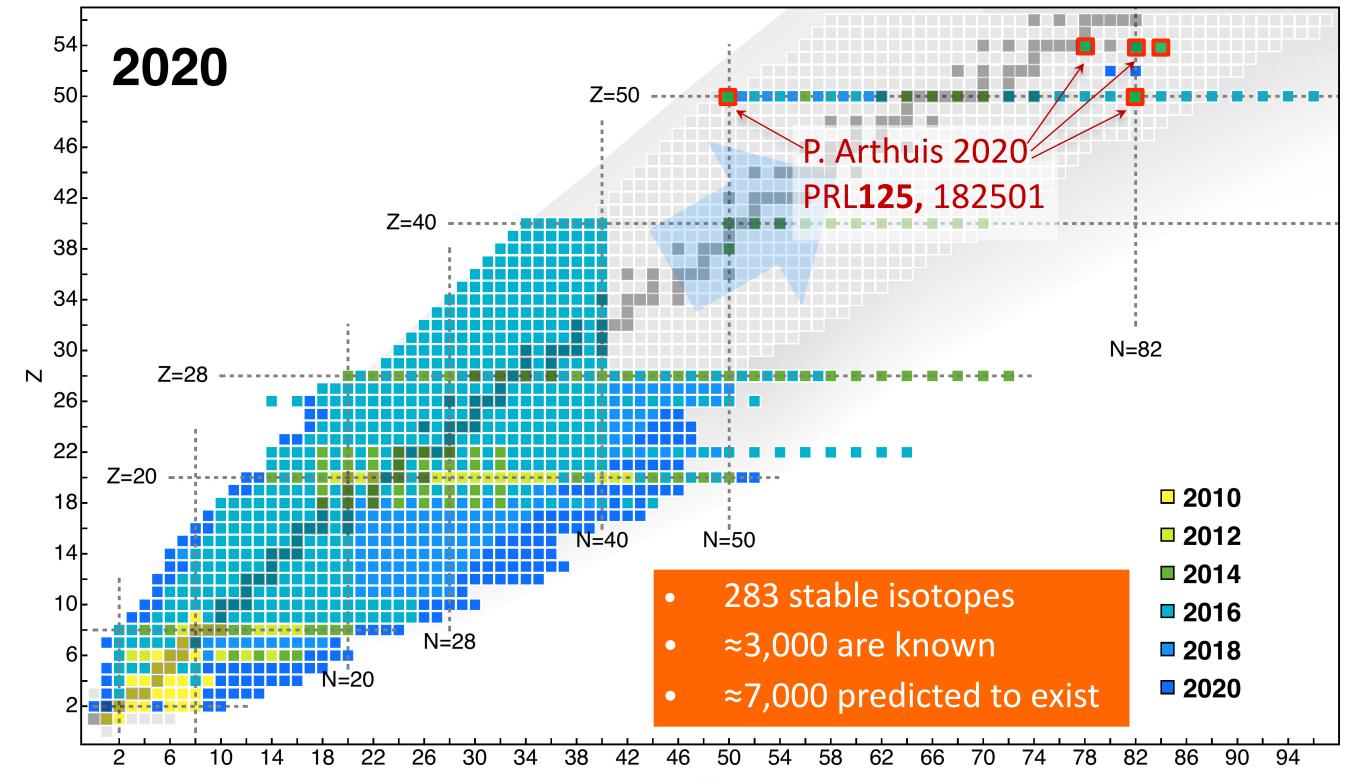
Ab Initio Structure and Reactions (in Milan)



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) 200 Early years Polynomial scaling Methods 3 number reached 150 2015 100 Mass 50h Wave Function-Based Methods 2000 1990 2010 2020

Open challenges:

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

Year



L. Coraggio, S. Pastore, CB, Frontiers in Phys 8, 626976 (2021)

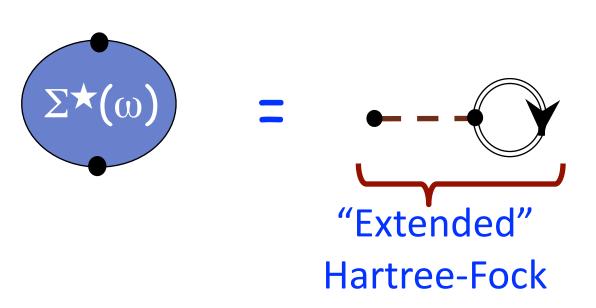


The Faddev-RPA and ADC(3) methods in a few words

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

F-RPA:

Both ladders and rings are needed for atomi nuclei:



R(2p1h)

R(2h1p)

Phys. Rev. C63, 034313 (2001) Phys. Rev. A76, 052503 (2007) Phys. Rev. A83, 042517 (2011)

ADC(3):

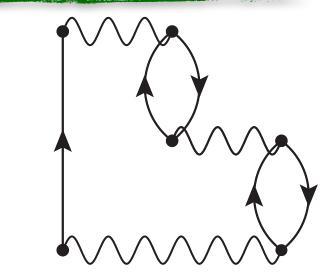
Lect. Notes in Phys 936 (2017)-Chapter 11.

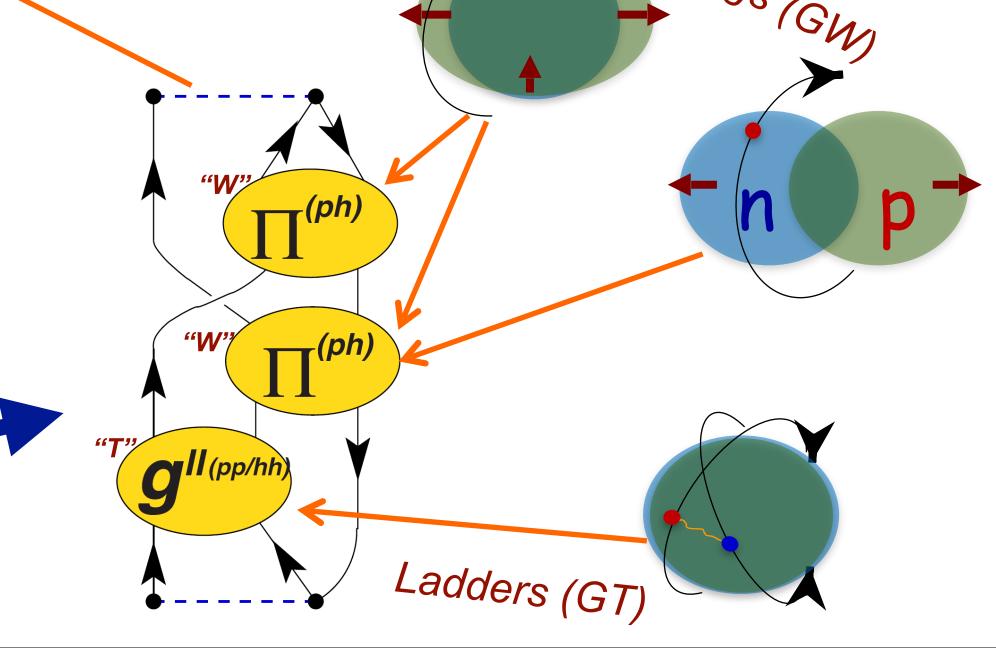
INFN

All Ladders (GT) and ring modes (GW) are coupled to all orders. Two approaches:

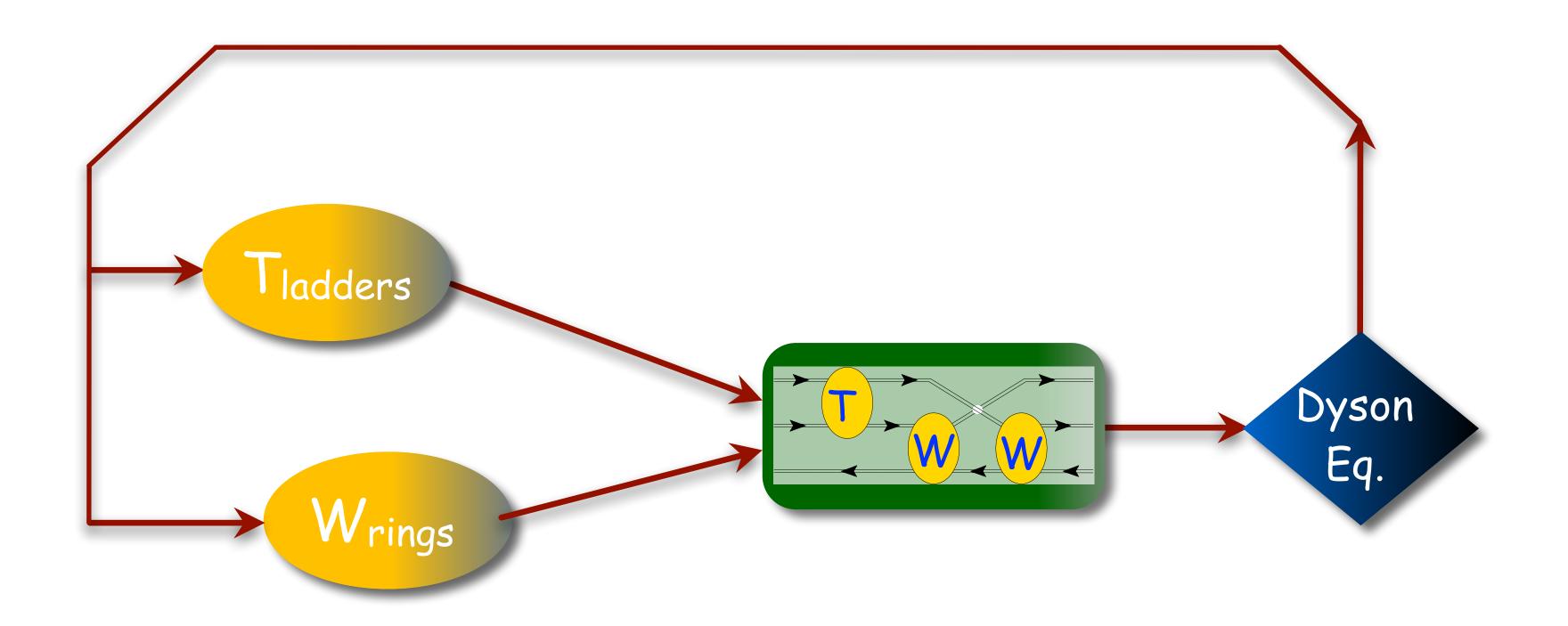
- Faddev-RPA allows for RPA modes
- ADC(3) Tamn-Dancoff version using 3rd order

diagrams as 'seeds':



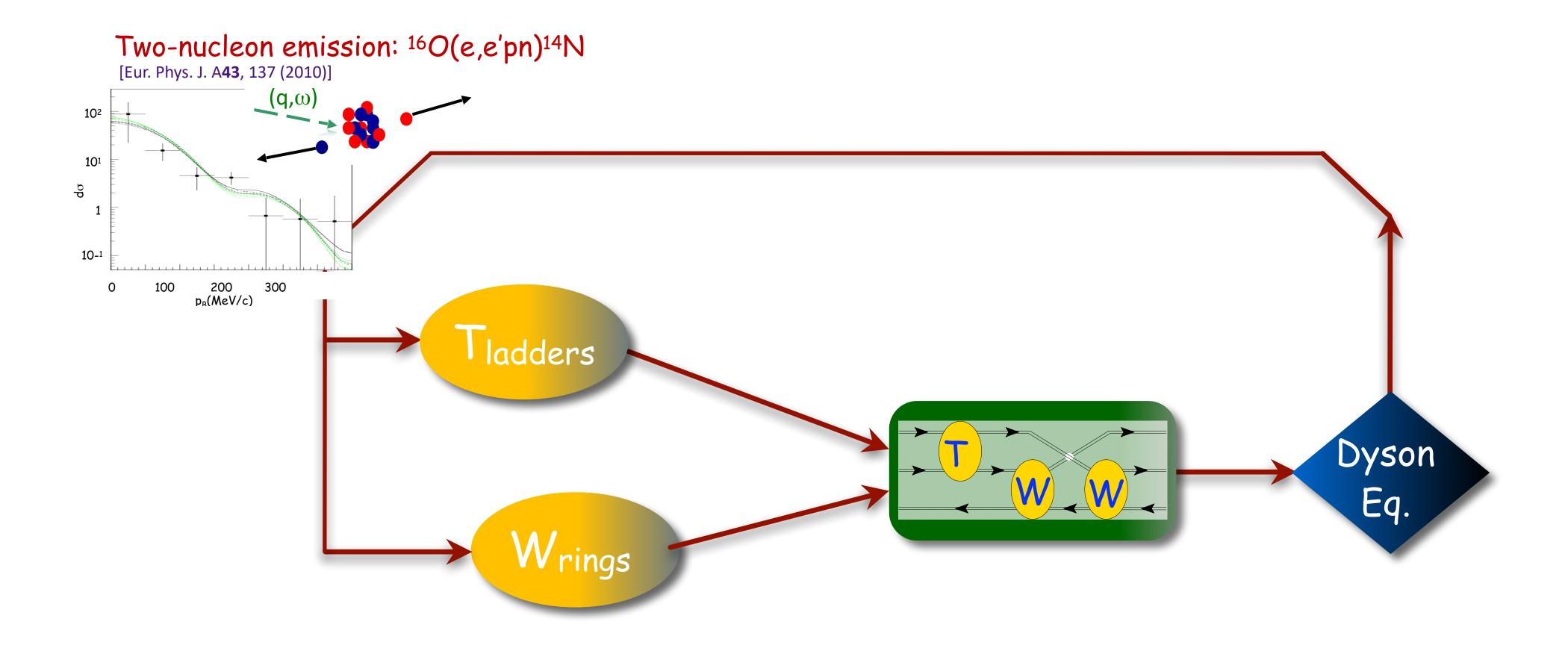






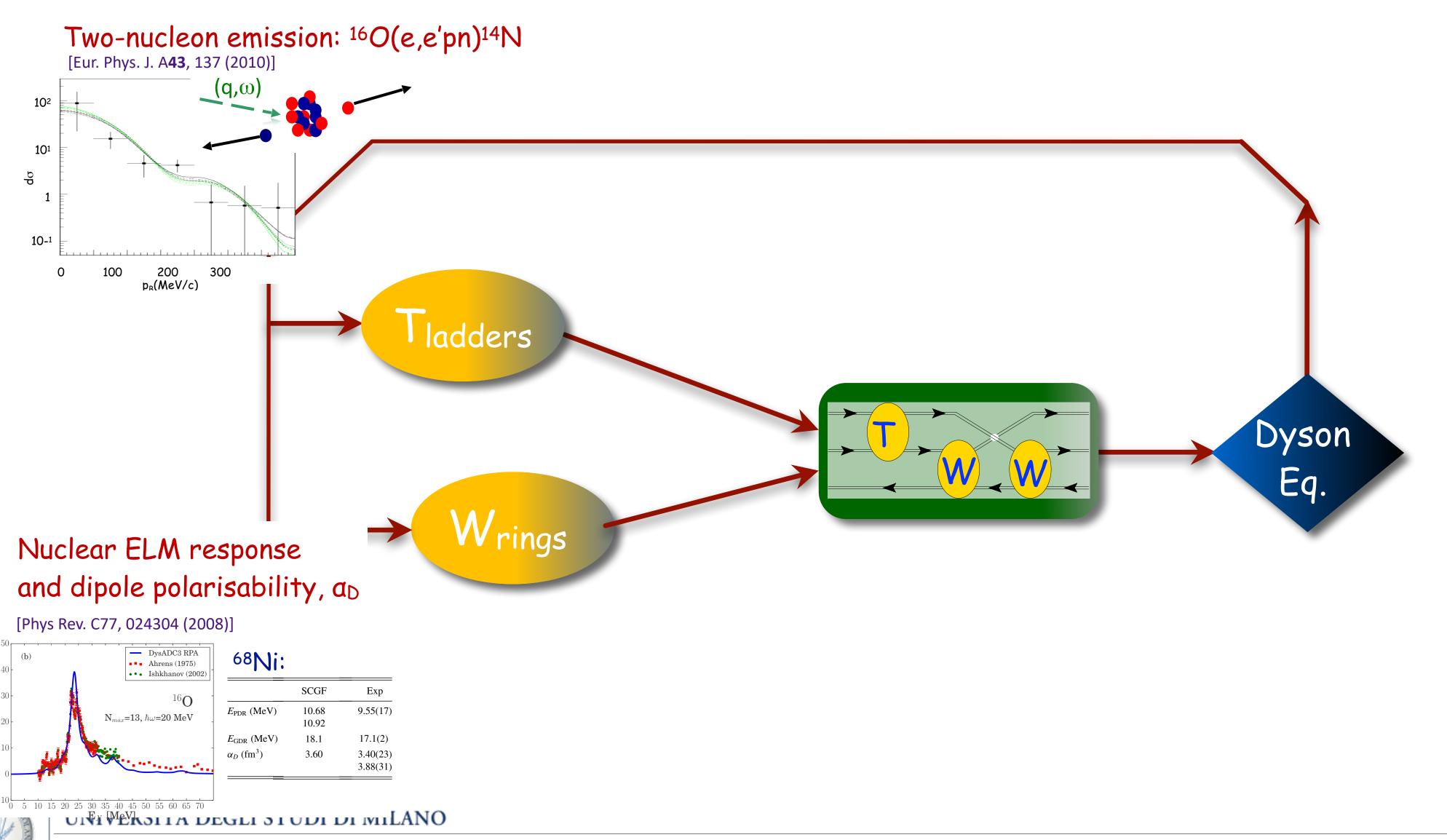




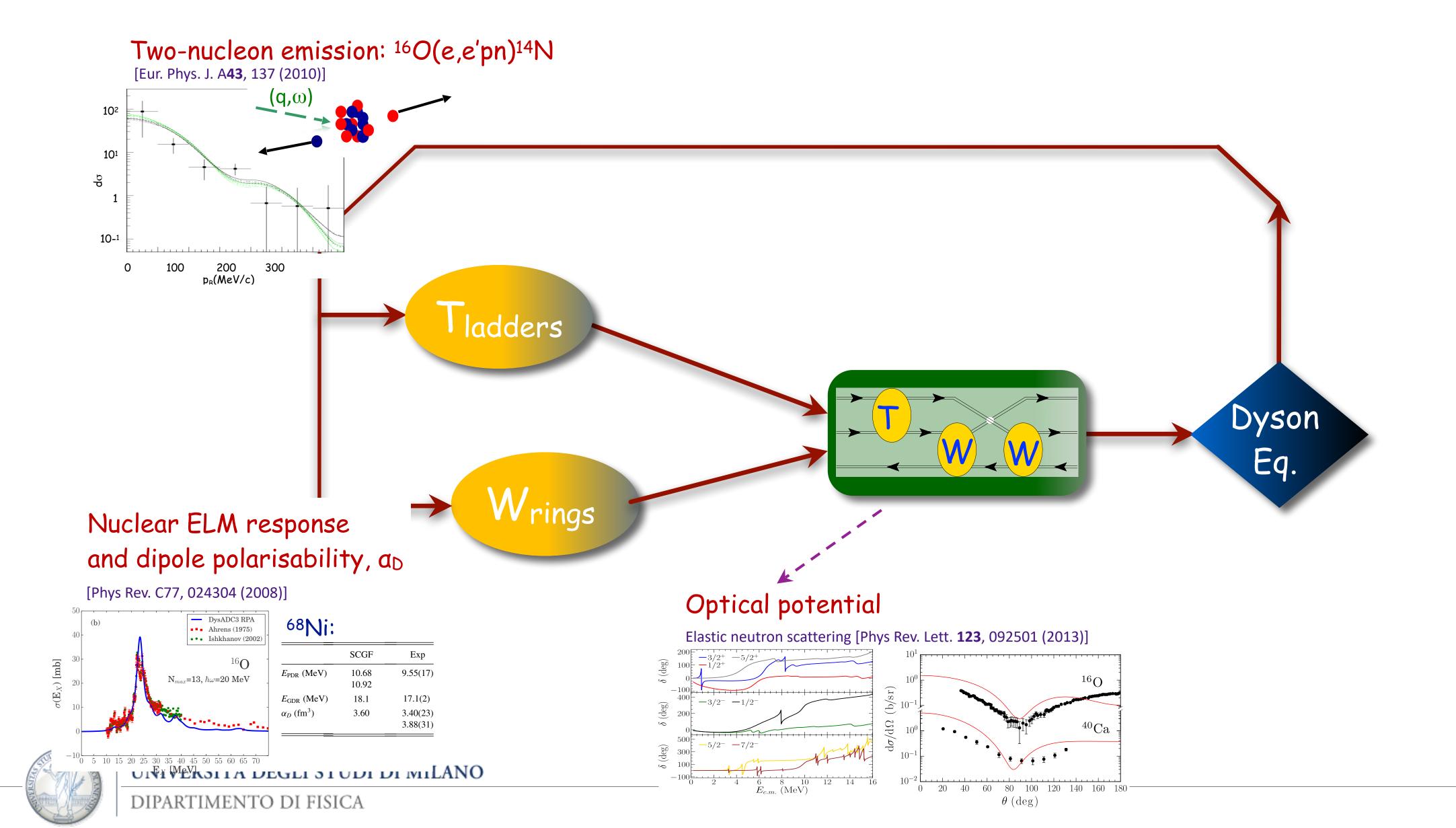




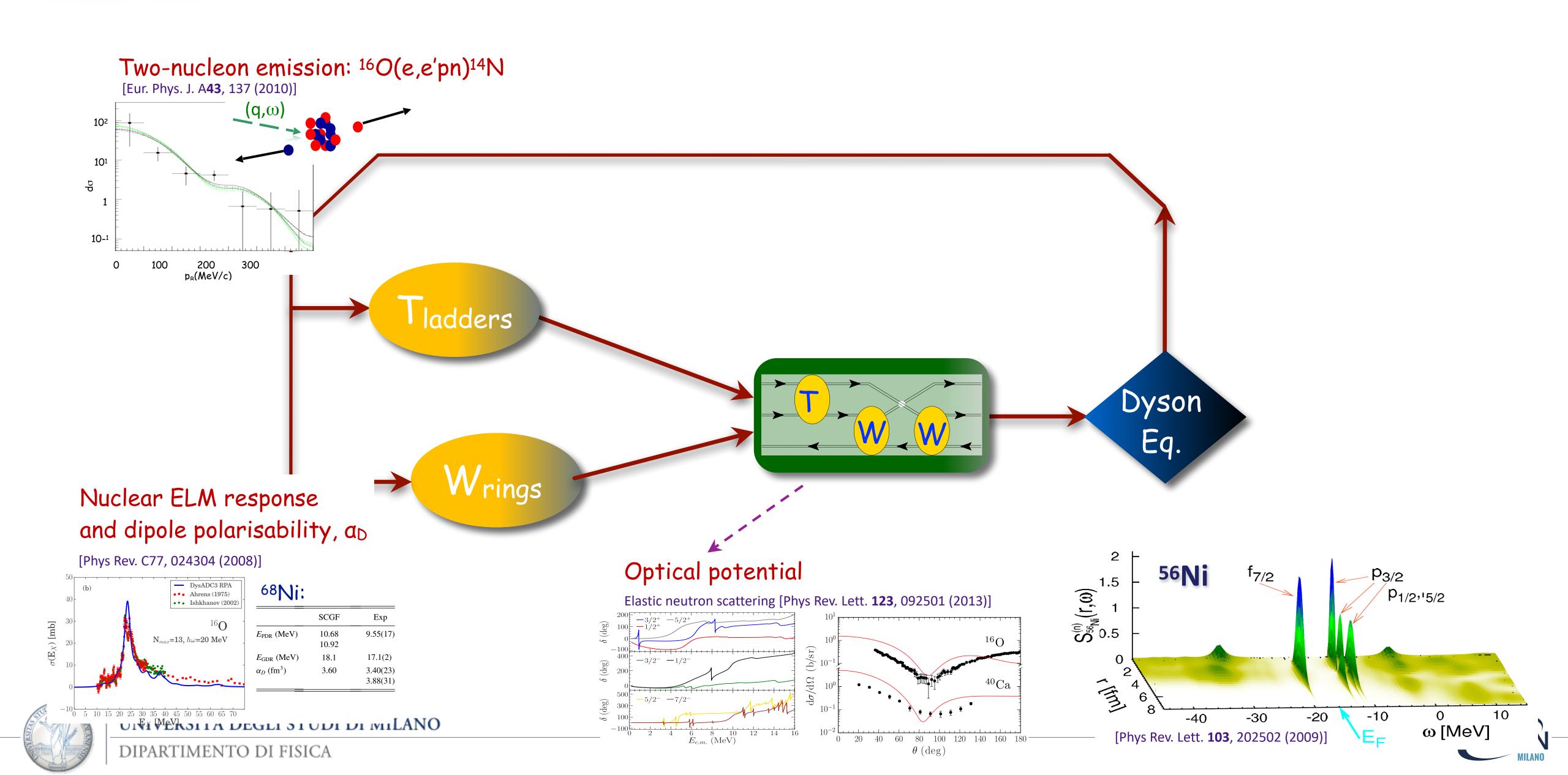


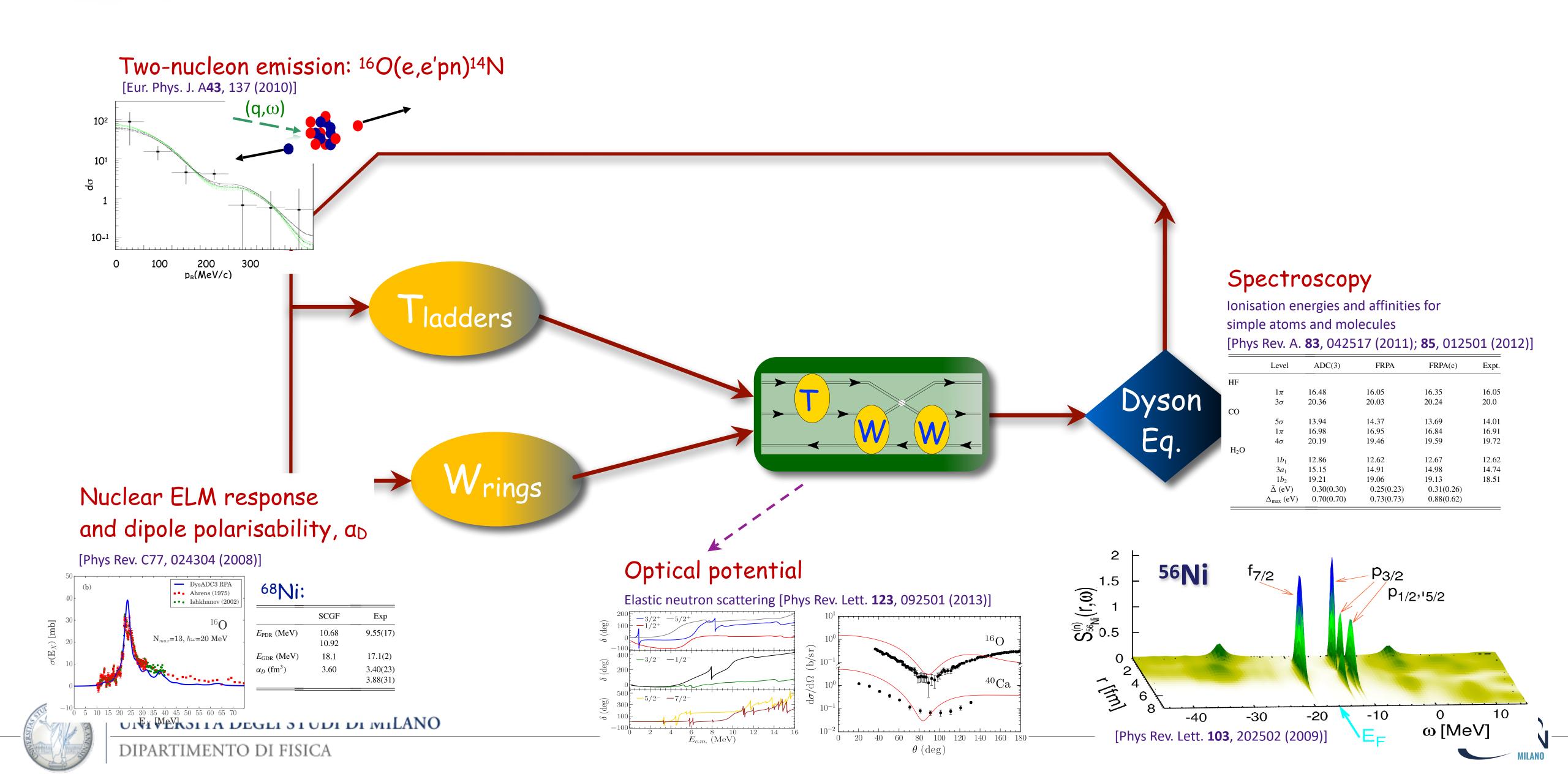


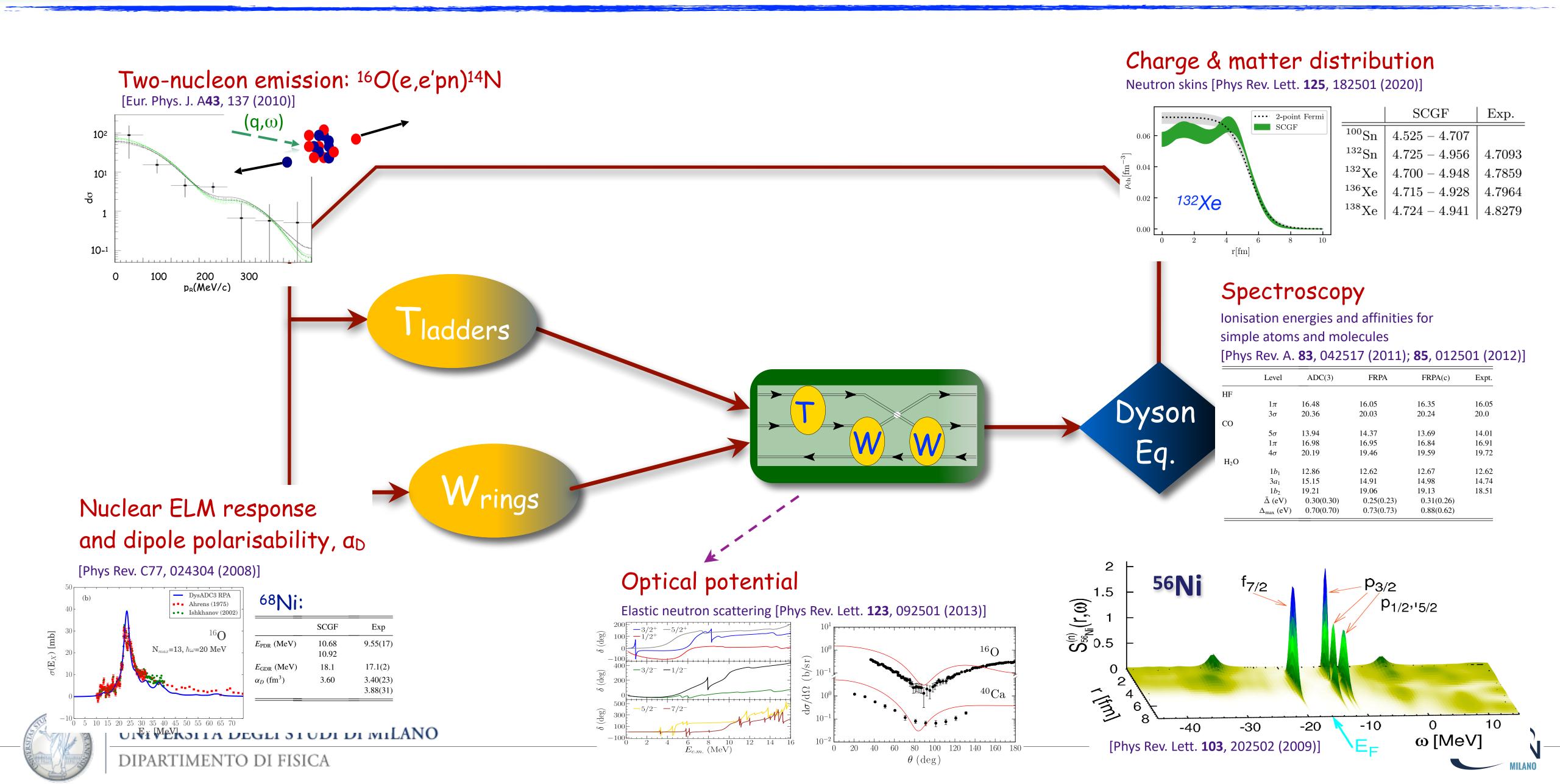


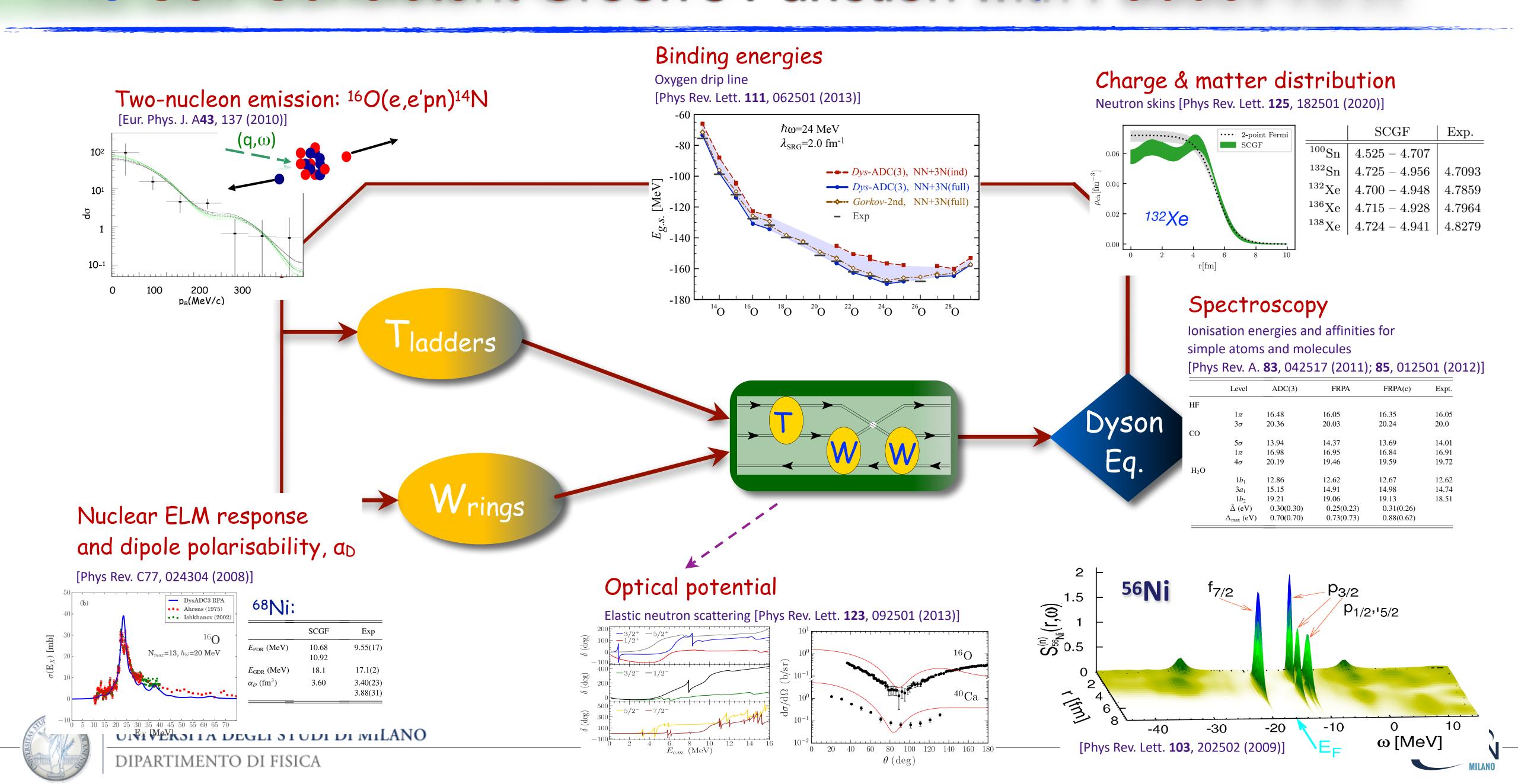






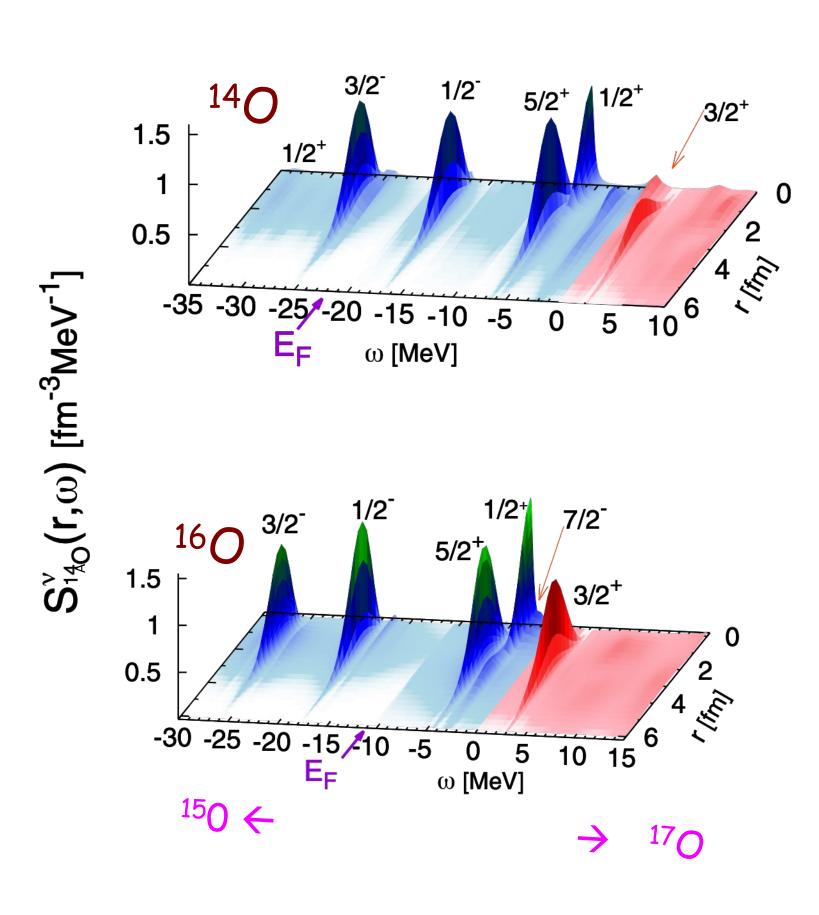


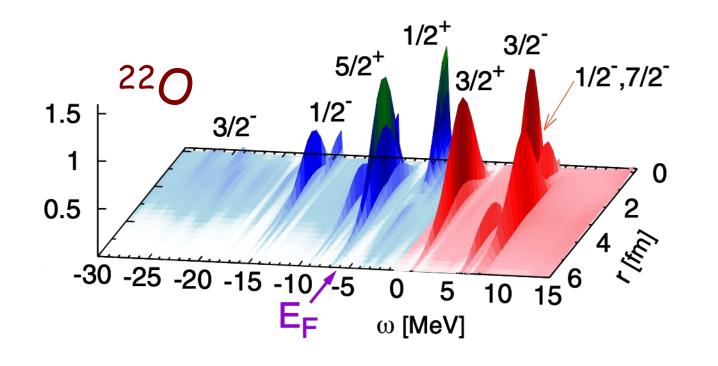


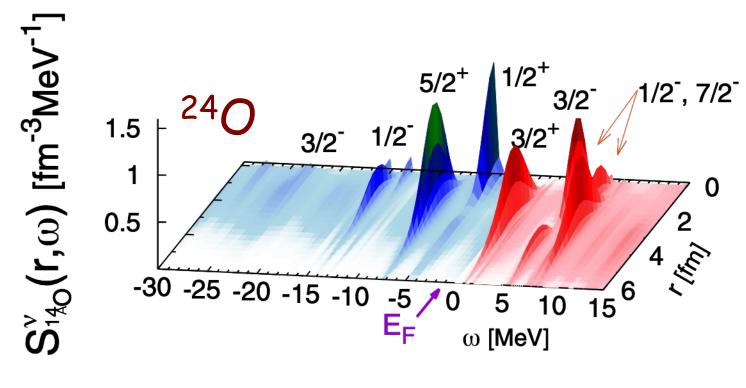


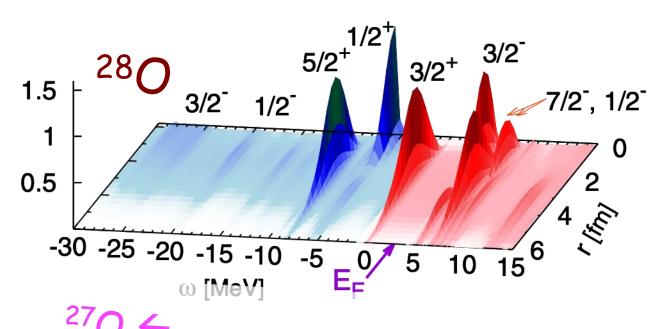
Neutron spectral function for oxygen isotopes

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

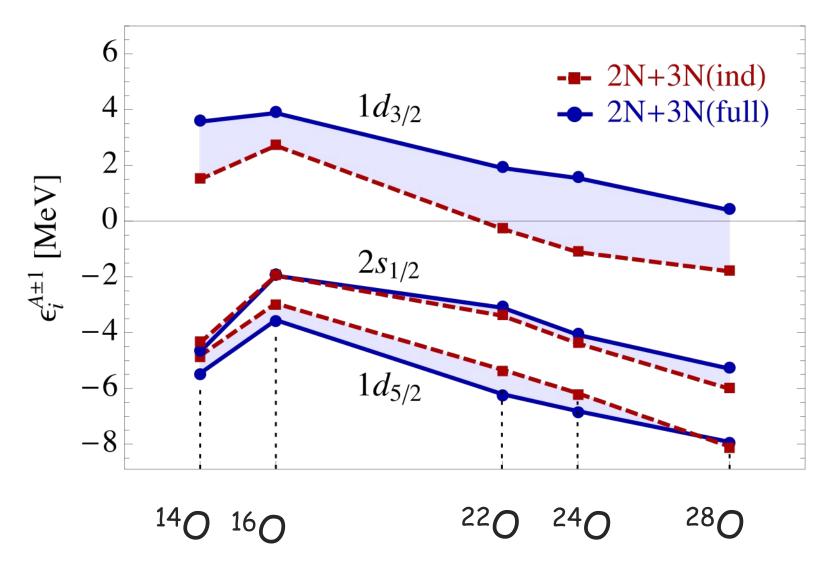








Neutron quasiparticle energies

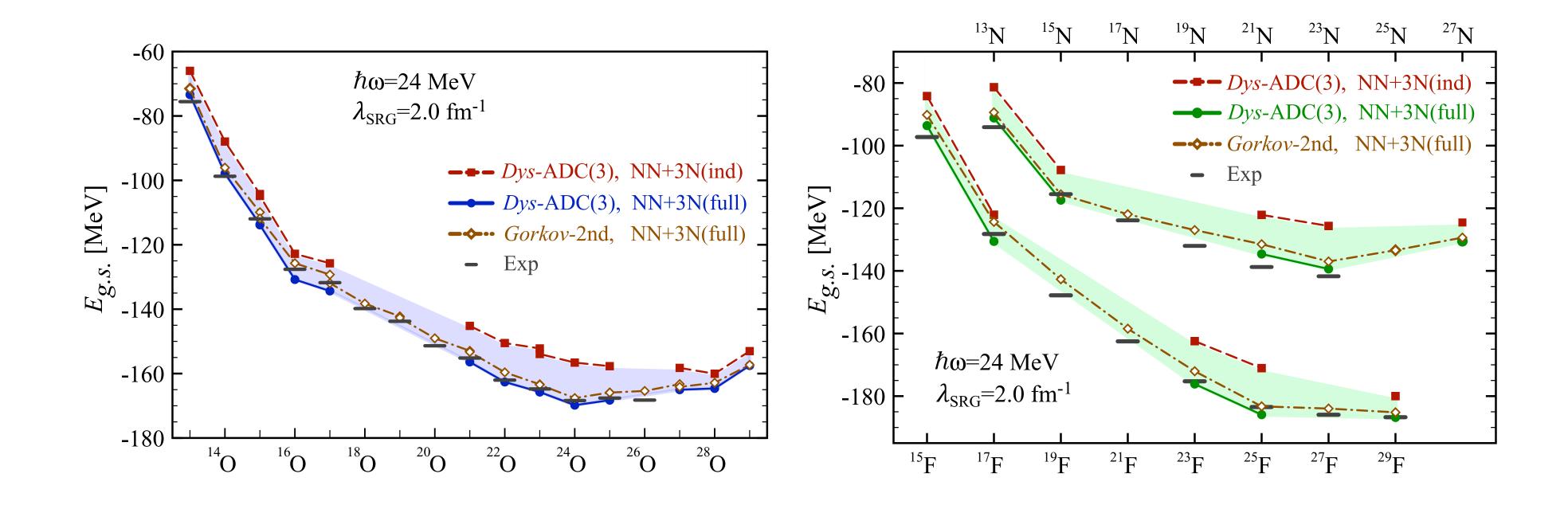






Results for the N-O-F chains

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



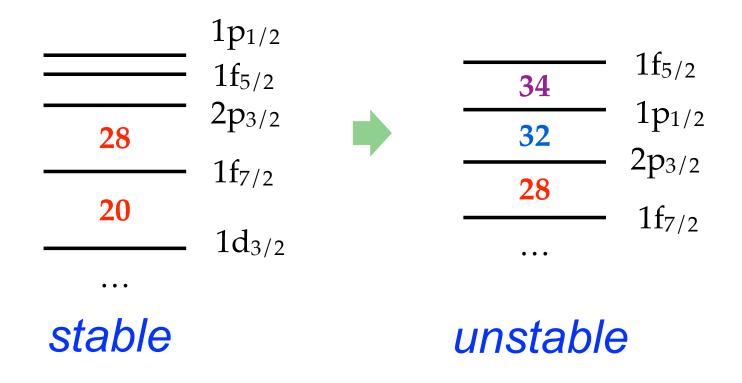
- > 3NF crucial for reproducing binding energies and driplines around oxygen
- > cf. microscopic shell model [Otsuka et al, PRL105, 032501 (2010).]



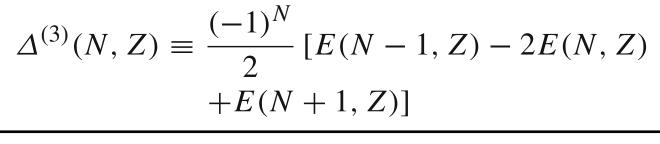


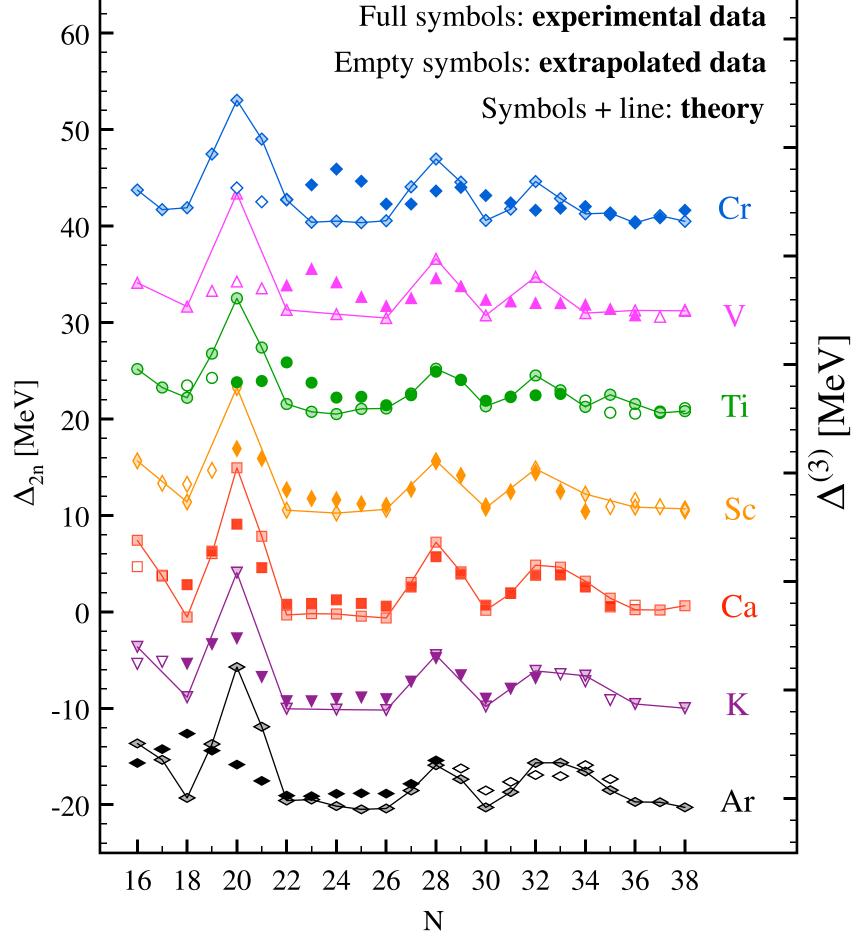
Magic numbers

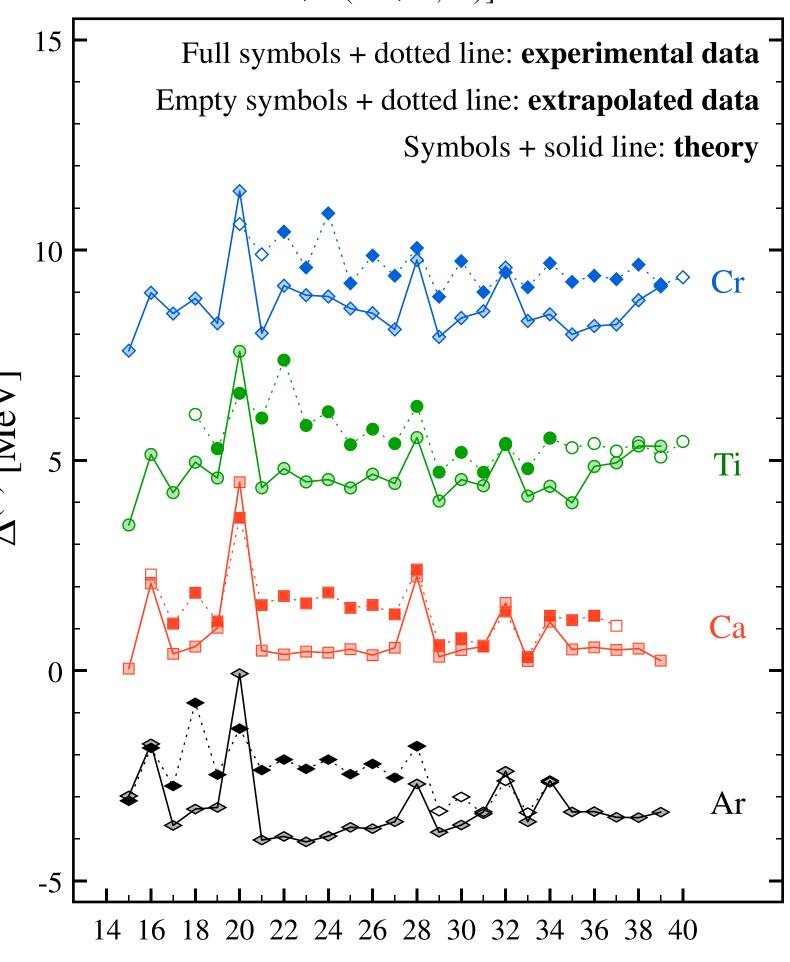
Magic numbers: extra-stable combinations of N & Z



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



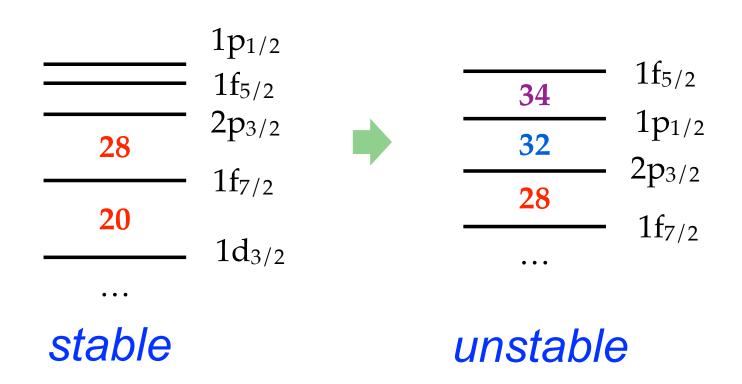




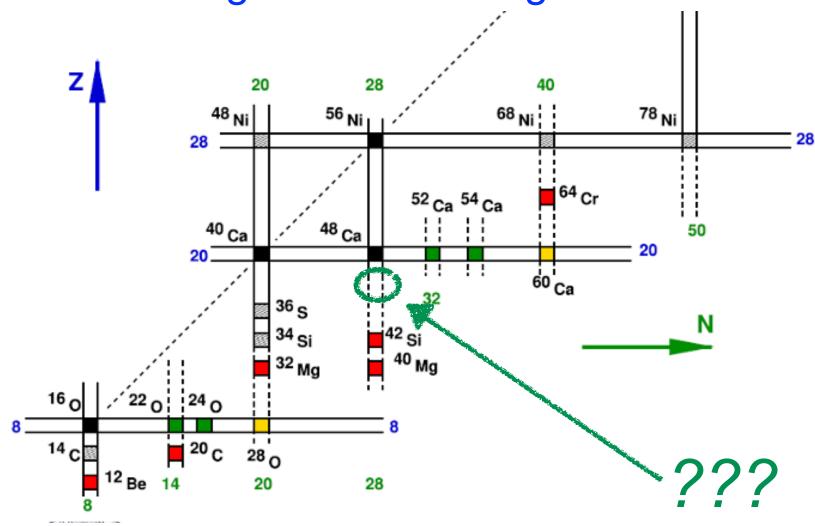


Magic numbers

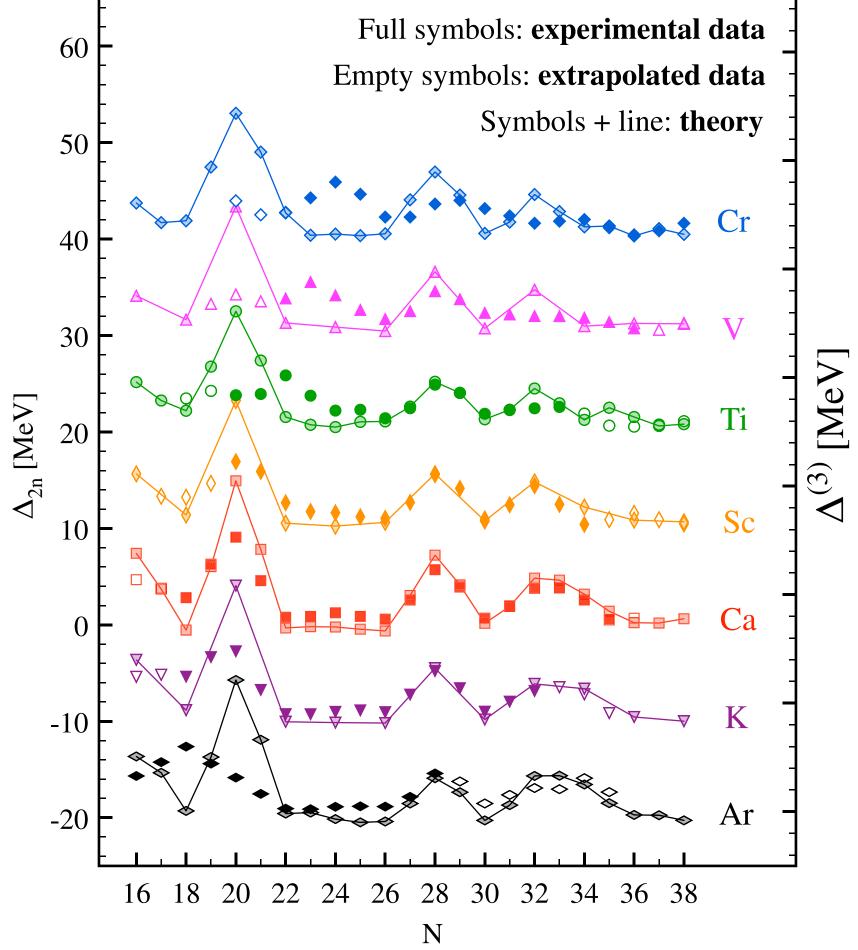
Magic numbers: extra-stable combinations of N & Z



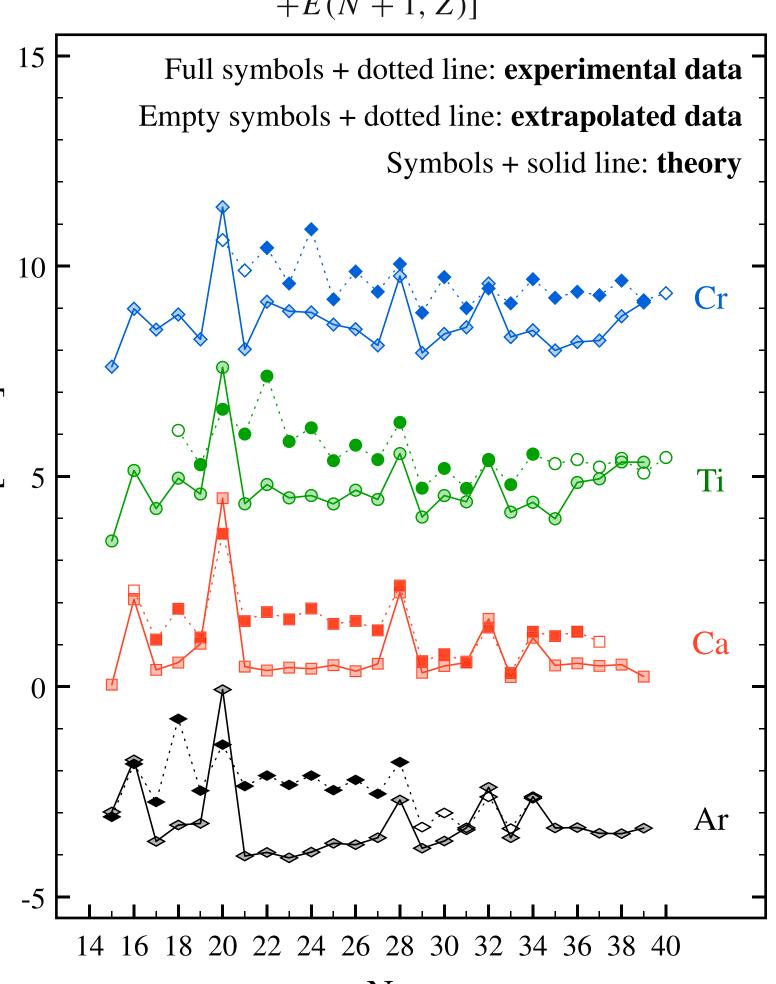
Known magic and semimagic nuclei:



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



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



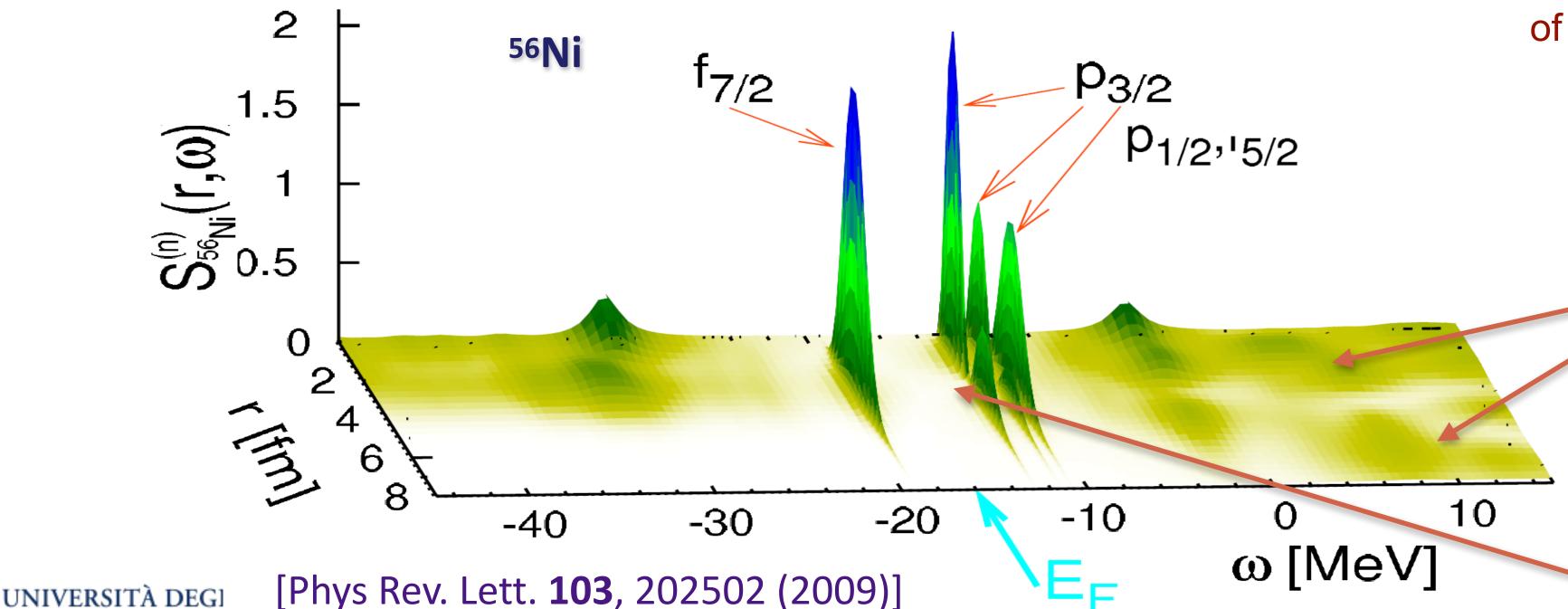
[Somà, CB et al. Eur. Phys. J. A 57, 135 (2021)]

The physics contained in the one-boby 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:
$$g_{\alpha\beta}(\omega)=g_{\alpha\beta}^{(0)}(\omega)+\sum_{\gamma\delta}g_{\alpha\gamma}^{(0)}(\omega)\Sigma_{\gamma\delta}^{\star}(\omega)g_{\delta\beta}(\omega)$$

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



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

==> Consistent computation of structure and reactions !!

Elastic scattering states

INFN

Low-E spectroscopy



DIPARTIMENTO DI FISICA

Ab initio optical potentials from propagator theory

Relation to Fesbach theory:

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

Escher & Jennings Phys. Rev. C66, 034313 (2002)

Previous SCGF work:

CB, B. Jennings, Phys. Rev. C72, 014613 (2005)

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

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

M. Vorabbi, CB, et al., in preparation

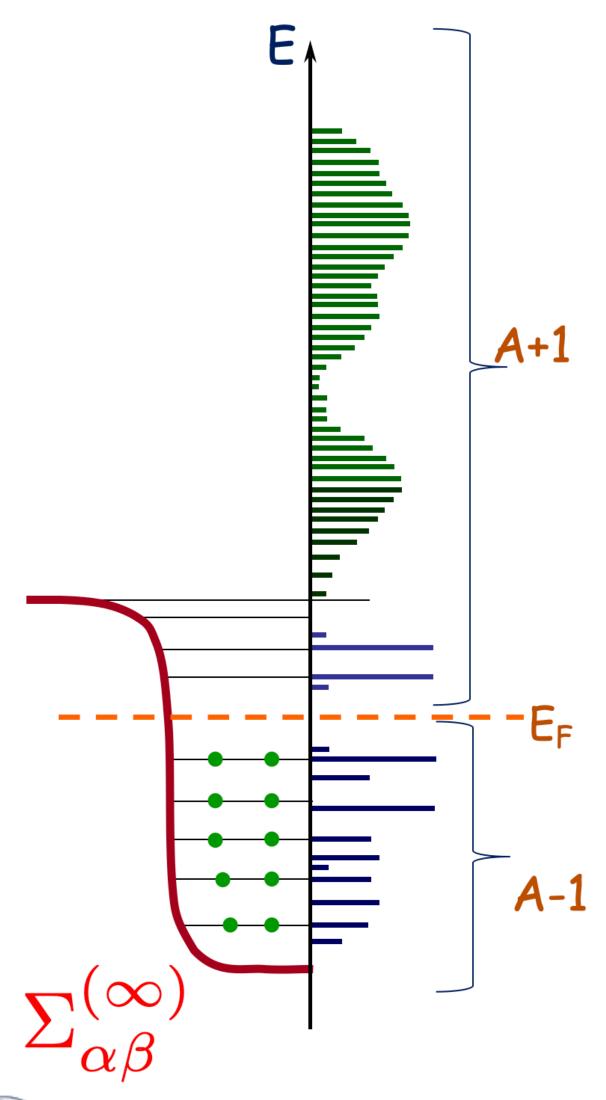
State-of-the-art of the field:

C. Hebborn, et al., CB, "Optical potentials for the rare-isotope beam era", arXiv:2210.07293 (WP) Jour. Phys. G (2023), in press.





Microscopic optical potential

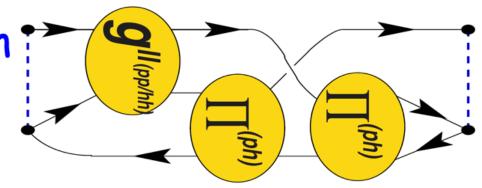


Nuclear self-energy $\Sigma^*(\mathbf{r}, \mathbf{r}'; \varepsilon)$:

- contains both particle and hole props.
- it is proven to be a Feshbach opt. pot., in general it is non-local!

$$\begin{split} \Sigma_{\alpha\beta}^{\star}(\omega) &= \Sigma_{\alpha\beta}^{(\infty)} + \sum_{i,j} \mathbf{M}_{\alpha,i}^{\dagger} \bigg(\frac{1}{E - (\mathbf{K}^{>} + \mathbf{C}) + i\Gamma}\bigg)_{i,j} \mathbf{M}_{j,\beta} \\ &+ \sum_{r,s} \mathbf{N}_{\alpha,r} \bigg(\frac{1}{E - (\mathbf{K}^{<} + \mathbf{D}) - i\Gamma}\bigg)_{r,s} \mathbf{N}_{s,\beta}^{\dagger} \end{split}$$
 mean-field

Particle-vibration couplings:



Solve scattering and overlap functions directly in momentum space:

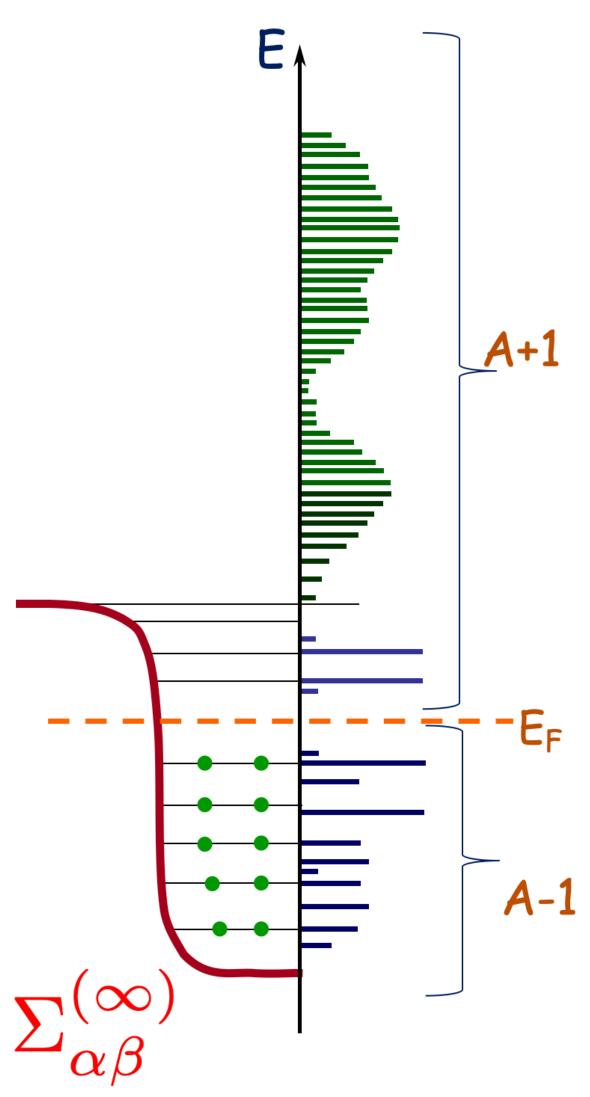
$$\Sigma^{* l,j}(k,k';E) = \sum_{n,n'} R_{n l}(k) \Sigma_{n,n'}^{* l,j} R_{n l}(k')$$

$$\frac{k^2}{2\mu} \psi_{l,j}(k) + \int dk' \, k'^2 \, \Sigma^{* l,j}(k,k';E_{c.m.}) \psi_{l,j}(k') = E_{c.m.} \psi_{l,j}(k)$$





Microscopic optical potential

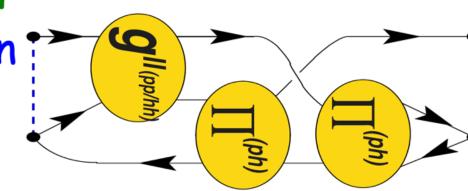


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$$\begin{split} \Sigma_{\alpha\beta}^{\star}(\omega) &= \Sigma_{\alpha\beta}^{(\infty)} + \sum_{i,j} \mathbf{M}_{\alpha,i}^{\dagger} \bigg(\frac{1}{E - (\mathbf{K}^{>} + \mathbf{C}) + i\Gamma} \bigg)_{i,j} \mathbf{M}_{j,\beta} \\ &+ \sum_{r,s} \mathbf{N}_{\alpha,r} \bigg(\frac{1}{E - (\mathbf{K}^{<} + \mathbf{D}) - i\Gamma} \bigg)_{r,s} \mathbf{N}_{s,\beta}^{\dagger} \end{split}$$

Particle-vibration couplings:

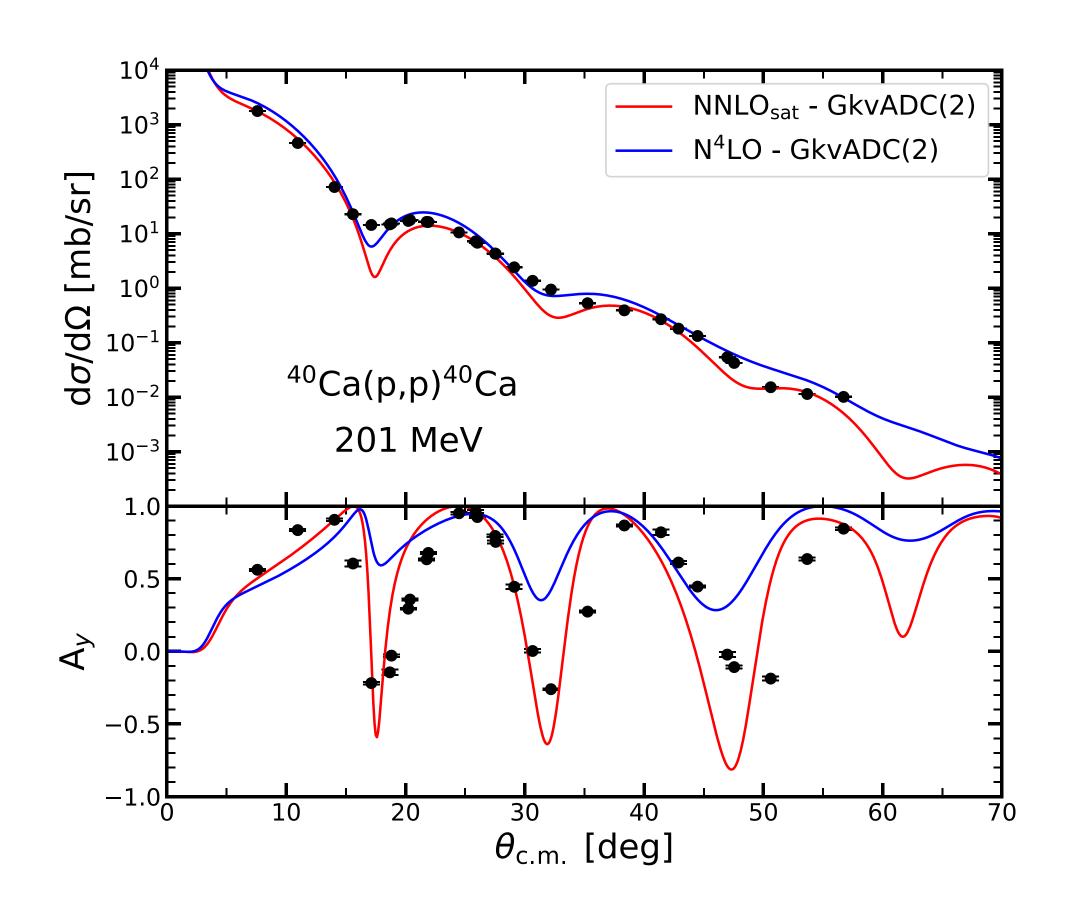


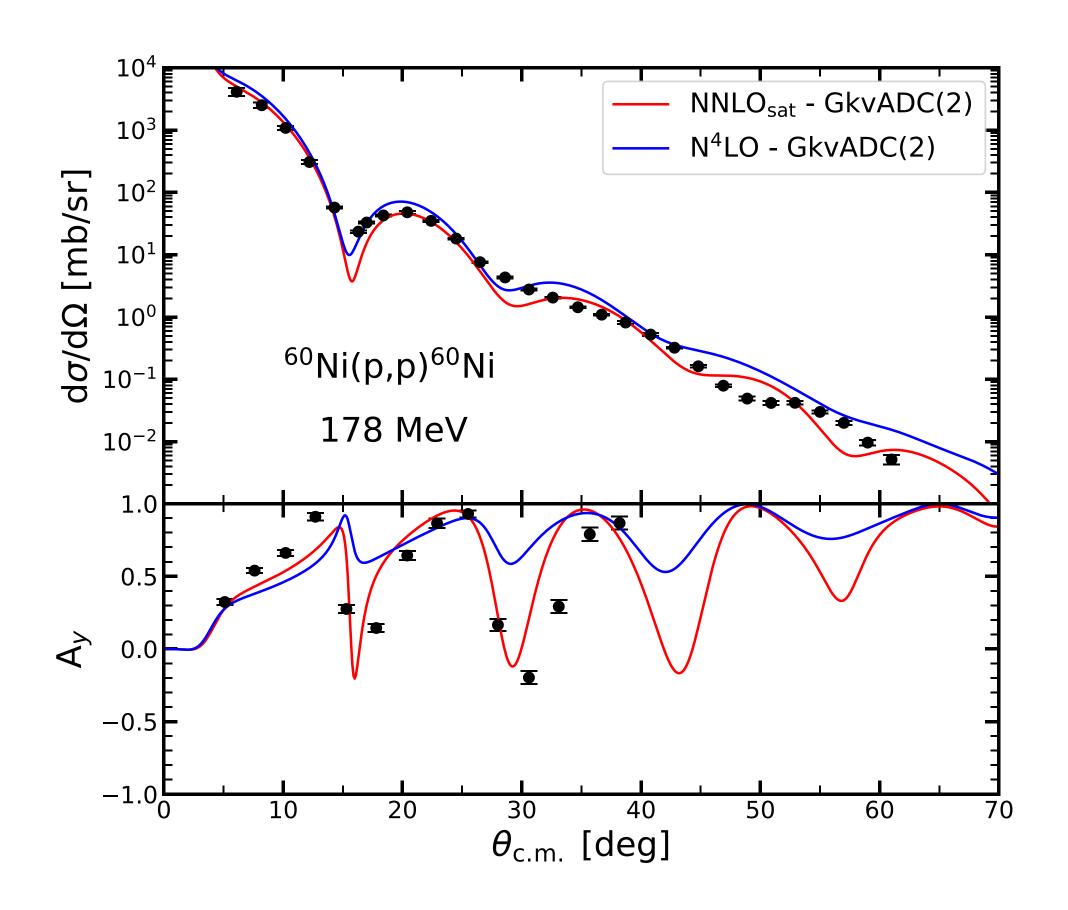
$$\sum_{\alpha\beta}^{(\infty)} = --$$





Elastic nucleon nucleus scattering







M. Vorabbi U. of surrey

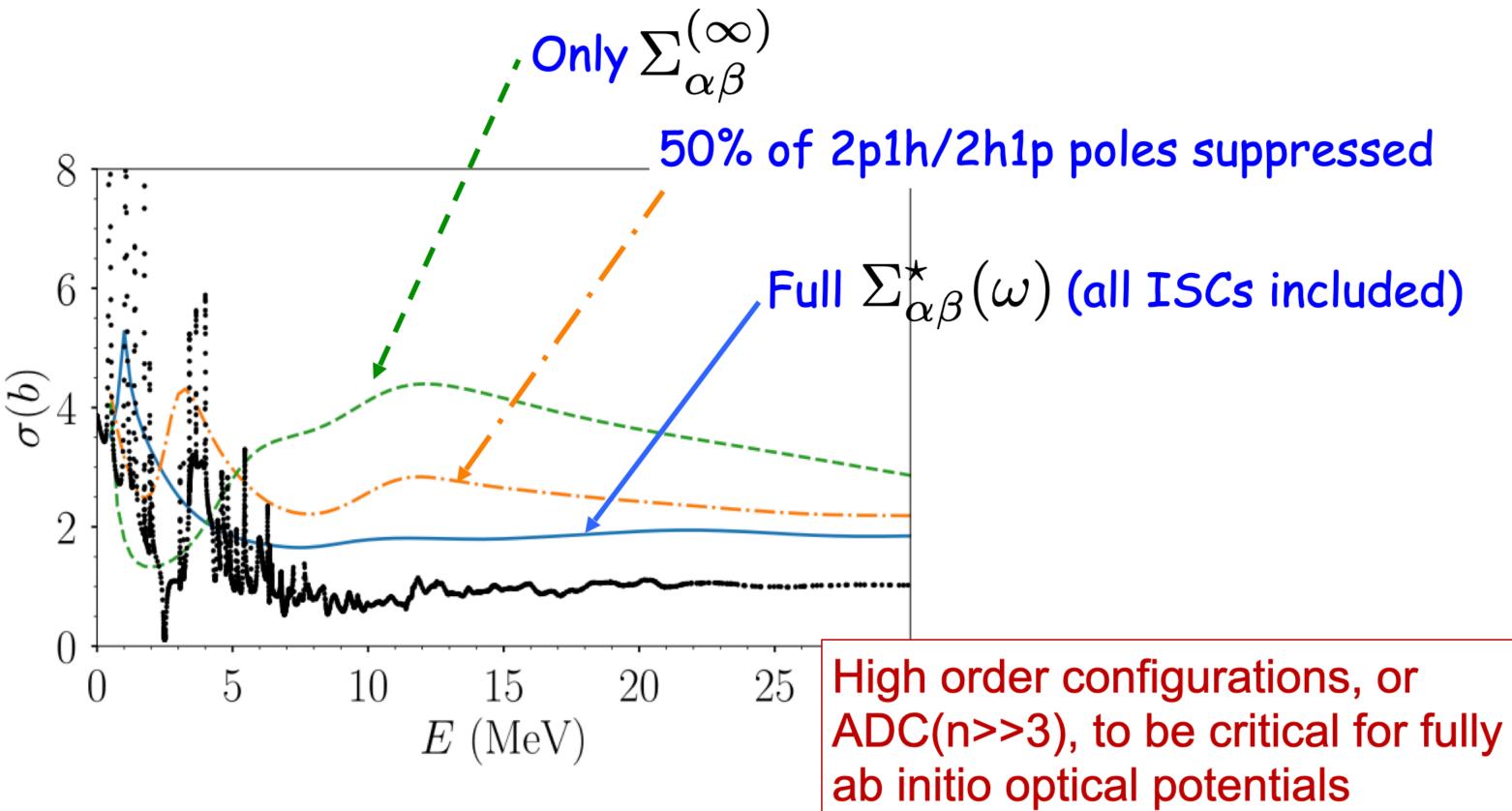


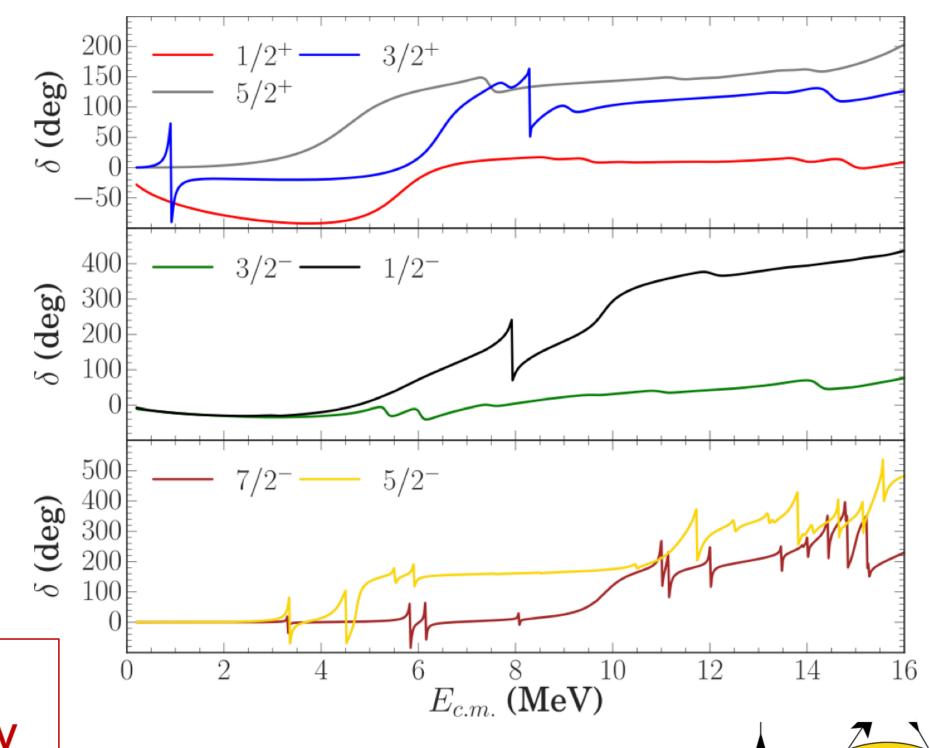


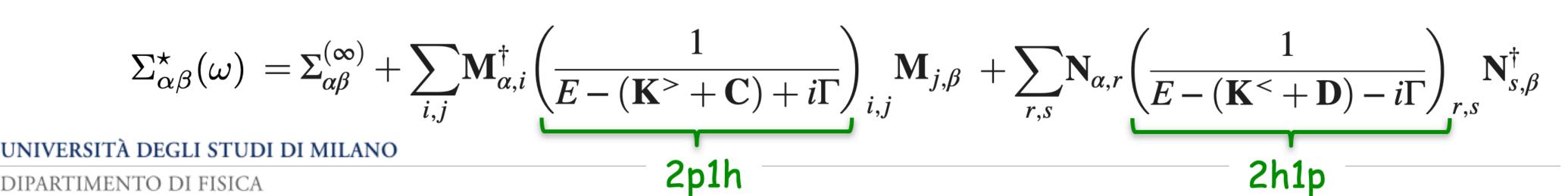
Role of intermediate state configurations (ISCs)



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







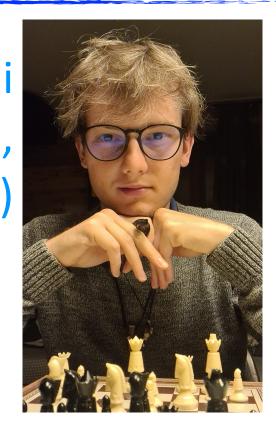
Green's function theory beyond ADC(3)?

DiagMC !!

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

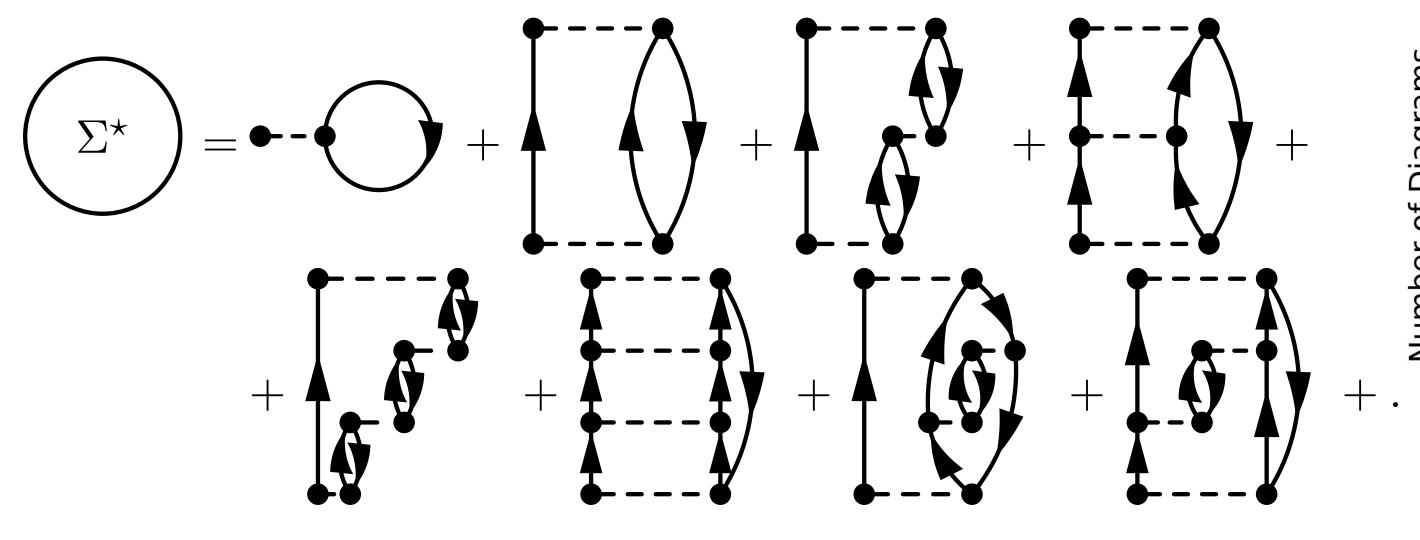
$$G_{\alpha\beta}(\omega) = G_{\alpha\beta}^{(0)}(\omega) + \sum_{\gamma\delta} G_{\alpha\gamma}^{(0)}(\omega) \Sigma_{\gamma\delta}^{\star}(\omega) G_{\delta\beta}(\omega)$$

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...

2

4

Order of Expansion

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...

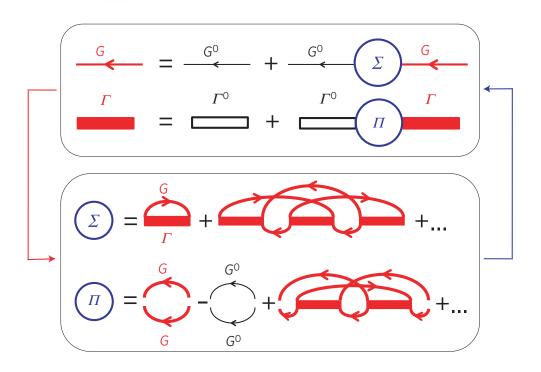


Figure 1 | **Bold diagrammatic Monte Carlo** The skeleton diagrammatic series for the self-energy Σ and the pair self-energy Π is evaluated

DiagMC:

Phys. Rev. Lett. 81, 2514 (1998)

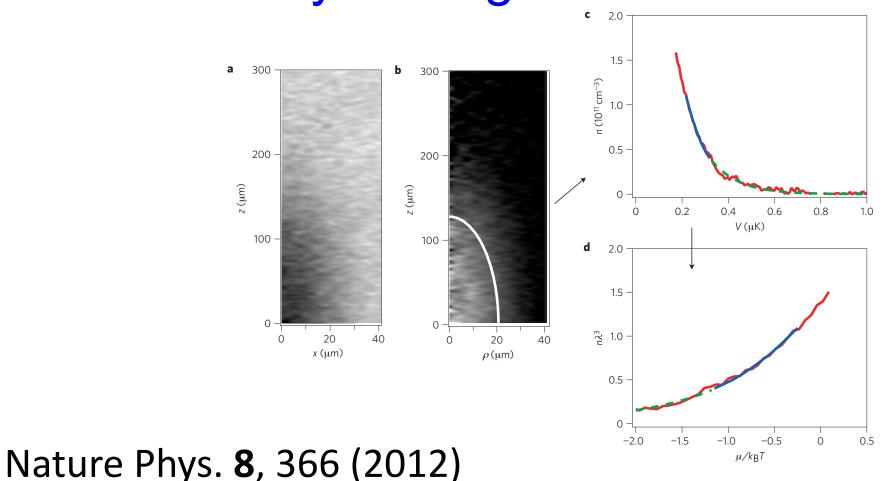
Phys. Rev. B 99, 035140 (2019)

•••

Mostly infinite matter at T≠0...

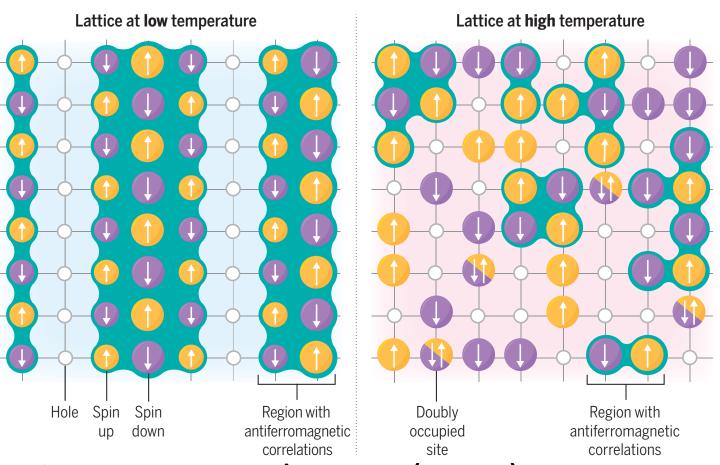
...what about finite nuclei??

EOS unitary fermi gas...



Science **385**, eade9194 (2024)

Spins in the Hubbard model...



 $\text{Im}\Sigma(\mathbf{k},i\omega_0)$

0.20

0.15

Fig. 2. Fingerprints of the different regimes. The momentum-resolved spectral function, $A(\mathbf{k})$ (left); the imaginary part of the self-energy, 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. A Im $\Sigma(\mathbf{k}, i\omega_0) = \text{Im } \Sigma(\mathbf{k}, i\omega_0)$ (right) are shown for





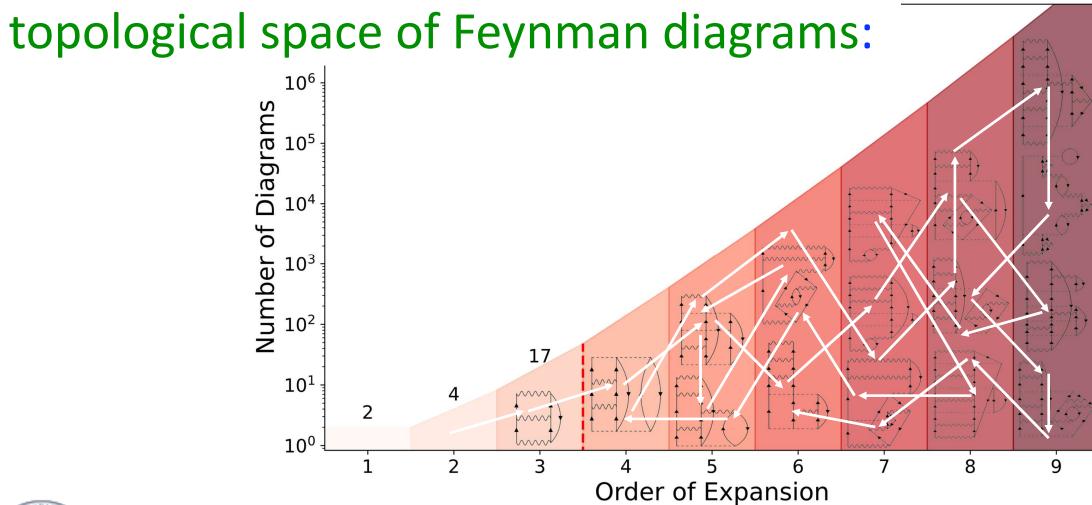
 $\Delta Im \Sigma(\mathbf{k})$

Diagrammatic Monte Carlo: overview

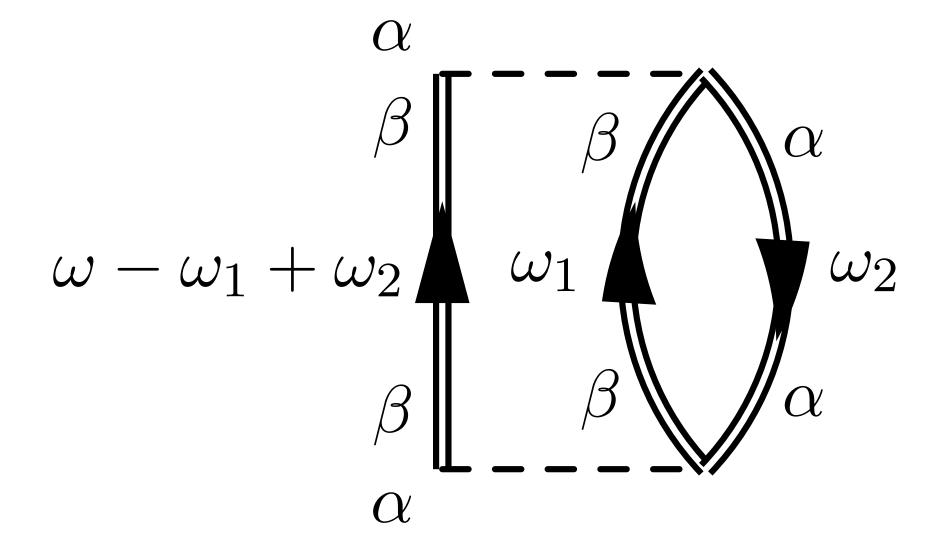
$$\Sigma_{\alpha\beta}^{\star}(\omega) = \sum_{\mathcal{T}} \sum_{\gamma_{1}...\gamma_{n}} \int d\omega_{1}...d\omega_{m} \,\mathcal{D}_{\alpha\beta}^{\omega} \left(\mathcal{T}; \gamma_{1}...\gamma_{n}; \omega_{1}...\omega_{m}\right) 1_{\mathcal{T} \in \mathcal{S}_{\Sigma^{\star}}}$$

Infinte Feynman series of diagrams

Monte Carlo integration in the



Monte Carlo integration - "101"







Diagrammatic Monte Carlo: overview

$$\Sigma_{\alpha\beta}^{\star}(\omega) = \sum_{\mathcal{T}} \sum_{\gamma_{1}...\gamma_{n}} \int d\omega_{1}...d\omega_{m} \,\mathcal{D}_{\alpha\beta}^{\omega}(\mathcal{T}; \gamma_{1}...\gamma_{n}; \omega_{1}...\omega_{m}) \, 1_{\mathcal{T} \in \mathcal{S}_{\Sigma^{\star}}}$$

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

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

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

- ullet $W_o(N)$ is an order dependent reweighting factor



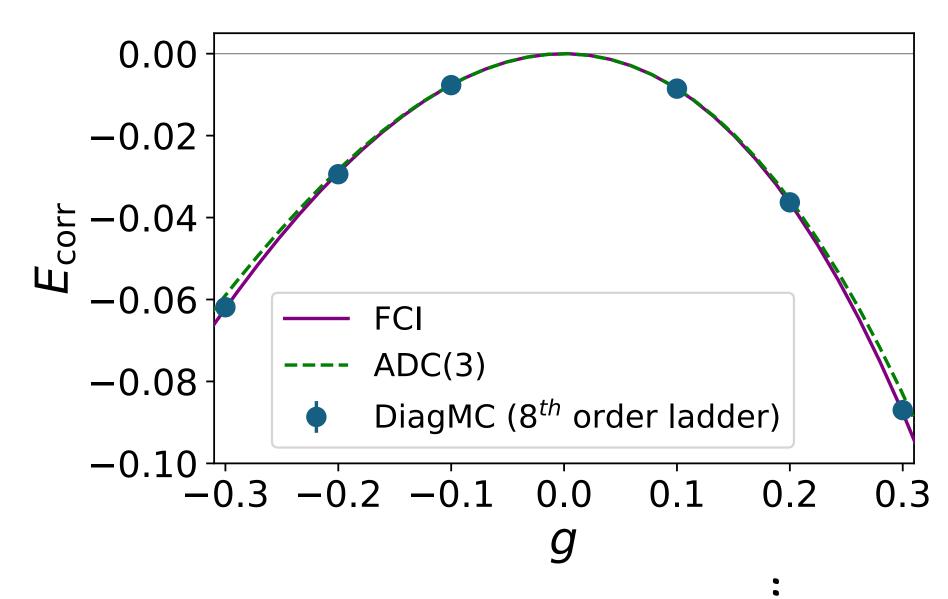


Results of the simulation for D=2-10 levels

S. Brolli (PhD Milan)



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



Spectroscopic function for *D*=10 levels :

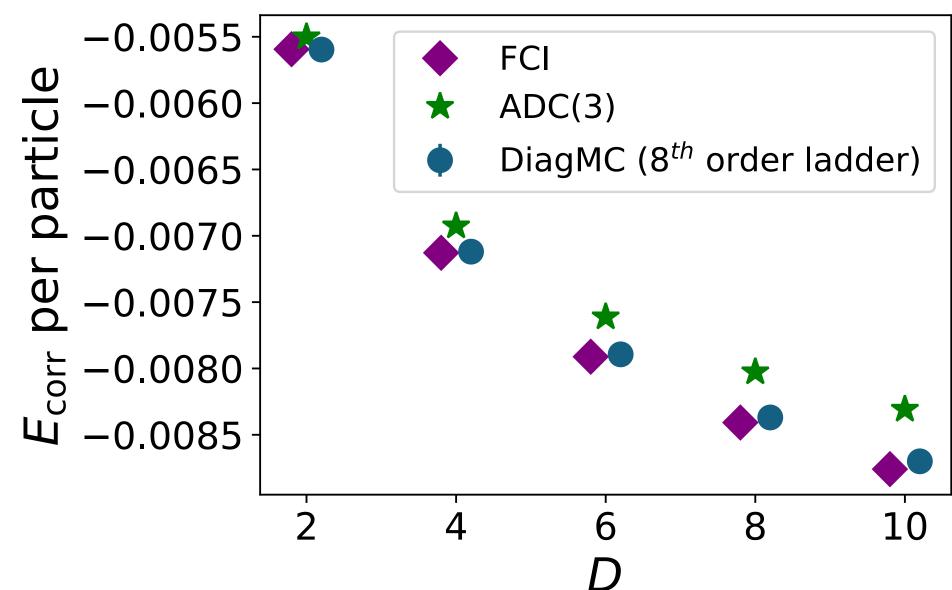
$$\alpha = 3$$

$$\alpha = 2$$

$$\alpha = 1$$

$$\alpha = 0$$

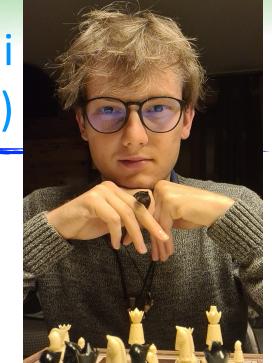
Accuracy for different model spaces model spaces (D=2-10 levels):



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



S. Brolli (PhD Milan)

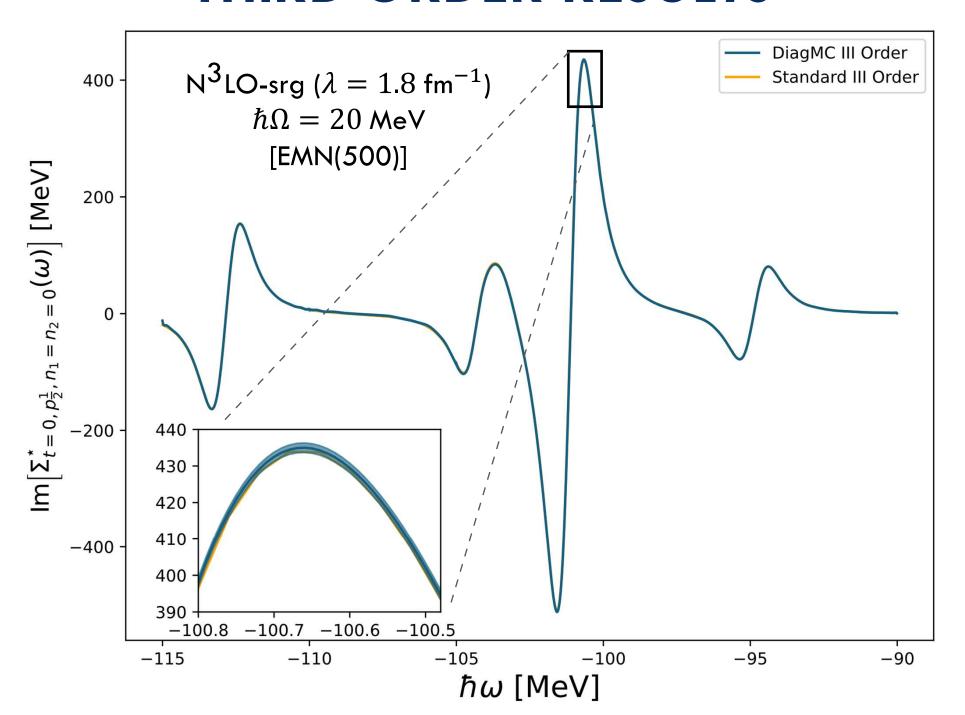


DiagMC is being extended to treat realistic microscopic nuclear Hamiltonians

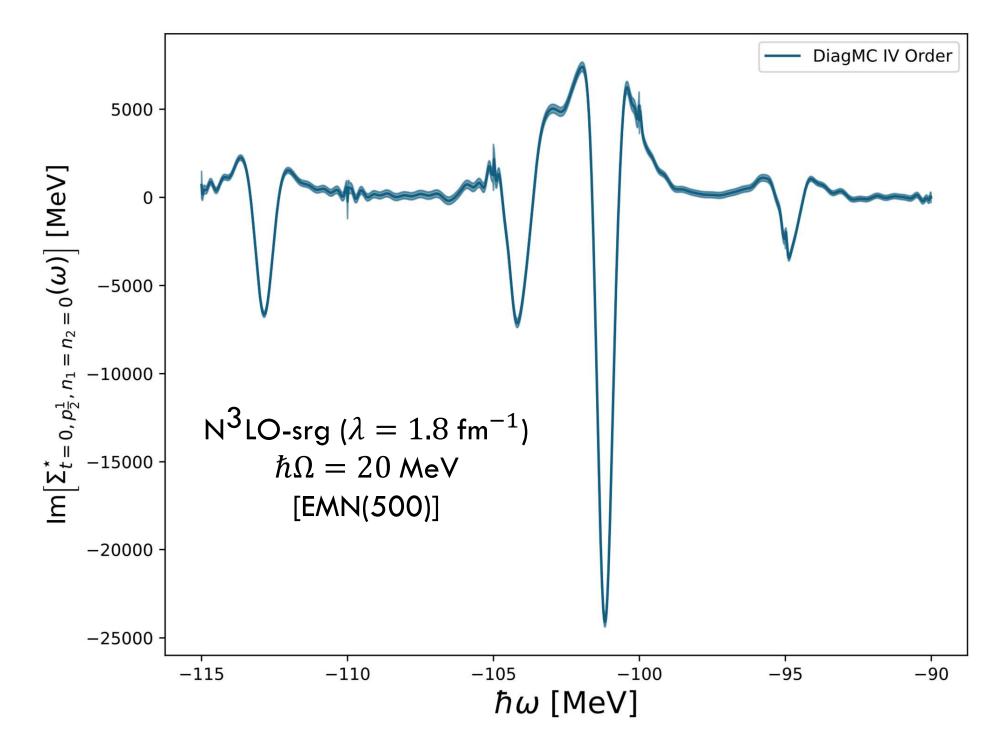
¹⁶O in harmonic oscillator space ($N_{max} = 2$, for now)

Example of neutron $p_{1/2}$ self-energy up to 3rd order

THIRD ORDER RESULTS



FOURTH ORDER RESULTS







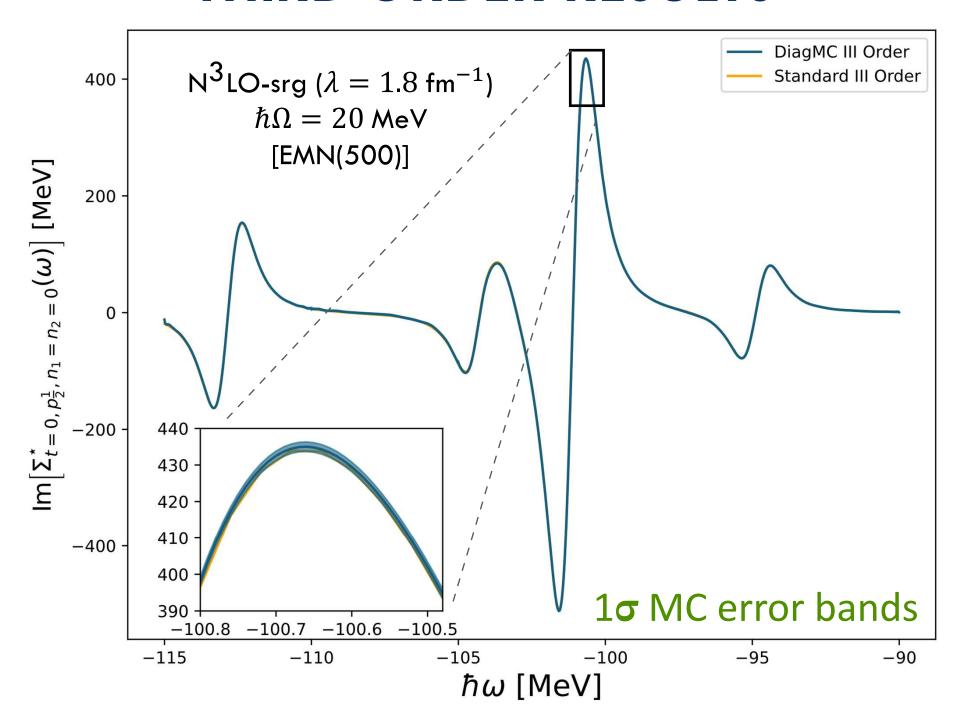
S. Brolli (PhD Milan)

DiagMC is being extended to treat realistic microscopic nuclear Hamiltonians

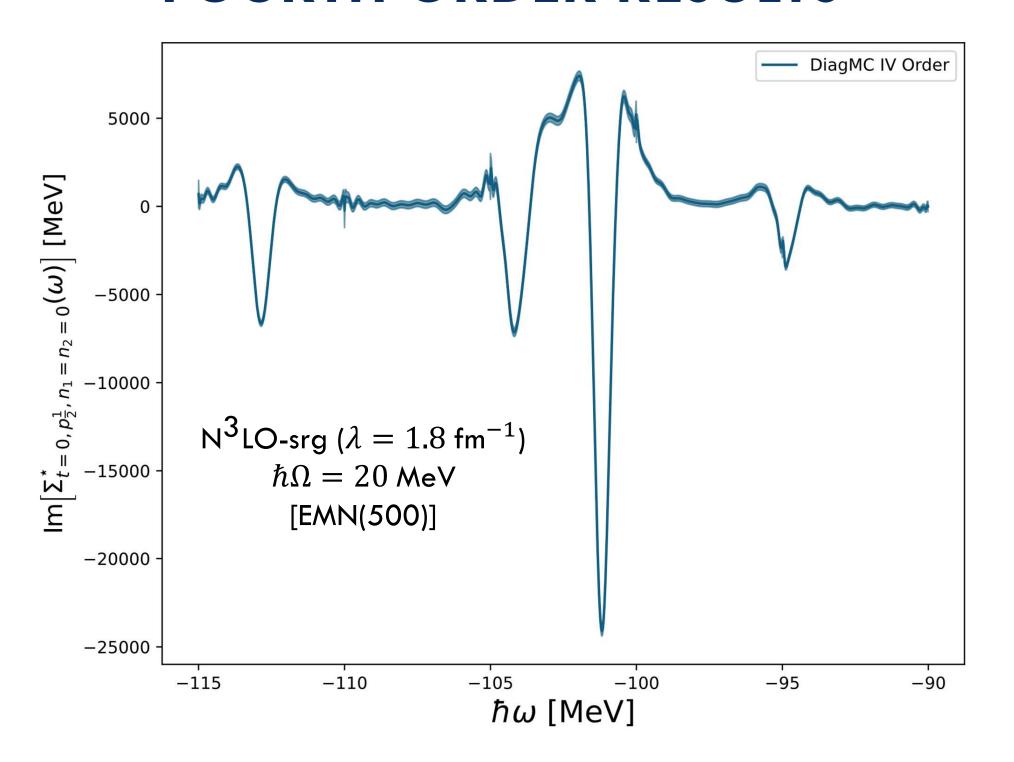
¹⁶O in harmonic oscillator space ($N_{max} = 2$, for now)

Example of neutron $p_{1/2}$ self-energy up to 3rd order

THIRD ORDER RESULTS



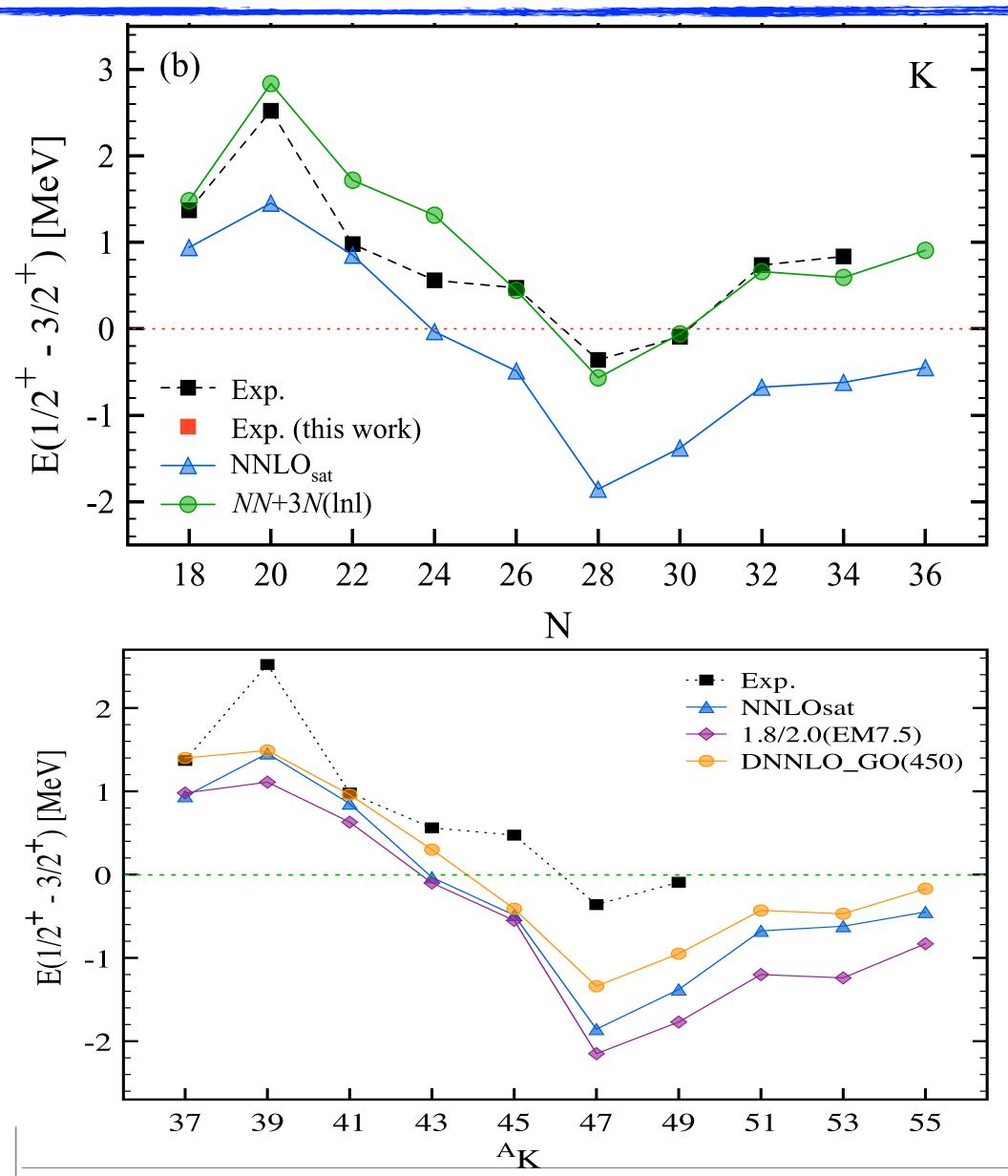
FOURTH ORDER RESULTS







$d_{3/2}$ — $s_{1/2}$ 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 form ACa

Papuga et al., PRL110, 172503 (2013); PRC90, 034321 (2014)

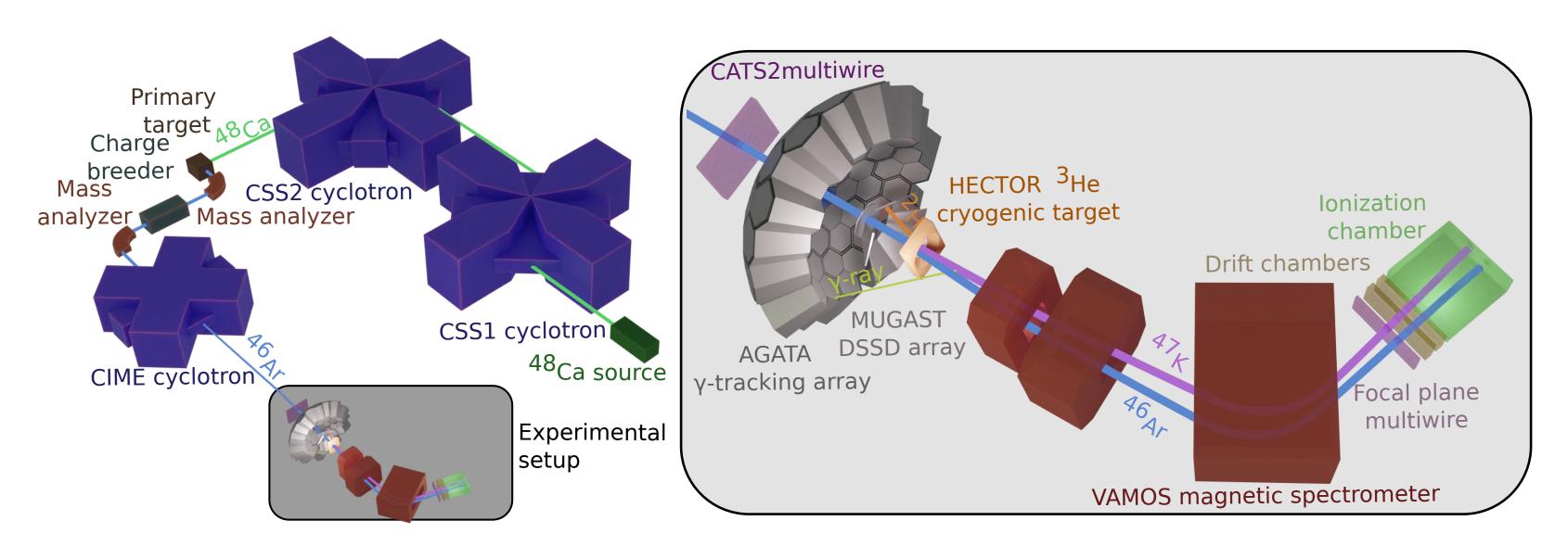
RIKEN, SEASTAR coll., Phys. Lett. **B802** 135215 (2020)

Linh, Gillibert, et al., PRC104, 044331 (2021)

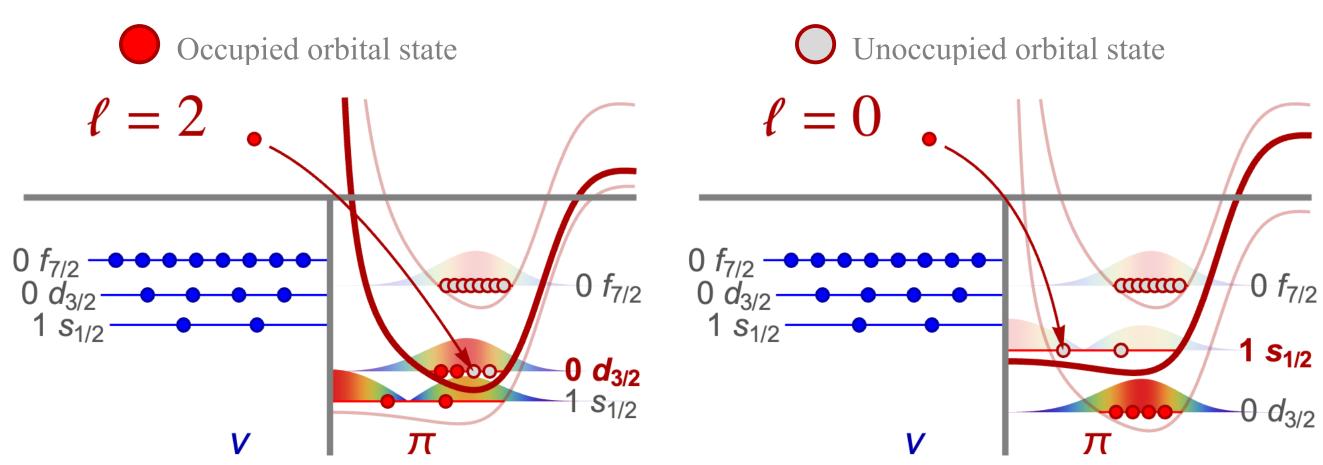


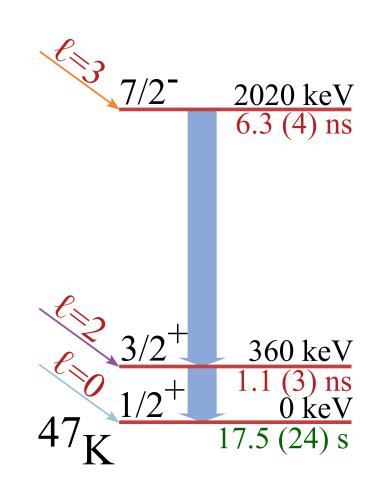


⁴⁶Ar(³He,d)⁴⁷K at GANIL



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

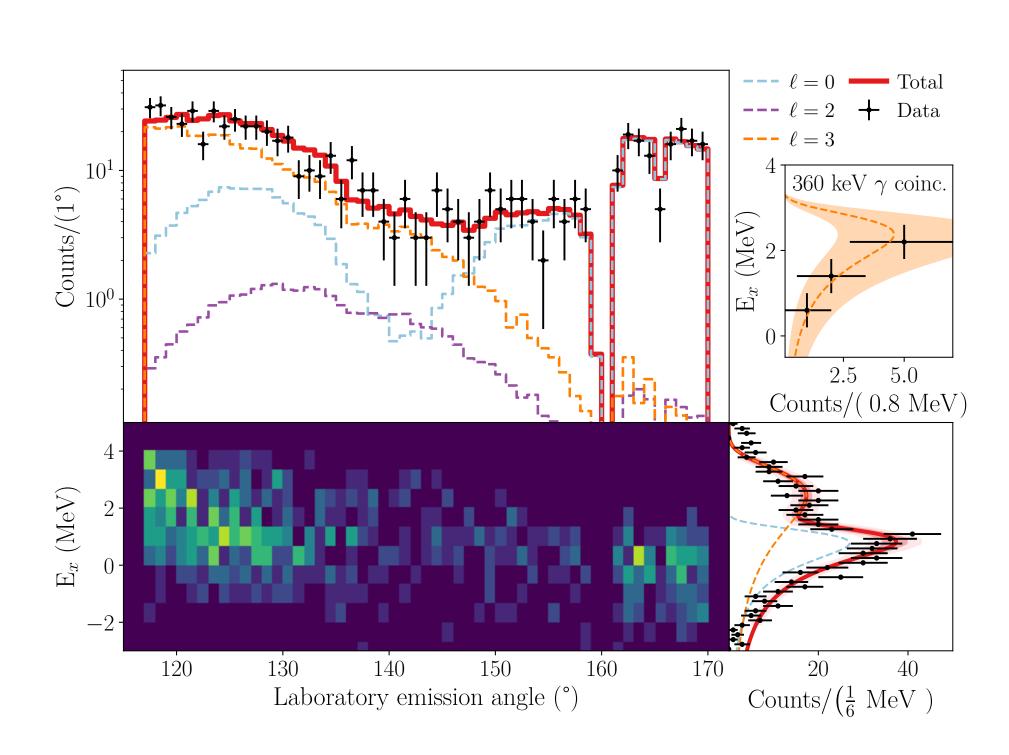


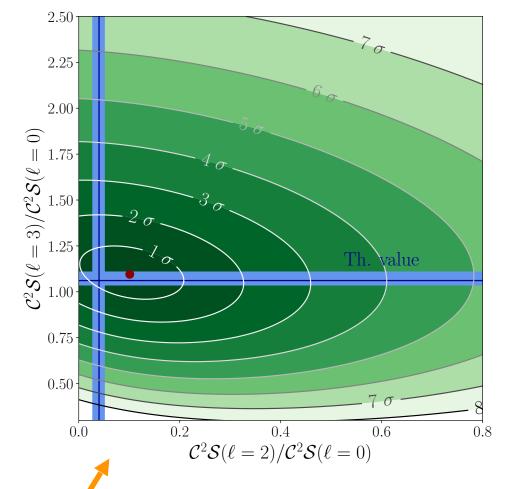




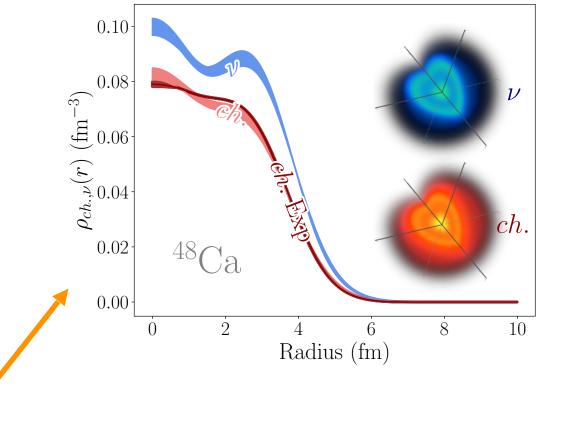


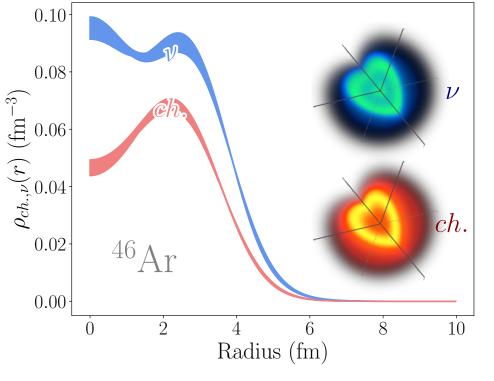
46Ar(3He,d)47K at GANIL: New charge bubble in 46Ar





 $\frac{d\sigma}{d\Omega} = \sum_{k} g_k \, \mathcal{C}^2 \mathcal{S}_k \, \frac{d\sigma_k^{SP}}{d\Omega}$





d3/2 - s1/2 inversion revisited from adding protons to ⁴⁶Ar

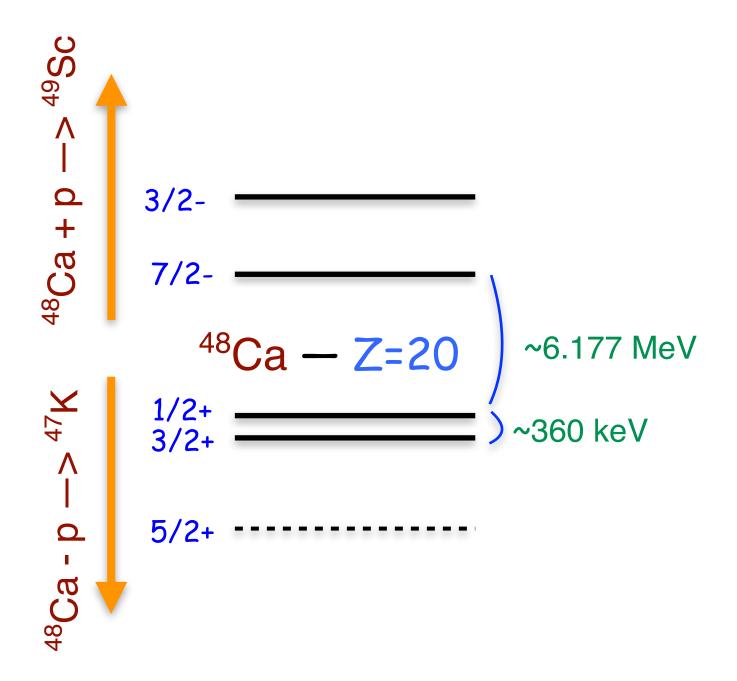
Theory & experiment for relative SFs agree within 1 sigma and confirms charge depletion in ⁴⁶Ar

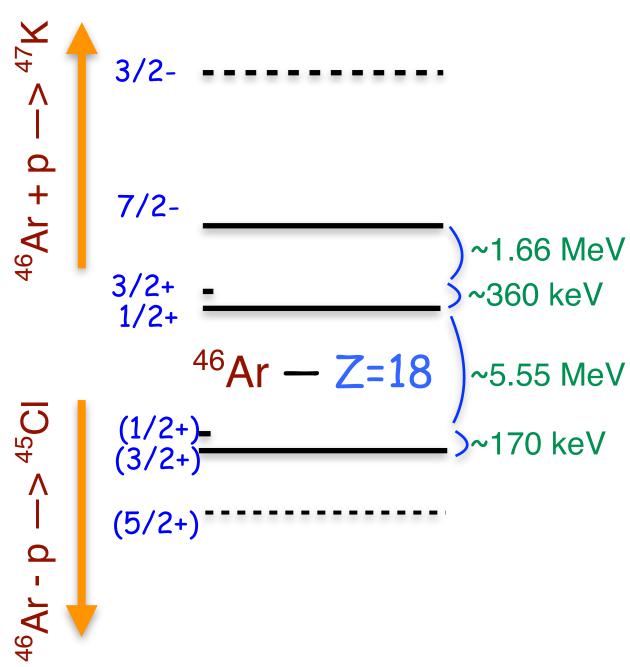
Theory bands are a combination of NNLOsat, Δ -full DN²LO(394) and DN²LO(450), as well as Darmstadt's saturating "magic force" 1.8/2.0 (7.5) —all of these have constrained LECs using the ¹⁶O radius and few other mid-mass nuclei data.

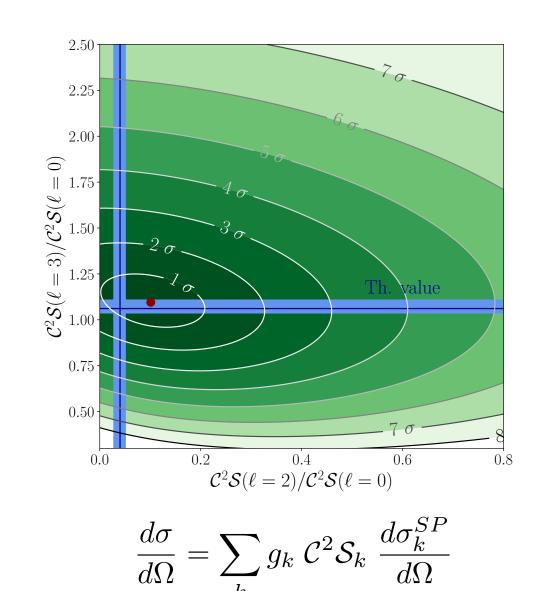


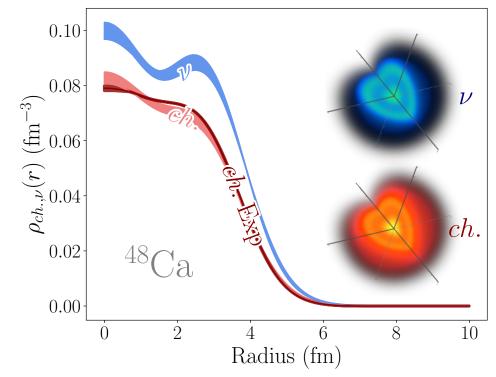


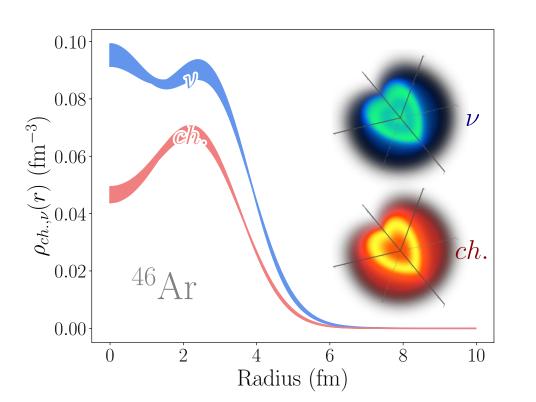
46Ar(3He,d)47K at GANIL: New charge bubble in 46Ar











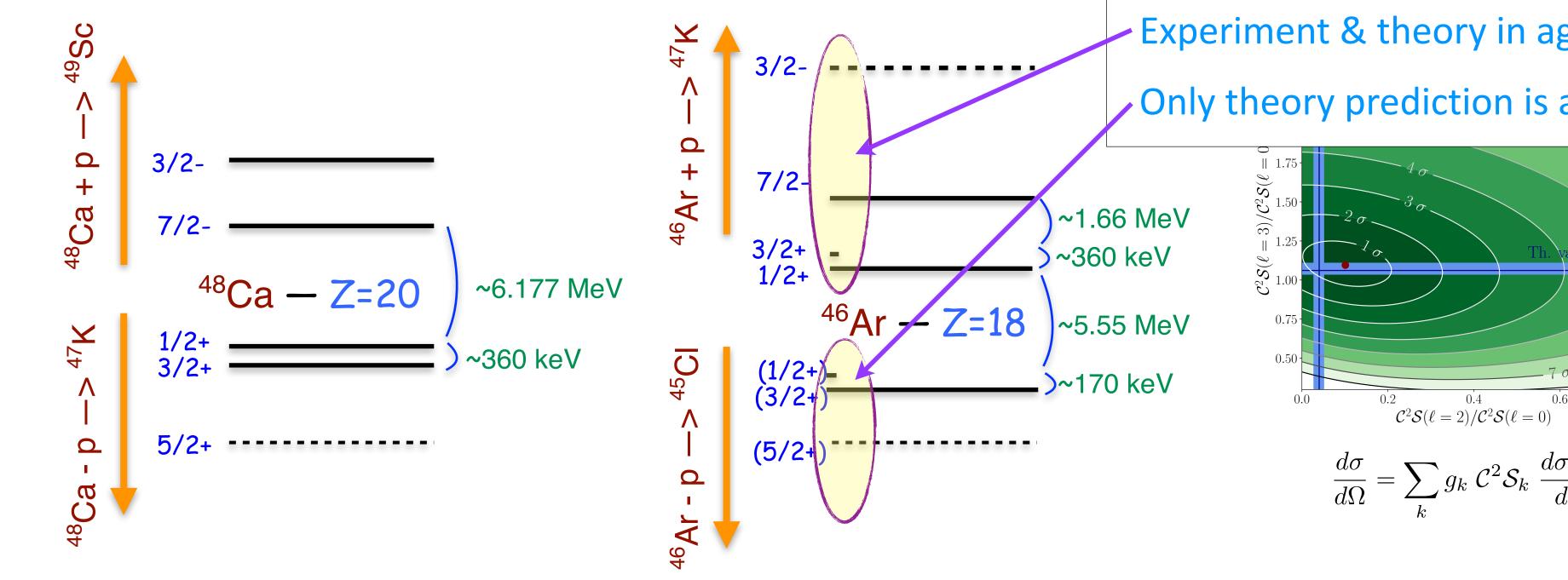
$$\Delta E_{1/2+-3/2+}$$
 (exp) = 360 keV

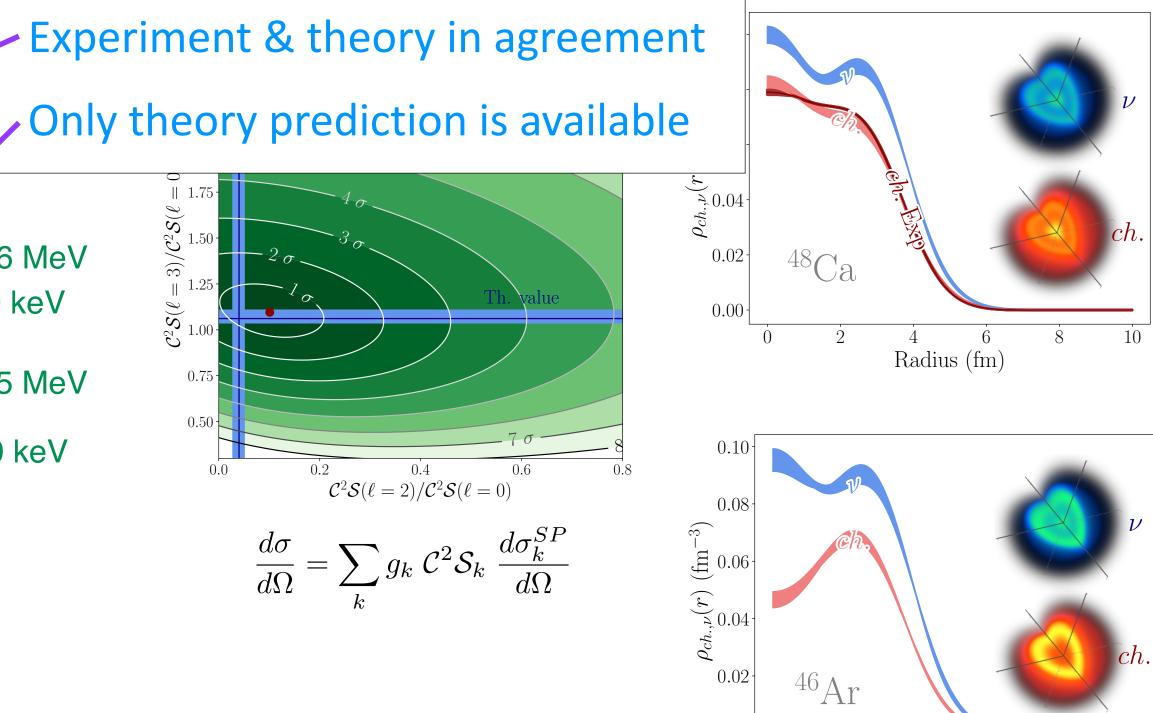
$$\Delta E_{1/2+-3/2+}$$
 (exp) = 5,55 MeV (theo) = 2,59 MeV

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



⁴⁶Ar(³He,d)⁴⁷K at GANIL: New charge bubble in ⁴⁶Ar





0.00

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

$$\Delta E_{1/2+-3/2+}$$
 (exp) = 5,55 MeV (theo) = 2,59 MeV

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



Radius (fm)

Nuclear Density Functional from Ab Initio Theory

See talk by G. Colò this morning

PHYSICAL REVIEW C 104, 024315 (2021)

Nuclear energy density functionals grounded in ab initio calculations

F. Marino, 1,2,* C. Barbieri, 1,2 A. Carbone, G. Colò, 1,2 A. Lovato, F. Pederiva, 5,5 X. Roca-Maza, 1,2 and E. Vigezzi

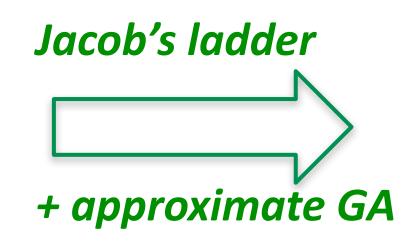
¹Dipartimento di Fisica "Aldo Pontremoli," Università degli Studi di Milano, 20133 Milano, Italy ²Istituto Nazionale di Fisica Nucleare, Sezione di Milano, 20133 Milano, Italy

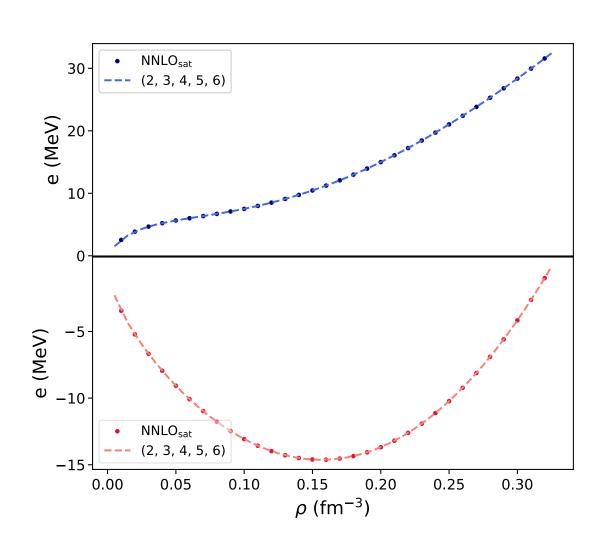
³Istituto Nazionale di Fisica Nucleare_CNAF Viale Carlo Rerti Pichat 6/2 40127 Rologna Italy



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





Benchmark in finite systems

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

F. Marino

(EPS PhD thesis

prize, 2025)

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

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





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

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

$$\rho = \frac{A}{I}$$

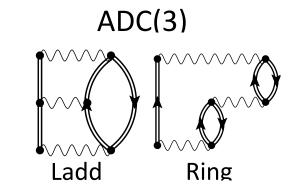
$$p_F = \sqrt[3]{\frac{6\pi^2\rho}{\nu_d}}$$

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

$$\Sigma^{11}(\omega) = \Sigma^{11(\infty)} + \tilde{\Sigma}(\omega)$$



$$\mathsf{ADC(3)} \text{ self energy:} \qquad \varSigma_{\alpha\beta}^{(\star)}(\omega) = -U_{\alpha\beta} \; + \; \varSigma_{\alpha\beta}^{(\infty)} \; + \; M_{\alpha,r}^{\dagger} \left[\frac{1}{\omega - [E^{>} + C]_{r,r'} + i\eta} \right]_{r,r'} M_{r',\beta} \; + N_{\alpha,s} \left[\frac{1}{\omega - (E^{<} + D) - i\eta} \right]_{s,s'} N_{s',\beta}^{\dagger}$$



Gorkov superfluid

formulation (at 1st order)

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

Normal self-energy

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

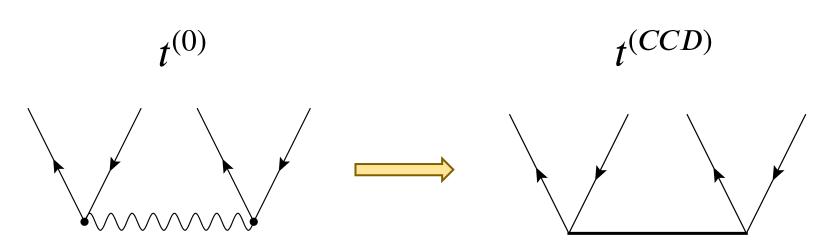
Extension of ADC(3)



ADC(3)-D

In
$$\widetilde{\Sigma}(\omega)$$
, replace $t^{(0)}$ with converged T_2 amplitudes $(t^{(0)})_{ij}^{ab} = \frac{\langle ab|v|ij\rangle_A}{\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b}$

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



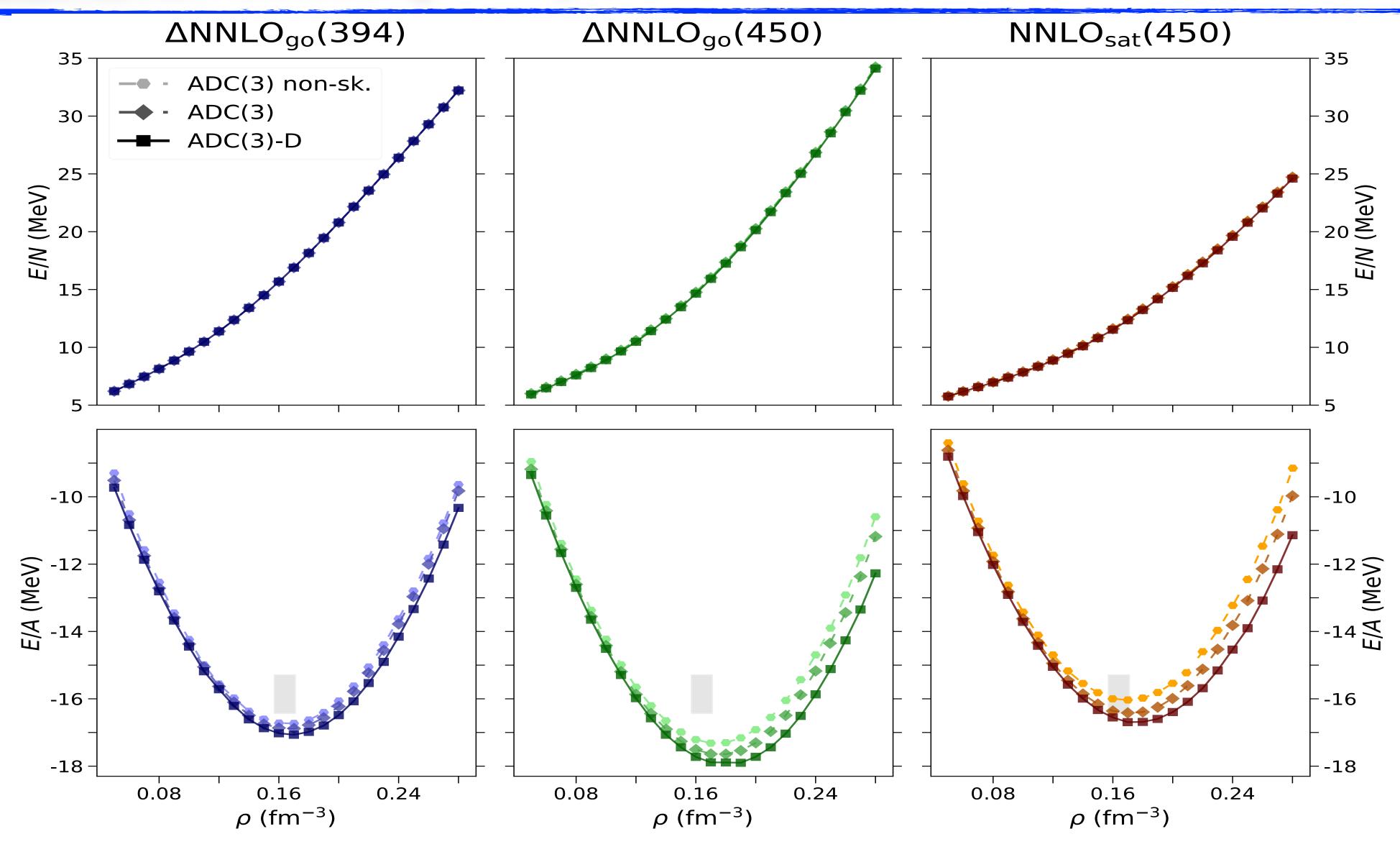
Somà et al., Phys. Rev. C 84, 064317 (2011) Raimondi et al., Phys Rev C 97, 054308 (2018) Barbieri et al., Lect. Notes Phys. 936, 571 (2017) - Ch 11 Barbieri et al., Phys. Rev. C **105**, 044330 (2022)

F. Marino, CB, and G. Colò, arXiv:2510.xxx, to be submitted

Pairing field



Equations of state (T=0)

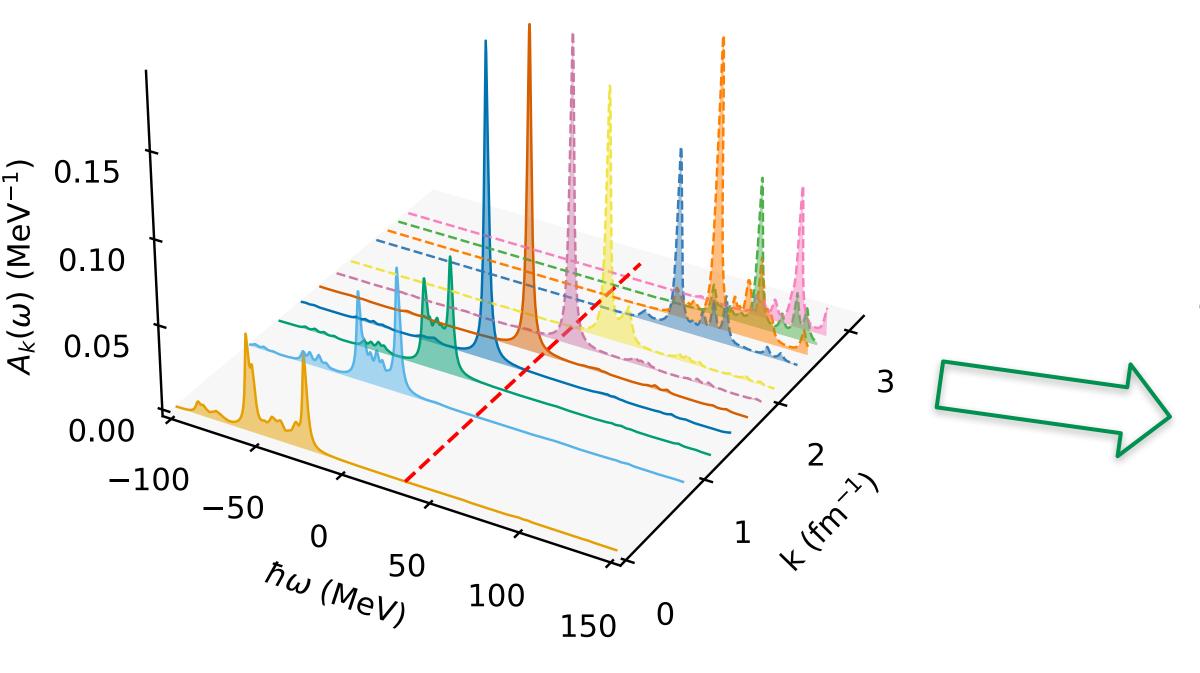






Removing finite size effects - Twisted Angle BC

Ordinary PBC

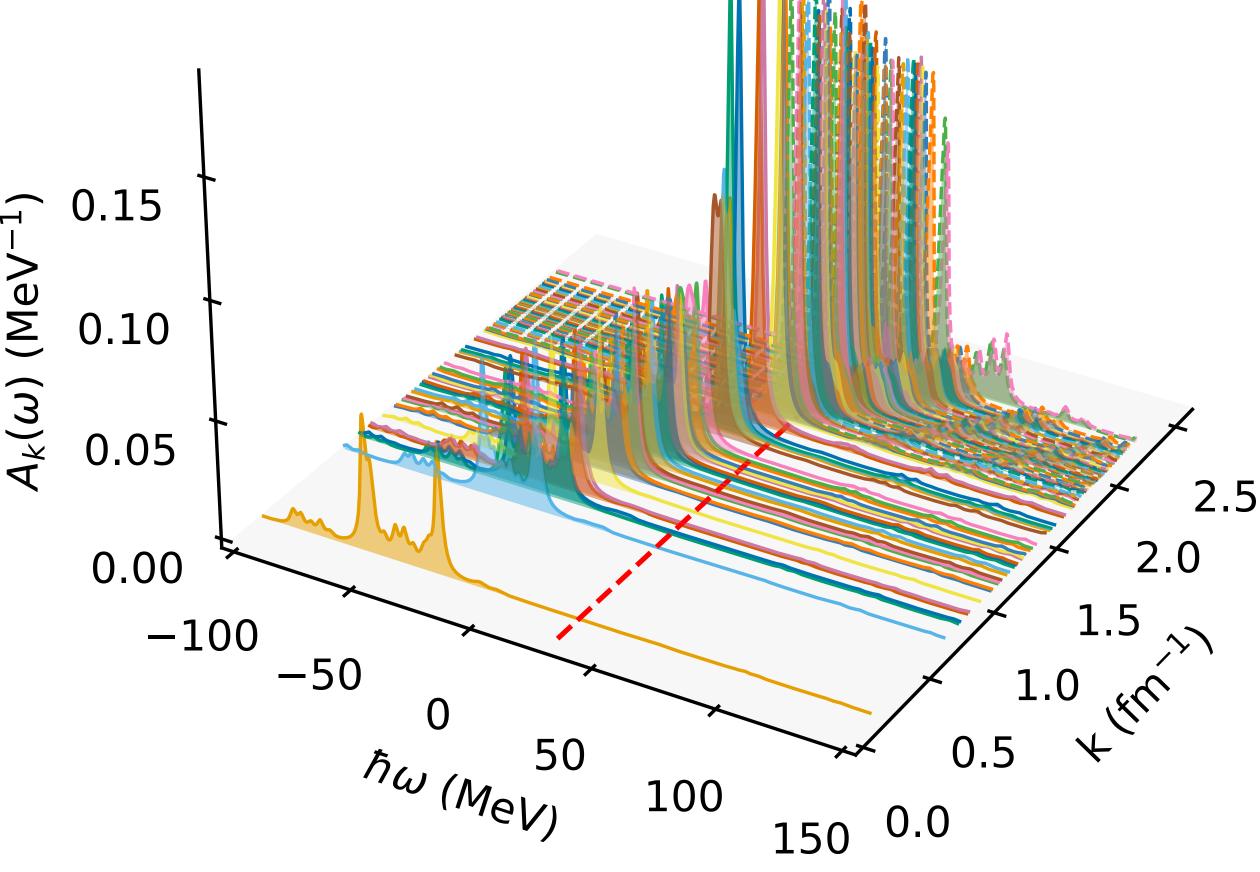


$$S^{p}(\mathbf{p},\omega) = \sum_{n} \left| \langle \Psi_{n}^{A+1} | \psi_{\mathbf{p}}^{\dagger} | \Psi_{0}^{A} \rangle \right|^{2} \delta \left(\hbar \omega - (E_{n}^{A+1} - E_{0}^{A}) \right)$$

$$S^{h}(\mathbf{p},\omega) = \sum_{k} \left| \langle \Psi_{k}^{A-1} | \psi_{\mathbf{p}} | \Psi_{0}^{A} \rangle \right|^{2} \delta \left(\hbar \omega - (E_{0}^{A} - E_{k}^{A-1}) \right)$$

Sp-TABC: chose just one set of twisted angles

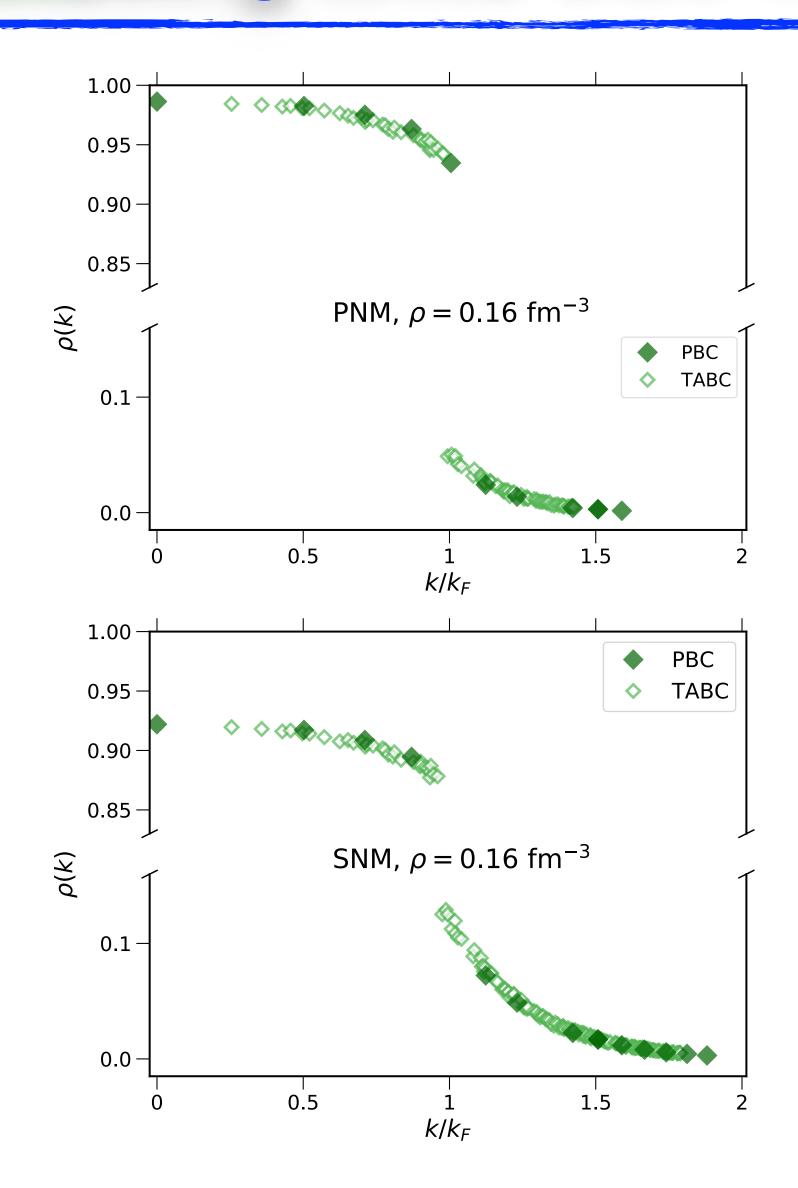
- Finer resolution in momenta
- Better description of the thermodynamic Limit

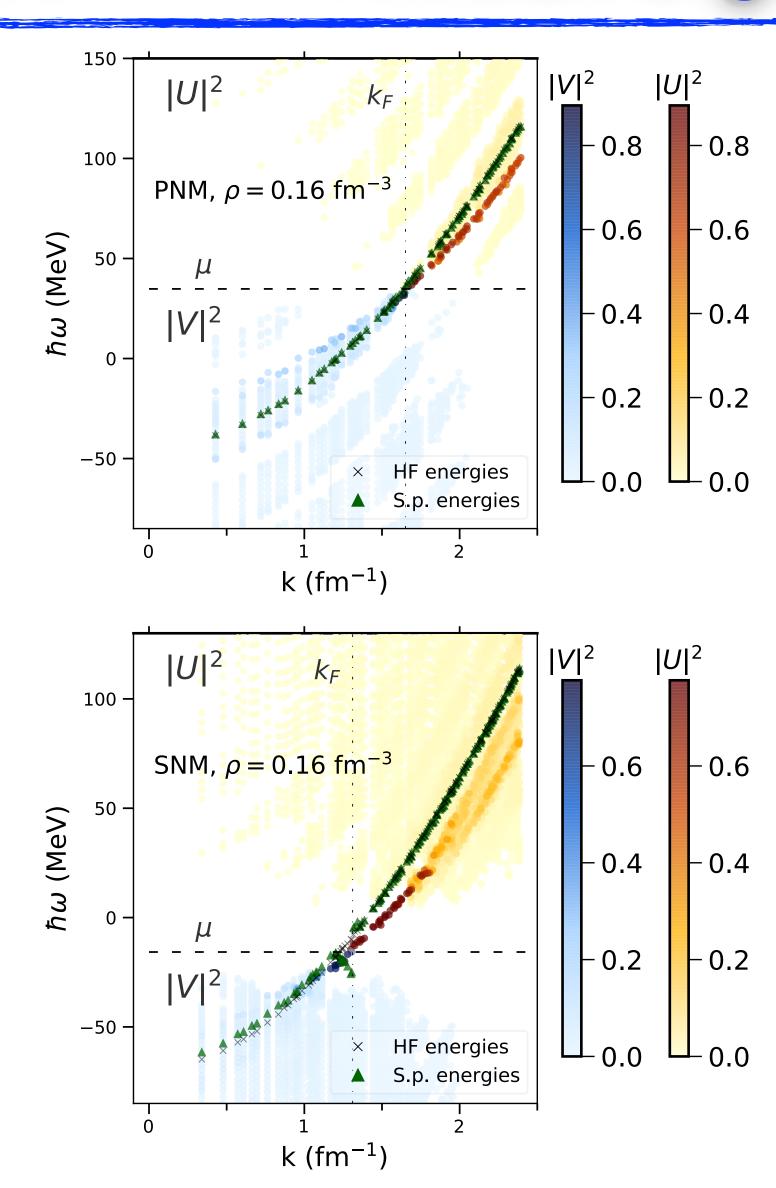






Removing finite size effects - Twisted Angle BC



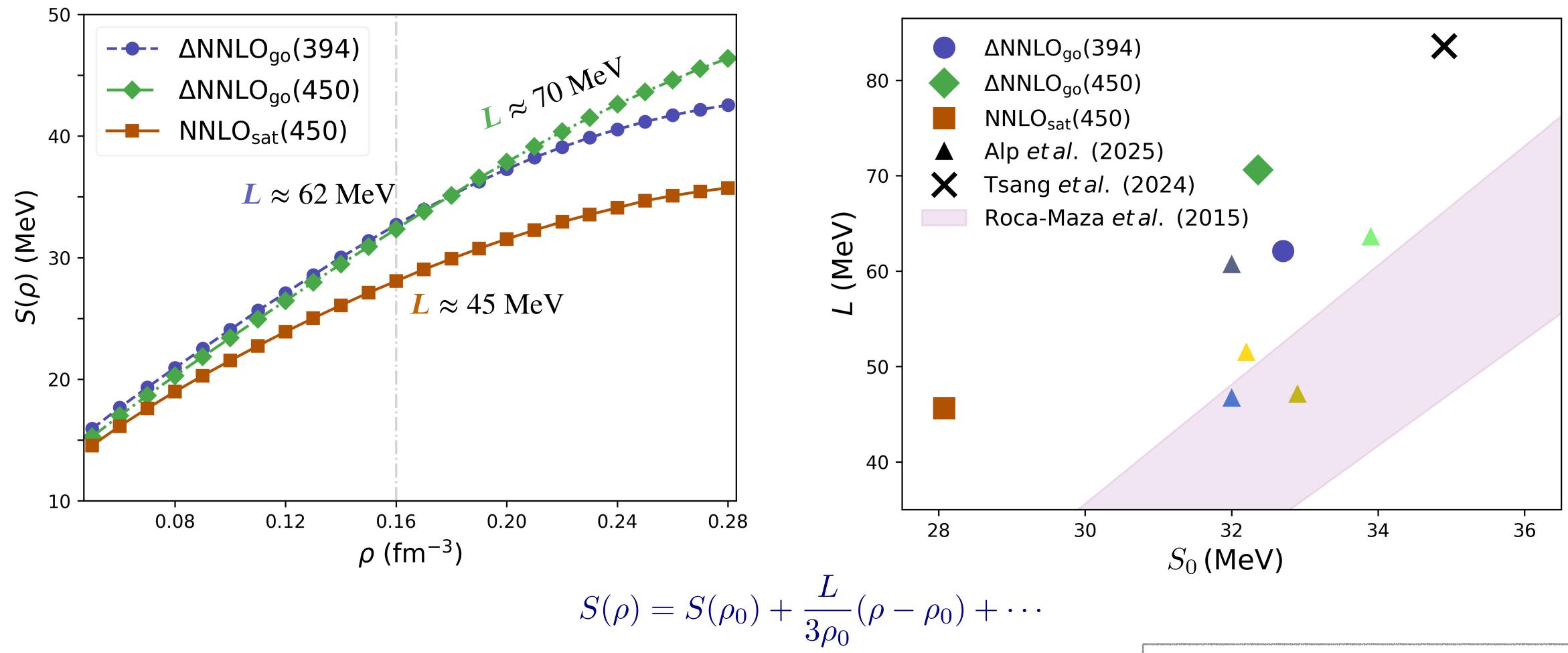


 $\Delta NNLO_{go}(450)$





Symmetry energy



F. Marino, CB, and G. Colò, arXiv:2510.xxx, to be submitted.



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)

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Upcoming 23rd conference on "Recent Progress in MAny-Body Theory" RPMBT-XXIII

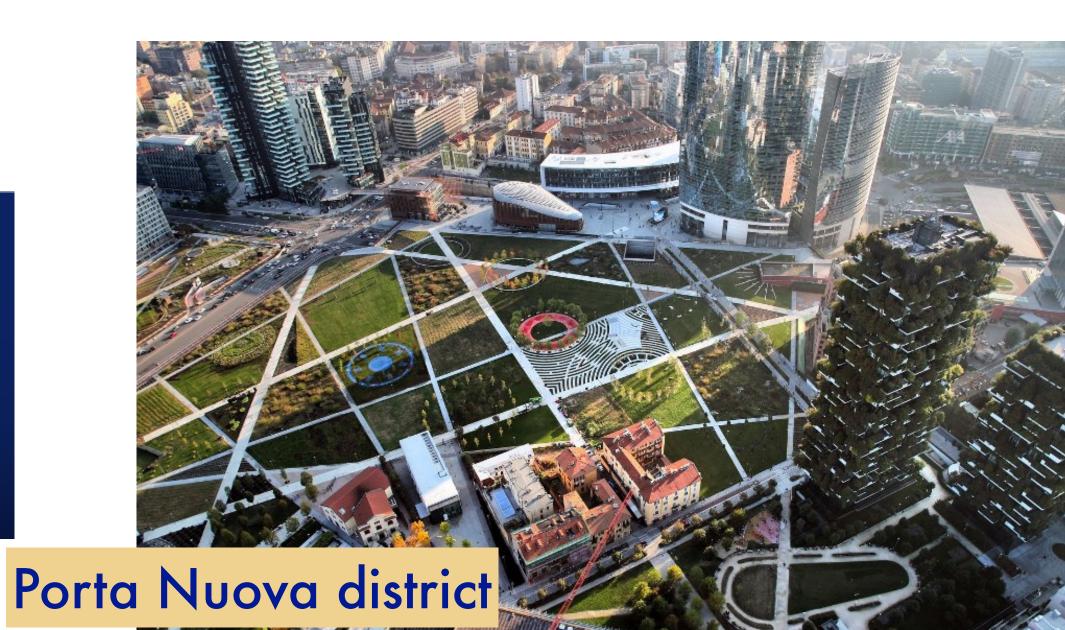
Milan, Italy:

14-18 Sept 2026 (main event)

9-11 Sept. (satellite school on QC)









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Thank you for your attention !!!



