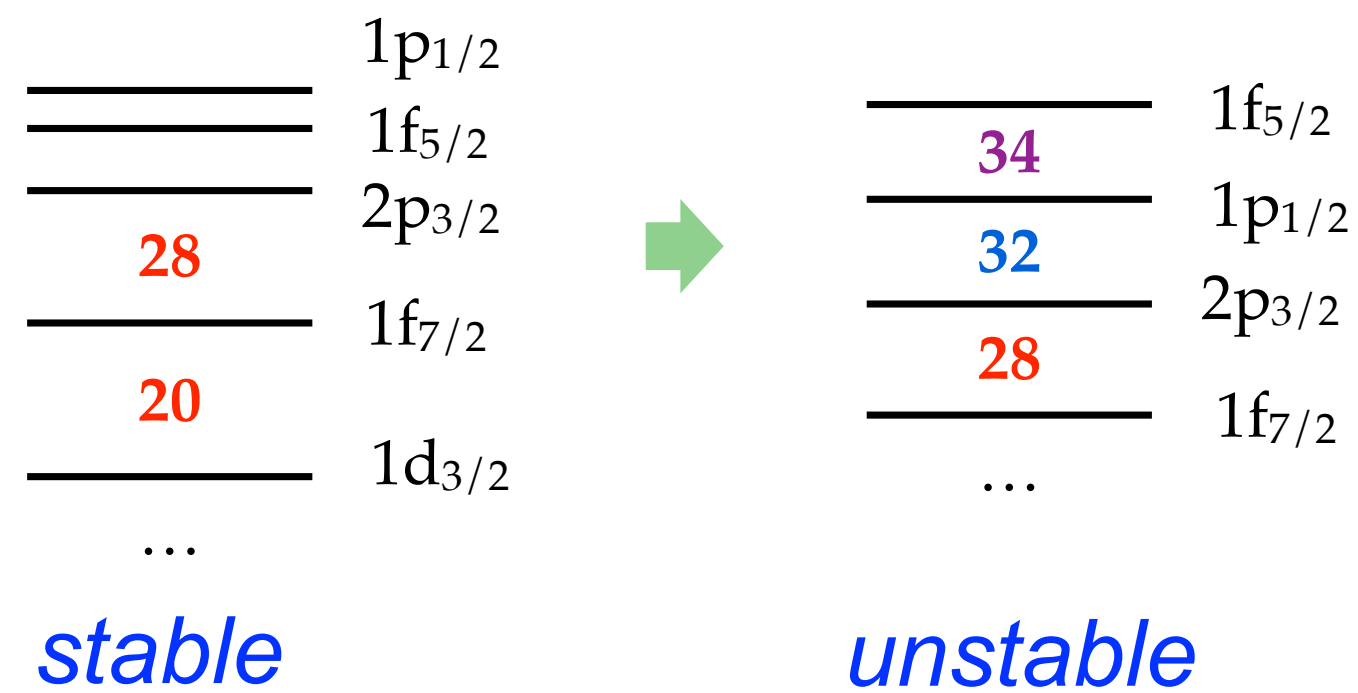
$$\Delta^{(3)}(N, Z) \equiv \frac{(-1)^N}{2} [E(N-1, Z) - 2E(N, Z) + E(N+1, Z)]$$



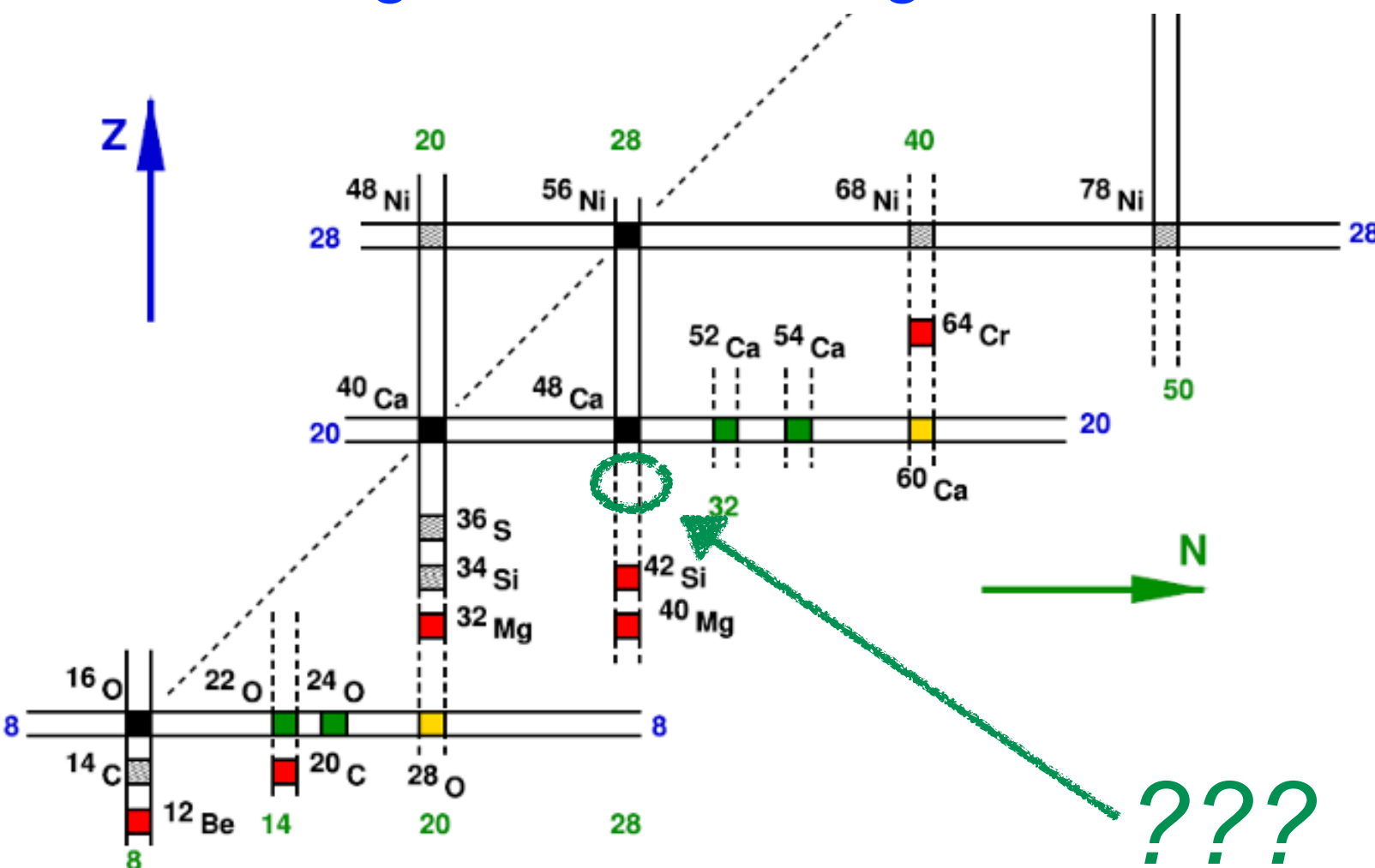


# Magic numbers

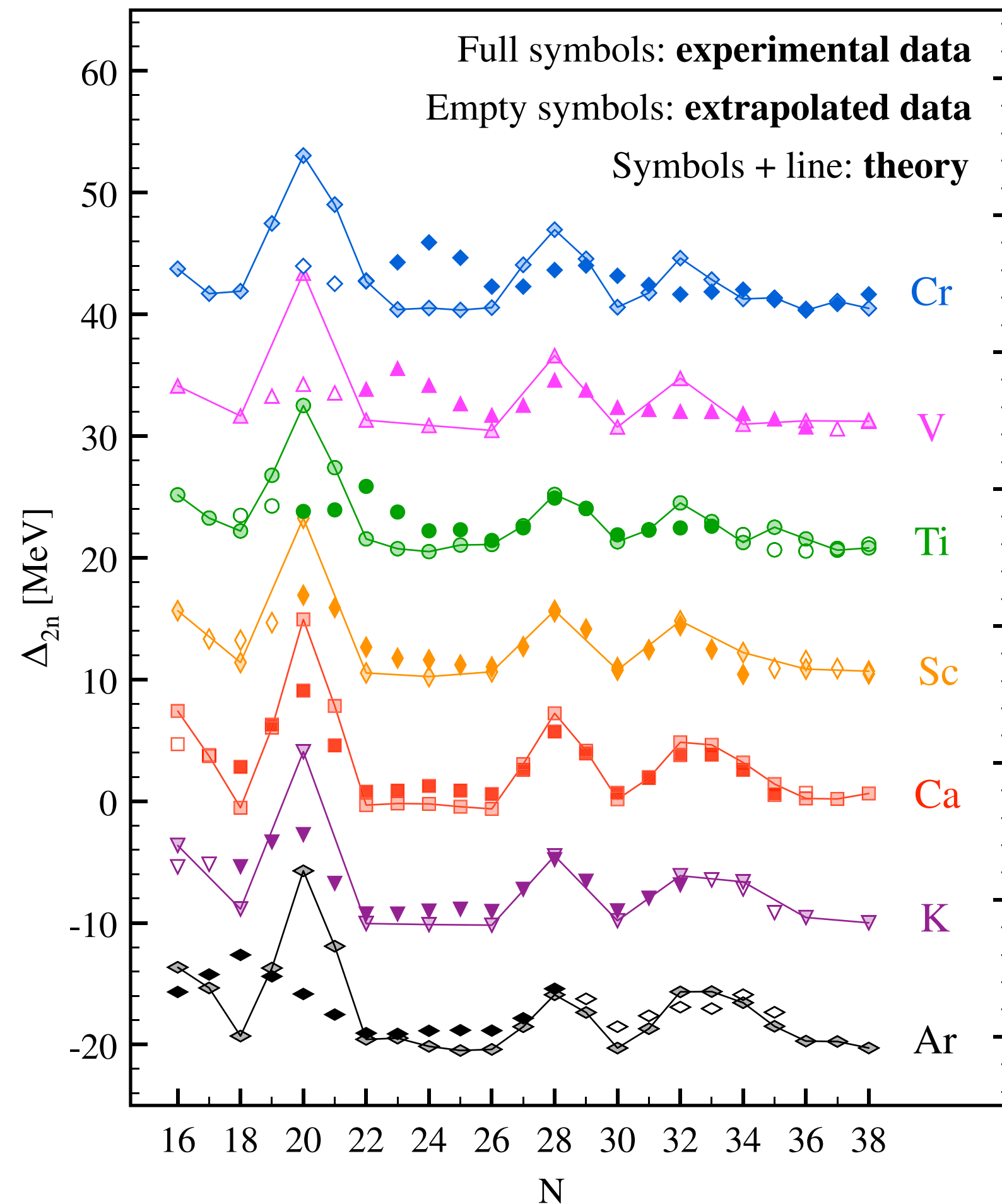
- Magic numbers: extra-stable combinations of N & Z



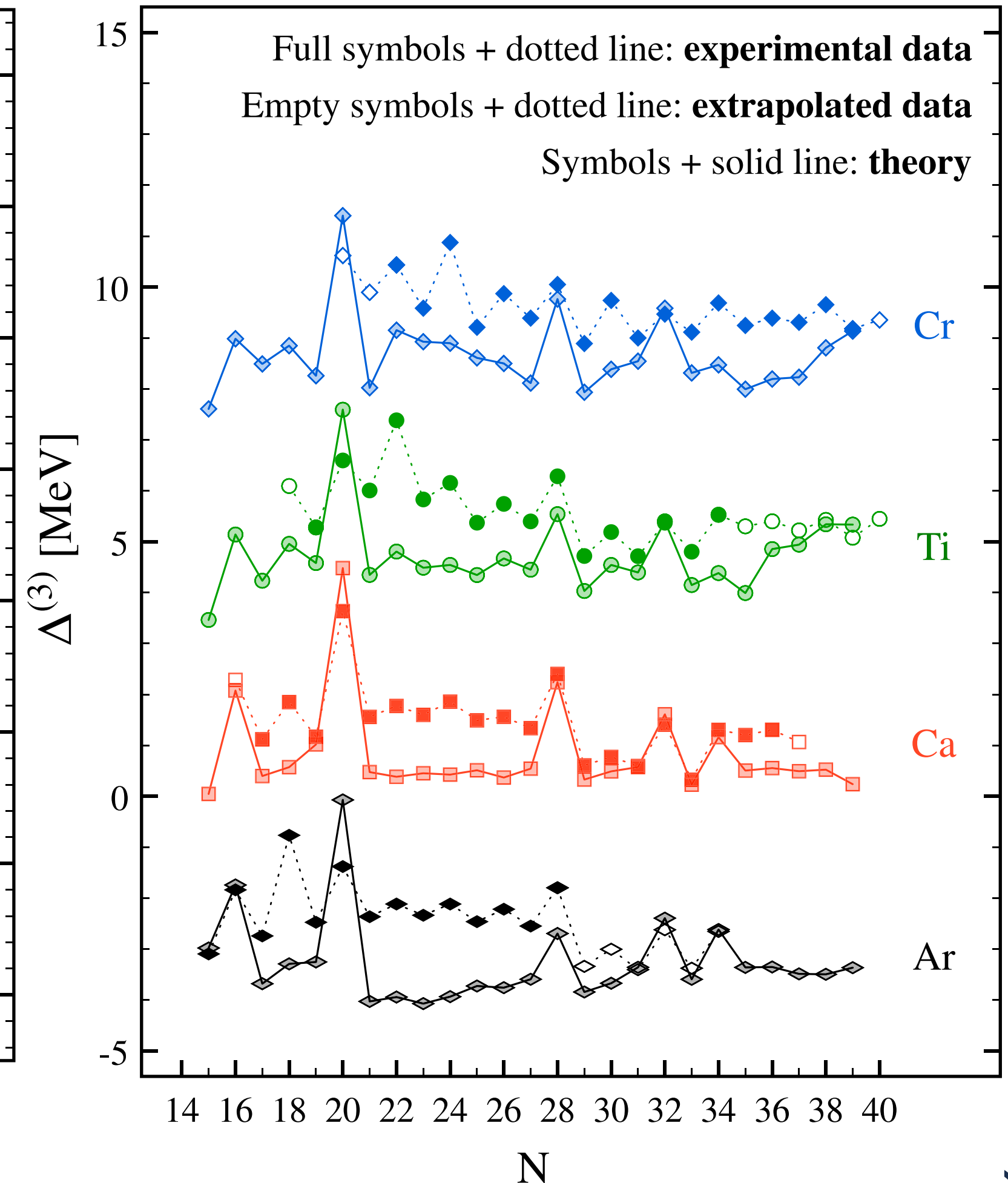
Known magic and semimagic nuclei:



$$\Delta_{2n}(N, Z) \equiv S_{2n}(N, Z) - S_{2n}(N + 2, Z)$$



$$\Delta^{(3)}(N, Z) \equiv \frac{(-1)^N}{2} [E(N-1, Z) - 2E(N, Z) + E(N+1, Z)]$$



[Somà, CB et al. Eur. Phys. J. A **57**, 135 (2021)]

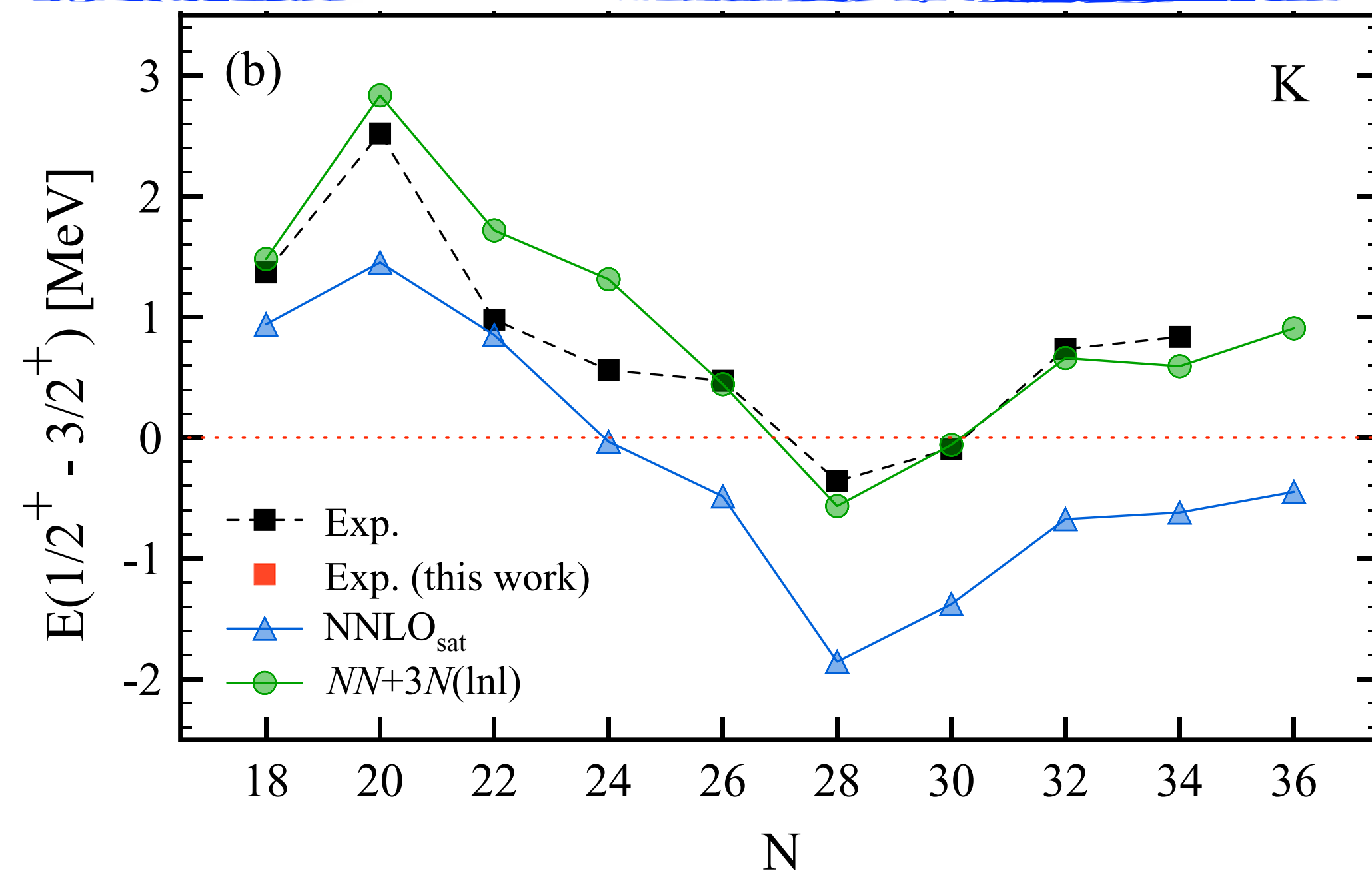
[Nowacki, Obertelli, Poves, PPNP 120, 103866 (2021)]



DIPARTIMENTO DI FISICA

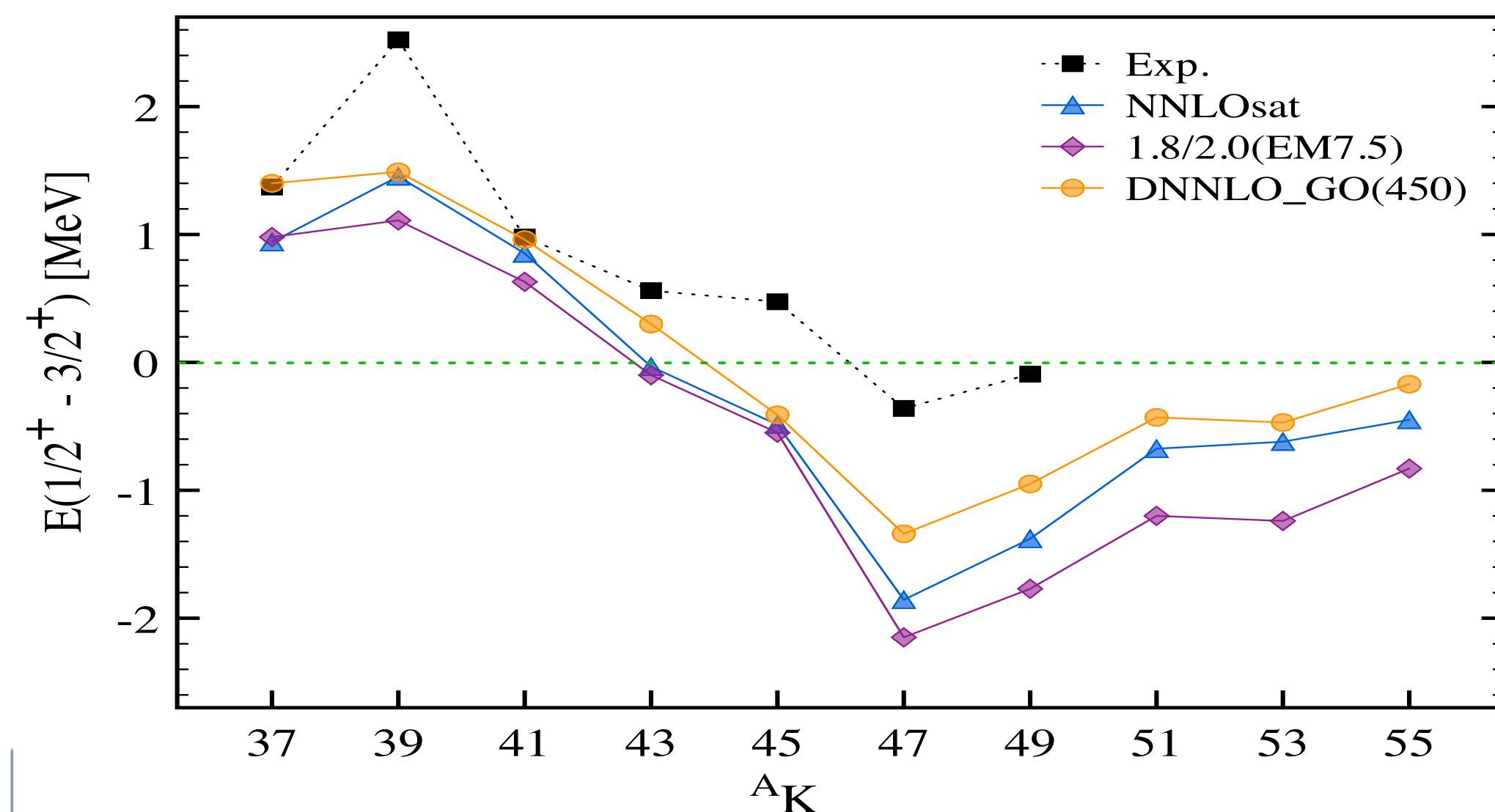


# $d_{3/2} - s_{1/2}$ inversion of protons at N=28



V. Somà, P. Navrátil, F. Raimondi, CB,  
T. Duguet, PRC**104**, 024315 (2021)

Both states populated by proton removal from  $^A\text{Ca}$



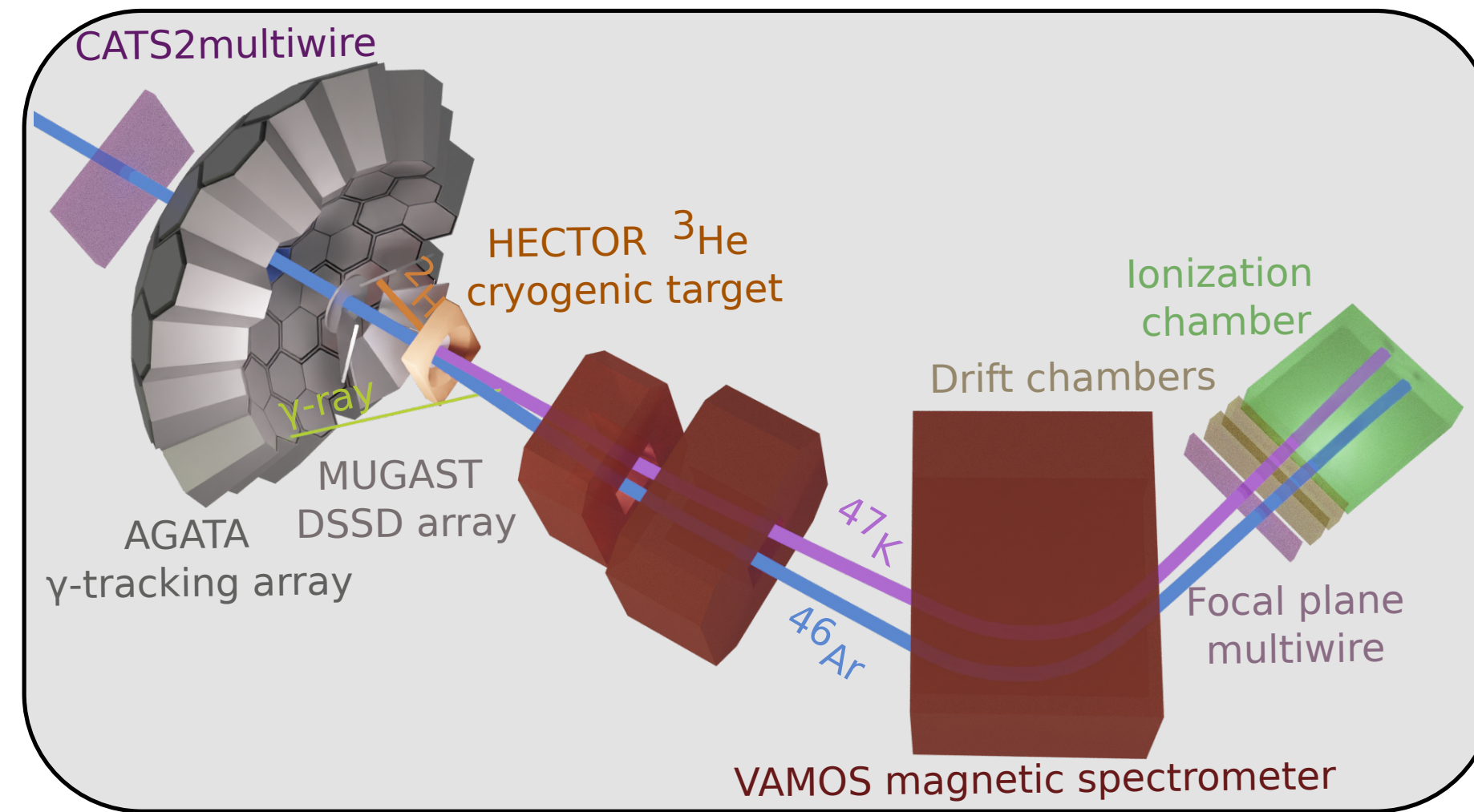
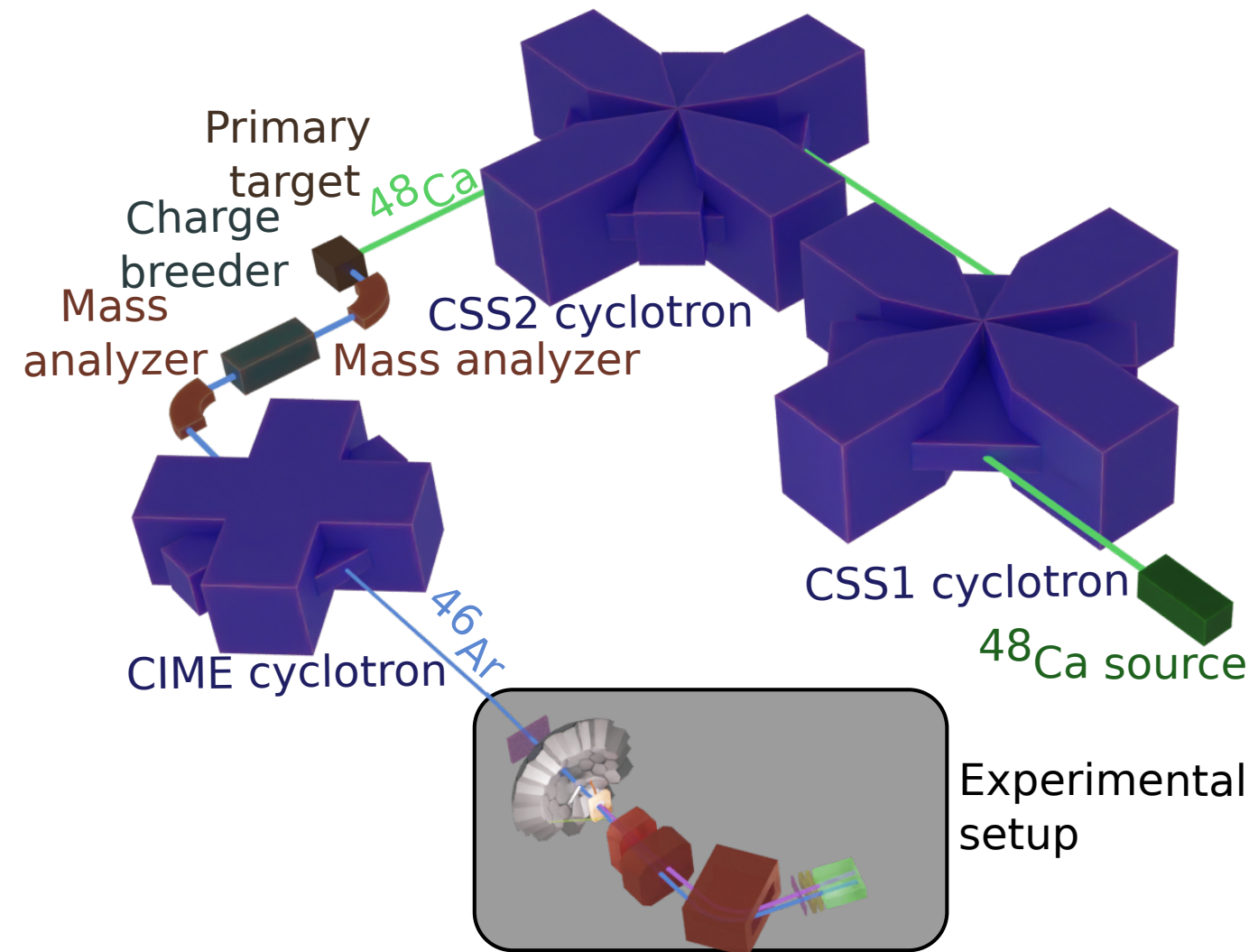
Papuga et al., PRL**110**, 172503 (2013); PRC**90**, 034321 (2014)

RIKEN, SEASTAR coll., Phys. Lett. **B802** 135215 (2020)

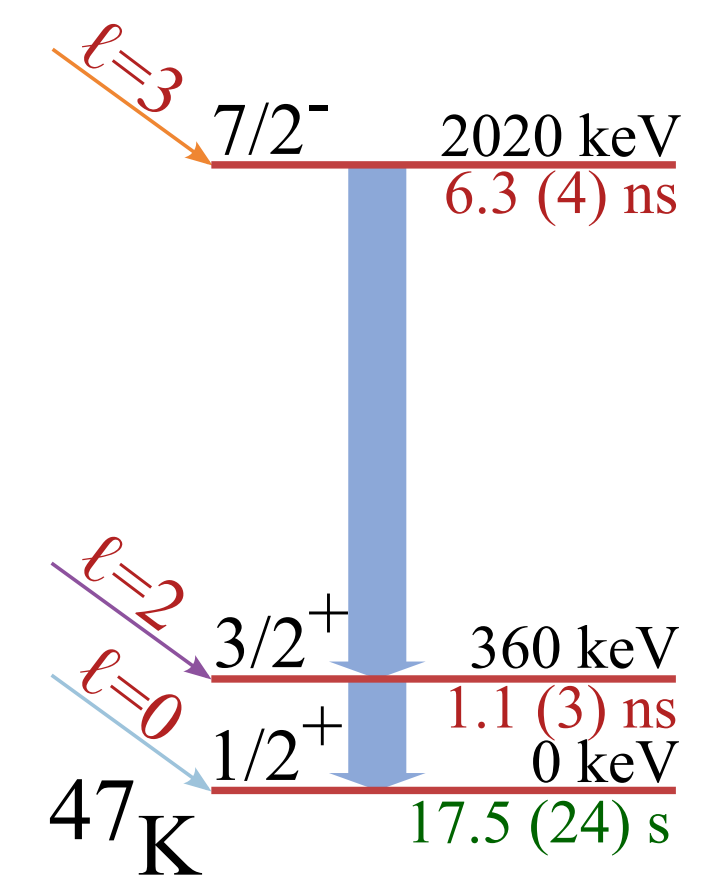
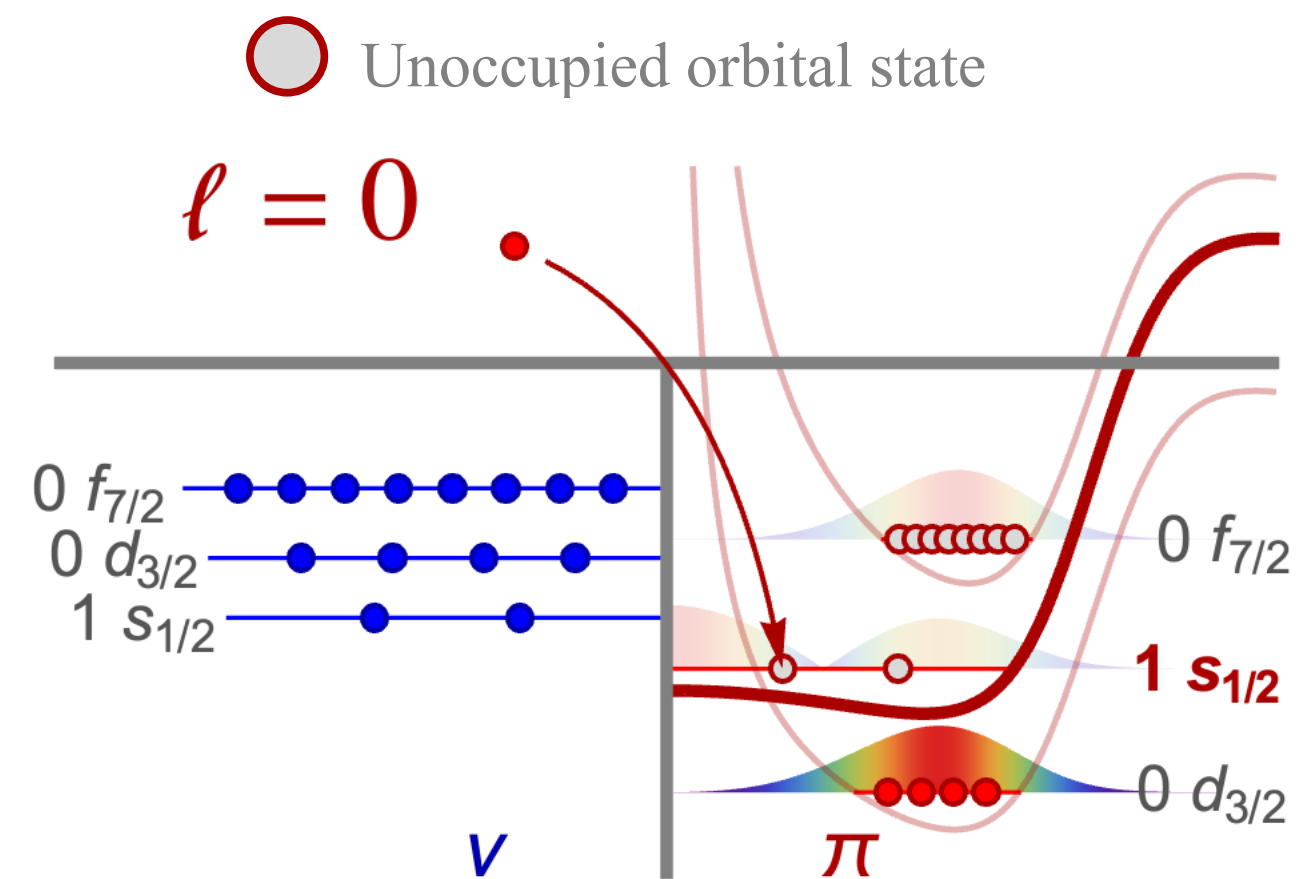
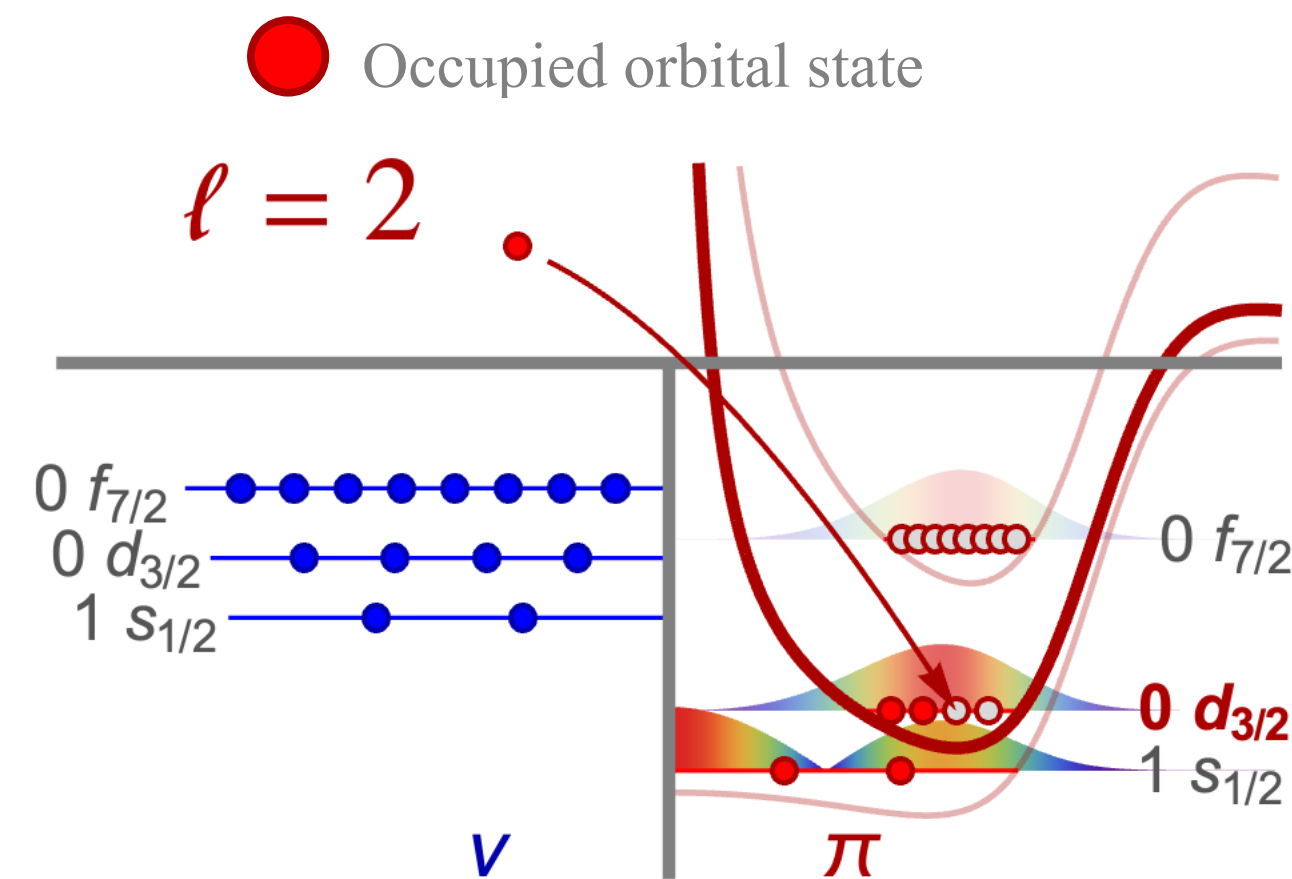
Linh, Gillibert, et al., PRC**104**, 044331 (2021)



# $^{46}\text{Ar}(^3\text{He},d)^{47}\text{K}$ at GANIL

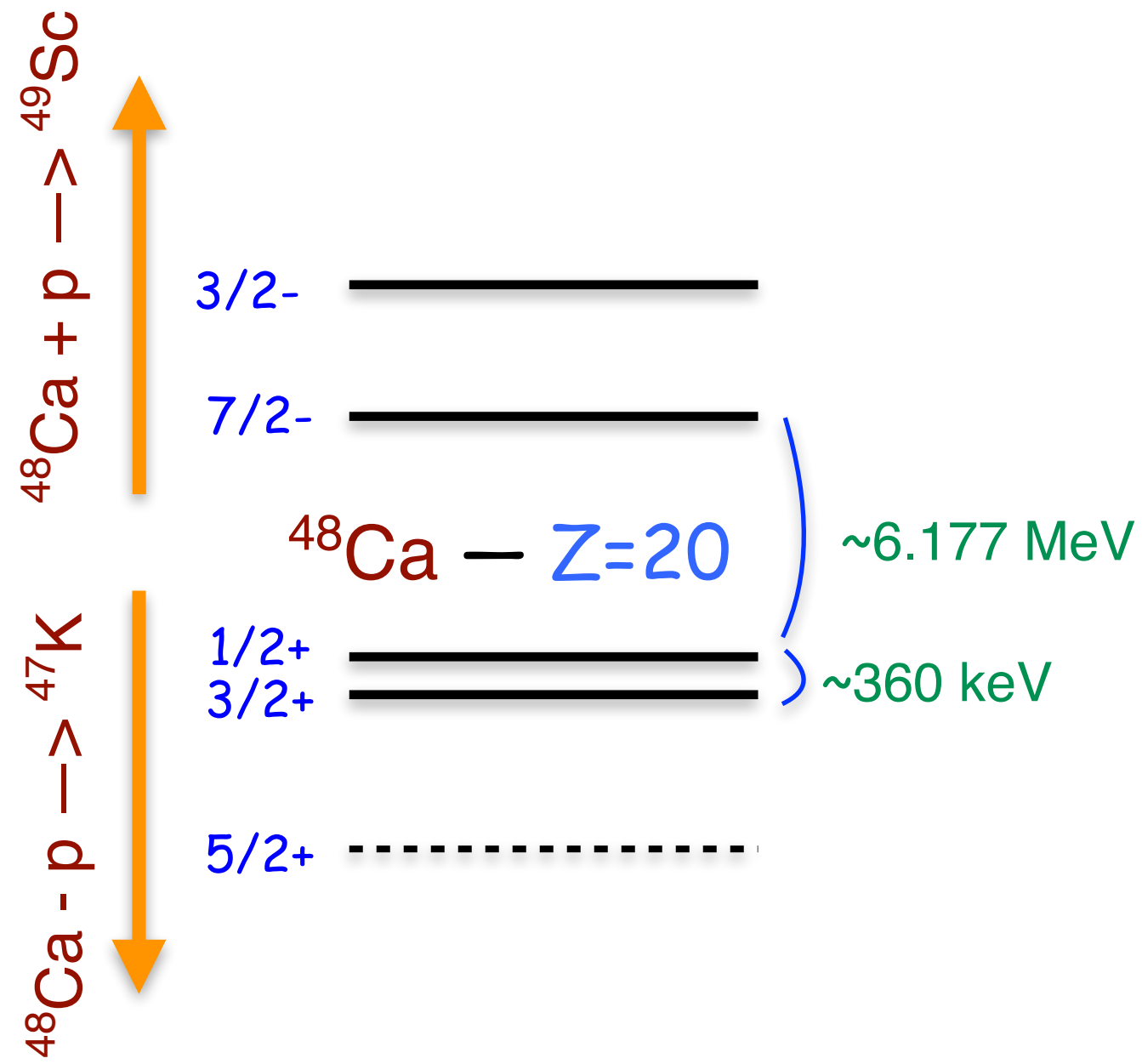


d3/2 - s1/2 inversion  
revisited from adding  
protons to  $^{46}\text{Ar}$

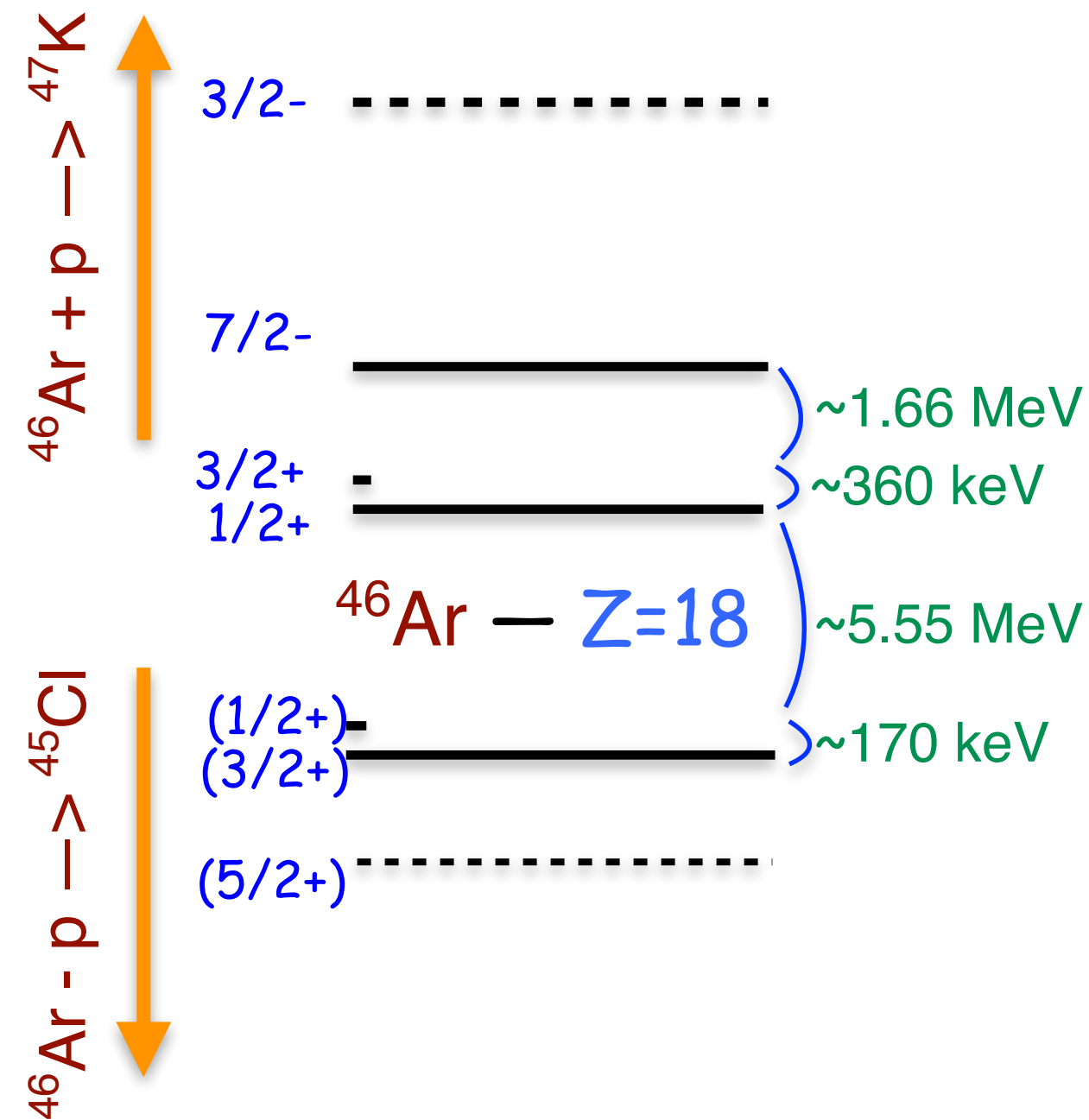




# $^{46}\text{Ar}(^3\text{He},d)^{47}\text{K}$ at GANIL : shell closure & charge bubble in $^{46}\text{Ar}$



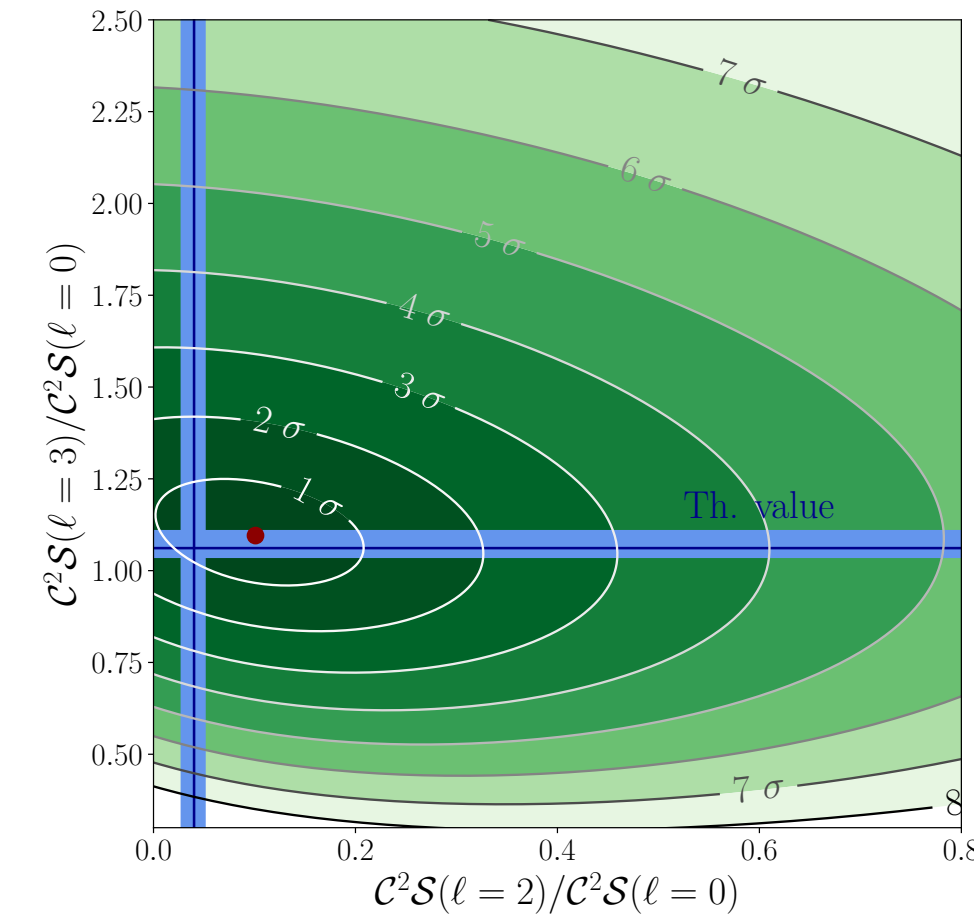
$$\Delta E_{1/2+ - 3/2+} (\text{exp}) = 360 \text{ keV}$$



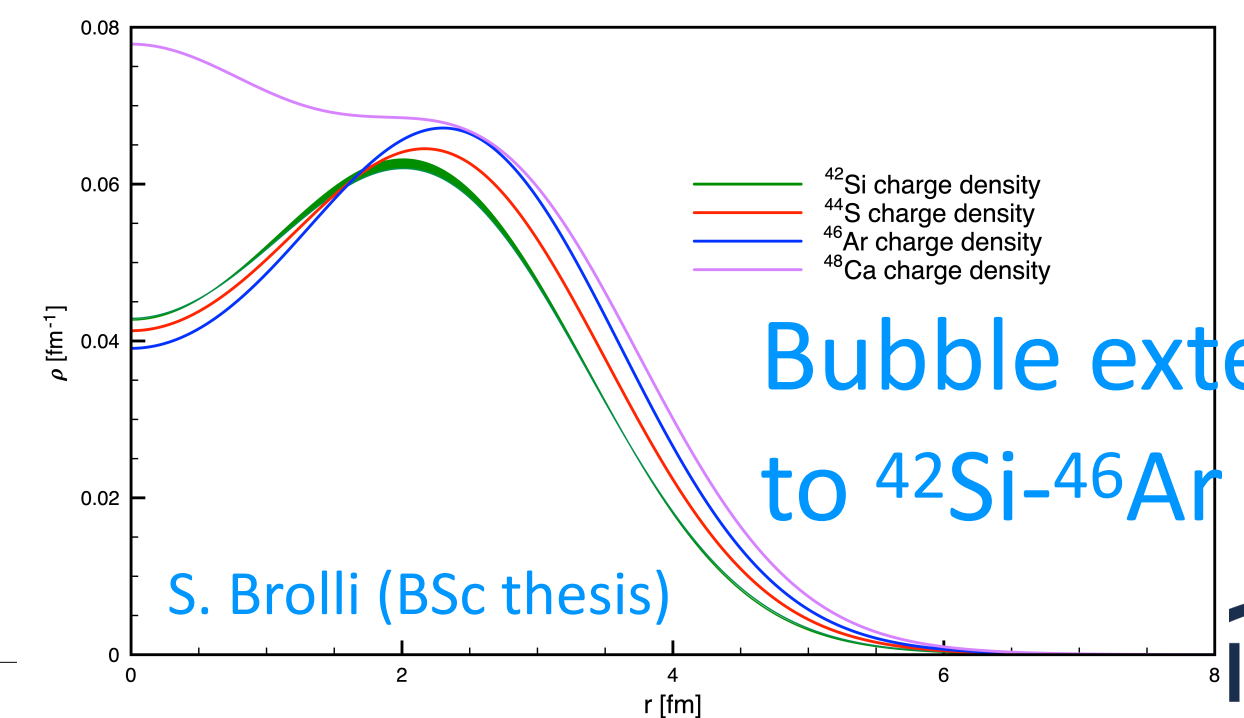
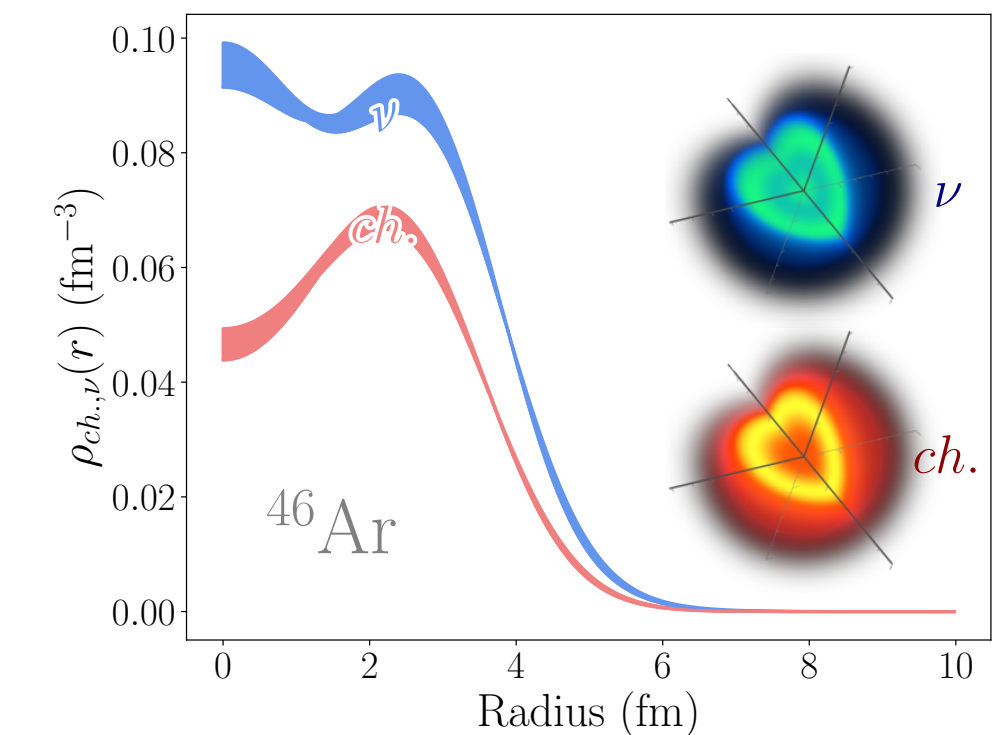
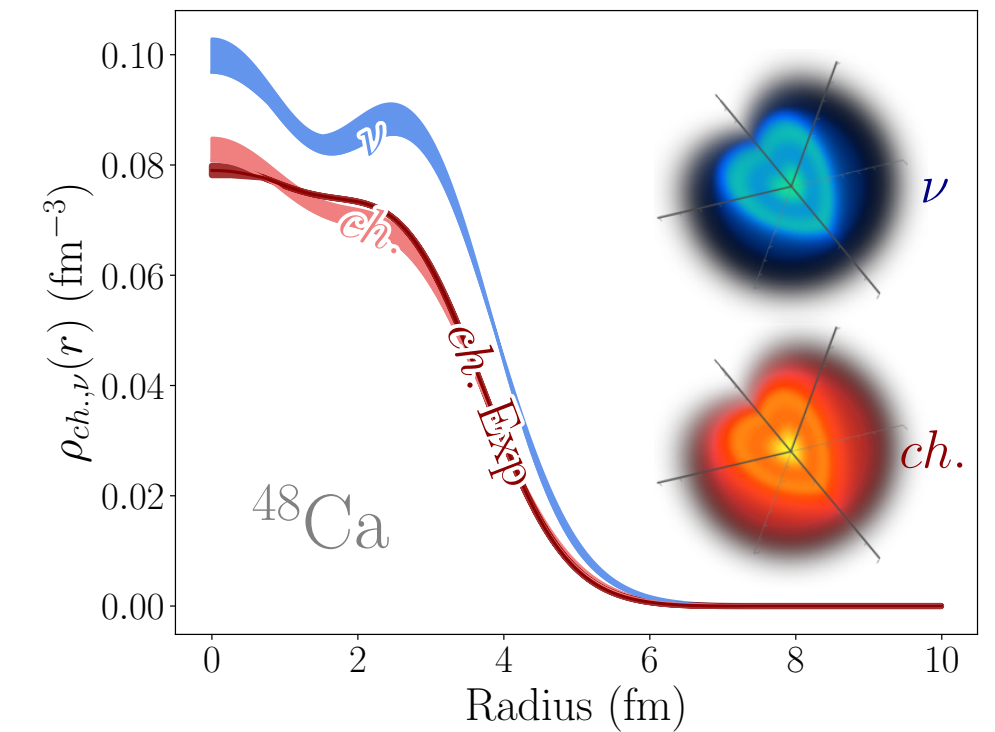
$$\Delta E_{1/2+ - 3/2+} (\text{exp}) = 5,55 \text{ MeV}$$

$$(\text{theo}) = 2,59 \text{ MeV}$$

The d3/2 - s1/2 gap opening and new shell closure at Z=18 !!



$$\frac{d\sigma}{d\Omega} = \sum_k g_k C^2 S_k \frac{d\sigma_k^{SP}}{d\Omega}$$



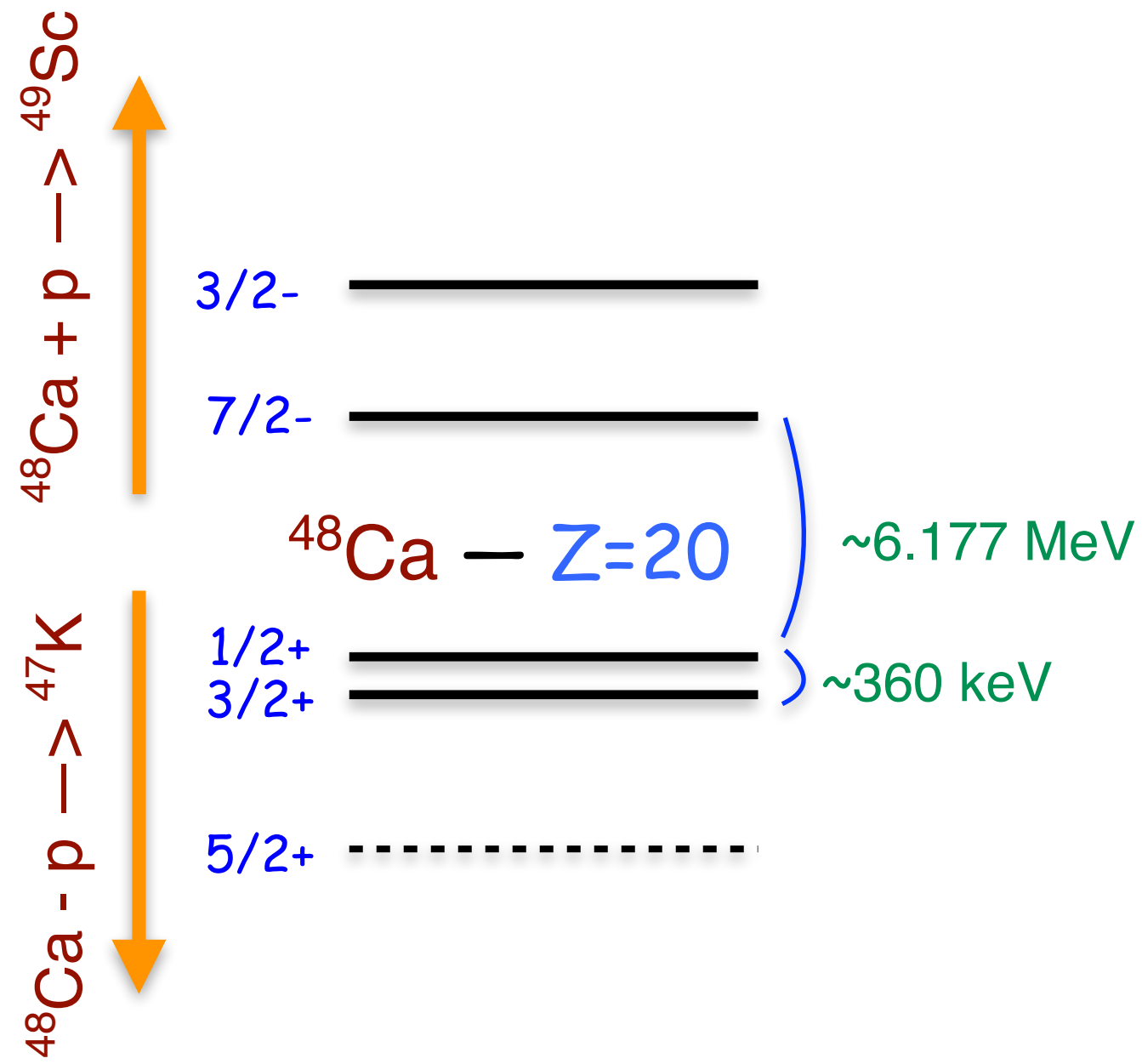
Bubble extends to  $^{42}\text{Si}$ - $^{46}\text{Ar}$  ??

S. Brolli (BSc thesis)

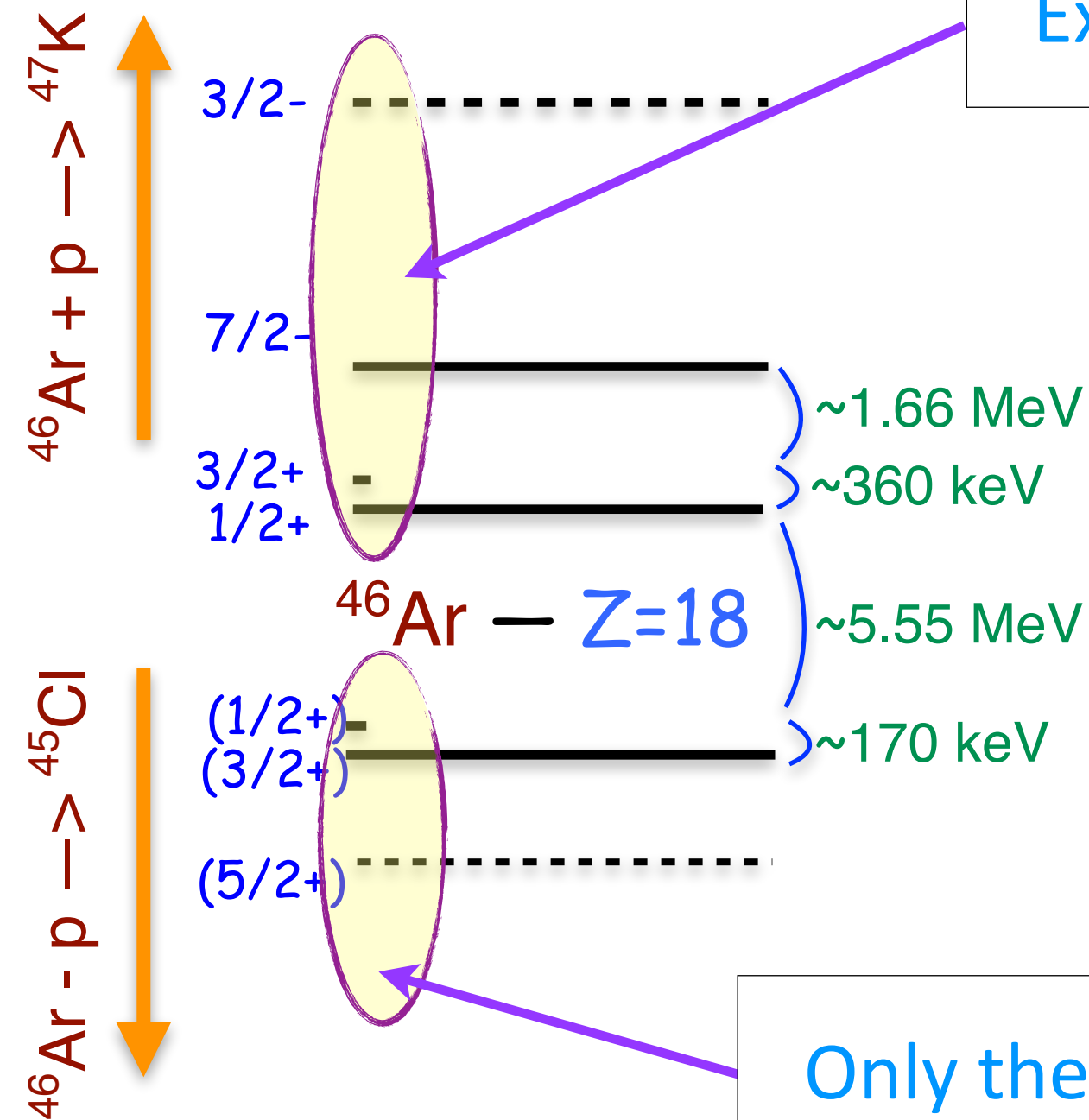




# $^{46}\text{Ar}(^3\text{He},d)^{47}\text{K}$ at GANIL : shell closure & charge bubble in $^{46}\text{Ar}$



$$\Delta E_{1/2+ - 3/2+} (\text{exp}) = 360 \text{ keV}$$

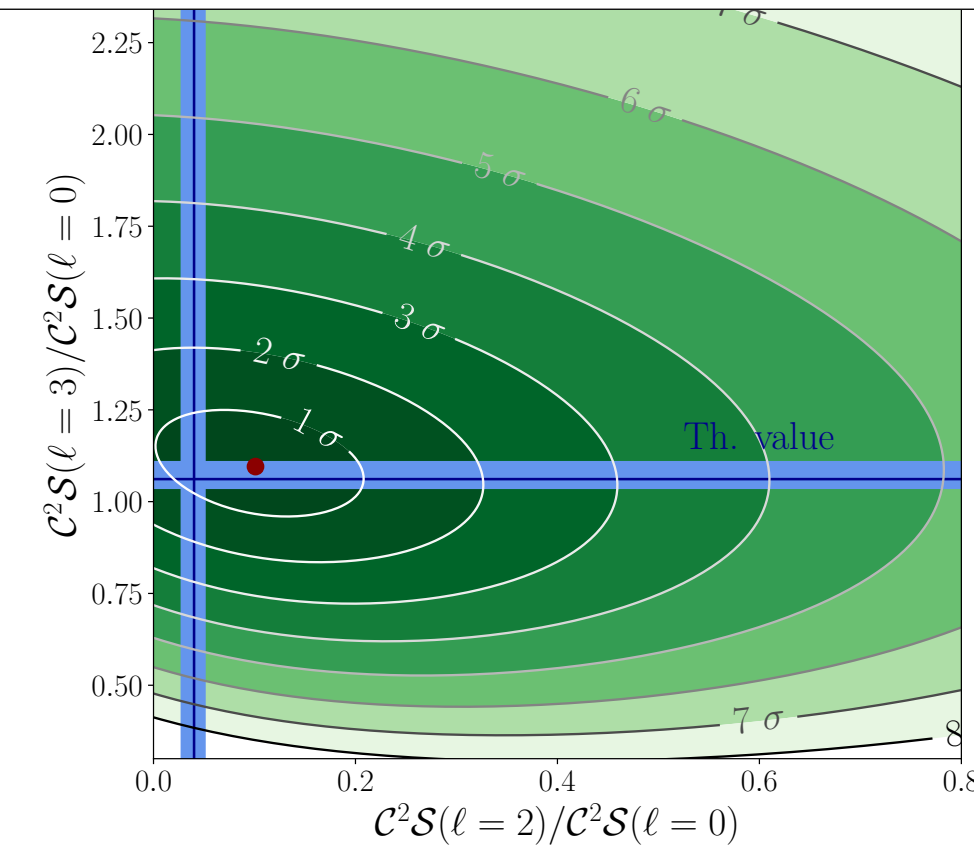


$$\Delta E_{1/2+ - 3/2+} (\text{exp}) = 5,55 \text{ MeV}$$

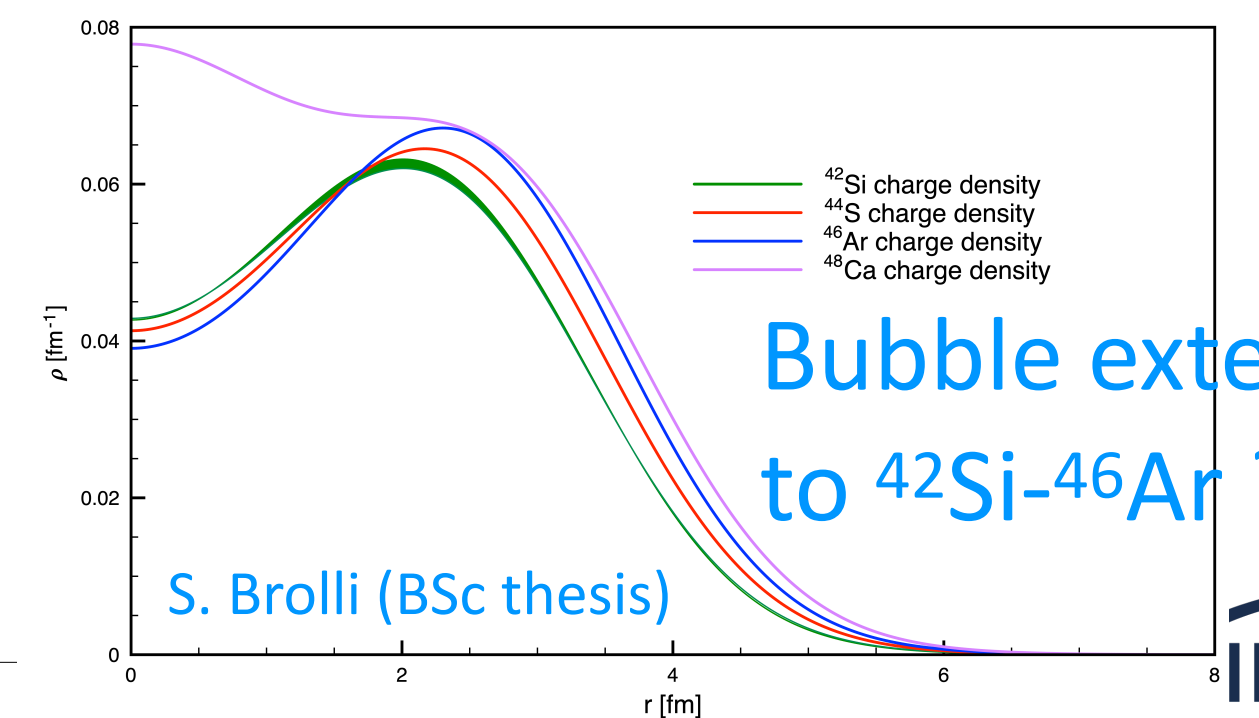
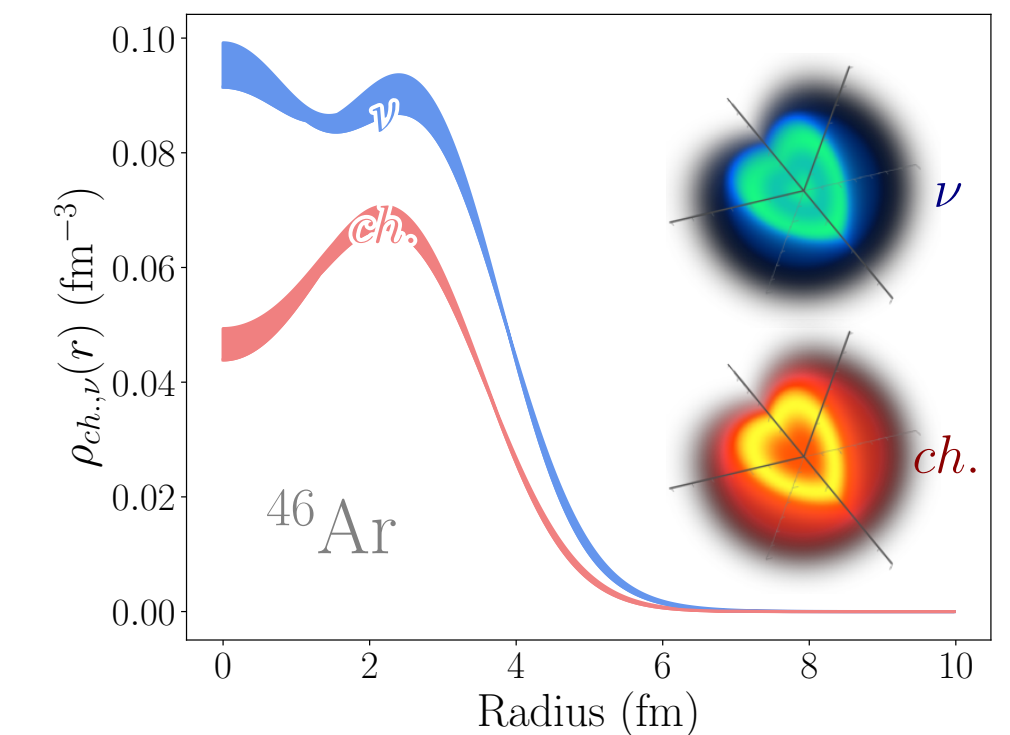
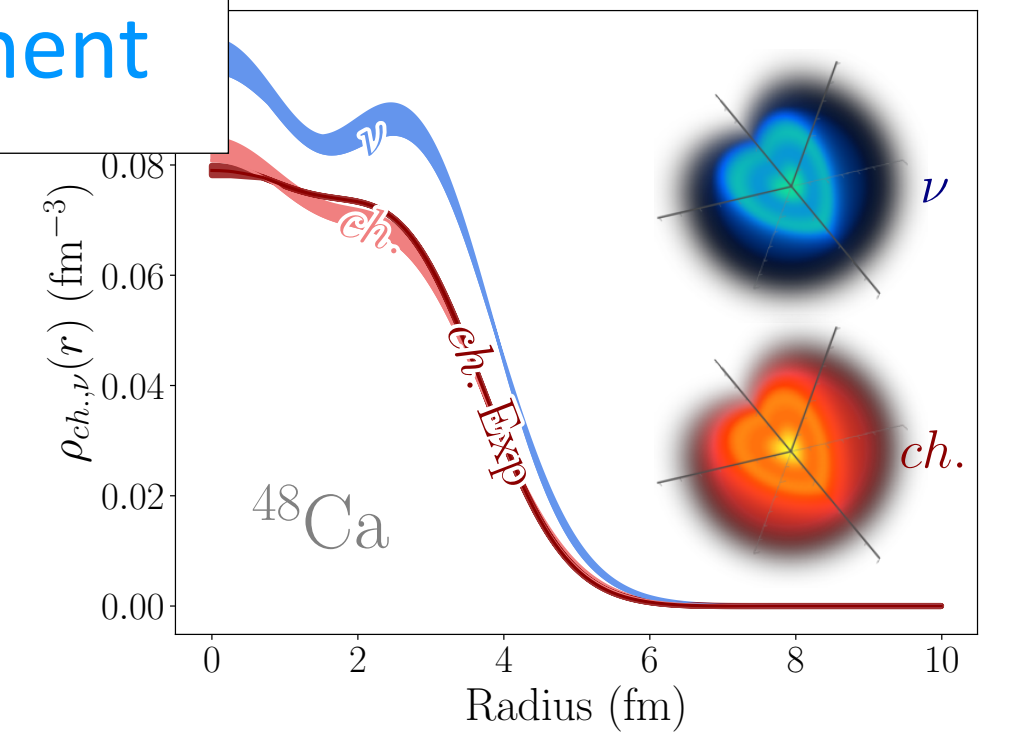
$$(\text{theo}) = 2,59 \text{ MeV}$$

The d3/2 - s1/2 gap opening and new shell closure at Z=18 !!

Experiment & theory in agreement



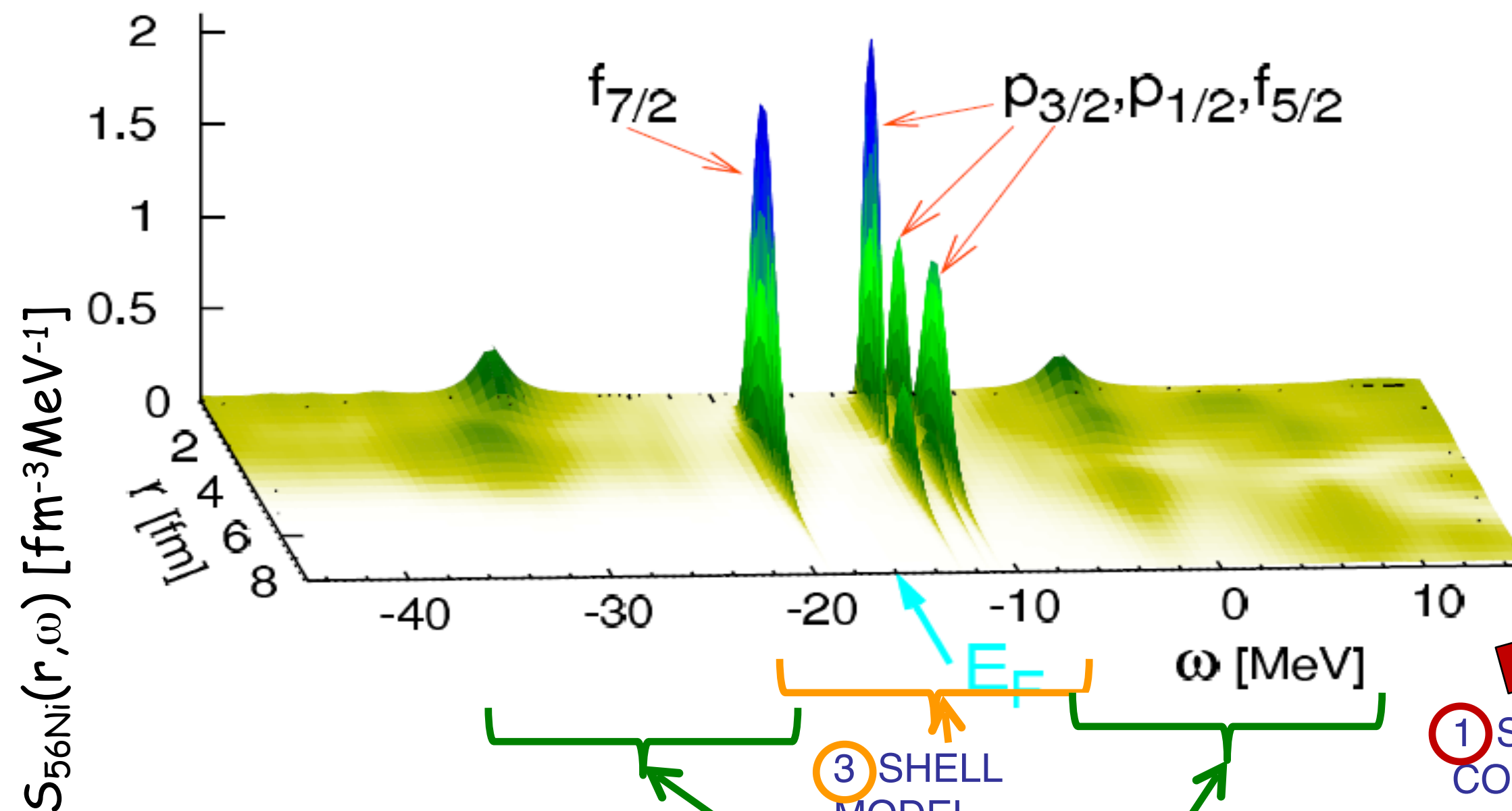
Only theory prediction is available



# Quenching of absolute spectroscopic factors

Overall quenching of spectroscopic factors is driven by:

SRC → ~10%  
 part-vibr. coupling → dominant!  
 “shell-model” → important for open shells



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

|                  |                    | 10 osc. shells |              | Exp. [30] | 1p0f space |      |                   |       |
|------------------|--------------------|----------------|--------------|-----------|------------|------|-------------------|-------|
|                  |                    | FRPA<br>(SRC)  | full<br>FRPA |           | FRPA       | SM   | $\Delta Z_\alpha$ |       |
| $^{57}\text{Ni}$ | $^{57}\text{Ni}$ : |                |              |           |            |      |                   |       |
|                  | $\nu 1p_{1/2}$     | 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 |
| $^{55}\text{Ni}$ | $^{55}\text{Ni}$ : |                |              |           |            |      |                   |       |
|                  | $\nu 0f_{7/2}$     | 0.95           | 0.72         | 0.69      |            | 0.89 | 0.86              | -0.03 |
|                  |                    | ①              | ② + ③        |           |            | ③    |                   |       |

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

(1) SHORT RANGE CORRELATIONS

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



# The physics contained in the **one-body** Green's function

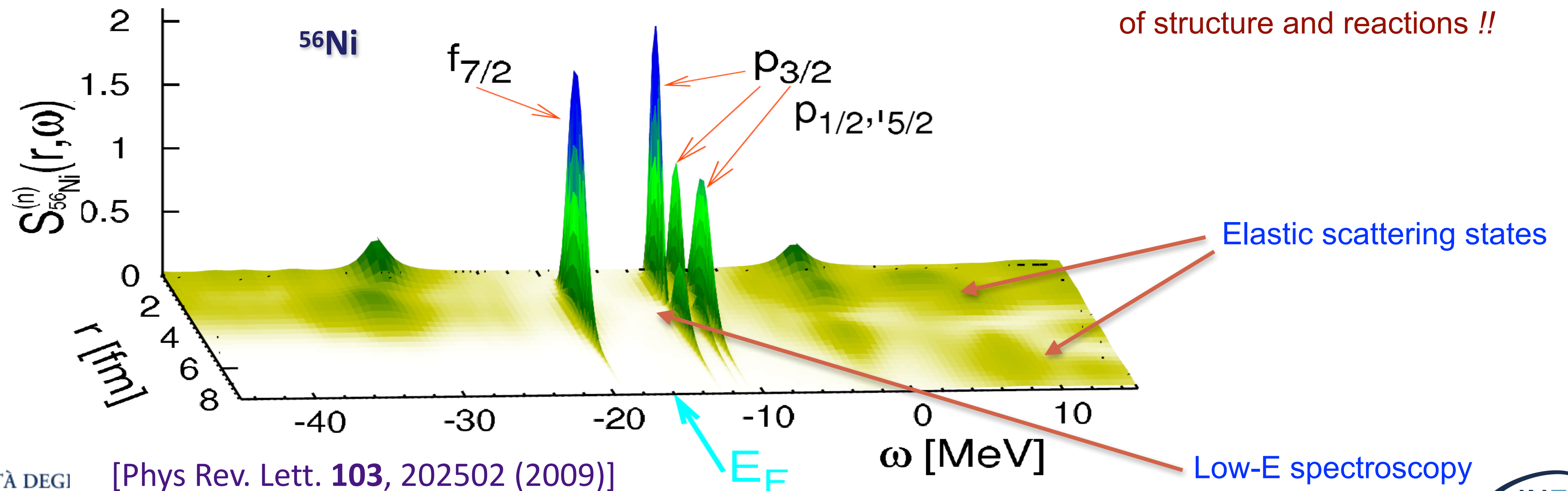
One-body propagator:  $g_{\alpha\beta}(t - t') = -i/\hbar \langle \Psi_0^A | T[c_\alpha(t) c_\beta^\dagger(t')] | \Psi_0^A \rangle$

Dyson Equation:  $g_{\alpha\beta}(\omega) = g_{\alpha\beta}^{(0)}(\omega) + \sum_{\gamma\delta} g_{\alpha\gamma}^{(0)}(\omega) \Sigma_{\gamma\delta}^*(\omega) g_{\delta\beta}(\omega)$

(One-body) spectral function:  $S(\alpha, \omega) := \pm \frac{1}{2\pi} \Im m \{ g_{\alpha\alpha}(\omega) \}$

The self-energy  $\Sigma_{\alpha\beta}^*(\omega)$  'decides' both ground state observables and elastic scattering.

==> Consistent computation of structure and reactions !!



# Ab initio optical potentials from propagator theory

## Relation to Feshbach theory:

Mahaux & Sartor, Adv. Nucl. Phys. 20 (1991)

Escher & Jennings Phys. Rev. C**66**, 034313 (2002)

## Previous SCGF work:

CB, B. Jennings, Phys. Rev. C**72**, 014613 (2005)

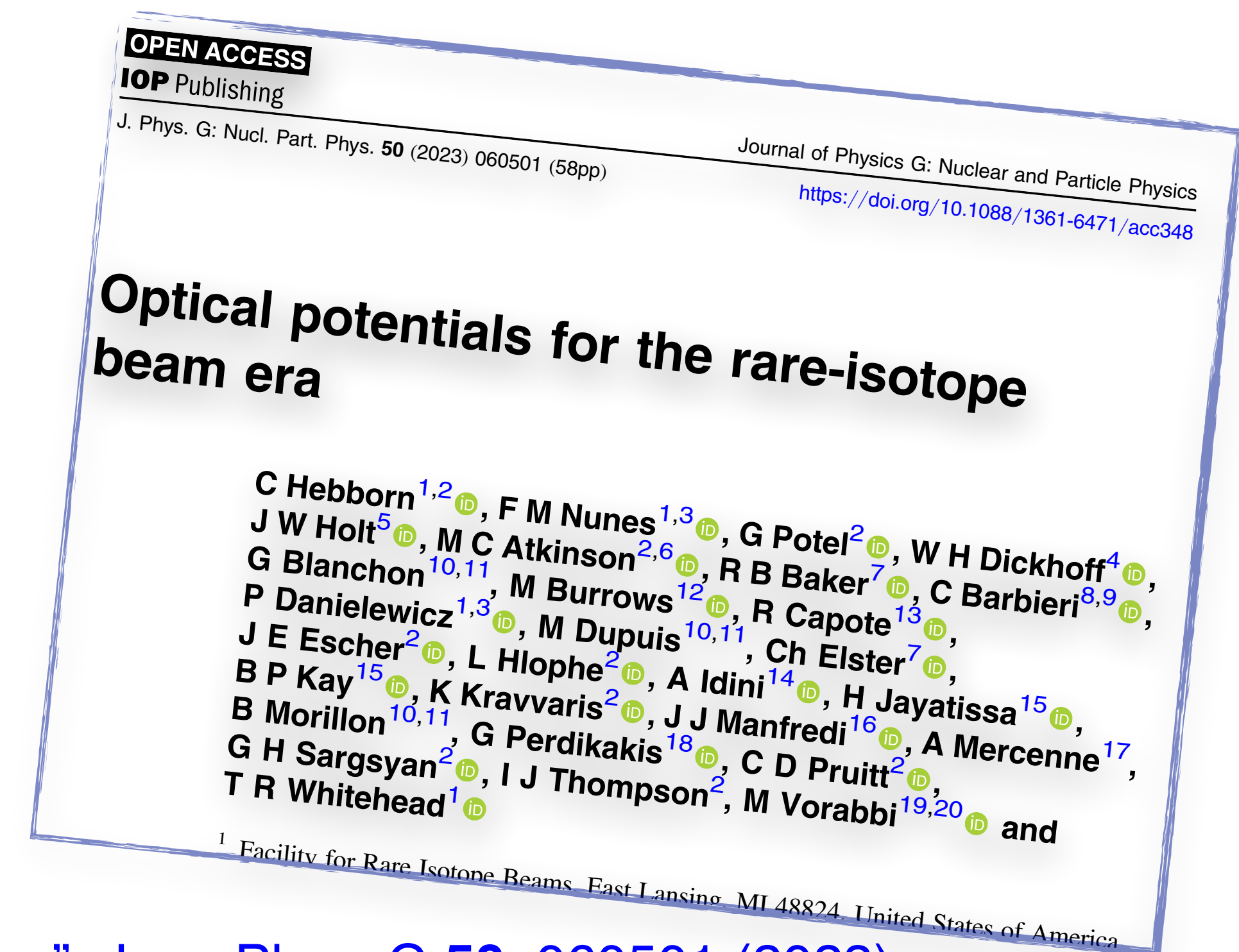
S. Waldecker, CB, W. Dickhoff, Phys. Rev. C**84**, 034616 (2011)

A. Idini, CB, P. Navrátil, Phys. Rev. Lett. **123**, 092501 (2019)

M. Vorabbi, CB, et al., Phys Rev C**109**, 034613 (2024)

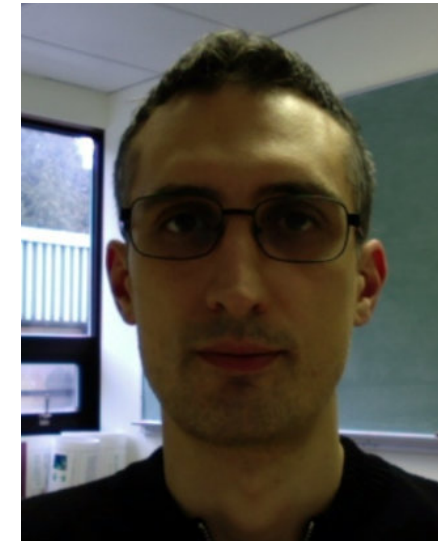
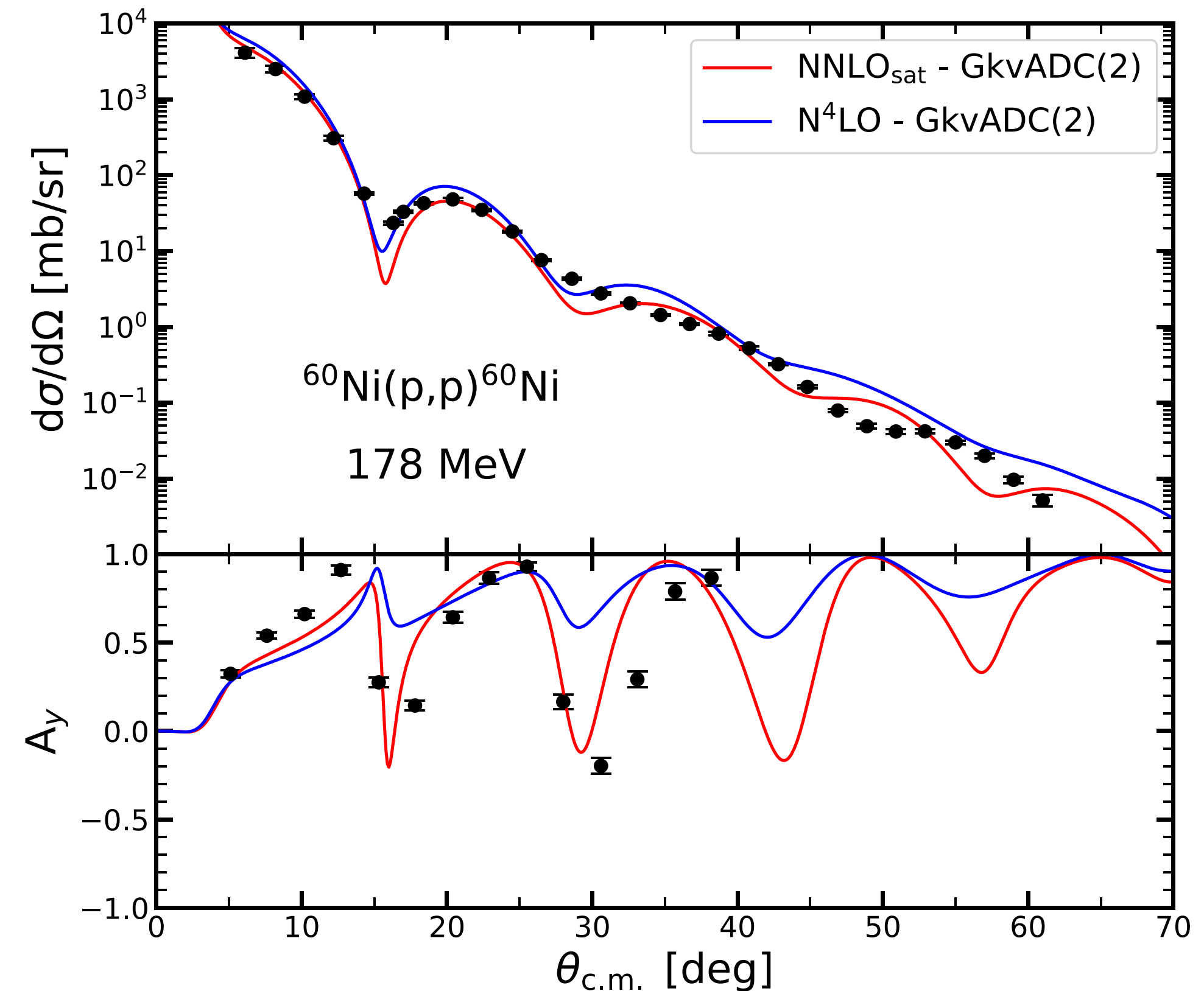
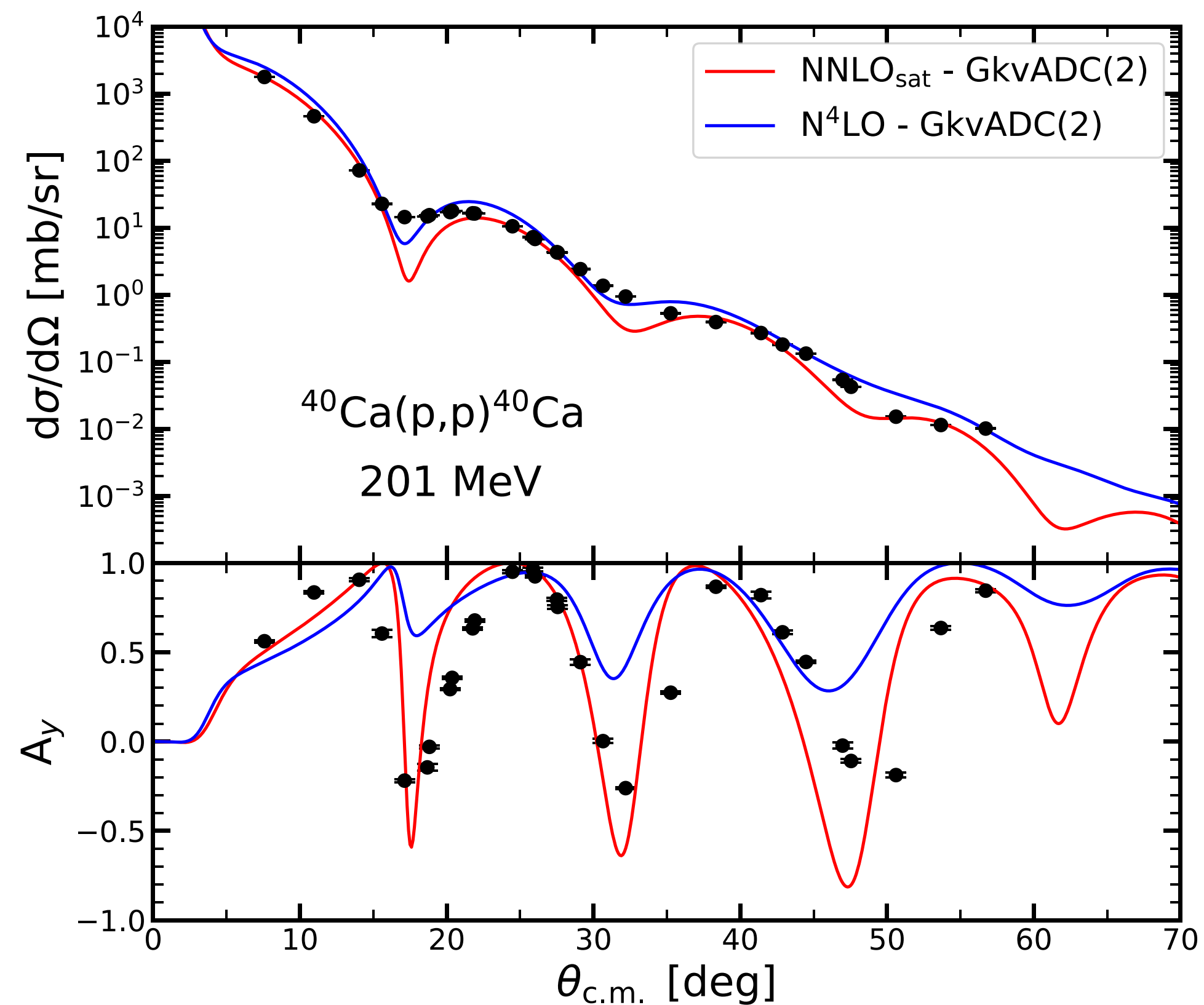
## State-of-the-art of the field:

C. Hebborn, et al., CB, “*Optical potentials for the rare-isotope beam era*”, Jour. Phys. G **50**, 060501 (2023)





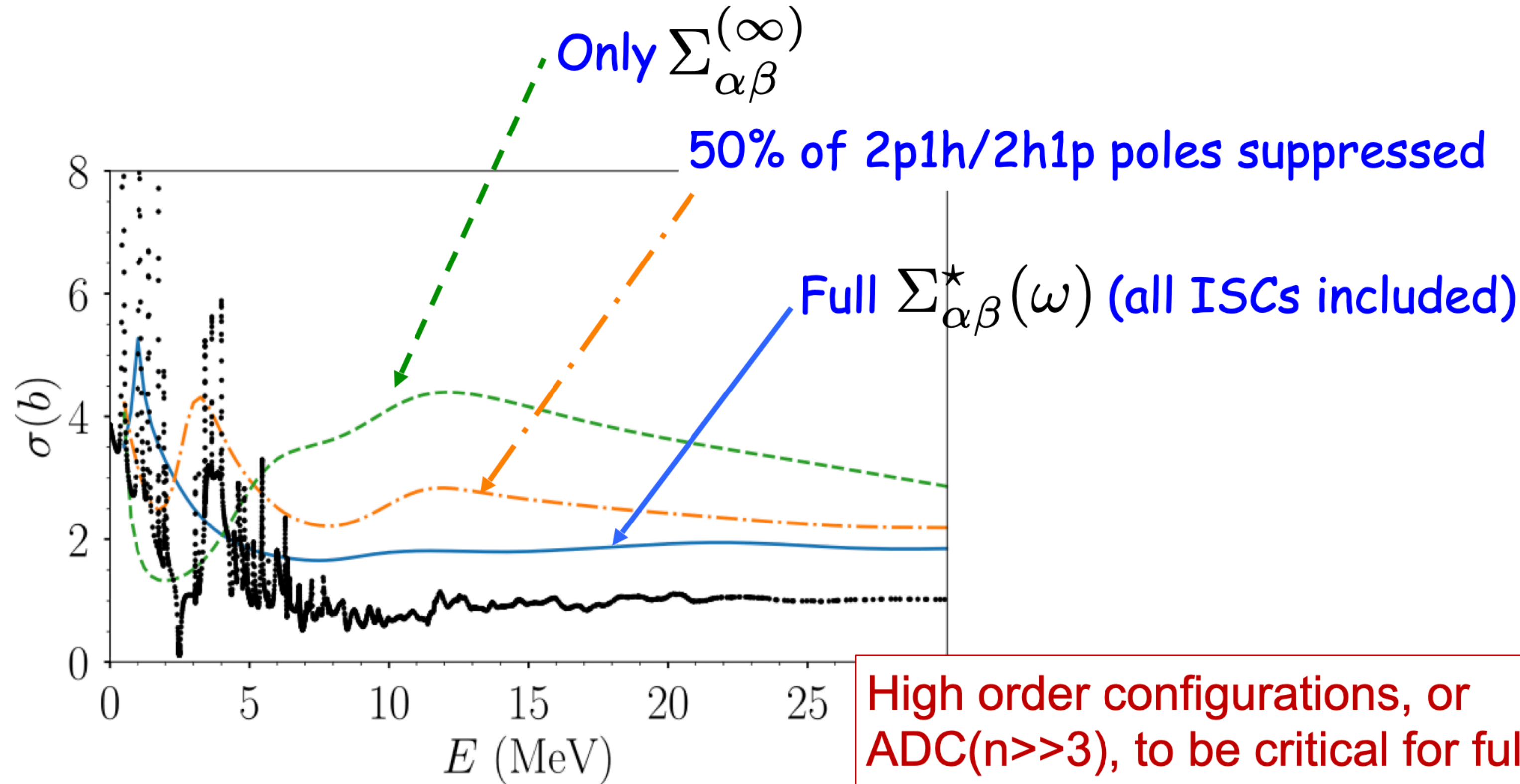
# Elastic nucleon nucleus scattering



M. Vorabbi  
U. of surrey

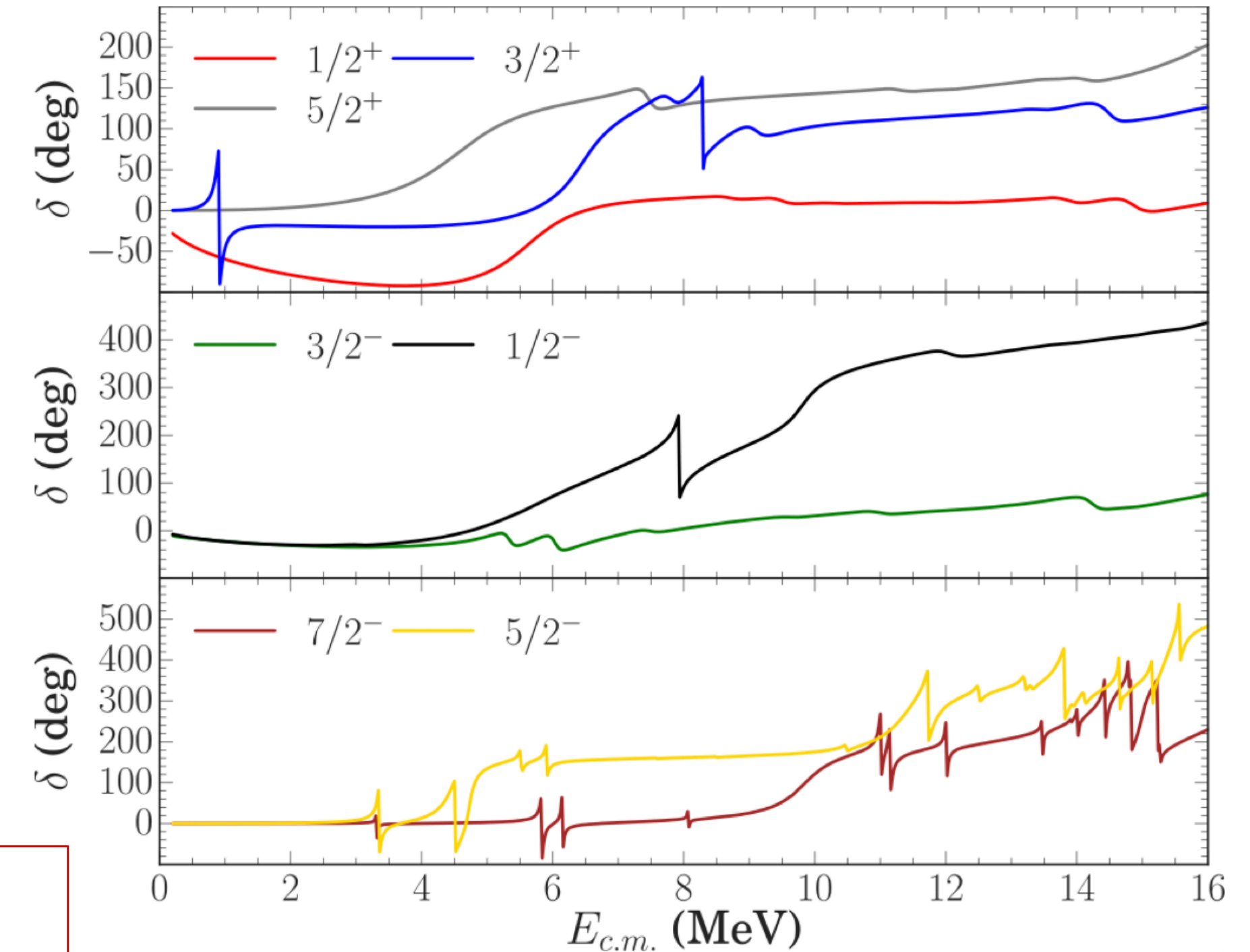
# Role of intermediate state configurations (ISCs)

$n$ - $^{16}\text{O}$ , total elastic cross section

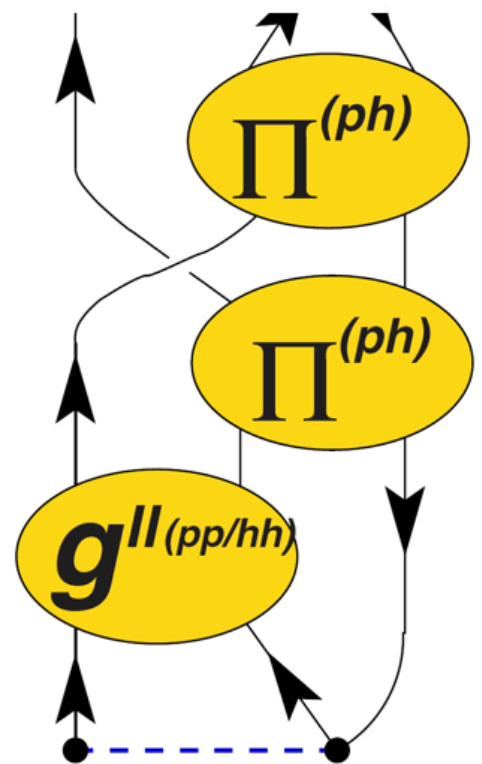


High order configurations, or ADC( $n \gg 3$ ), to be critical for fully ab initio optical potentials

[A. Idini, CB, Navrátil, Phys. Rev. Lett. **123**, 092501 (2019)]



$$\Sigma_{\alpha\beta}^*(\omega) = \Sigma_{\alpha\beta}^{(\infty)} + \underbrace{\sum_{i,j} \mathbf{M}_{\alpha,i}^\dagger \left( \frac{1}{E - (\mathbf{K}^> + \mathbf{C}) + i\Gamma} \right)_{i,j} \mathbf{M}_{j,\beta}}_{2p1h} + \underbrace{\sum_{r,s} \mathbf{N}_{\alpha,r} \left( \frac{1}{E - (\mathbf{K}^< + \mathbf{D}) - i\Gamma} \right)_{r,s} \mathbf{N}_{s,\beta}^\dagger}_{2h1p}$$





# Diagrammatic Monte Carlo for nuclei



# Green's function theory beyond ADC(3)? **DiagMC !!**

The Green's function is found as the exact solution of the Dyson equation:

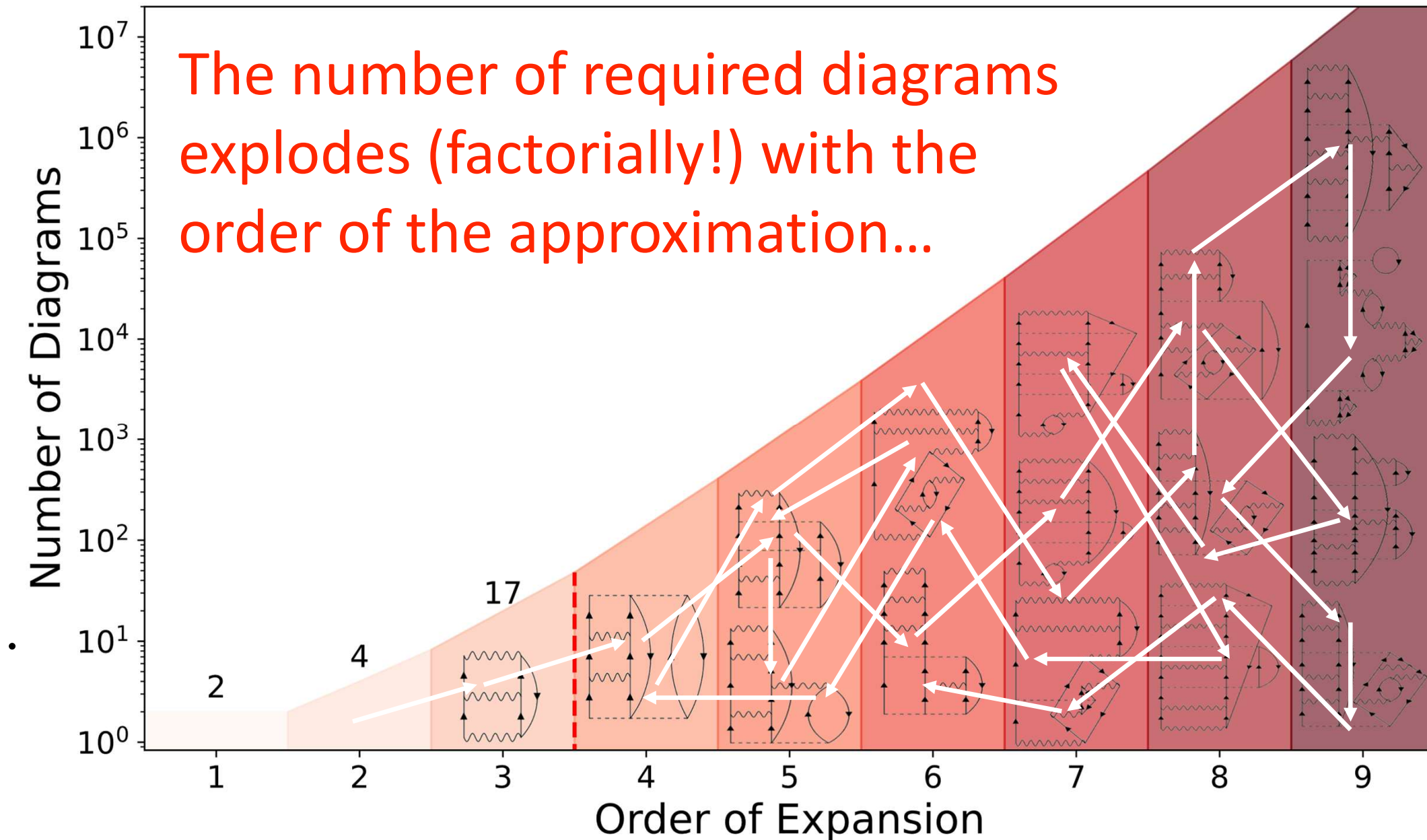
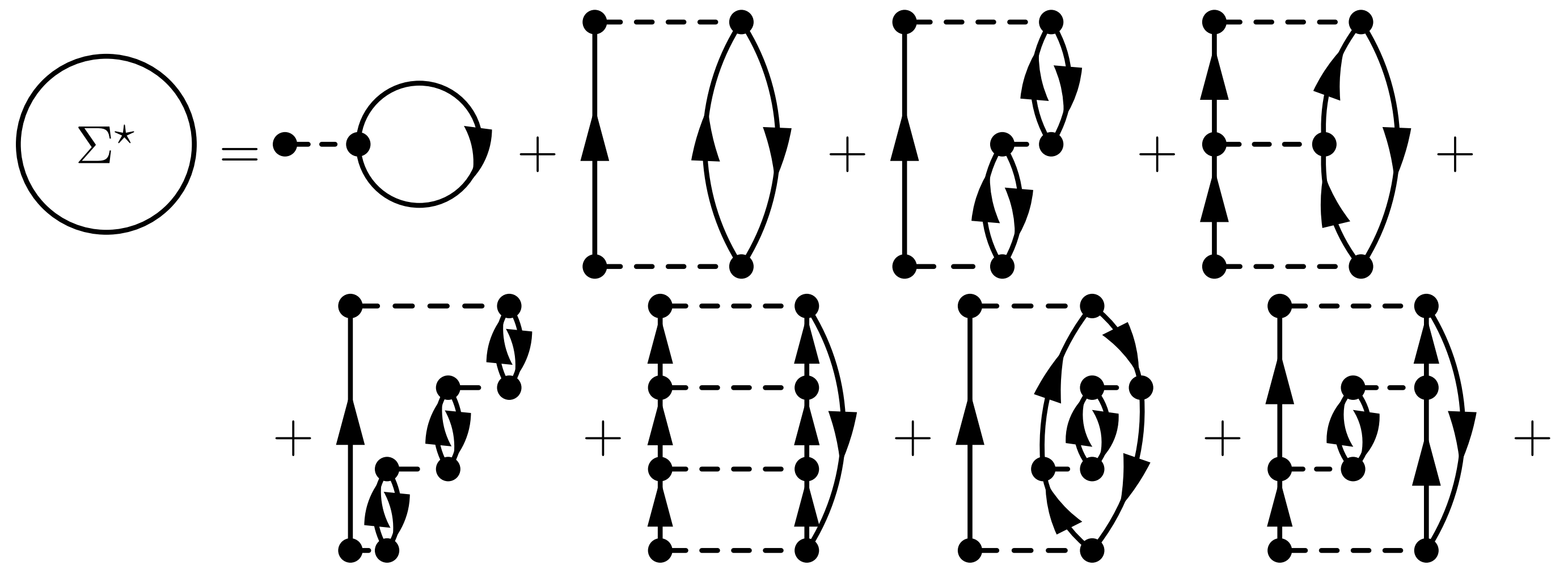
$$G_{\alpha\beta}(\omega) = G_{\alpha\beta}^{(0)}(\omega) + \sum_{\gamma\delta} G_{\alpha\gamma}^{(0)}(\omega) \Sigma_{\gamma\delta}^*(\omega) G_{\delta\beta}(\omega)$$

S. Brolli

(PhD candidate,  
Milan)



It requires knowing the self-energy which is the sum of an *infinite series* of Feynman diagrams:



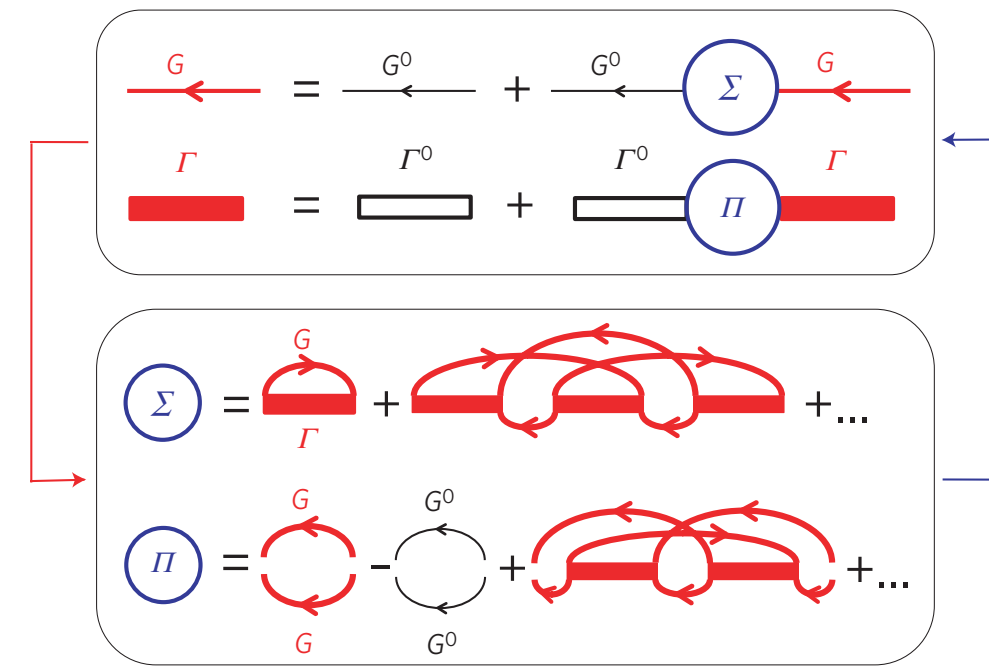
The number of required diagrams explodes (factorially!) with the order of the approximation...

Diagrammatic Monte Carlo (DiagMC) *samples diagrams in their topological space* using a Markov chain.

[Brolli, CB, Vigezzi, Phys. Rev. Lett. **134**, 182502 (2025)]



# Diagrammatic MC in solid state physics...



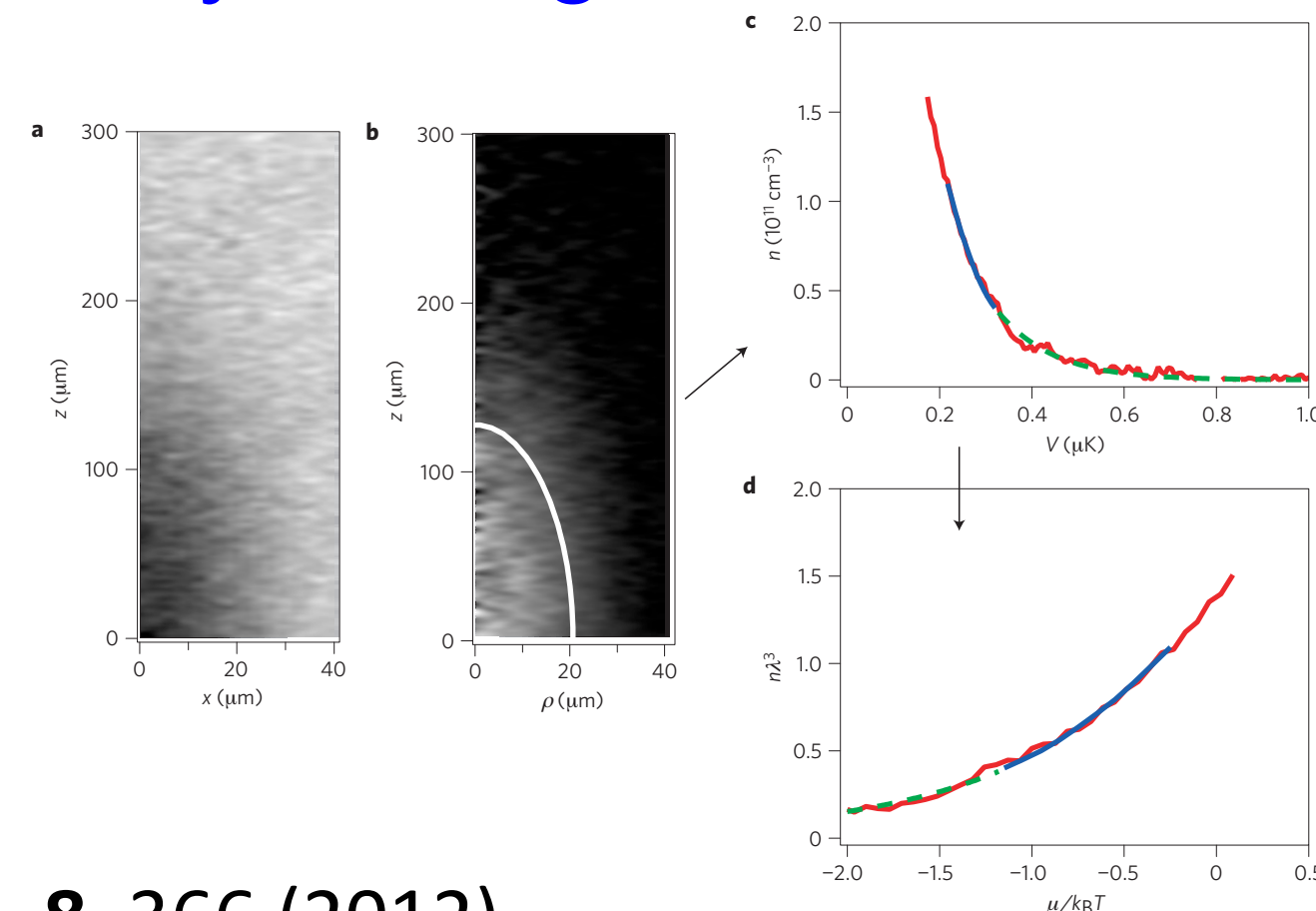
DiagMC:  
Phys. Rev. Lett. 81, 2514 (1998)  
Phys. Rev. B 99, 035140 (2019)  
...

Mostly infinite matter at  $T \neq 0$ ...

...what about finite nuclei??

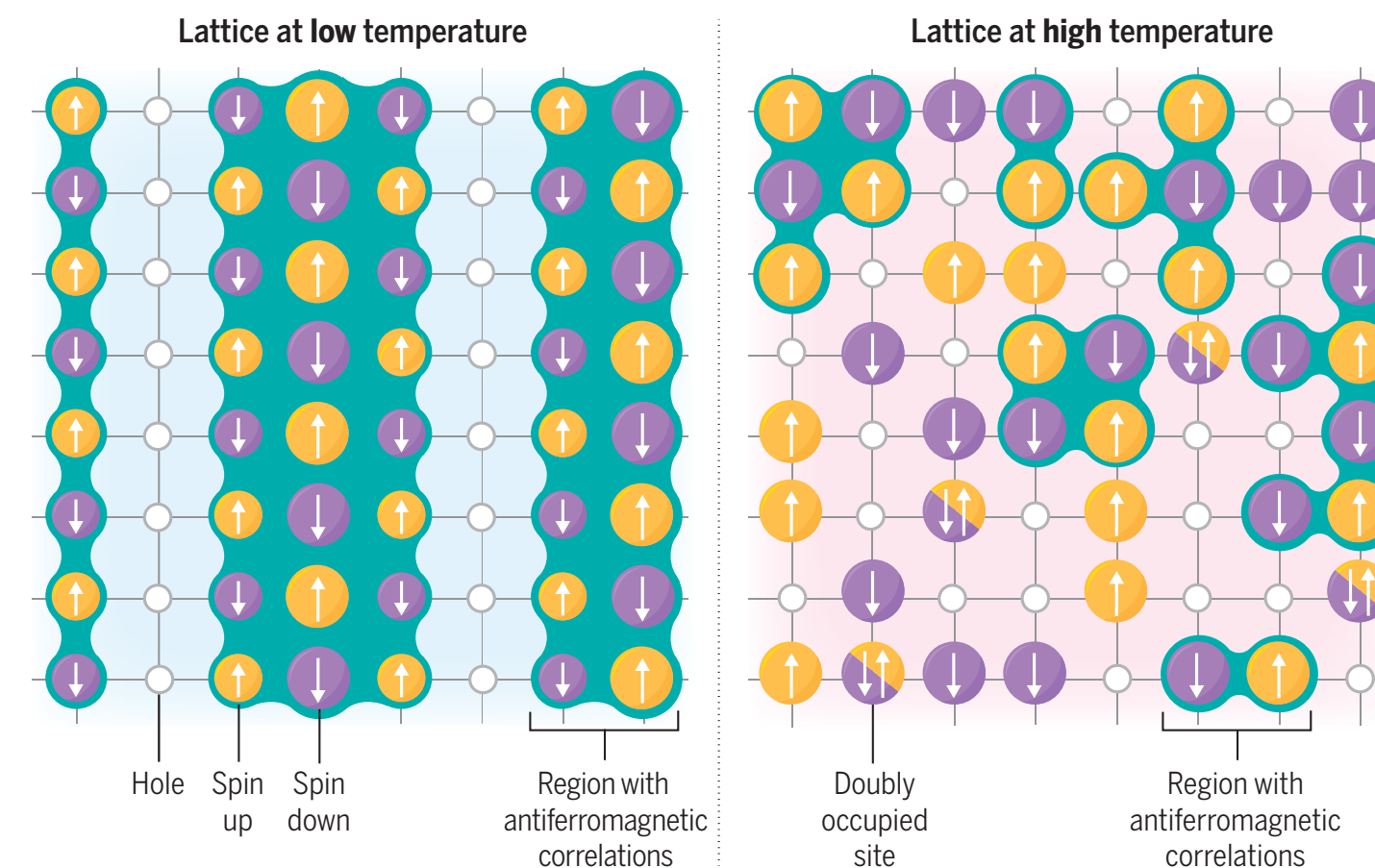
**Figure 1 | Bold diagrammatic Monte Carlo** The skeleton diagrammatic series for the self-energy  $\Sigma$  and the pair self-energy  $\Pi$  is evaluated

## EOS unitary fermi gas...

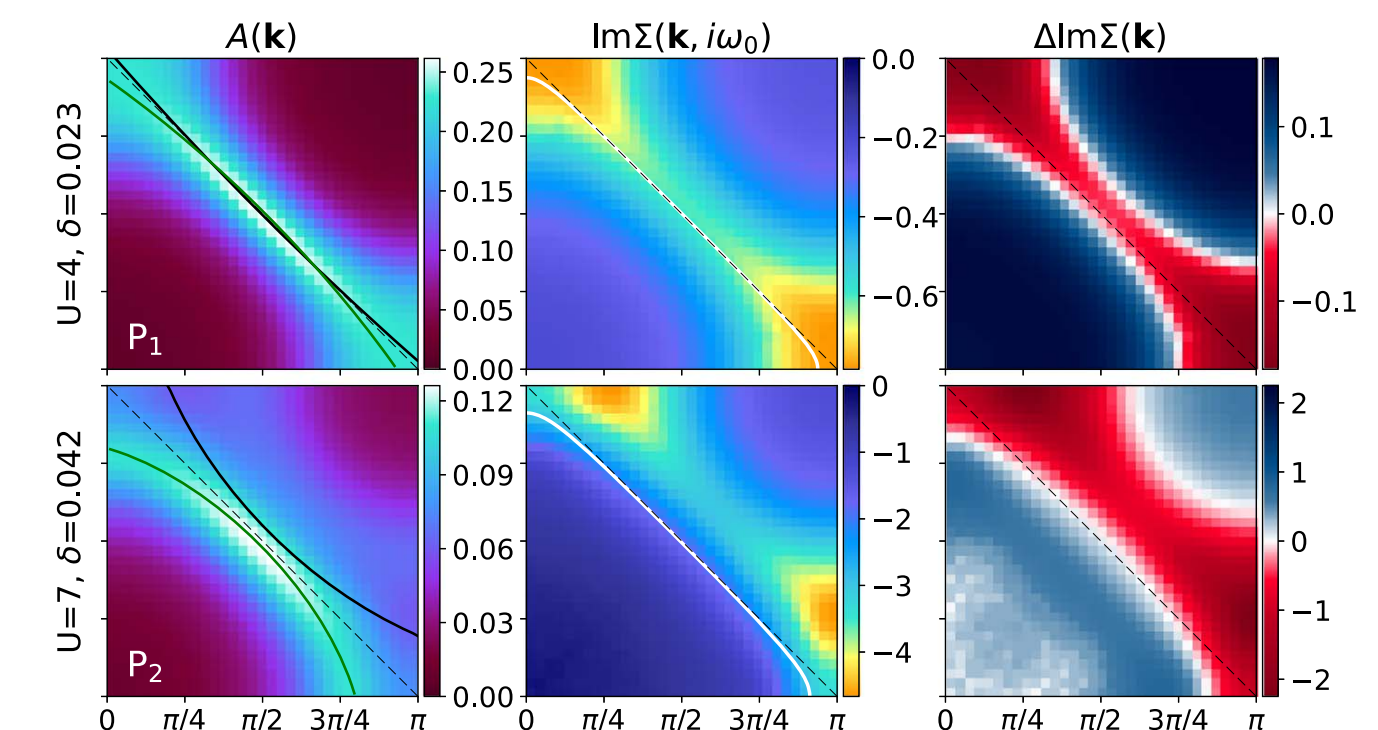


Nature Phys. **8**, 366 (2012)

## Spins in the Hubbard model...



Science **385**, eade9194 (2024)



**Fig. 2. Fingerprints of the different regimes.** The momentum-resolved spectral function,  $A(\mathbf{k})$  (left); the imaginary part of the self-energy,  $\text{Im}\Sigma(\mathbf{k}, i\omega_0)$  (middle); and the difference between the imaginary part of the self-energy at the two lowest Matsubara frequencies,  $\Delta\text{Im}\Sigma(\mathbf{k}) = \text{Im}\Sigma(\mathbf{k}, i\omega_0) - \text{Im}\Sigma(\mathbf{k}, i\omega_1)$  (right) are shown for

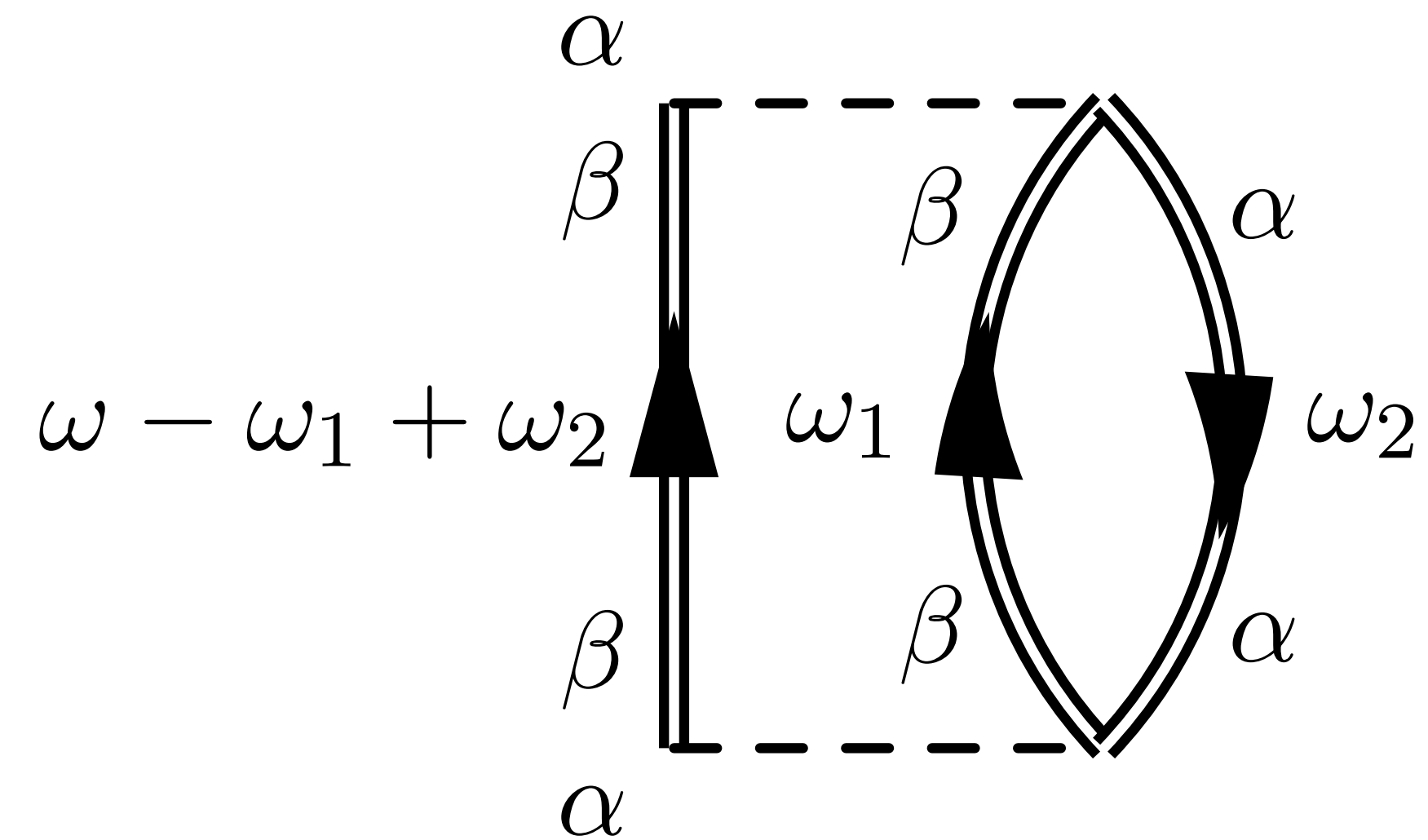
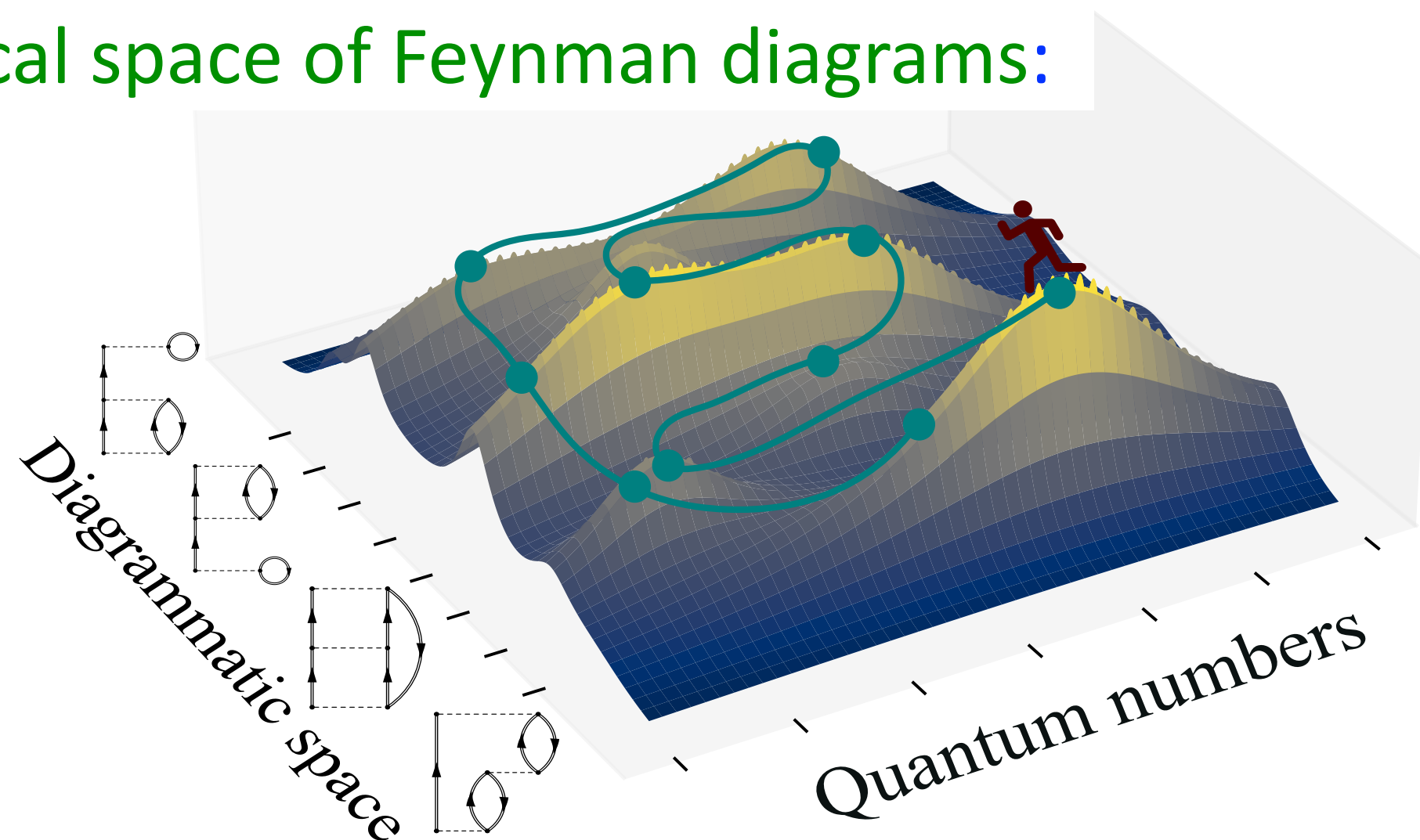
# Diagrammatic Monte Carlo: overview

$$\Sigma_{\alpha\beta}^*(\omega) = \sum_{\mathcal{T}} \sum_{\gamma_1 \dots \gamma_n} \int d\omega_1 \dots d\omega_n \mathcal{D}_{\alpha\beta}^{\omega}(\mathcal{T}; \gamma_1 \dots \gamma_n; \omega_1 \dots \omega_n) 1_{\mathcal{T} \in \mathcal{S}_{\Sigma^*}}$$

Infinte Feynman  
series of diagrams

Monte Carlo integration - "101"

Monte Carlo integration in the  
topological space of Feynman diagrams:





# Diagrammatic Monte Carlo: overview

$$\Sigma_{\alpha\beta}^*(\omega) = \sum_{\mathcal{T}} \sum_{\gamma_1 \dots \gamma_n} \int d\omega_1 \dots d\omega_m \mathcal{D}_{\alpha\beta}^{\omega}(\mathcal{T}; \gamma_1 \dots \gamma_n; \omega_1 \dots \omega_m) 1_{\mathcal{T} \in \mathcal{S}_{\Sigma^*}}$$

We define  $\mathcal{C} := (\mathcal{T}; \gamma_1 \dots \gamma_n; \omega_1 \dots \omega_m)$

$$\Sigma_{\alpha\beta}^*(\omega) = \int d\mathcal{C} |\mathcal{D}_{\alpha\beta}^{\omega}(\mathcal{C})| e^{i \arg[\mathcal{D}_{\alpha\beta}^{\omega}(\mathcal{C})]} 1_{\mathcal{T} \in \mathcal{S}_{\Sigma^*}}$$

$$\Sigma_{\alpha\beta}^*(\omega) = \mathcal{Z}_{\alpha\beta}^{\omega} \int d\mathcal{C} \frac{|\mathcal{D}_{\alpha\beta}^{\omega}(\mathcal{C})| W_o(N)}{\mathcal{Z}_{\alpha\beta}^{\omega}} \frac{e^{i \arg[\mathcal{D}_{\alpha\beta}^{\omega}(\mathcal{C})]}}{W_o(N)} 1_{\mathcal{T} \in \mathcal{S}_{\Sigma^*}}$$

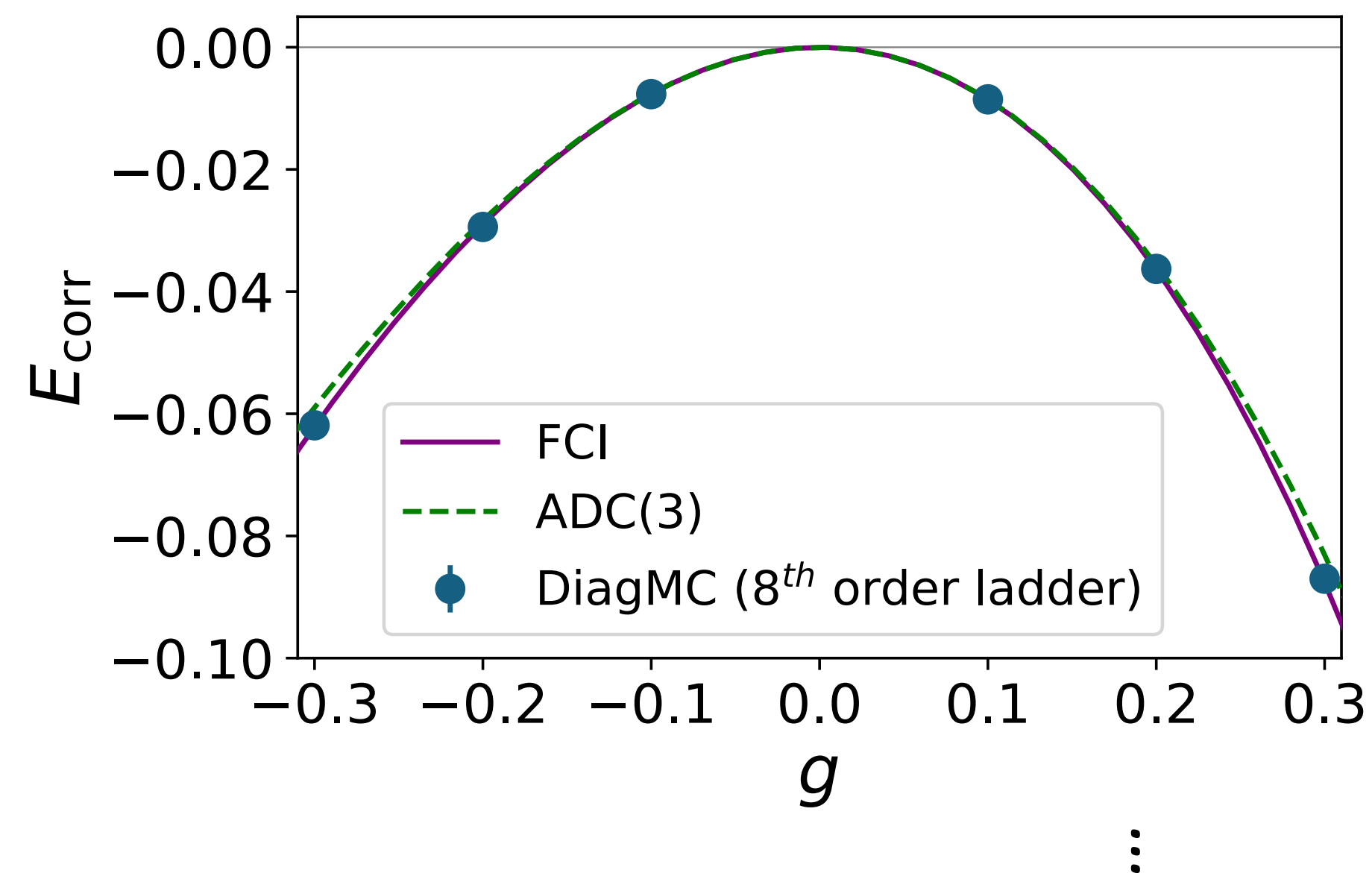
- $W_o(N)$  is an order dependent reweighting factor
- $\mathcal{Z}_{\alpha\beta}^{\omega} = \int d\mathcal{C} |\mathcal{D}_{\alpha\beta}^{\omega}(\mathcal{C})| W_o(N)$  is a normalization factor
- $w_{\alpha\beta}^{\omega}(\mathcal{C}) := \frac{|\mathcal{D}_{\alpha\beta}^{\omega}(\mathcal{C})| W_o(N)}{\mathcal{Z}_{\alpha\beta}^{\omega}}$  is a probability distribution function

# Results of the simulation for $D=2-10$ levels

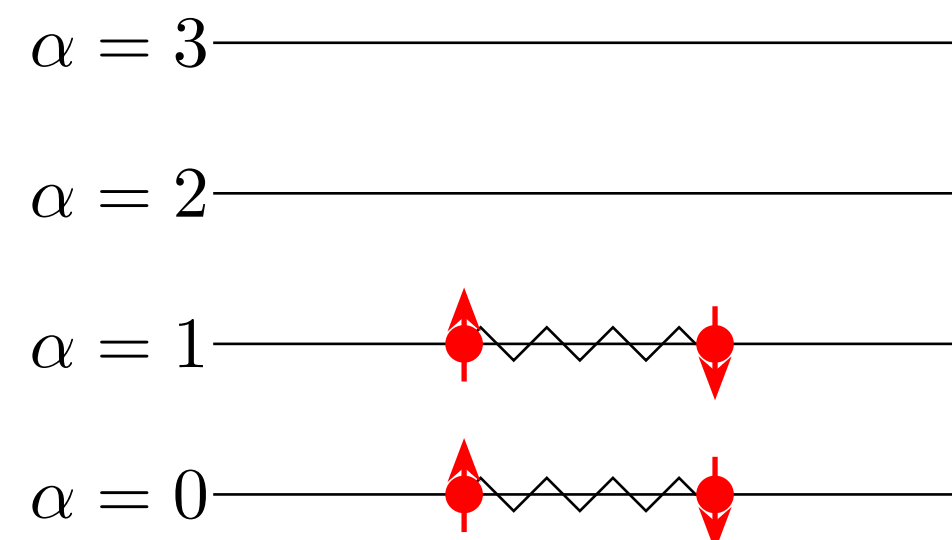
S. Brolli  
(PhD Milan)



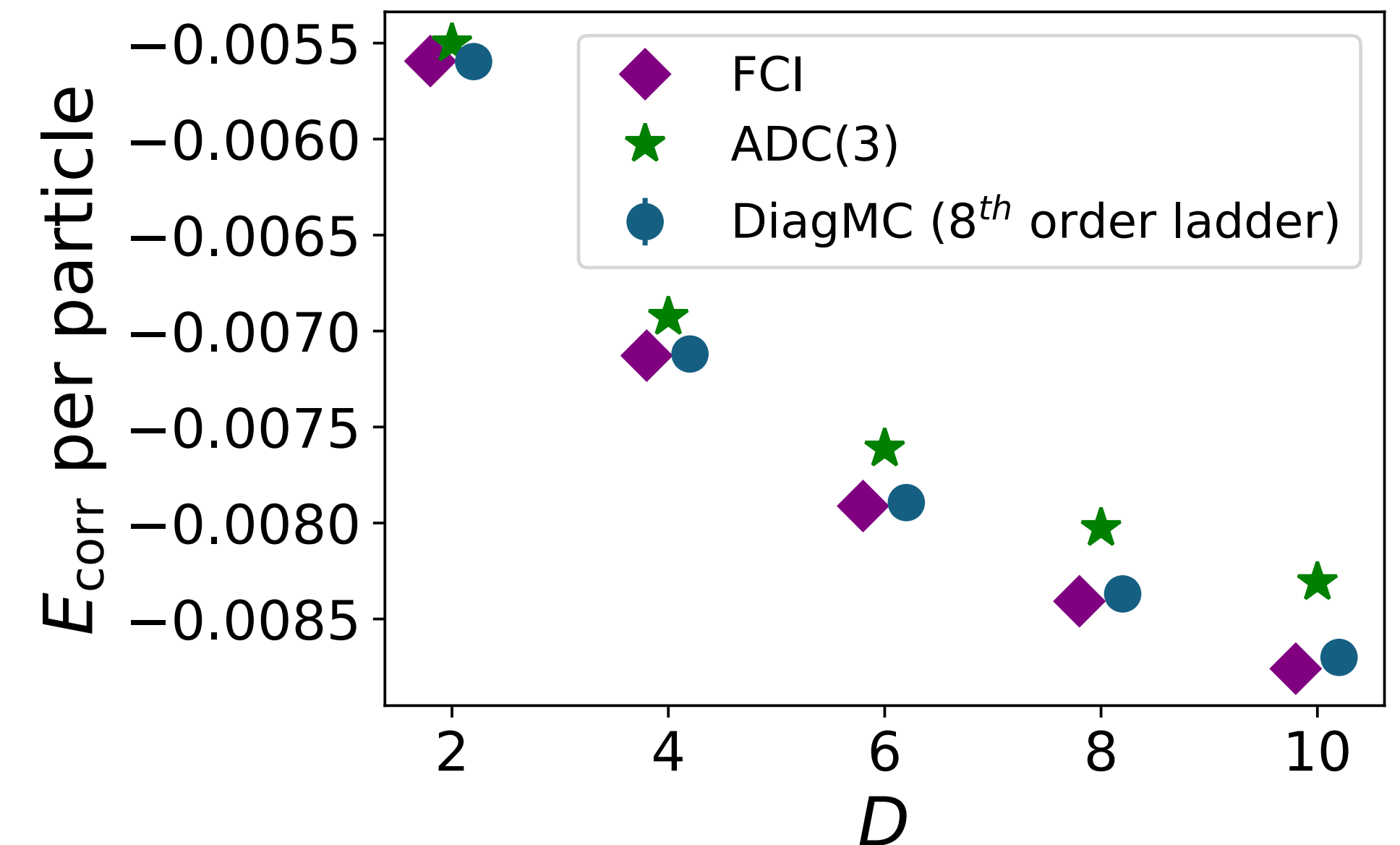
Correlation energy  $\Delta E = E - E_{HF}$  as a function of interaction strength ( $g$ ):



Spectroscopic function  
for  $D=10$  levels :



Accuracy for different model spaces model spaces ( $D=2-10$  levels):



$$H = \xi \sum_{\alpha=0}^{D-1} \sum_{\sigma=+,-} \alpha c_{\alpha\sigma}^{\dagger} c_{\alpha\sigma} - \frac{g}{2} \sum_{\alpha,\beta=0}^{D-1} c_{\alpha+}^{\dagger} c_{\alpha-}^{\dagger} c_{\beta-} c_{\beta+}$$



# Time-ordered DiagMC for atomic nuclei ( $^{16}\text{O}$ )

## Time-ordered Diagrammatic Monte Carlo for $^{16}\text{O}$

Stefano Brolli<sup>1,2,\*</sup> and Carlo Barbieri<sup>1,2,†</sup>

<sup>1</sup>Dipartimento di Fisica “Aldo Pontremoli,” Università degli Studi di Milano, via Celoria 16, I-20133 Milano, Italy  
<sup>2</sup>INFN, Sezione di Milano, via Celoria 16, I-20133 Milano, Italy  
 (Dated: May 8, 2026)

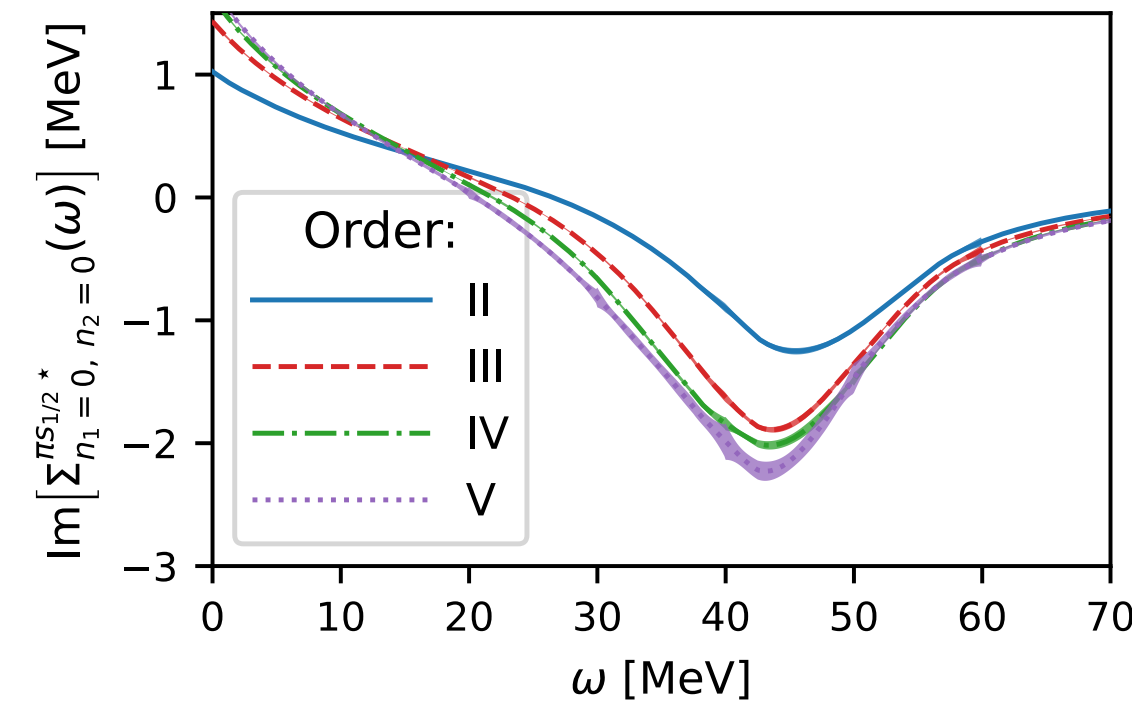
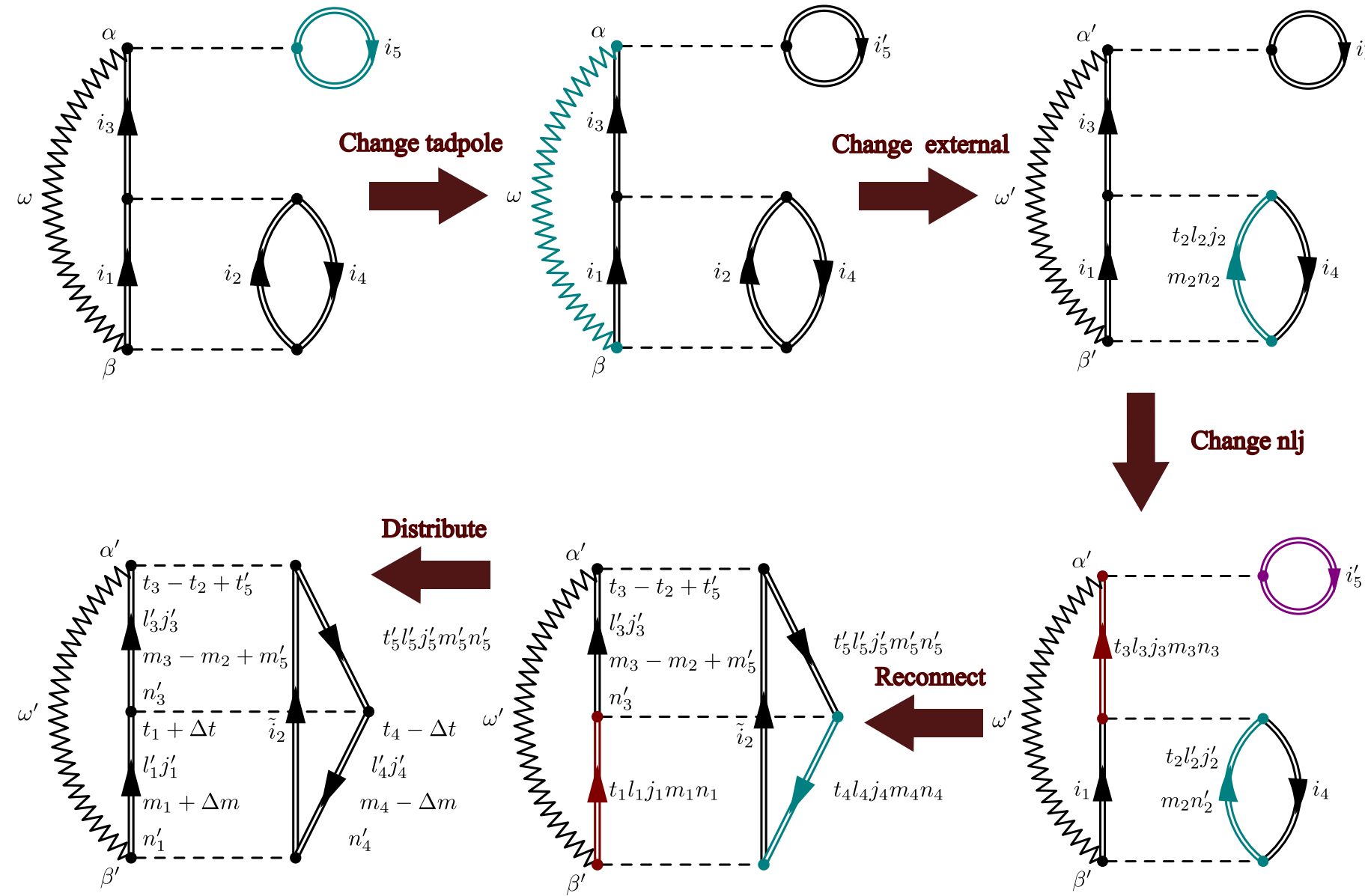


FIG. 4. Imaginary part of the  $n_1 = n_2 = 0$  component of the self-energy in the proton  $s_{1/2}$  partial wave, computed in the HF basis with  $\eta = 10$  MeV. The real part can be reconstructed via a dispersion relation. Monte Carlo uncertainties are shown as a band and are only visible at fifth order.

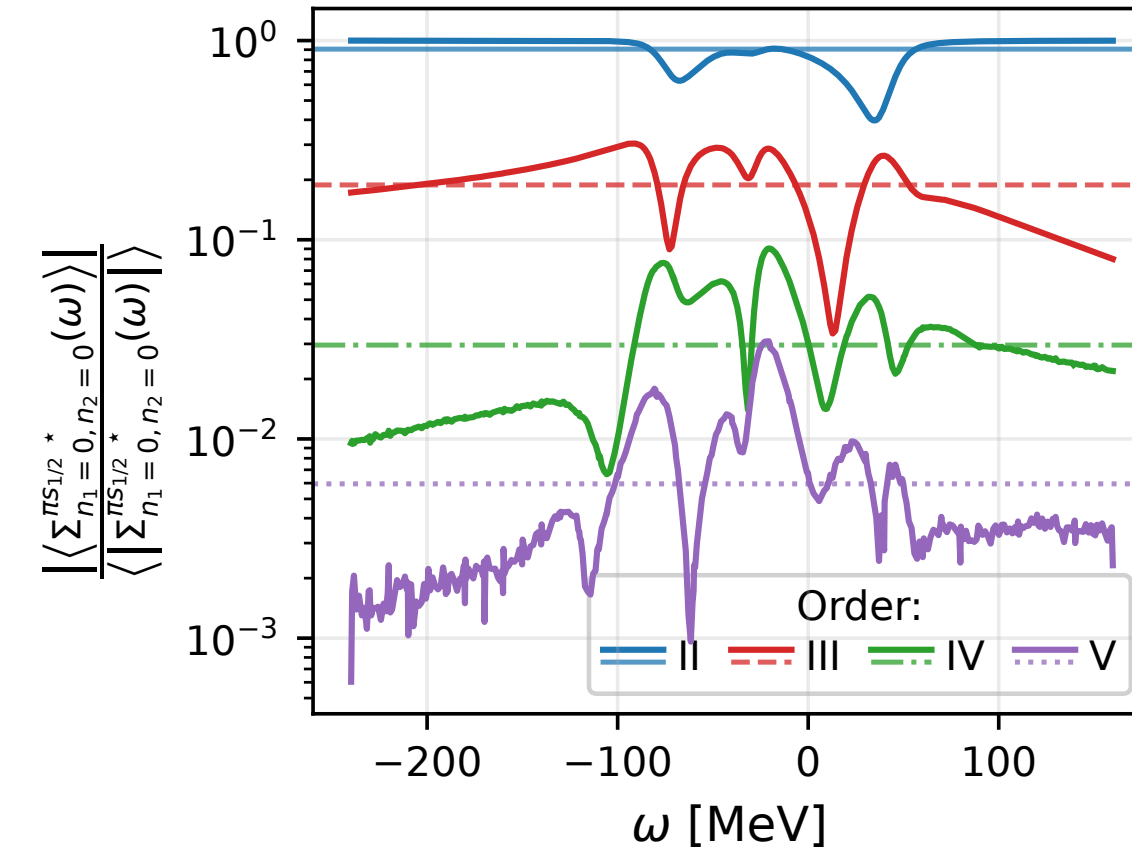


FIG. 3. Average sign of the self-energy contributions as a function of the energy  $\omega$ . The results are shown for different perturbative orders for the component  $n_1 = n_2 = 0$  of the protonic  $s_{1/2}$  wave and  $\eta = 10$  MeV. The horizontal lines represent the average sign contributions for each order.

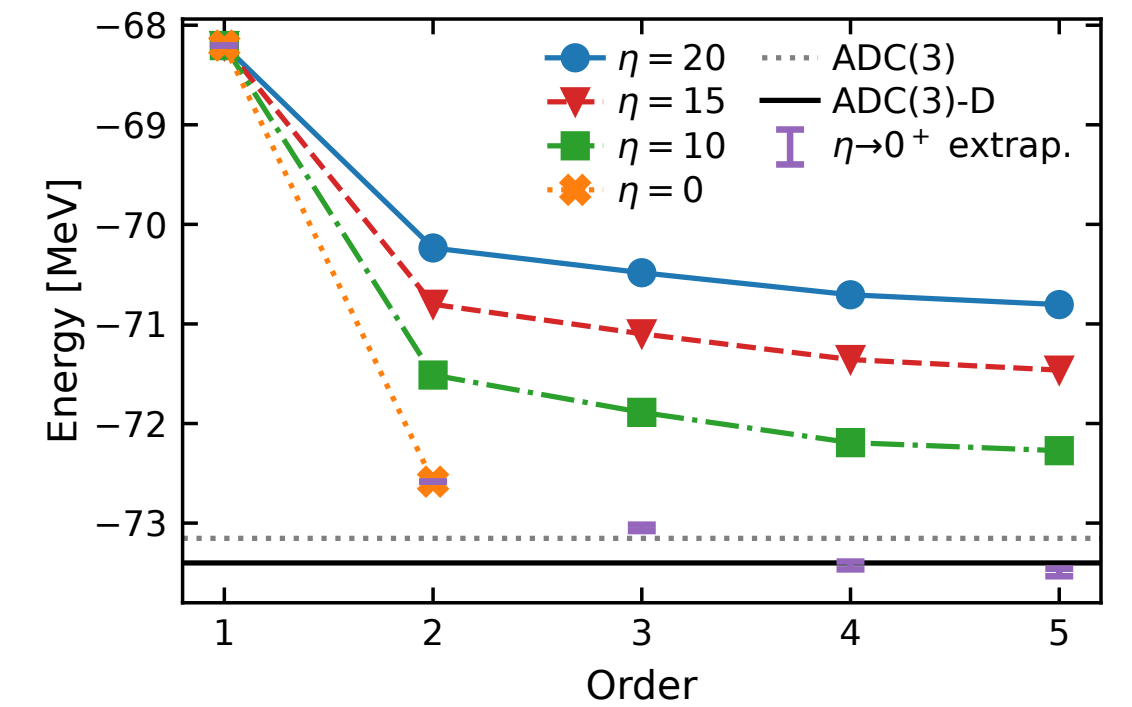


FIG. 5. Top: Proton  $s_{1/2}$  spectral function computed at successive perturbative orders within TO-DMC, using a regulator  $\eta = 10$  MeV. Bottom: Ground-state energy as a function of perturbative order in the self-energy for different values of the regulator  $\eta$ . Results at  $\eta = 20, 15$ , and  $10$  MeV are obtained from TO-DMC simulations, while the second-order point at  $\eta = 0$  is obtained with the SCGF framework of Refs. [33, 48]. Extrapolations to  $\eta \rightarrow 0^+$  are performed from the TO-DMC data as described in the main text.

# SCGF for infinite Matter





# Rooting Nuclear Density Functional into Ab Initio Theory

PHYSICAL REVIEW C **104**, 024315 (2021)

## Nuclear energy density functionals grounded in *ab initio* calculations

F. Marino <sup>1,2,\*</sup> C. Barbieri <sup>1,2</sup> A. Carbone,<sup>3</sup> G. Colò <sup>1,2</sup> A. Lovato <sup>4,5</sup> F. Pederiva,<sup>6,5</sup> X. Roca-Maza <sup>1,2</sup>  
and E. Viguzzi <sup>2</sup>

<sup>1</sup>Dipartimento di Fisica “Aldo Pontremoli,” Università degli Studi di Milano, 20133 Milano, Italy

<sup>2</sup>Istituto Nazionale di Fisica Nucleare, Sezione di Milano, 20133 Milano, Italy

<sup>3</sup>Istituto Nazionale di Fisica Nucleare—CNAF Viale Carlo Rortti Pichat 6/2 40127 Bologna, Italy



F. Marino  
(EPS PhD thesis  
prize, 2025)

DFT is in principle exact – but the energy  
density functional (EDF) is not known

For nuclear physics this is even more  
demanding: need to link the EDF to  
theories rooted in QCD!

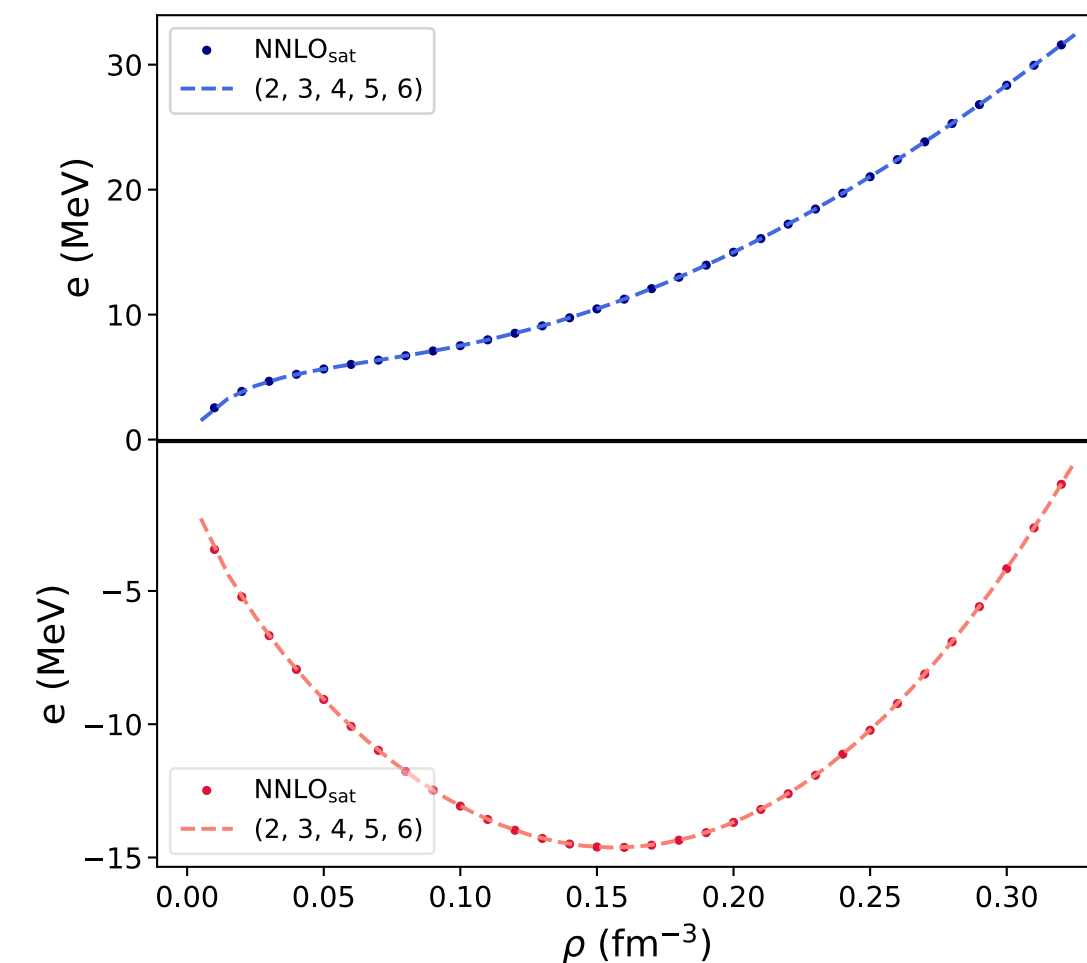
Machine-learn DFT functional  
on the nuclear equation of state

Jacob's ladder



+ approximate GA

Benchmark in finite systems



$$E = \int d\mathbf{r} \mathcal{E}(\mathbf{r}) = E_{\text{kin}} + E_{\text{pot}} + E_{\text{Coul}}$$

$$E_{\text{GA}} = E_{\text{LDA}} + E_{\text{surf}}$$

$$E_{\text{surf}} = \int d\mathbf{r} \left[ \sum_{t=0,1} C_t^\Delta \rho_t \Delta \rho_t - \frac{W_0}{2} \left( \rho \nabla \cdot \mathbf{J} + \sum_q \rho_q \nabla \cdot \mathbf{J}_q \right) \right]$$

# Benchmark on finite systems

Machine-learn DFT functional  
on the nuclear equation of state

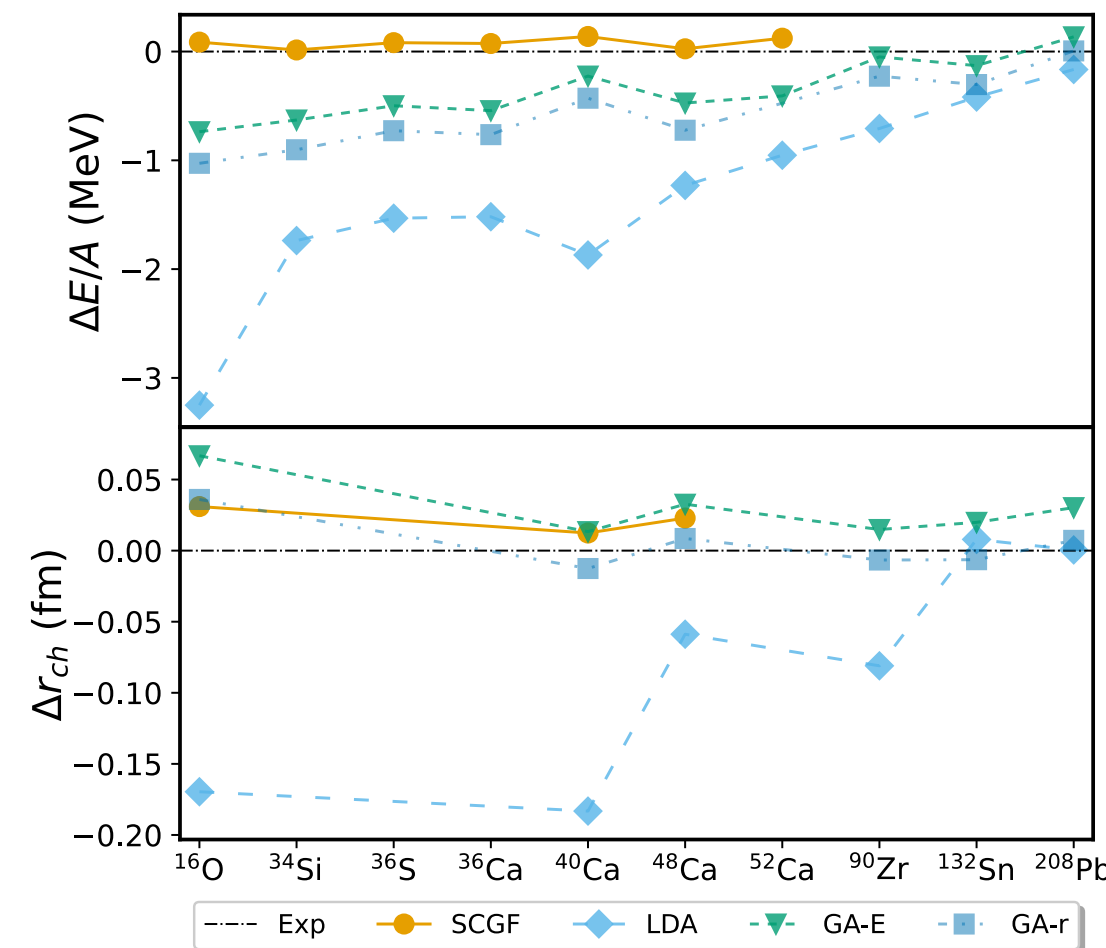
Jacob's ladder



+ approximate GA

Benchmark in finite systems

Gradient terms are important!



Problem: gradients here were added ad hoc to the EDF, so far.

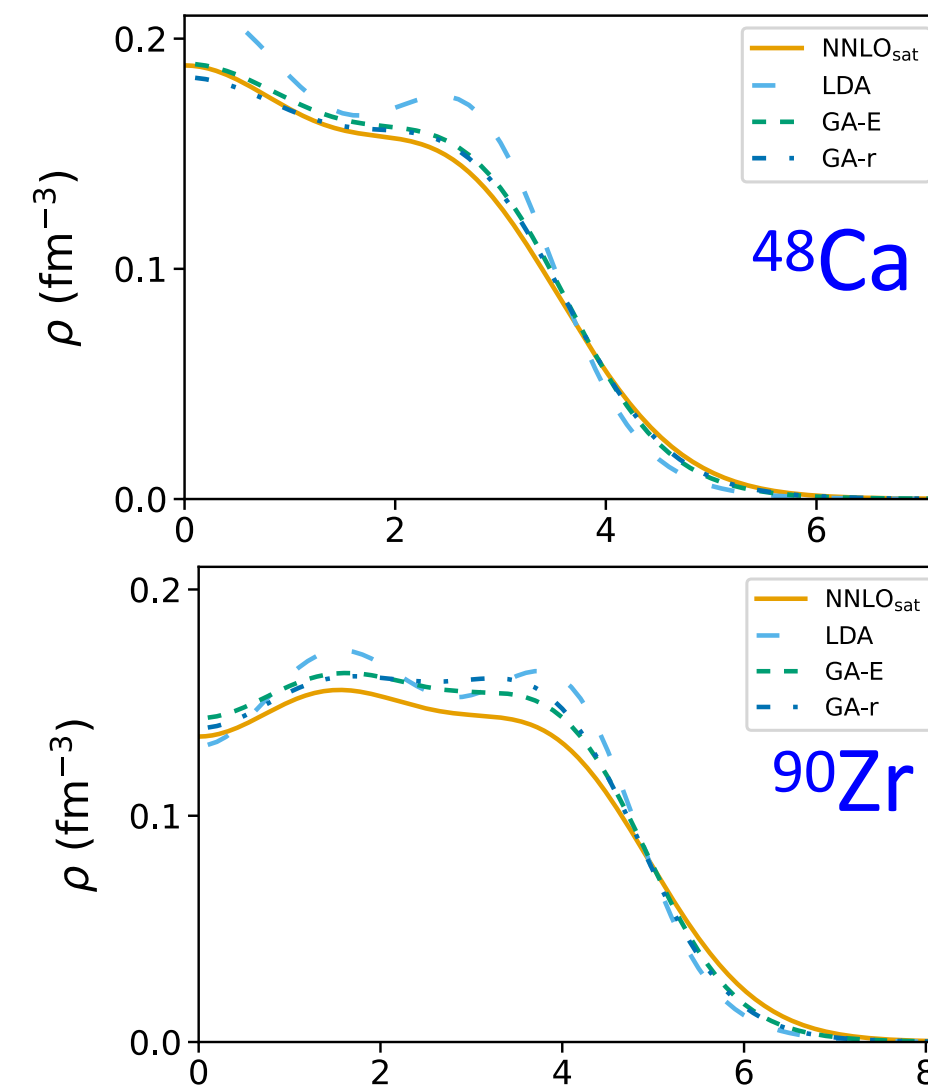
→

Need to extract gradient information from  
non-uniform matter. E.g., external  
(monochromatic) perturbations:

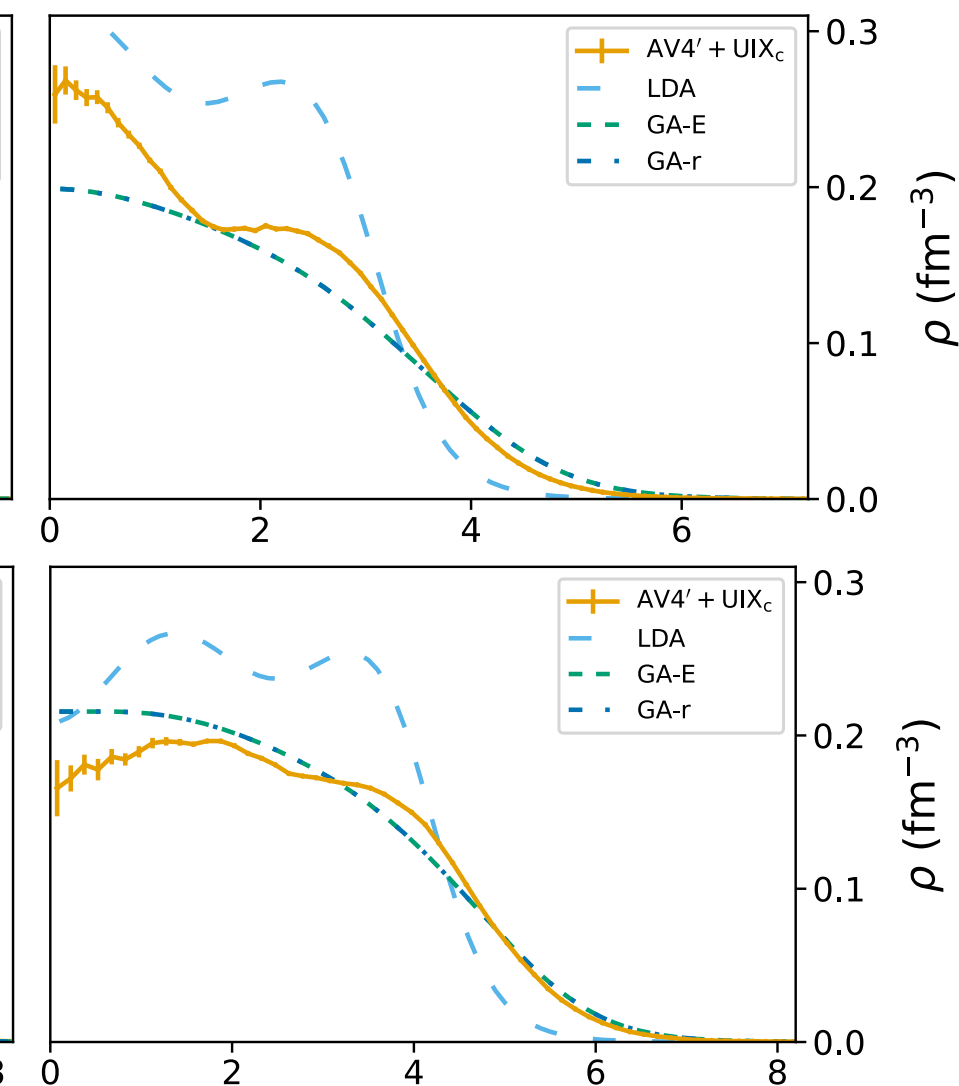
$$v(\mathbf{x}) = v_q e^{i\mathbf{q} \cdot \mathbf{x}} + c.c. = 2v_q \cos(\mathbf{q} \cdot \mathbf{x})$$

$$\delta\rho(\mathbf{x}) = 2\rho_q \cos(\mathbf{q} \cdot \mathbf{x})$$

SCGF/NNLO-sat :



AFDMC/AV4' :





# Gorkov ansatz... for atomic nuclei

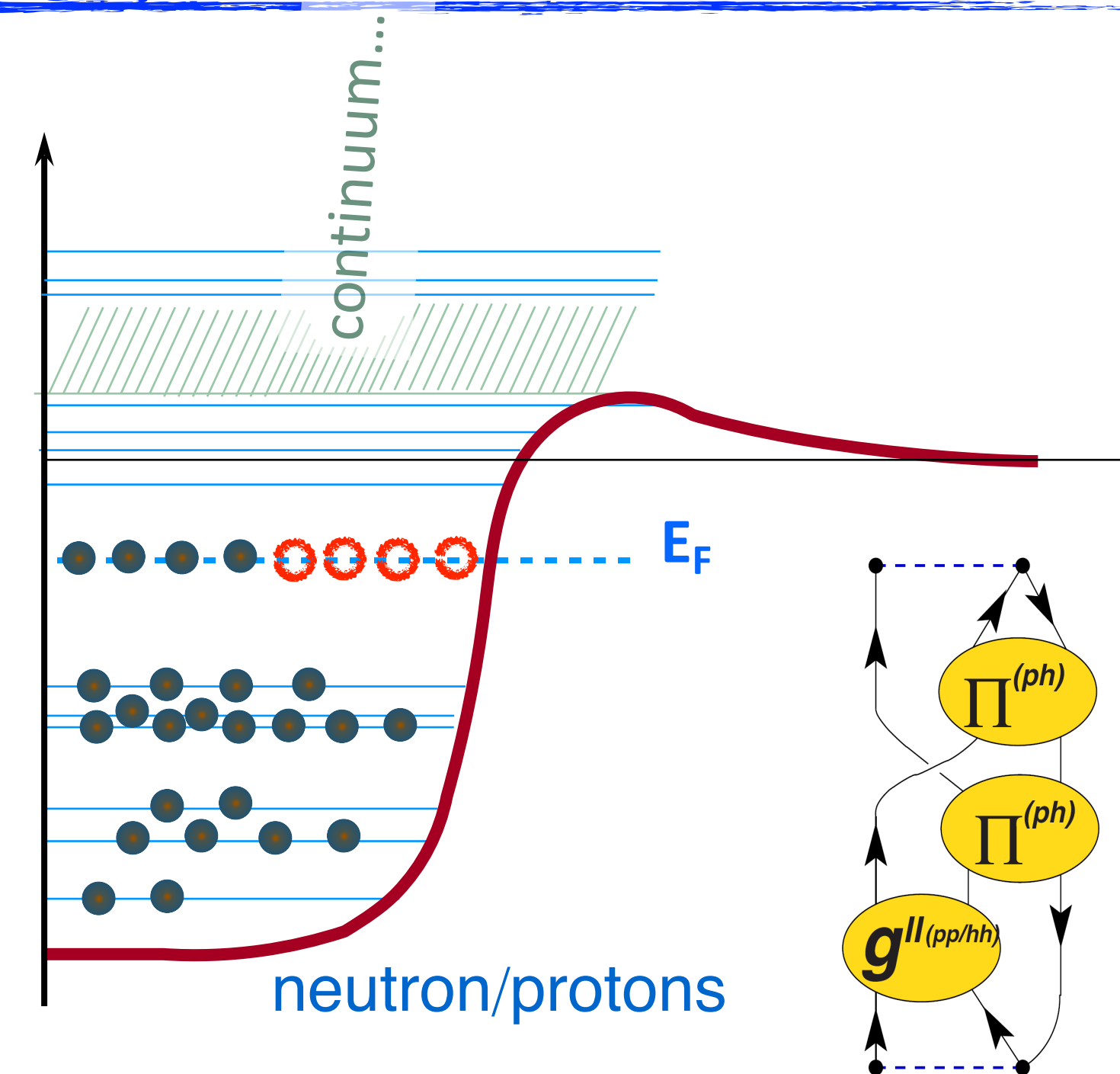
- In the presence of degeneracies (vanishing ph- gaps), enforce (two nucleon) pairing to mitigate instabilities:

- Ansatz many-body state:  $|\Psi_0\rangle = \sum_{n=0}^{\infty} c_{2n} |\psi^{2n}\rangle$

→ Introduce a “grand-canonical” potential  $\Omega \equiv H - \mu N$

→  $|\Psi_0\rangle$  minimizes  $\Omega_0 = \min_{|\Psi_0\rangle} \{\langle \Psi_0 | \Omega | \Psi_0 \rangle\}$  under the constraint  $N = \langle \Psi_0 | N | \Psi_0 \rangle$

- Generates a set of two normal and two anomalous self-energies:



$$\Sigma_{\alpha\beta}^*(\omega) = \Sigma_{\alpha\beta}^{\infty} + \tilde{\Sigma}_{\alpha\beta}(\omega) = \begin{pmatrix} \Sigma_{\alpha\beta}^{11,\infty} & \Sigma_{\alpha\beta}^{12,\infty} \\ \left(\Sigma_{\beta\alpha}^{12,\infty}\right)^* & -\Sigma_{\beta\alpha}^{11,\infty} \end{pmatrix} + \begin{pmatrix} \tilde{\Sigma}_{\alpha\beta}^{11}(\omega) & \tilde{\Sigma}_{\alpha\beta}^{12}(\omega) \\ -\left(\tilde{\Sigma}_{\beta\alpha}^{12}(-\omega)\right)^* & -\tilde{\Sigma}_{\beta\alpha}^{11}(-\omega) \end{pmatrix}$$

[Gorkov 1958]



# Gorkov ansatz... for atomic nuclei

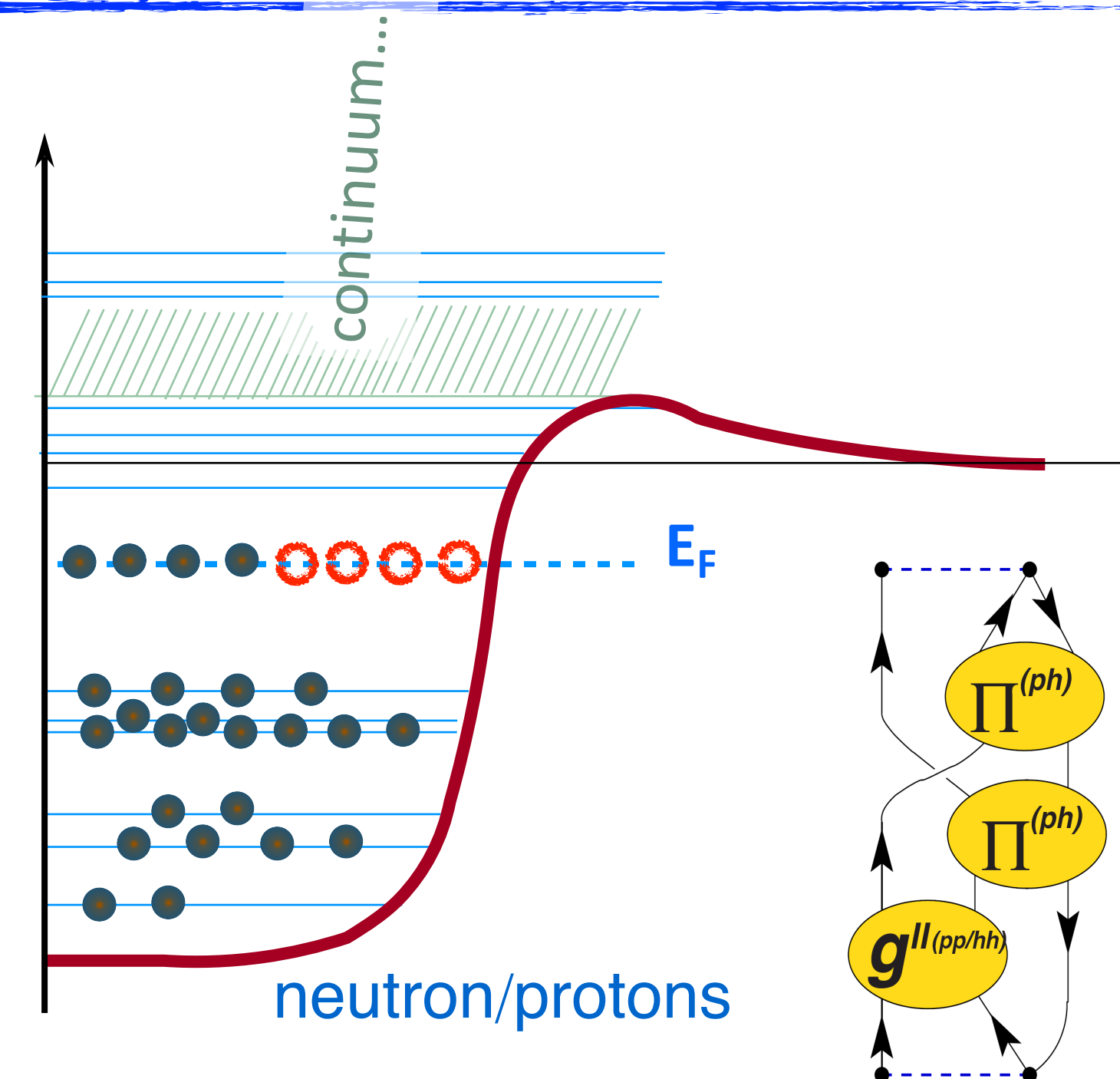
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[Gorkov 1958]

In the limit of particle number restoration:

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

V. Somà, CB, T. Duguet, Phys. Rev. C **89**, 024323 (2022)

CB, T. Duguet, V. Somà, Phys. Rev. C **105**, 044330 (2022)





# Algebraic diagrammatic construction [ADC(3)] for infinite matter

Finite size box (of length  $L$ ) with periodic Boundary conditions:

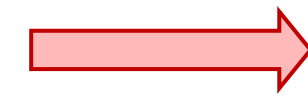
$$\rho = \frac{A}{L} \quad p_F = \sqrt[3]{\frac{6\pi^2\rho}{v_d}} \quad \mathbf{k} = \frac{1}{L} \left( 2\pi\mathbf{n} + \boldsymbol{\theta} \right), \quad |\mathbf{k}|^2 = k_x^2 + k_y^2 + k_z^2 \leq \frac{4\pi^2}{L^2} N_{max}$$

## Gorkov superfluid formulation

$$\mathbf{g}(\omega) = \mathbf{g}^{(0)}(\omega) + \mathbf{g}^{(0)}(\omega) \mathbf{\Sigma}^*(\omega) \mathbf{g}(\omega)$$

Normal self-energy      Pairing field

$$\mathbf{\Sigma}^*(\omega) = \begin{pmatrix} \Sigma^{11}(\omega) & \Delta \\ -\Delta^* & \Sigma^{22}(\omega) \end{pmatrix}$$



$$\left( \begin{array}{ccc|c} T+\Lambda-1\mu_q & M^\dagger & N & \Delta \\ M & E^>+C-1\mu_q & & \\ N^\dagger & & E^<+D-1\mu_q & \\ \hline \Delta^\dagger & -(T+\Lambda)^*+1\mu_q & -M^T & -N^* \\ & -M^* & -(E^>+C)^*+1\mu_q & \\ & -N^T & & -(E^<+D)^*+1\mu_q \end{array} \right) \begin{pmatrix} \mathcal{U}^q \\ \mathcal{W}^q \\ \mathcal{Z}^q \\ \mathcal{V}^q \\ \mathcal{R}^q \\ \mathcal{S}^q \end{pmatrix} = \hbar\omega_q \begin{pmatrix} \mathcal{U}^q \\ \mathcal{W}^q \\ \mathcal{Z}^q \\ \mathcal{V}^q \\ \mathcal{R}^q \\ \mathcal{S}^q \end{pmatrix}$$

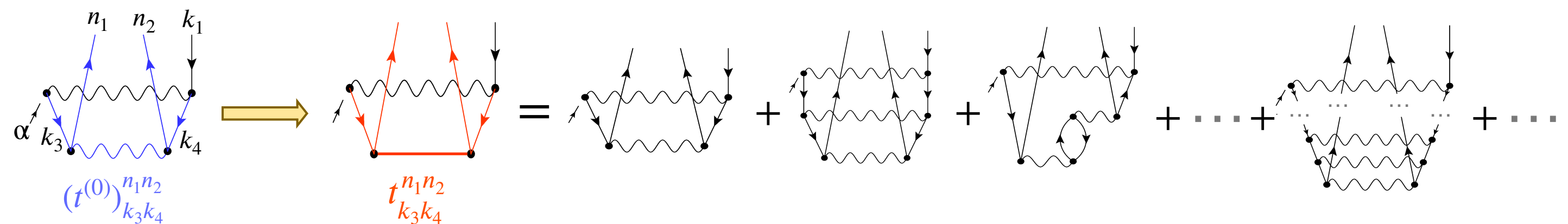
Normal self-energy in full ADC(3) but use pairing only at 1st order

Extension of ADC(3)



ADC(3)-D

In  $\tilde{\Sigma}(\omega)$ , replace  $t^{(0)}$  with converged  $T_2$  amplitudes

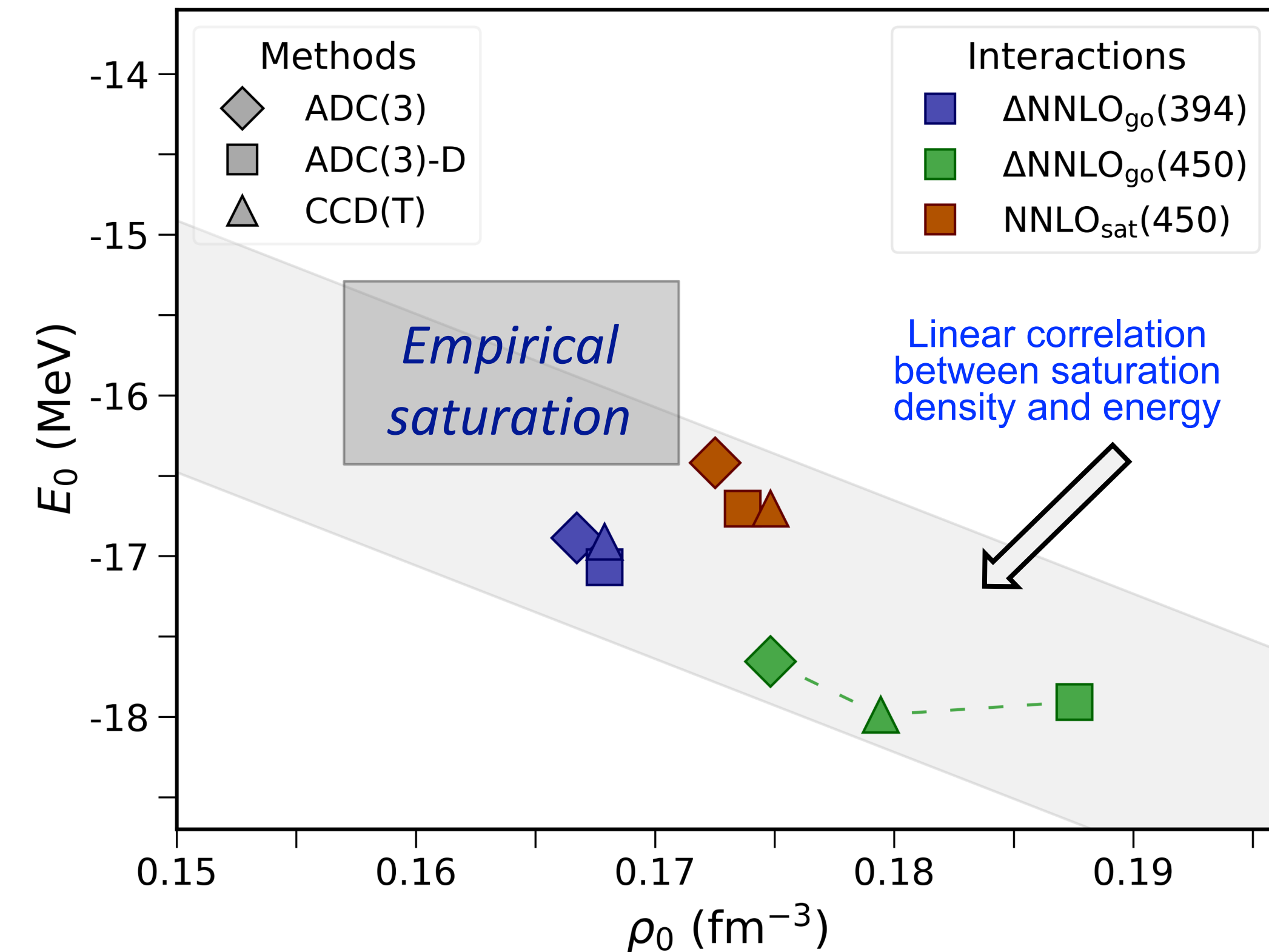


$$(t^{(0)})_{ij}^{ab} = \frac{\langle ab|v|ij\rangle_A}{\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b}$$



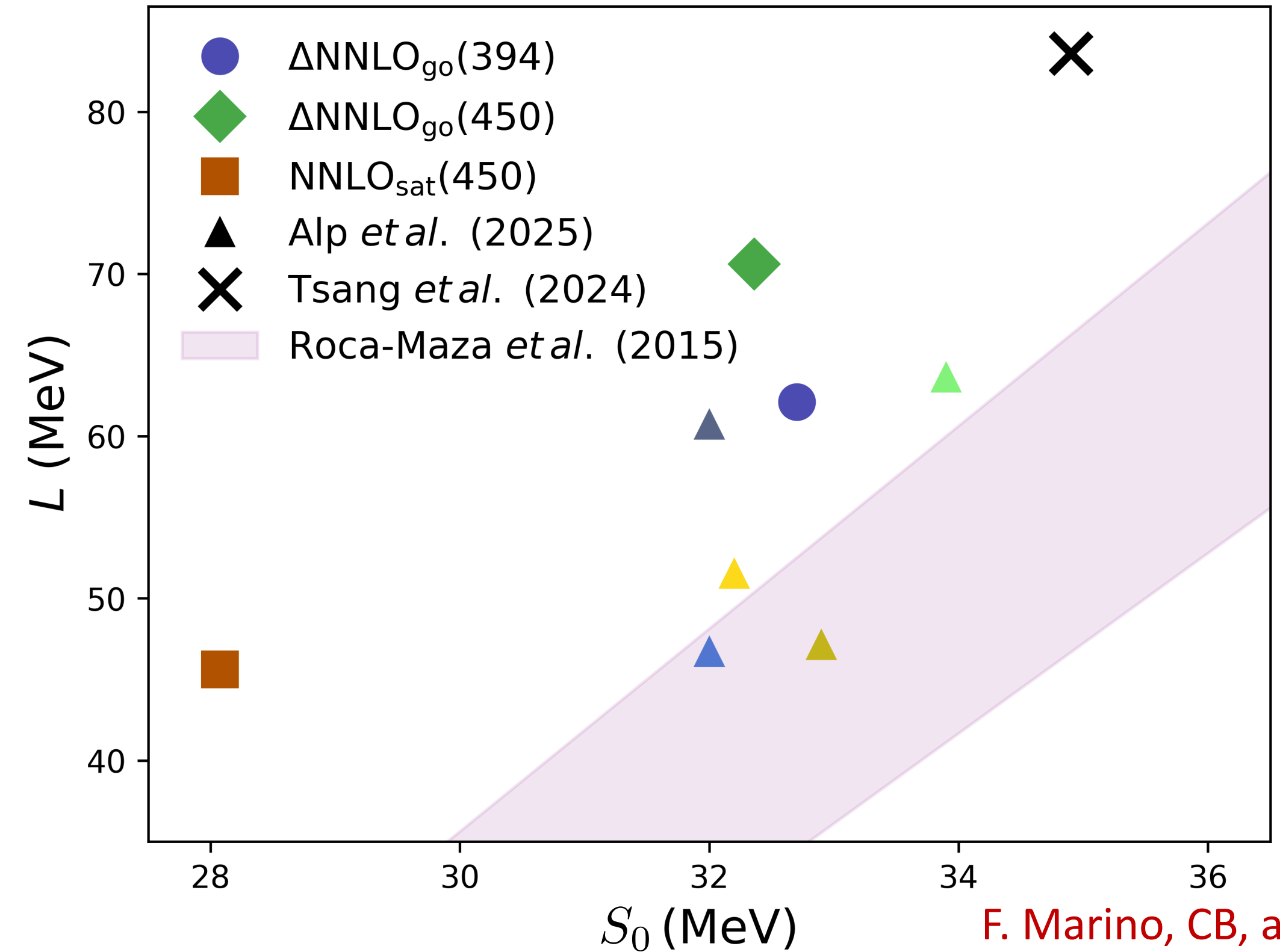
# Bulk properties of nucleonic matter

## Saturation



- ◆ Generally good agreement across many-body methods
- ◆ Interaction-dependence is the dominant uncertainty

## Symmetry energy



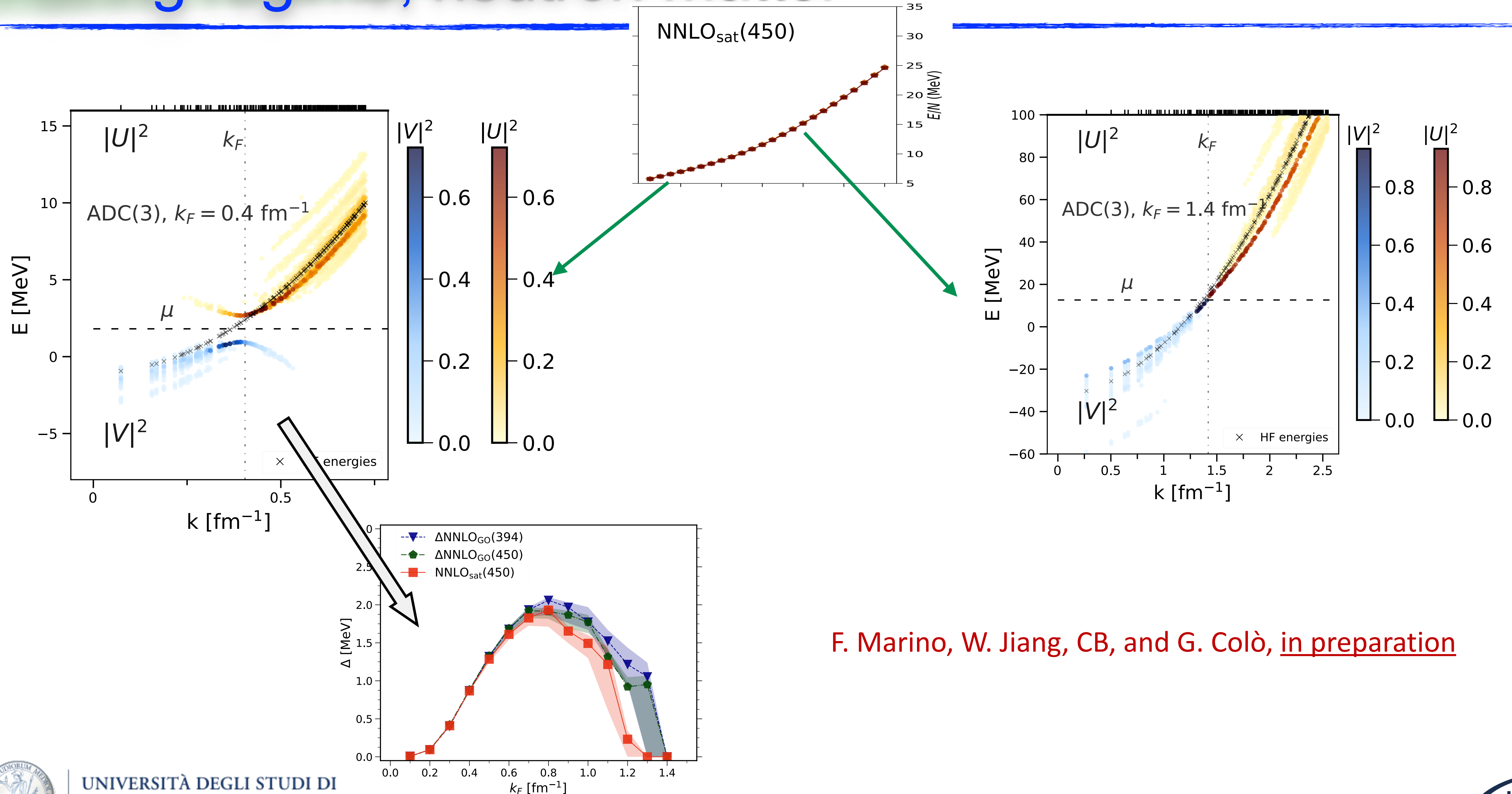
F. Marino, CB, and G. Colò,  
Phys. Rev. C **113**,  
064301 (2026).

$$S(\rho) = S(\rho_0) + \frac{L}{3\rho_0}(\rho - \rho_0) + \dots$$

Alp *et al.*, arXiv:2504.18259  
Burgio *et al.*, Front. Astron. Space Sci. **11**, 1505560 (2024)  
Lynch and Tsang, Phys. Lett. B **830**, 137098 (2022)  
Roca-Maza *et al.*, Phys. Rev. C **92**, 064304 (2015)



# Pairing regime, neutron matter



F. Marino, W. Jiang, CB, and G. Colò, in preparation

# Neural Network Quantum States





# Neural Network Quantum States (NQS):

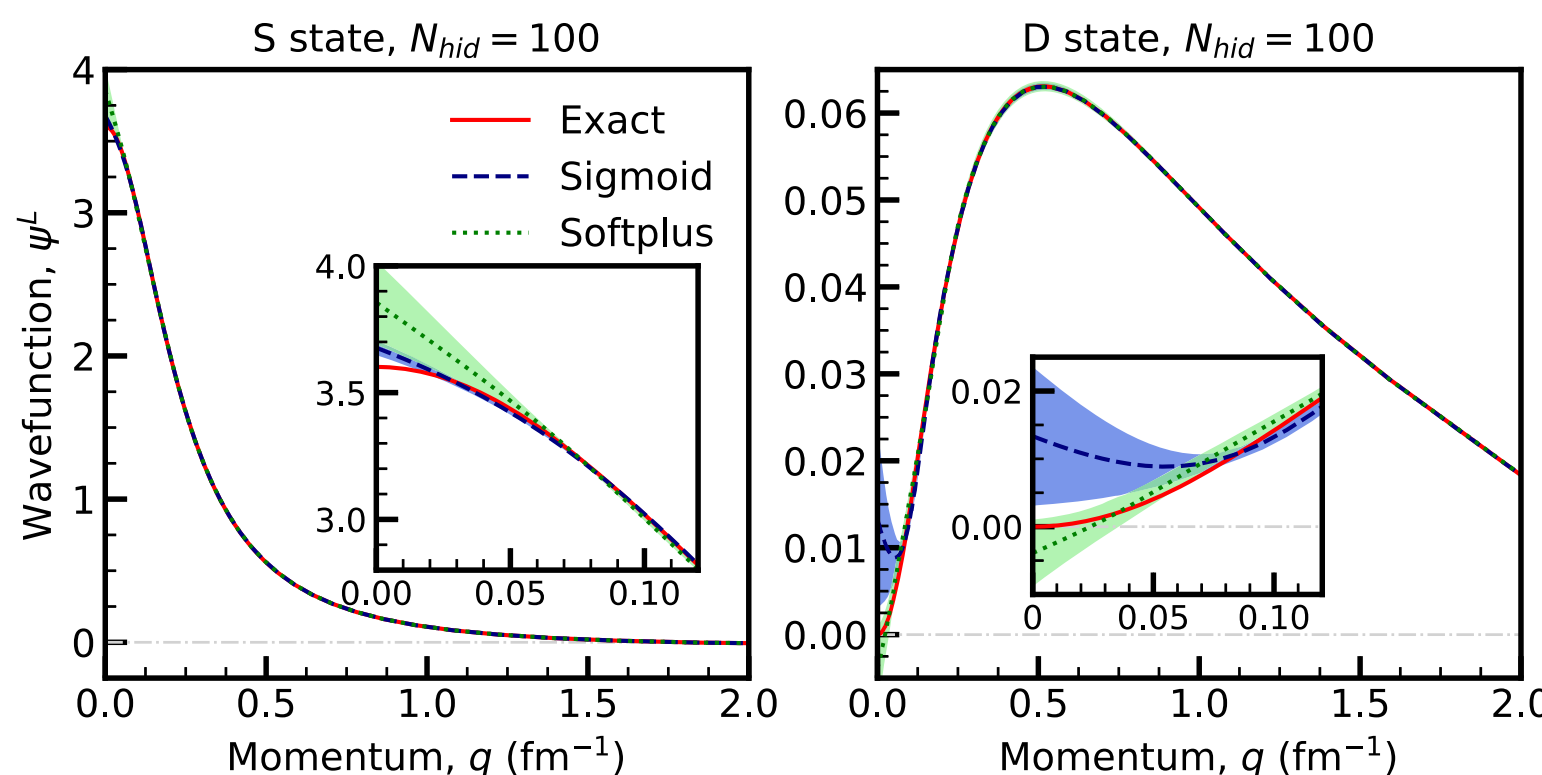
$$\frac{\langle \Psi_V | H | \Psi_V \rangle}{\langle \Psi_V | \Psi_V \rangle} = E_V \geq E_0$$

$$|\Psi_V^J\rangle = \prod_{i<j<k} \left( 1 - \sum_{\text{cyc}} u(r_{ij}) u(r_{jk}) \right) \prod_{i<j} f(r_{ij}) |\Phi\rangle$$

In short: a VMC with a NN trial wave function!

*neural networks*

The  
deuteron:



Light nuclei:

|                 | $\Lambda$           | VMC-ANN     | VMC-JS      | GFMC        | GFMC <sub>c</sub> |
|-----------------|---------------------|-------------|-------------|-------------|-------------------|
| ${}^2\text{H}$  | $4 \text{ fm}^{-1}$ | $-2.224(1)$ | $-2.223(1)$ | $-2.224(1)$ | -                 |
|                 | $6 \text{ fm}^{-1}$ | $-2.224(4)$ | $-2.220(1)$ | $-2.225(1)$ | -                 |
| ${}^3\text{H}$  | $4 \text{ fm}^{-1}$ | $-8.26(1)$  | $-7.80(1)$  | $-8.38(2)$  | $-7.82(1)$        |
|                 | $6 \text{ fm}^{-1}$ | $-8.27(1)$  | $-7.74(1)$  | $-8.38(2)$  | $-7.81(1)$        |
| ${}^4\text{He}$ | $4 \text{ fm}^{-1}$ | $-23.30(2)$ | $-22.54(1)$ | $-23.62(3)$ | $-22.77(2)$       |
|                 | $6 \text{ fm}^{-1}$ | $-24.47(3)$ | $-23.44(2)$ | $-25.06(3)$ | $-24.10(2)$       |

Keeble, Rios, Phys. Lett. B **809**, 135743 (2020)

Rozalén Sarmiento, Keeble, EPJ Plus **139**, 189 (2024)

C. Adams, G. Carleo, A. Lovato, N. Rocco,  
Phys. Rev. Lett. **127**, 022502 (2021)



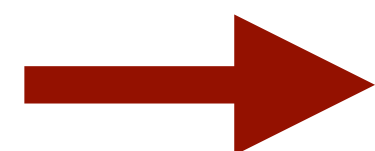
# Neural Network Quantum States (NQS):

$$\frac{\langle \Psi_V | H | \Psi_V \rangle}{\langle \Psi_V | \Psi_V \rangle} = E_V \geq E_0 \quad |\Psi_V^J\rangle = \prod_{i < j < k} \left( 1 - \sum_{\text{cyc}} u(r_{ij}) u(r_{jk}) \right) \prod_{i < j} f(r_{ij}) |\Phi\rangle$$

In short: a VMC with a NN trial wave function!

*neural networks*

- **NQS often surpass traditional VMC**, with accuracy similar to GFMC/DMC but at a fraction of the cost
- Sometimes referred as “**science driven learning**”: it is not supervised and the cost function is the variational principle.
- However: the **variational principle is the only guiding principle** exploited, what about the rest??



Use Physics Informed Neural Networks (PINN) !



# Physics Informed Neural Networks

- ◆ Generally used for solving ODE and PDE: NN represent the solution  $f(\mathbf{x})$ ,  $\partial f(\mathbf{x})/\partial x_i, \dots$
- ◆ General PINN cost function:

$$\mathcal{L}_{PINN} = \mathcal{L}_{PDE} + \mathcal{L}_{phys} + \mathcal{L}_{data}$$

constraint from  
diff. equations

Physics constraints  
(e.g. boundary conditions)

Any known (measured) data

# Physics Informed Neural Networks for nuclei

- ♦ The Schrödinger problem is an integro-differential eq.: use NN to represent  $\Psi(\mathbf{x}_1, \mathbf{x}_2, \dots)$
- ♦ Many-body PINN cost function:

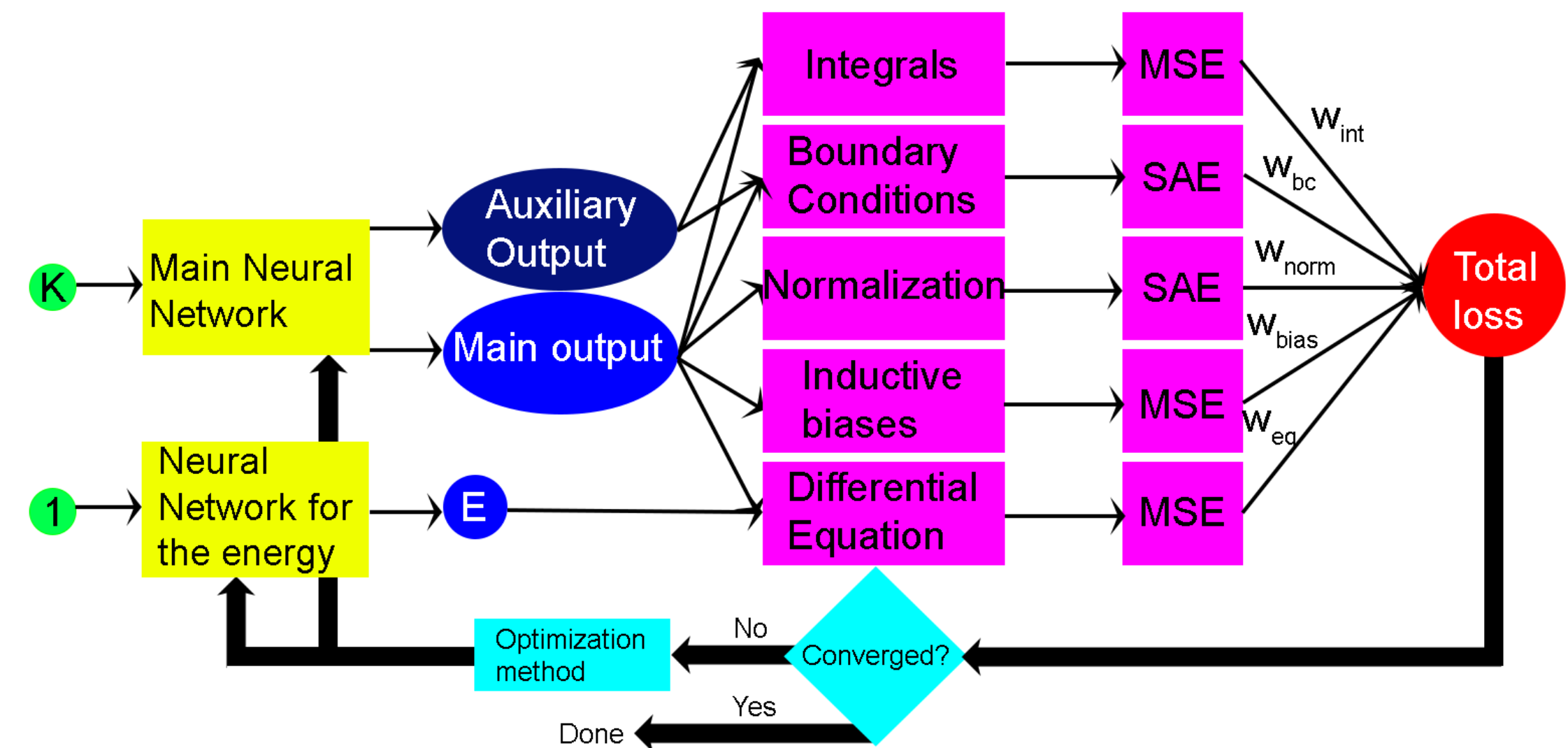
$$\mathcal{L}_{PINN} = \mathcal{L}_{PDE} + \mathcal{L}_{phys} + \cancel{\mathcal{L}_{data}}$$

Schrod. eq.

$$\mathcal{L}_{PDE} = \sum_{i=0}^{N_c} |[H\psi](x_i) - E\psi(x_i)|^2 \quad \text{with} \quad E = \frac{\langle \psi | H | \psi \rangle}{\mathcal{I}[\psi]}$$

Physics constraints

$$\mathcal{L}_{phys} = w_{int} \mathcal{L}_{int} + w_{BCs} \mathcal{L}_{BCs} + w_{norm} \mathcal{L}_{norm} + w_{var} \mathcal{L}_{var} + \dots$$



- ♦ Through boundary conditions, one may target excited (and scattering) states.

L. Brevi, A. Mandarino, E. Prati,  
Technologies 12, 174 (2024); New J. Phys. **26**, 103015 (2024).

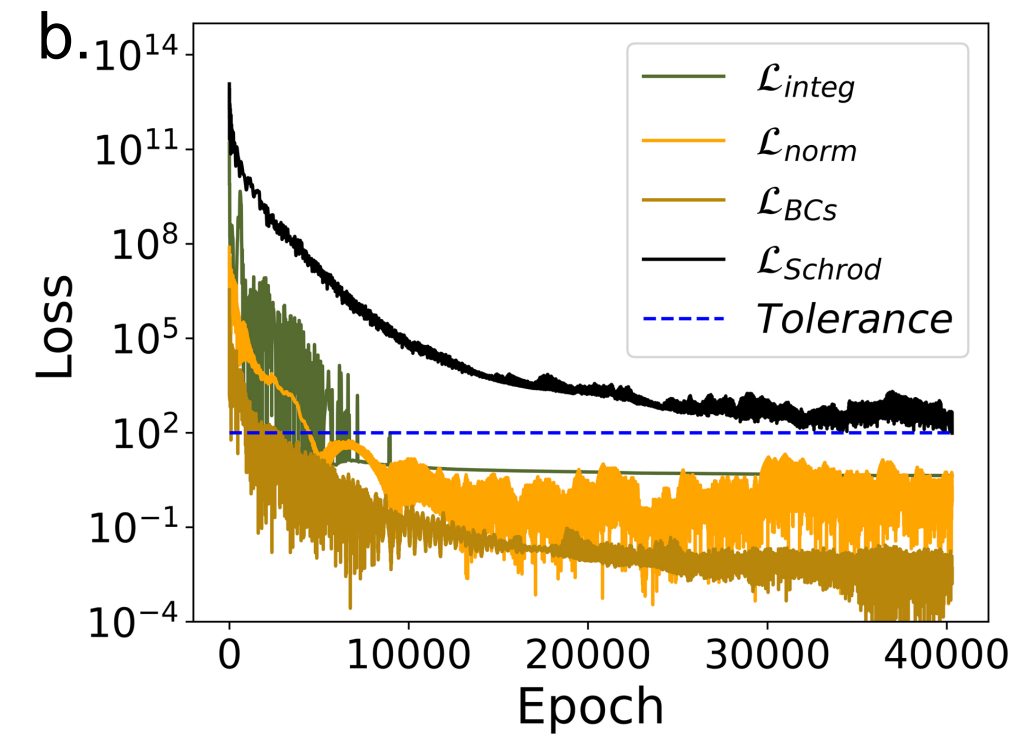
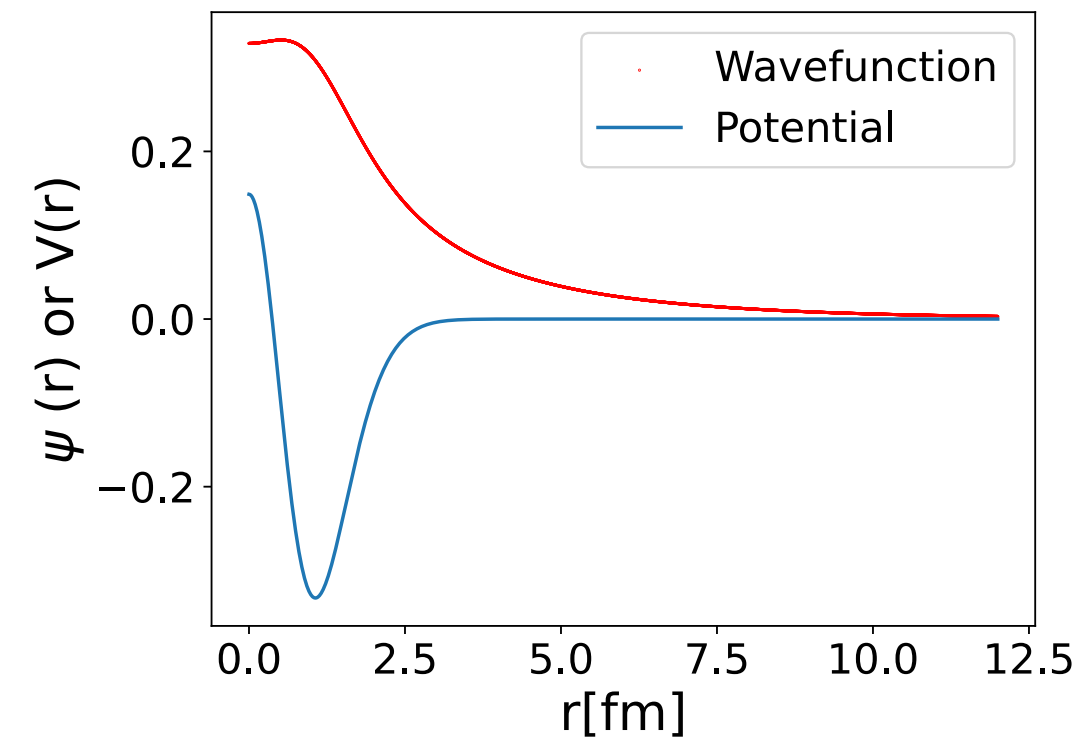
L. Brevi, A. Mandarino, CB, E. Prati, arXiv:2602.11193



# Physics Informed Neural Networks for the deuteron

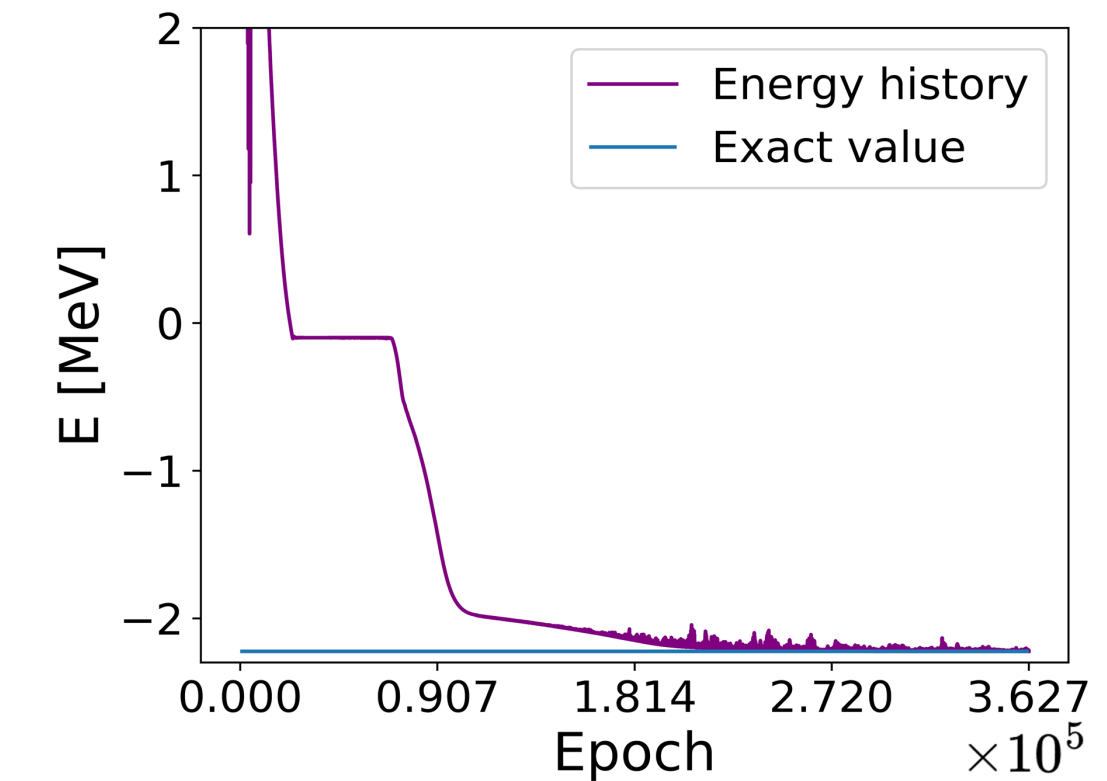
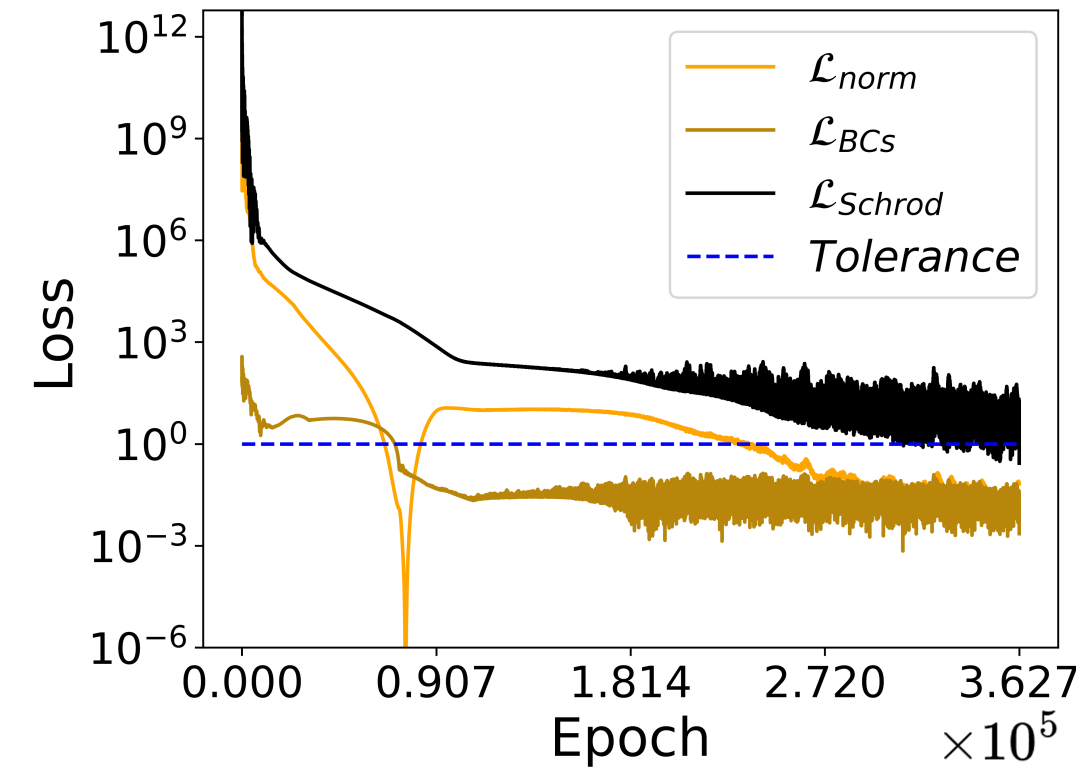
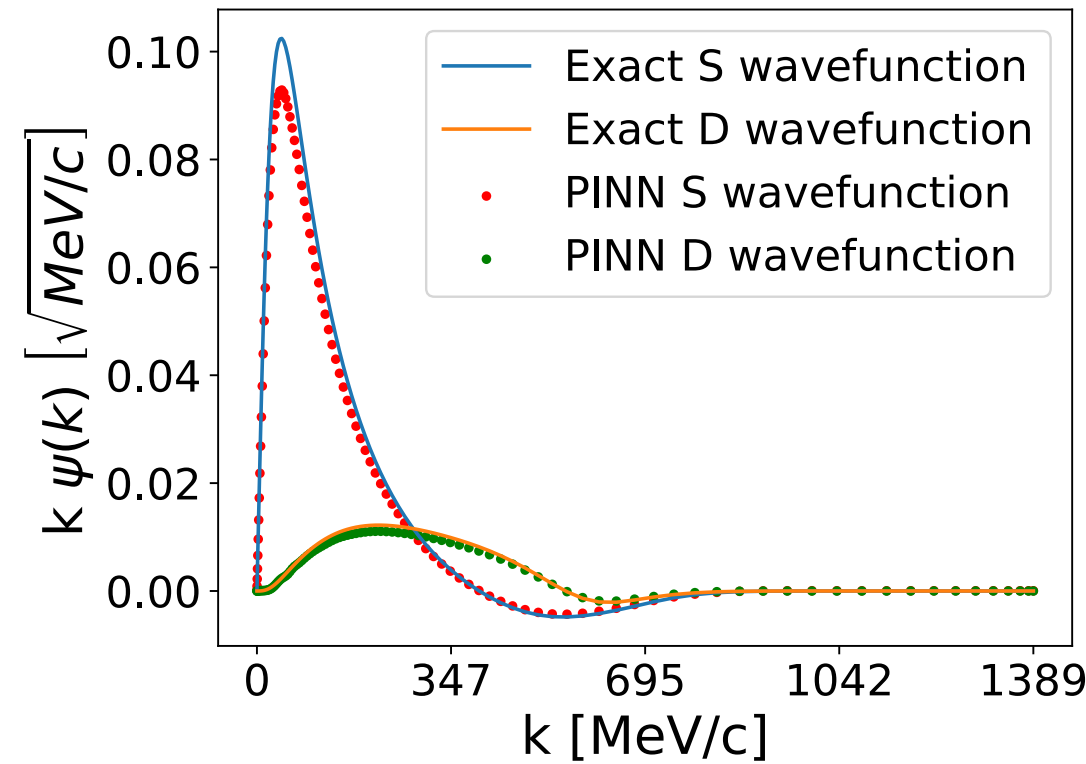
L. Brevi, A. Mandarino, CB, E. Prati, arXiv:2602.11193

## ◆ Coordinate space, Minnesota potential:



|           | $Err_{E,exp}$          | $Err_{E,Num}$          | $1 - \mathcal{F}_\psi$ |
|-----------|------------------------|------------------------|------------------------|
| Minnesota | 0.01                   | $1 \times 10^{-8}$     |                        |
| N4LO(550) | $-5.96 \times 10^{-6}$ | $-5.21 \times 10^{-5}$ | $1 \times 10^{-5}$     |
| CD-Bonn   | $-6.01 \times 10^{-4}$ | $-2.76 \times 10^{-7}$ | $1 \times 10^{-9}$     |

## ◆ Momentum space with N4LO(550) from EMN:



$$\mathcal{L}_{phys} = w_{ODE} \mathcal{L}_{ODE} + (w_{int} \mathcal{L}_{int} + w_{norm} \mathcal{L}_{norm}) + w_{BCs} \mathcal{L}_{BCs} + w_{var} \mathcal{L}_{var}$$

# Conclusions

- ◆ Applications of SCGF approaches to finite nuclei — shell evolution, **new Z=18 shell closure** for  $^{46}\text{Ar}$
- ◆ Applications of SCGF to scattering — **optical potentials** from first principles
- ◆ Novel developments: breakthrough in DiagrammaticMC for nuclei (*Time Ordered DiagMC* algorithm)
- ◆ EoS and response for infinite matter, also important to advance nuclear DFT functionals.
- ◆ The ADC Green's functions method combined with gorkov is a powerful ab initio tool to study the EOS and single-particle properties of nuclear matter.
- ◆ Novel developments: Physics Informed Neural Network (PINN) as an alternative to NQS (network quant. States)

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

