Ab initio computations of the nuclear spectral function

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Probing exotic structure of short-lived nuclei by electron scattering

ECT* Trento
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Collaborators:
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Outline

- **Introduction**
- **Calculation set-up**
  - Many-body method: self-consistent Green's functions
  - Hamiltonian
- **Results**
  - Ground-state properties
  - Spectral function
- **Conclusions**

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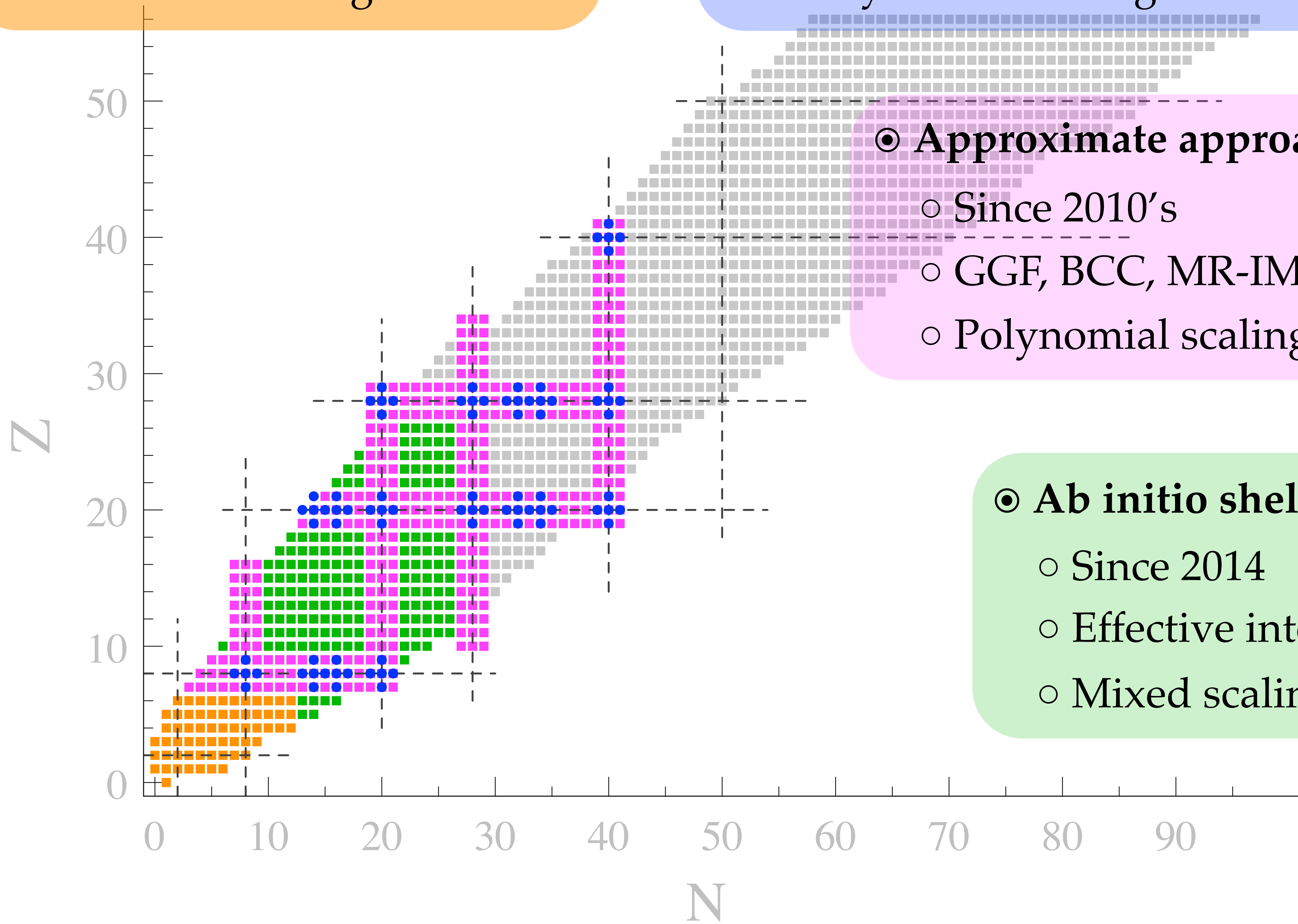
Evolution of ab initio nuclear chart

- **"Exact" approaches**
  - Since 1980's
  - Monte Carlo, CI, …
  - Factorial scaling

- **Approximate approaches for closed-shell nuclei**
  - Since 2000's
  - SCGF, CC, IMSRG
  - Polynomial scaling

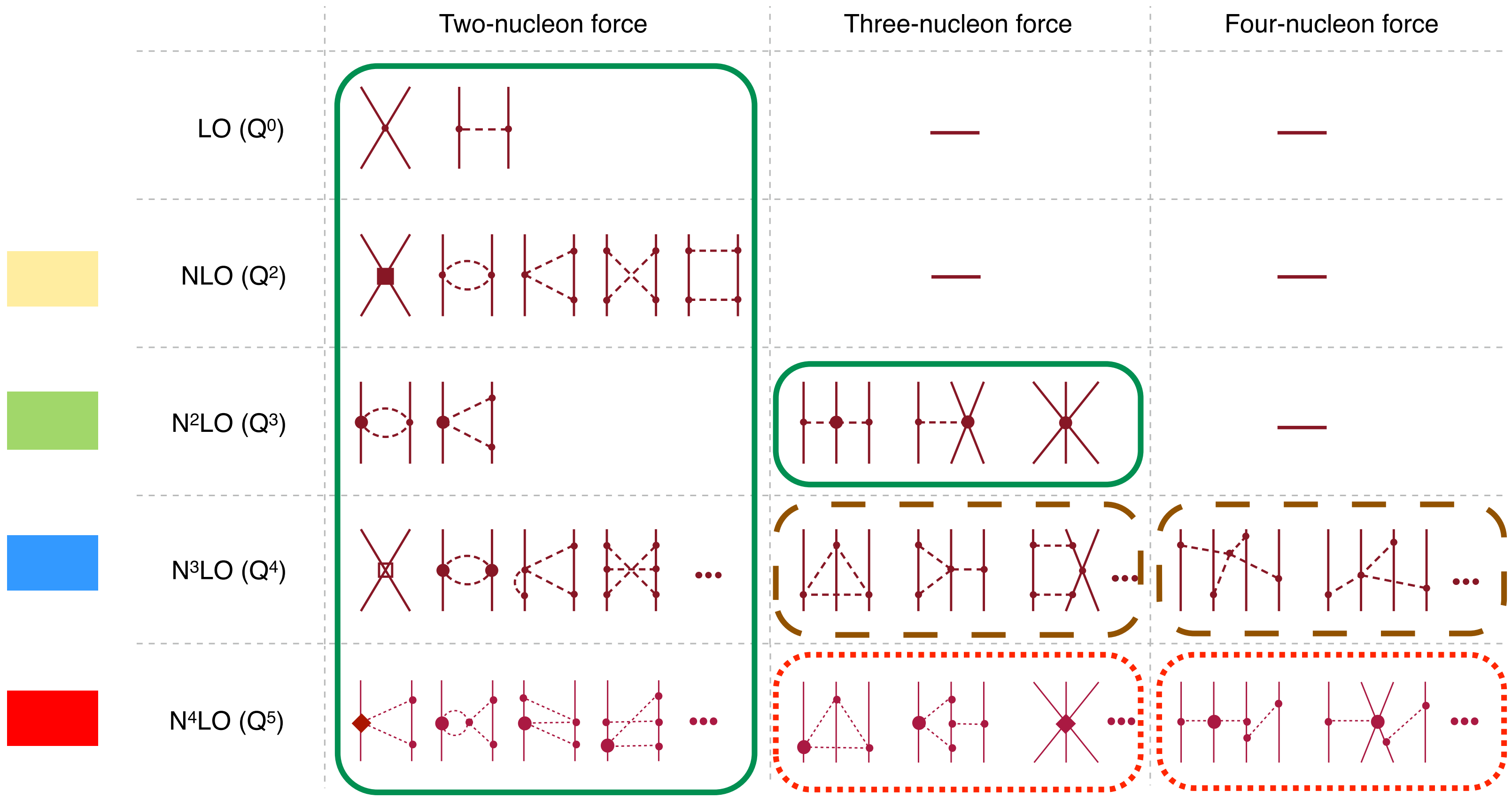


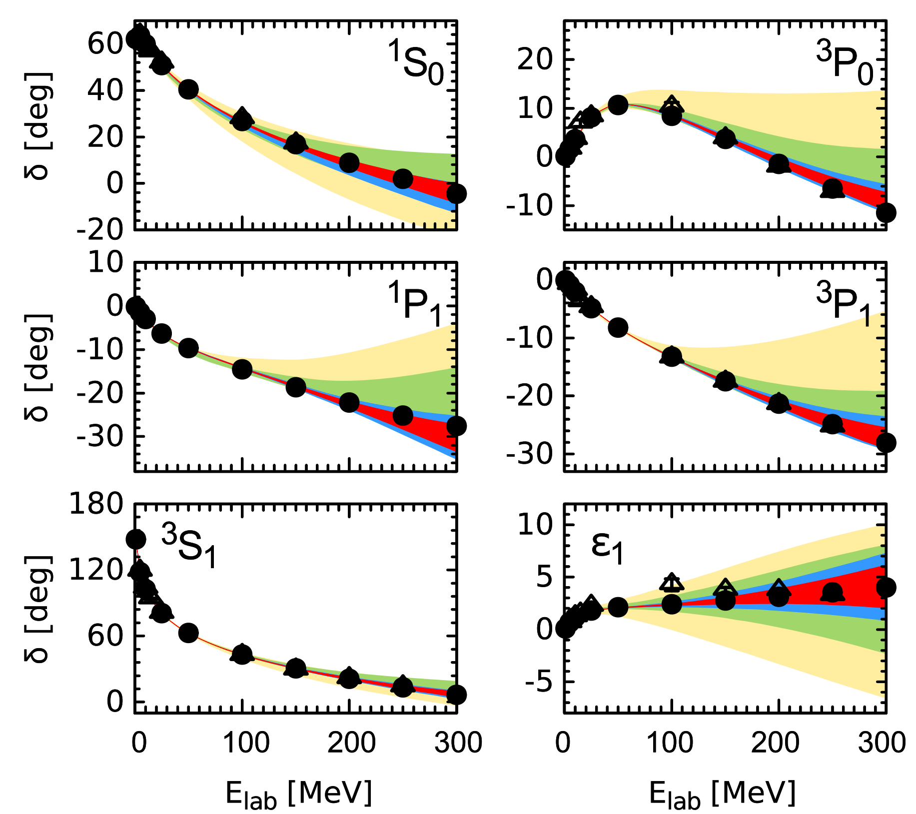
- **Approximate approaches for open-shells**
  - Since 2010's
  - GGF, BCC, MR-IMSRG
  - Polynomial scaling

- **Ab initio shell model**
  - Since 2014
  - Effective interaction via CC/IMSRG
  - Mixed scaling

Chiral effective field theory & nuclear interactions

- Chiral EFT provides a **systematic** framework to construct AN interactions (A=2, 3, …)
- Main features:
  - High-energy physics unresolved → **soft potentials** → improved many-body convergence
  - Many-body forces and currents consistently derived
  - A **theoretical error** can be, in principle, assigned to each order in the expansion



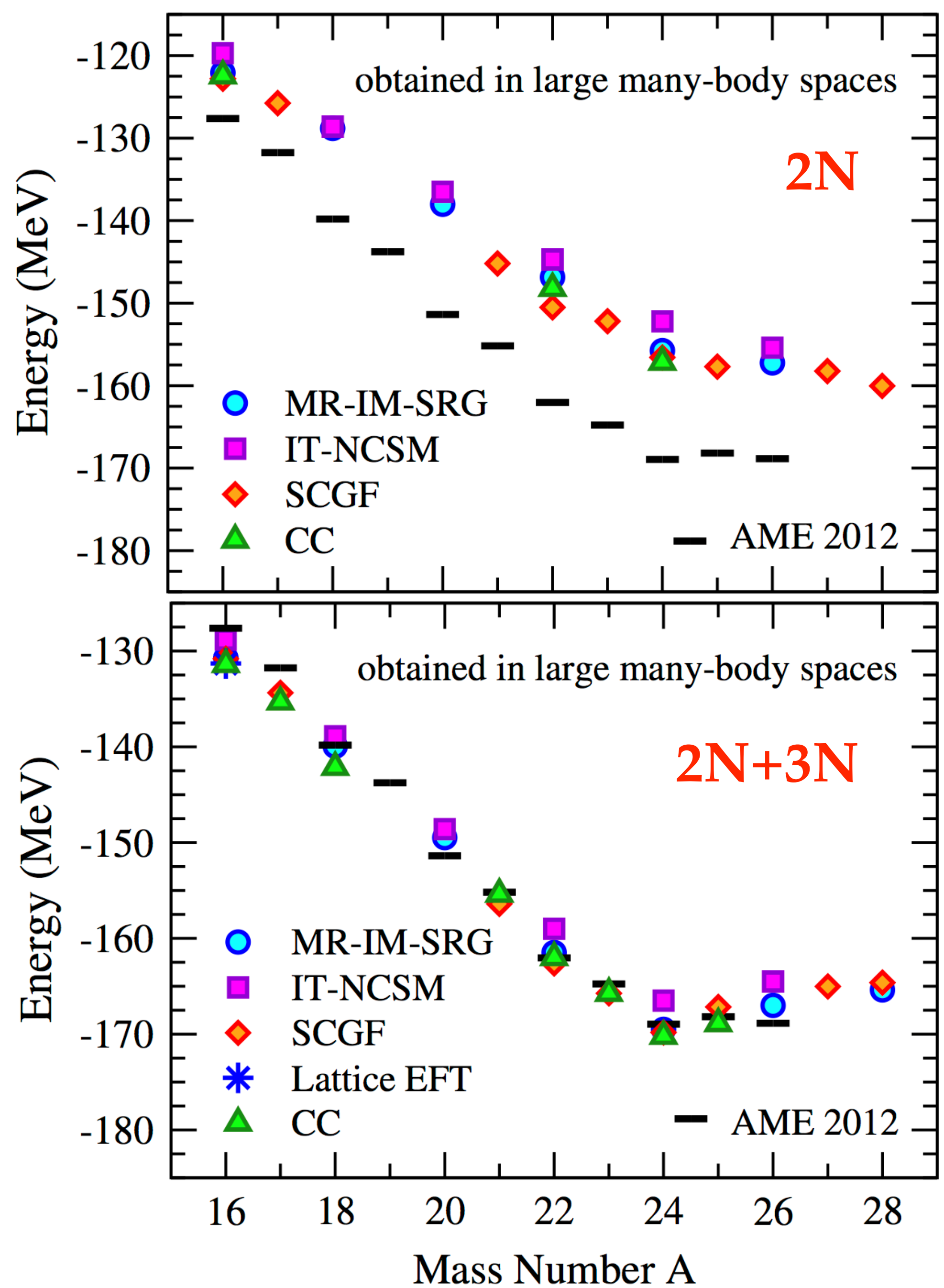


[Meißner 2016]

➪ **Ideally: apply to the many-nucleon system (and propagate the theoretical error)**

Benchmarks and diagnostics

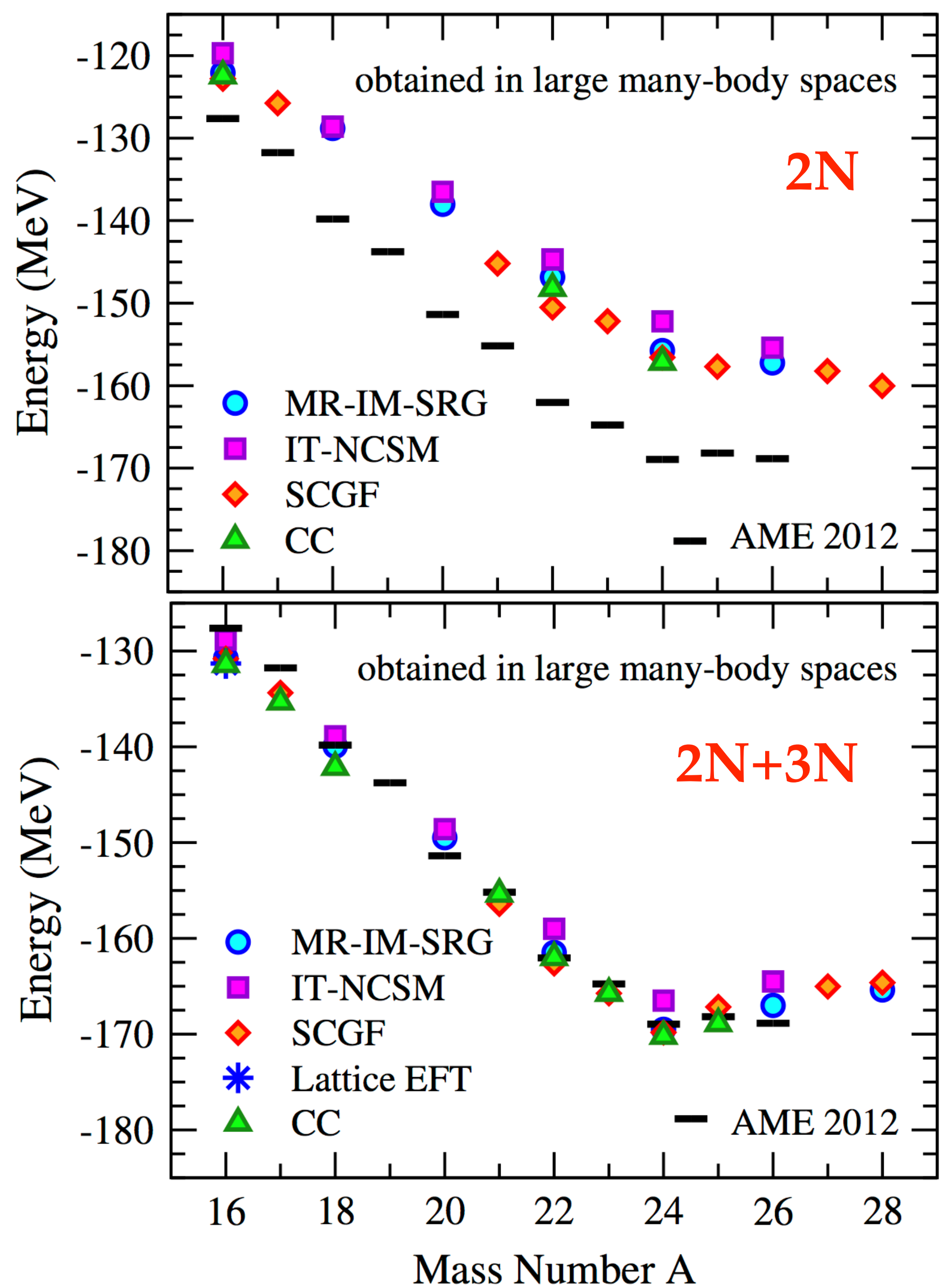
Benchmark between various methods



[Hebeler *et al.* 2015]

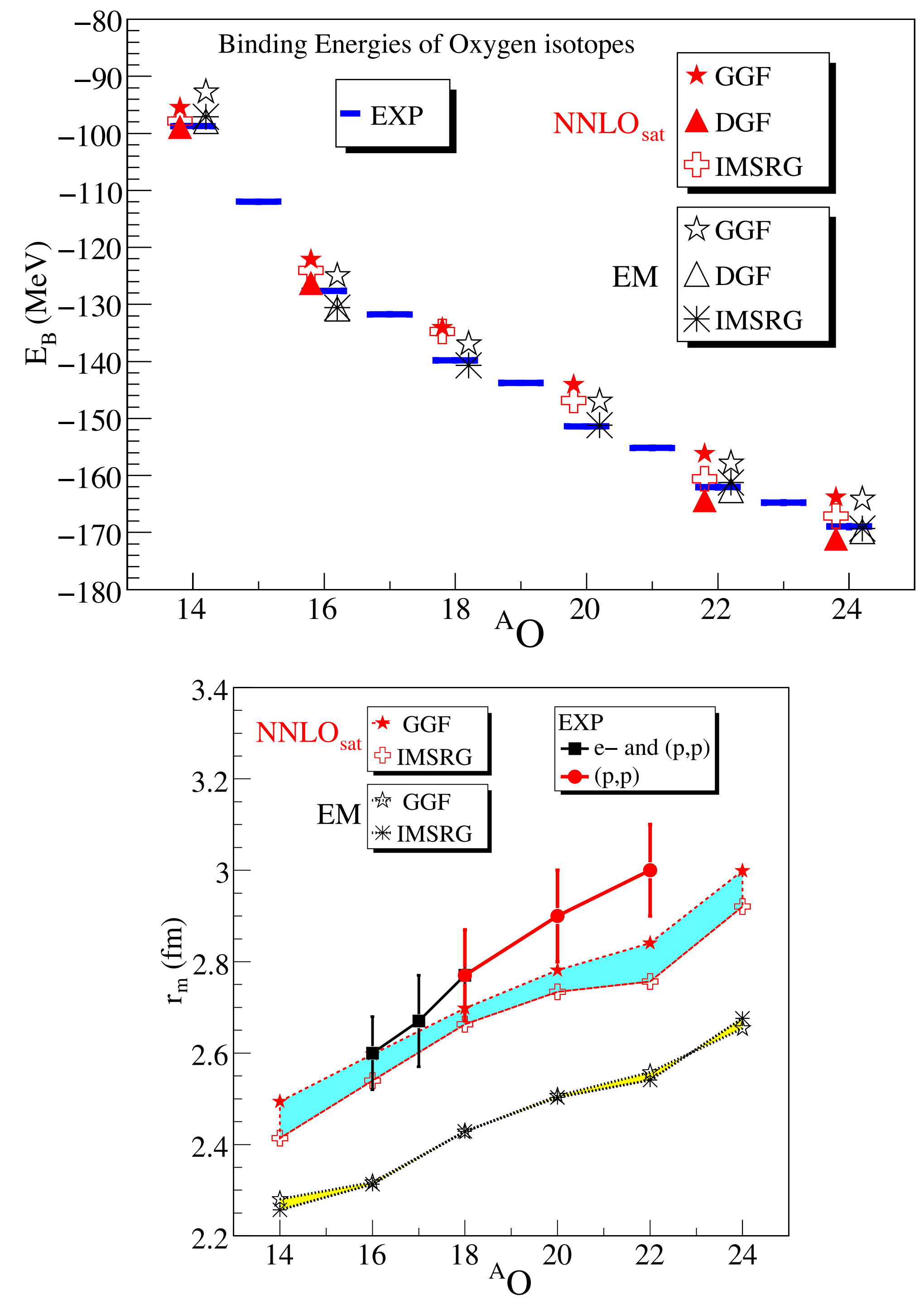
Benchmarks and diagnostics

Benchmark between various methods



[Hebeler *et al.* 2015]

Diagnostics of nuclear interactions



[Lapoux *et al.* 2016]

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Self-consistent Green's function approach

⊙ **Solution of the *A*-body Schrödinger equation** $H|\Psi_k^A\rangle = E_k^A|\Psi_k^A\rangle$ **achieved by**

1) Rewriting it in terms of **1-, 2-, …. *A*-body objects** $G_1{=}G$, G_{2}, … G_A (**Green's functions**)

2) Expanding these objects in perturbation (in practise **G** ➟ **one-body observables**, etc..)

- **Self-consistent** schemes resum (infinite) subsets of perturbation-theory contributions

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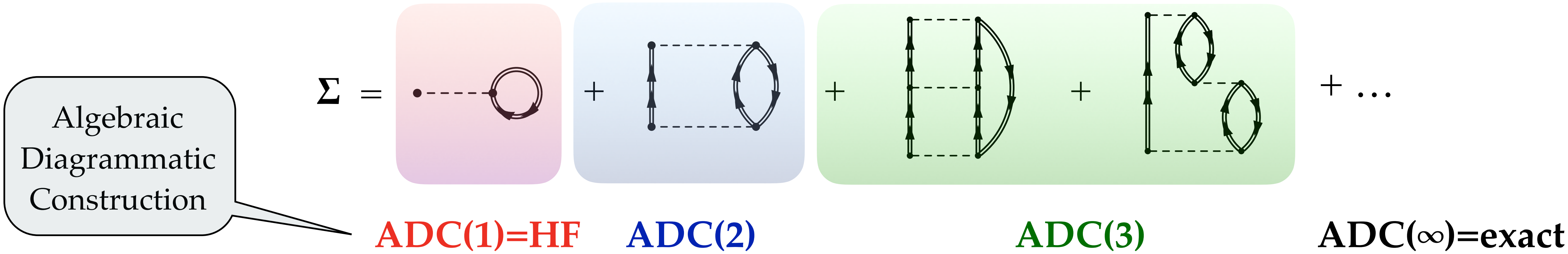
⊙ **Self-energy expansion**



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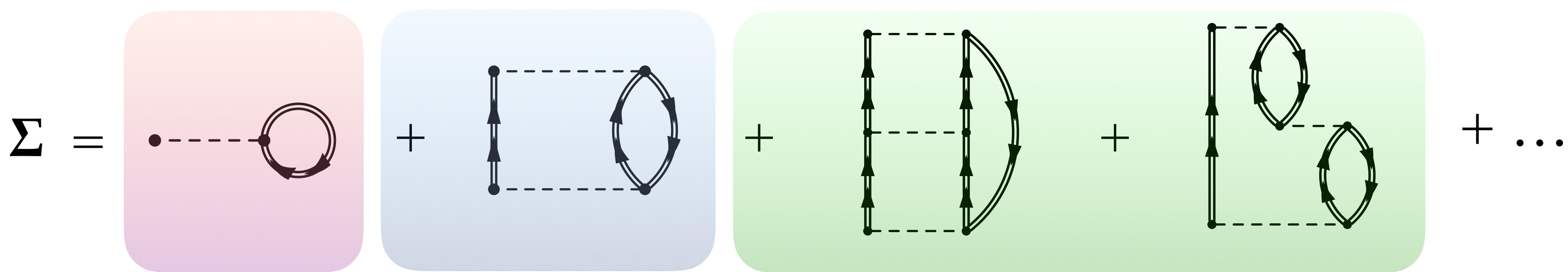
⦿ **Self-energy expansion**

Algebraic Diagrammatic Construction



ADC(1)=HF ADC(2) ADC(3) ADC(∞)=exact

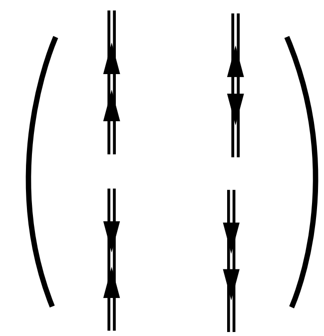
⦿ **Access a variety of quantities**

○ One-body GF → Ground-state properties of even-even A + spectra of odd-even neighbours

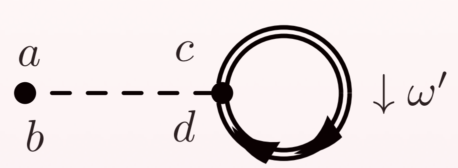
○ Two-body GF → Excited spectrum of even-even A

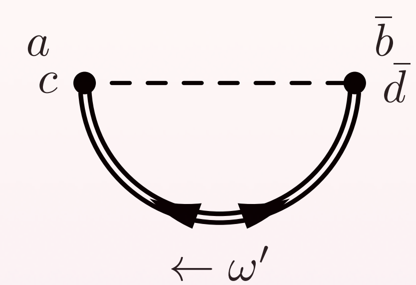
○ Self-energy → Optical potential for nucleon-nucleus scattering

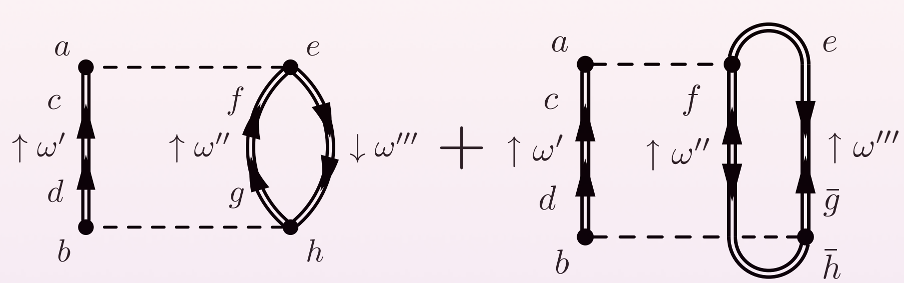
Gorkov-Green's functions for open-shell systems

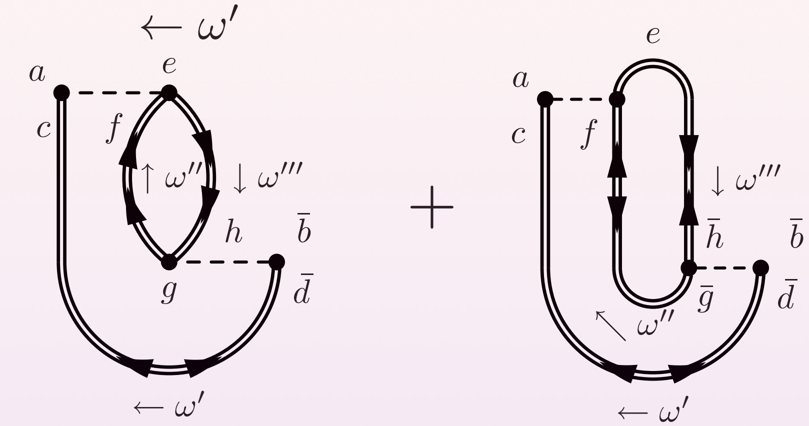
- Standard expansion schemes fail to account for superfluidity
- **Gorkov scheme generalises GF theory to superfluid systems** [Gorkov 1958]
  - Use **symmetry breaking** (particle number) to effectively include pairing correlations
  - Start expansion from symmetry-breaking reference $|\Psi_0\rangle \equiv \sum_{A}^{\text{even}} c_A \, |\psi_0^A\rangle$
  - 4 one-body Gorkov propagators $\mathbf{G}_{ab} = \begin{pmatrix} G^{11}_{ab} & G^{12}_{ab} \\ G^{21}_{ab} & G^{22}_{ab} \end{pmatrix} =$ 
  - Symmetry must be eventually restored

- **Current implementation: ADC(2)** [Somà, Duguet & Barbieri 2011]

$\Sigma^{11\,(1)}_{ab} =$ 

$\Sigma^{12\,(1)}_{ab} =$ 

$\Sigma^{11\,(2)}_{ab}(\omega) =$ 

$\Sigma^{12\,(2)}_{ab}(\omega) =$ 

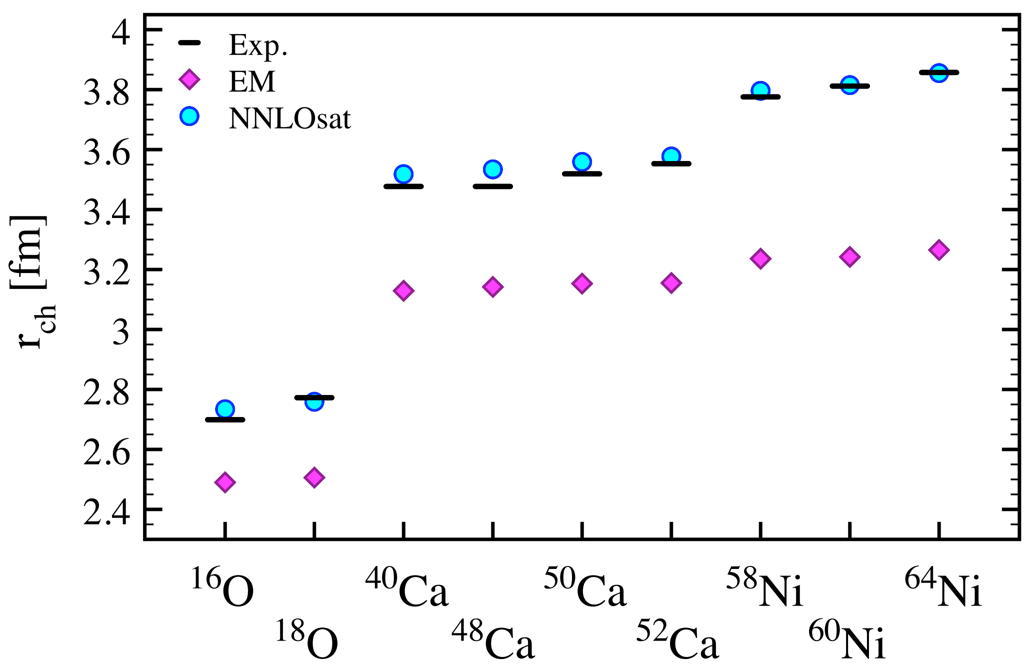
NNLO$_{\text{sat}}$ interaction

- **Development of a new ChEFT-inspired Hamiltonian: NNLO$_{\text{sat}}$**
  - Simultaneous fit of low-energy constants in 2- and 3-body sectors
  - Data from light nuclei included in fit of low-energy constants

[Ekström *et al.* 2015]

TABLE I. Binding energies (in MeV) and charge radii (in fm) for ^{3}H, ^{3,4}He, ^{14}C, and ^{16,22,23,24,25}O employed in the optimization of NNLO$_{\text{sat}}$.

	$E_{\text{g.s.}}$	Expt. [69]	r_{ch}	Expt. [65,66]
^{3}H	8.52	8.482	1.78	1.7591(363)
^{3}He	7.76	7.718	1.99	1.9661(30)
^{4}He	28.43	28.296	1.70	1.6755(28)
^{14}C	103.6	105.285	2.48	2.5025(87)
^{16}O	124.4	127.619	2.71	2.6991(52)
^{22}O	160.8	162.028(57)		
^{24}O	168.1	168.96(12)		
^{25}O	167.4	168.18(10)		



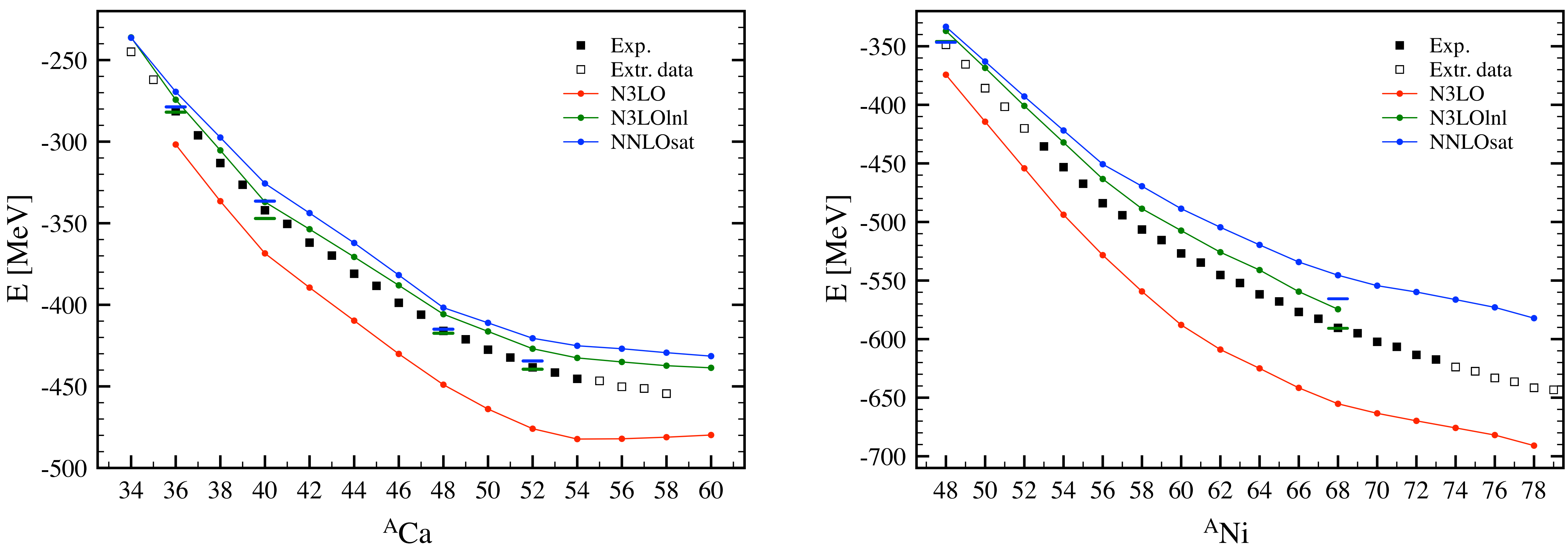
[Somà, *et al.* unpublished]

- **Generated debate in the community**
  - Ab initio philosophy?
  - EFT philosophy?
  - Which data should we use to fix the parameters of the interaction?
  - *Optimistic* view: NNLO$_{\text{sat}}$ indicates that ChEFT strategy is feasible

N3LO *NN* + 3*N* (LNL) interaction

⦿ **Novel version of the 'standard' N3LO interaction**

- ○ "Local/nonlocal" (LNL) regulators [Navrátil 2018]
- ○ Follows traditional ab initio strategy (fit *X*-body sector on *X*-body data)



[Somà, *et al.* in preparation]

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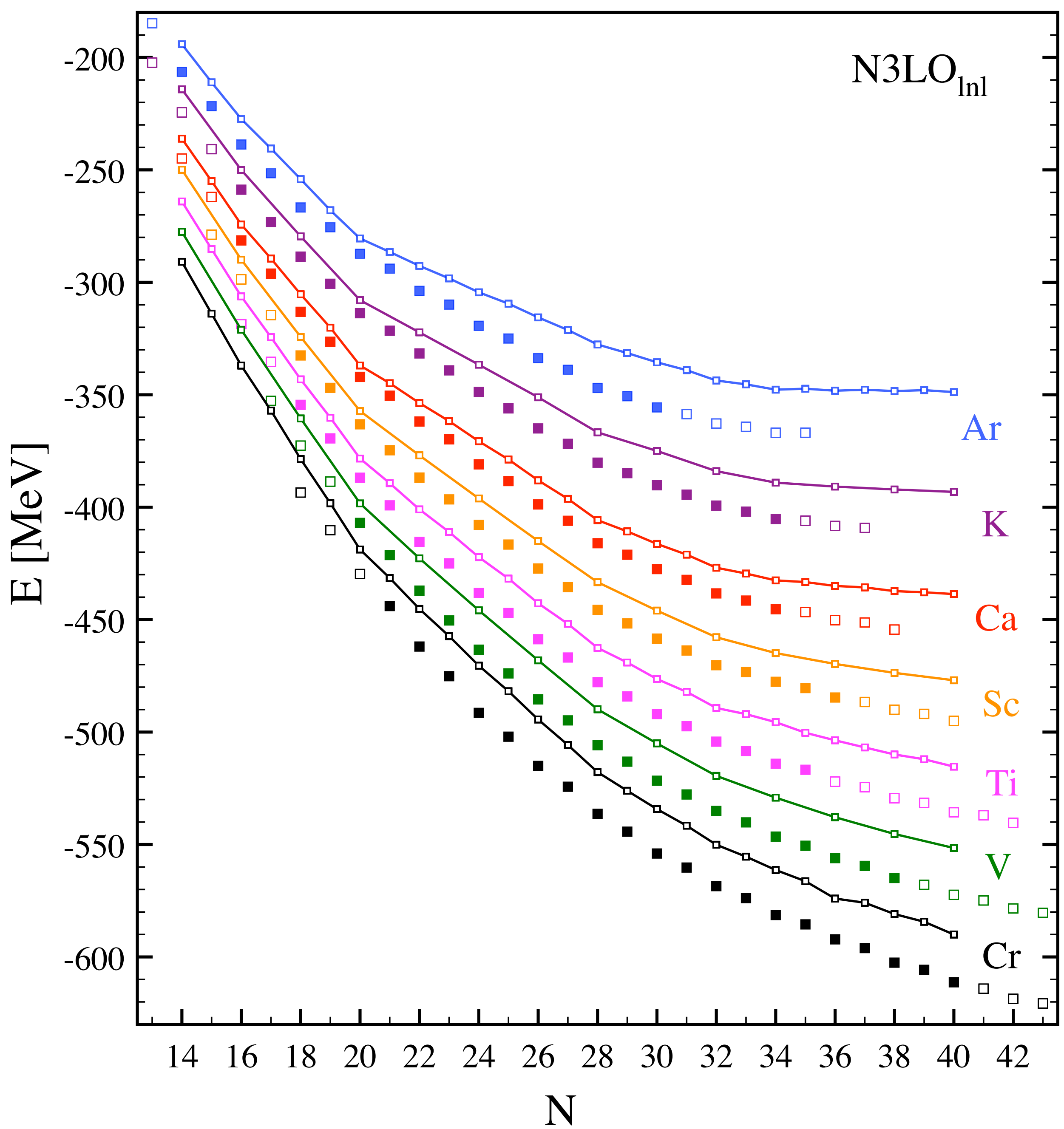
Systematics in mid-mass nuclei

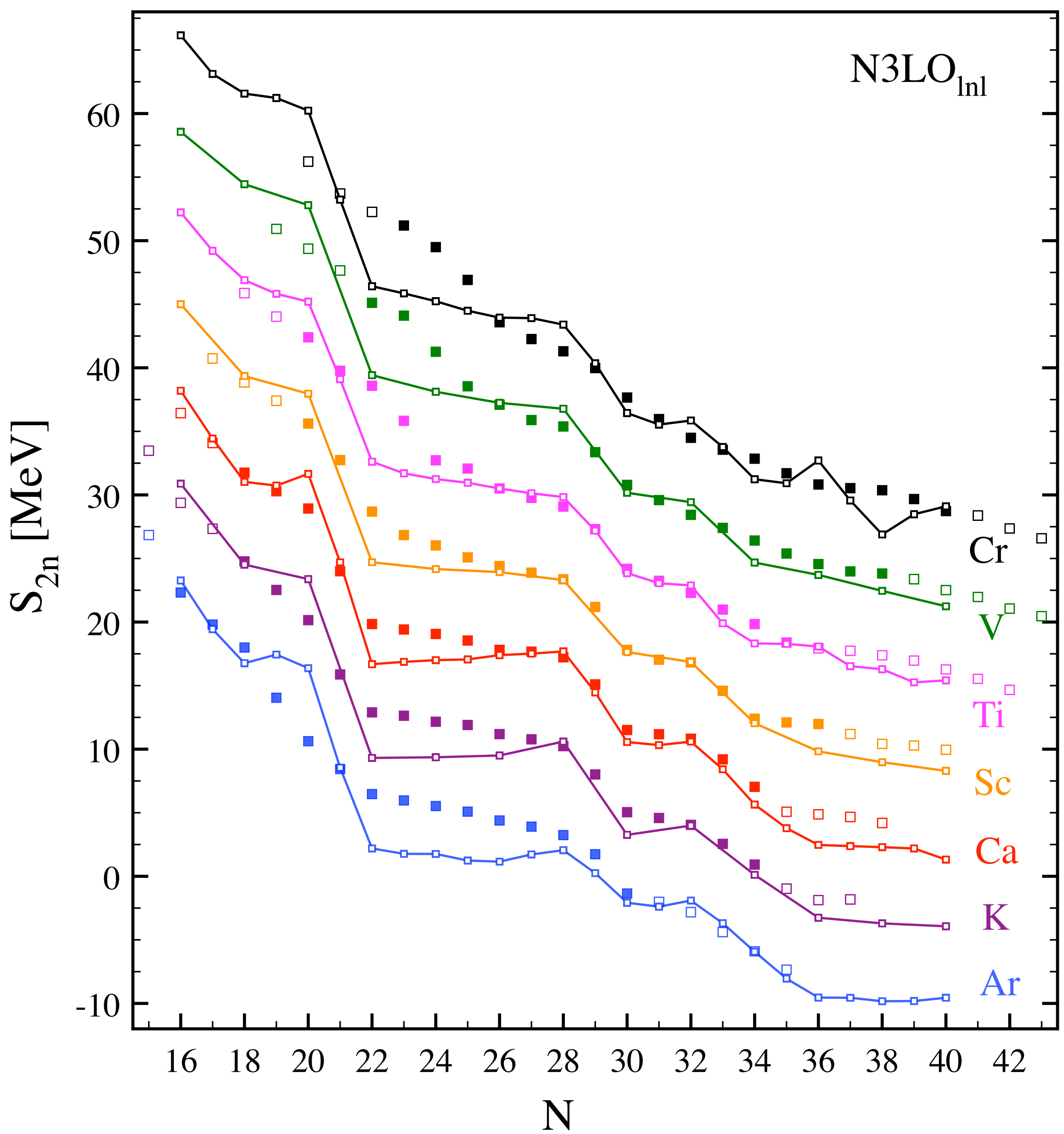
- **Systematic investigation of *Z*=18-24 region**



Binding energies

Systematics in mid-mass nuclei

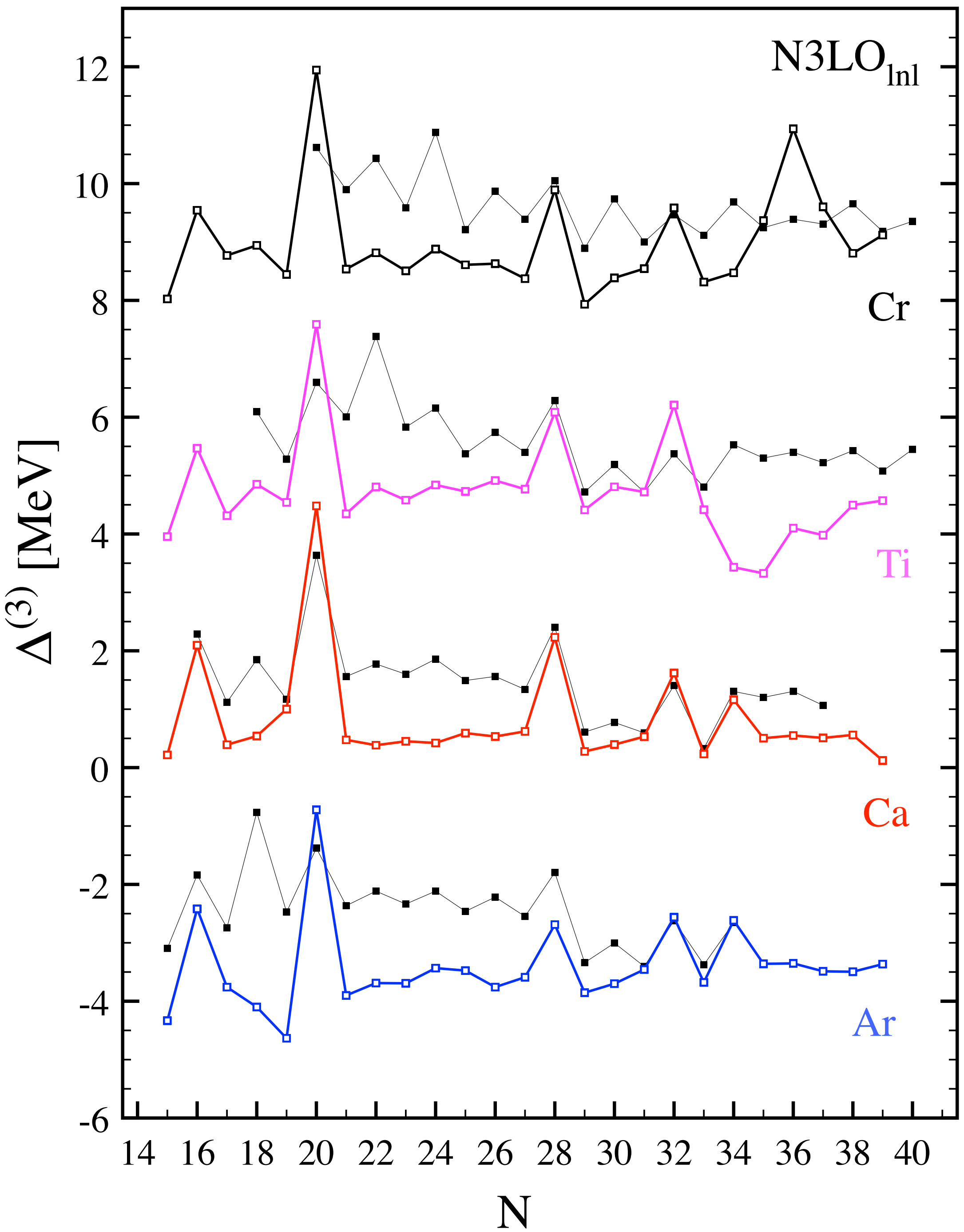
⦿ **Systematic investigation of *Z*=18-24 region**



Two-neutron separation energies

Systematics in mid-mass nuclei

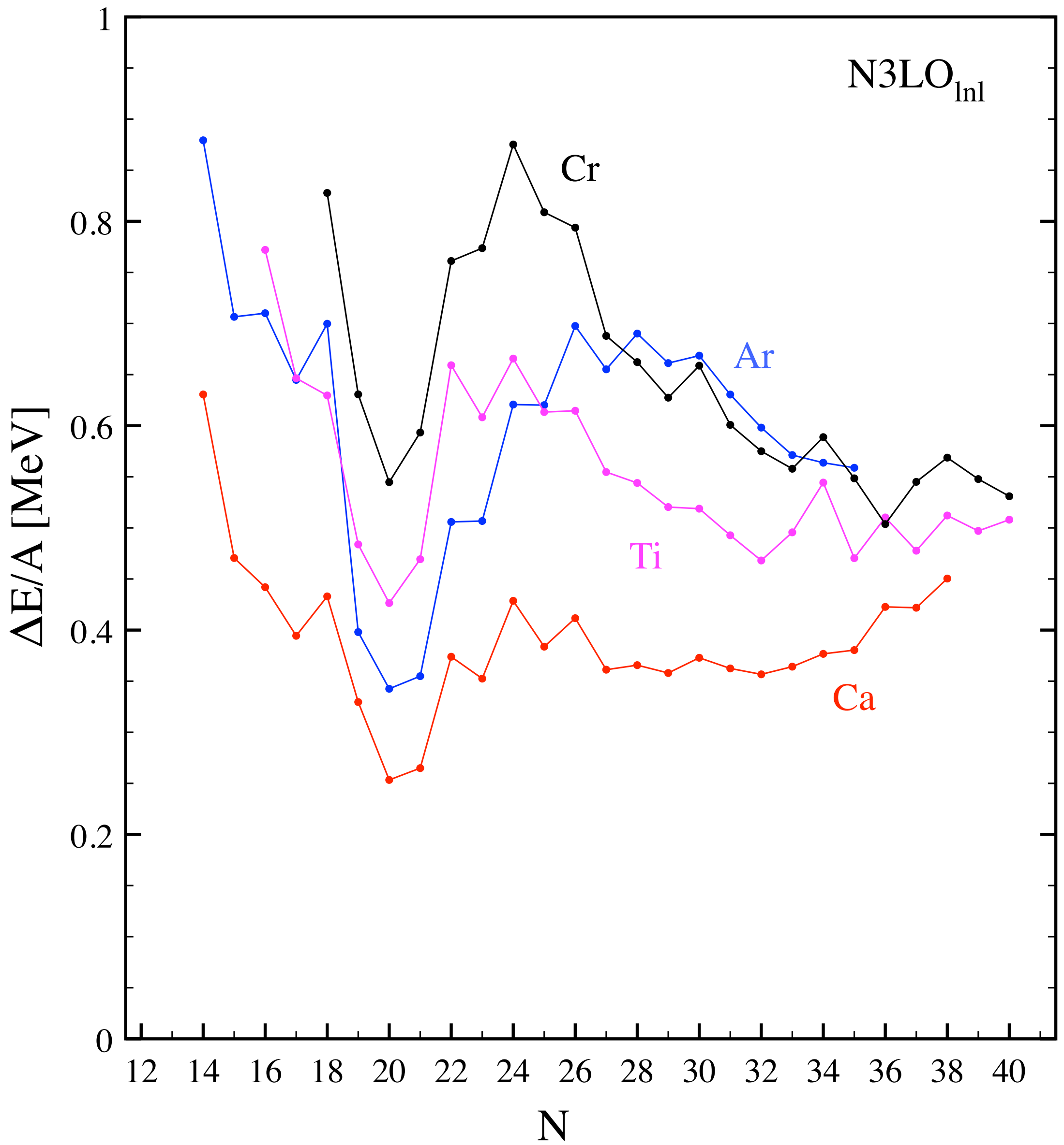
- **Systematic investigation of *Z*=18-24 region**



Three-point mass differences

Doubly open-shell nuclei

⊙ **Currently, description of doubly open-shell nuclei quantitatively worsens with deformation**



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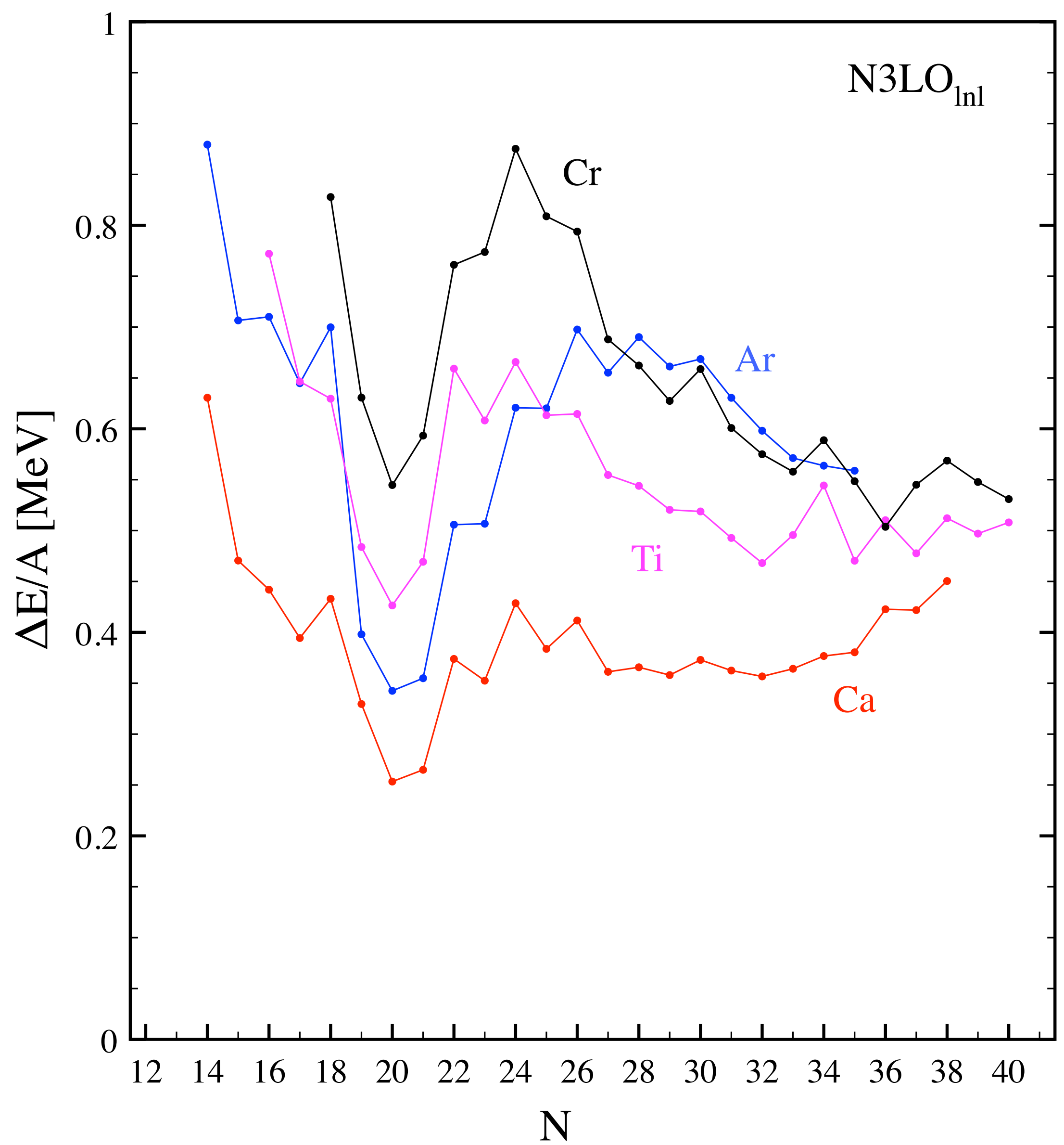
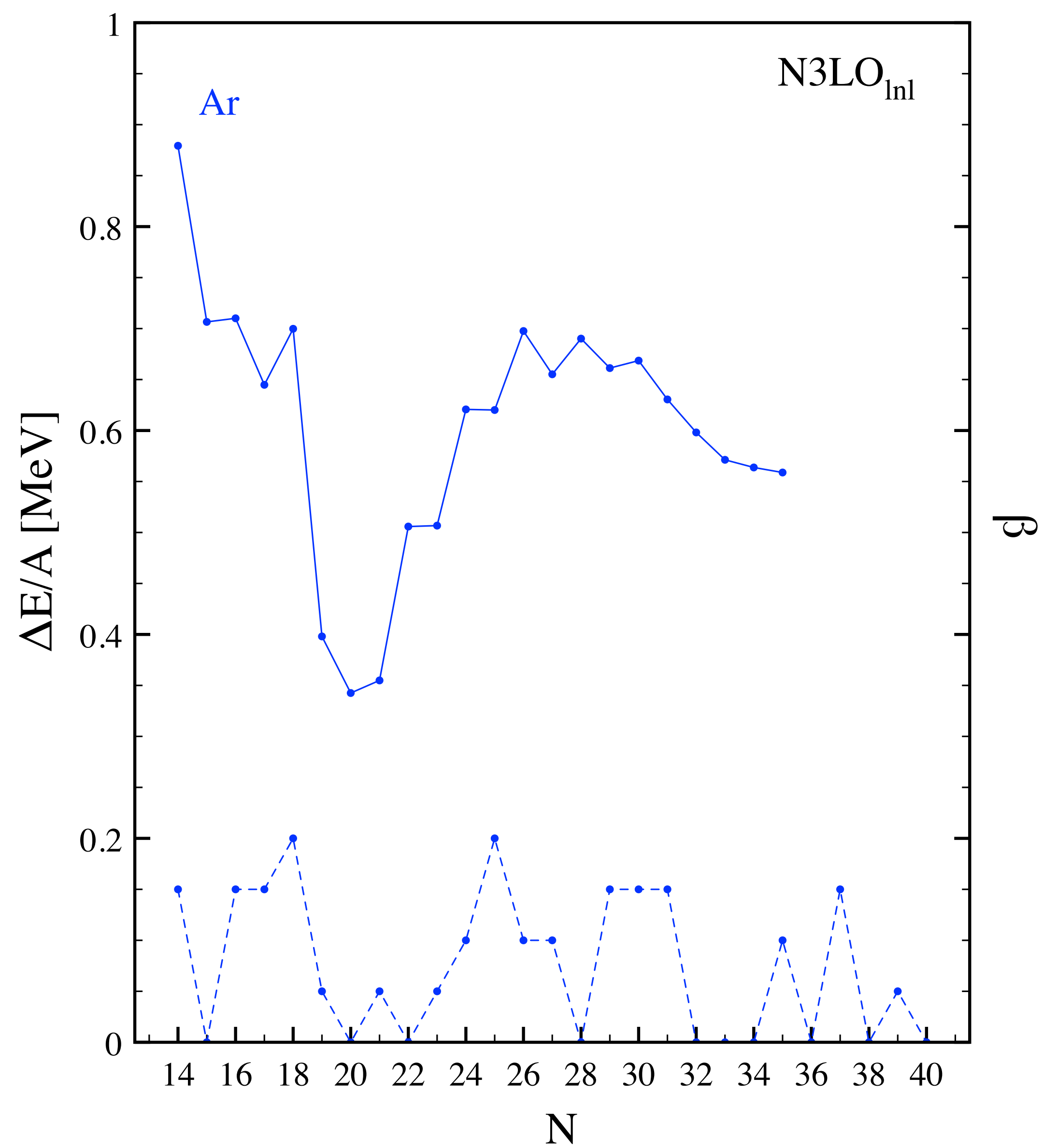
➪ Correlation with deformation parameter β





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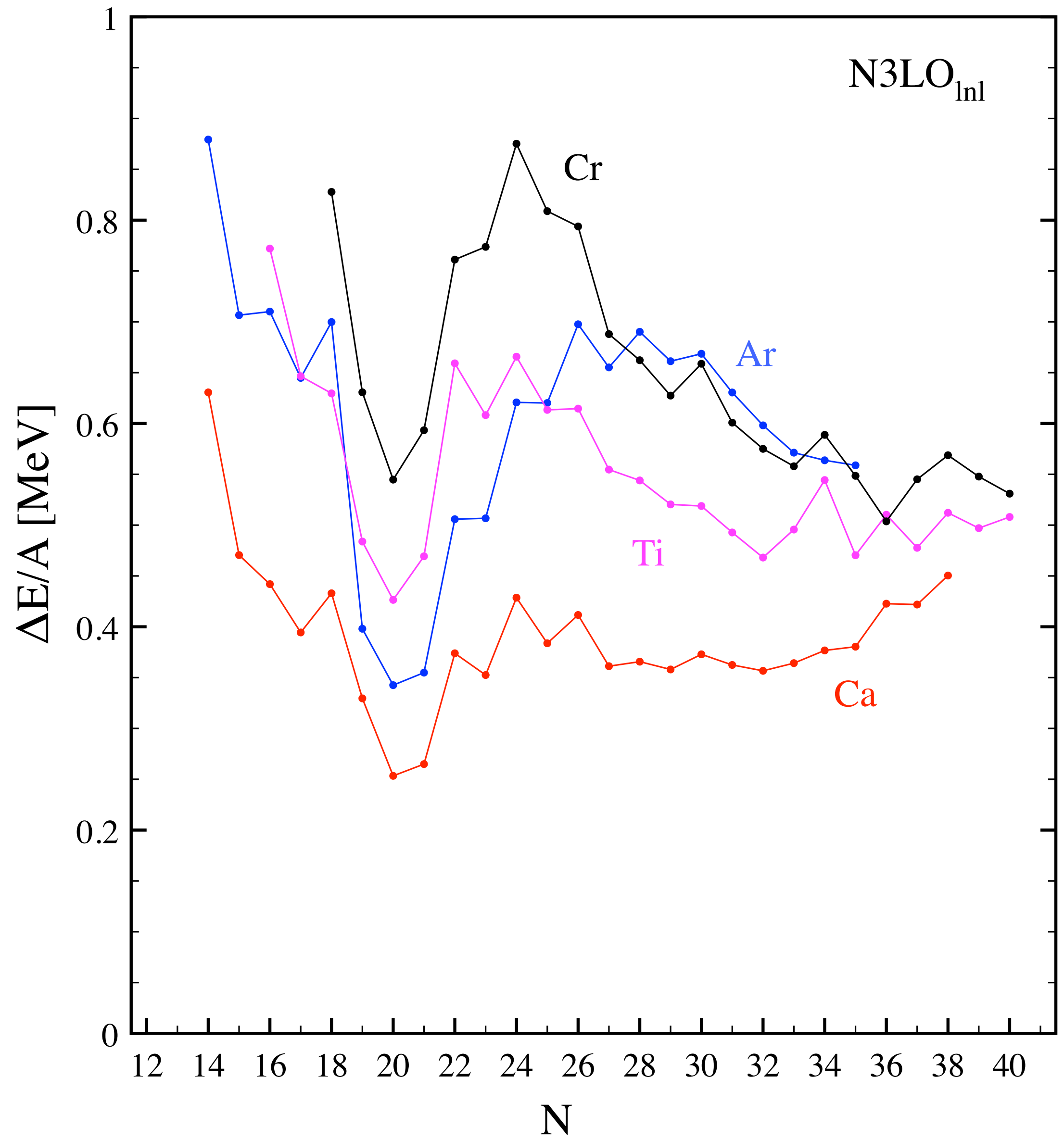

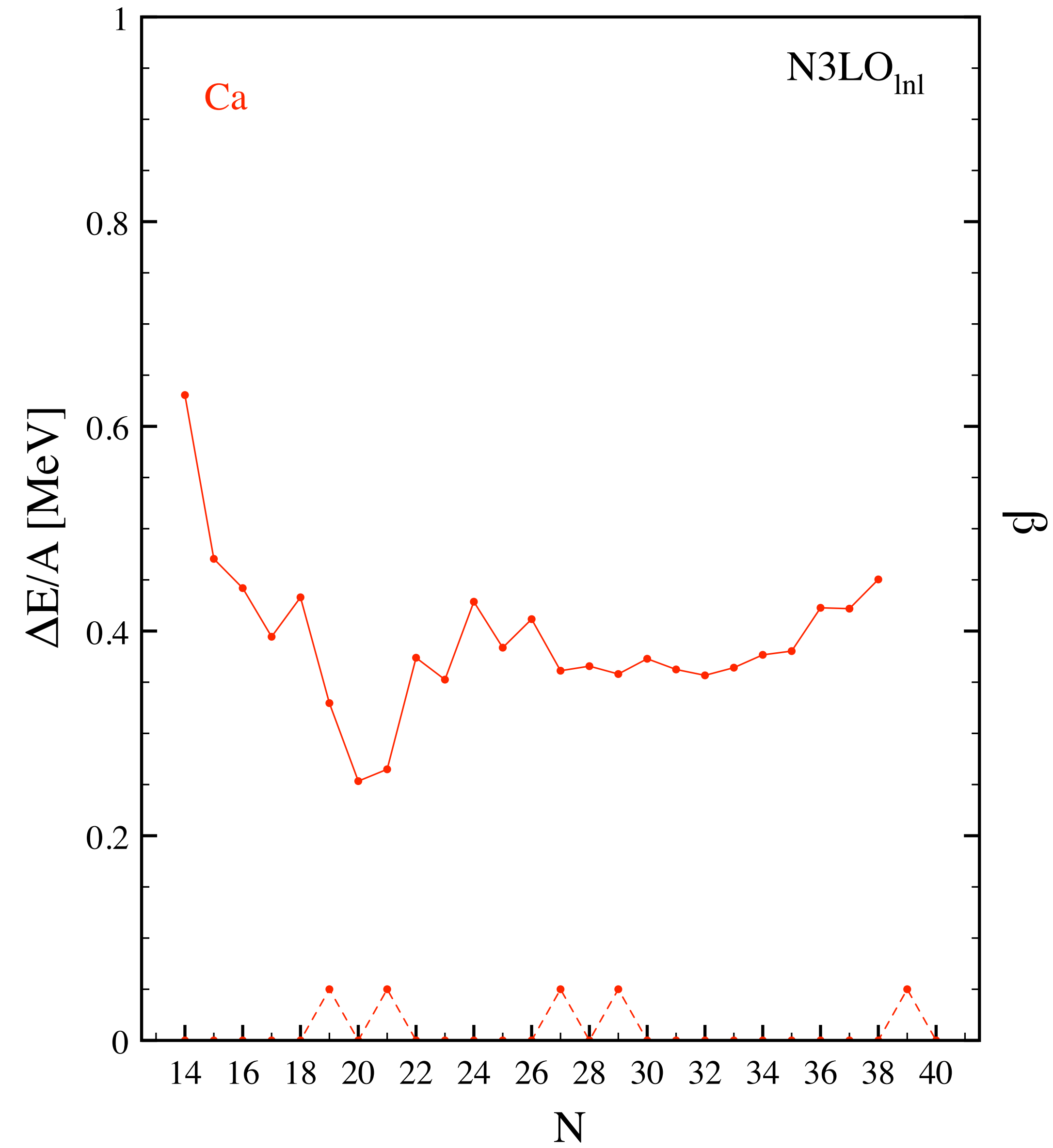

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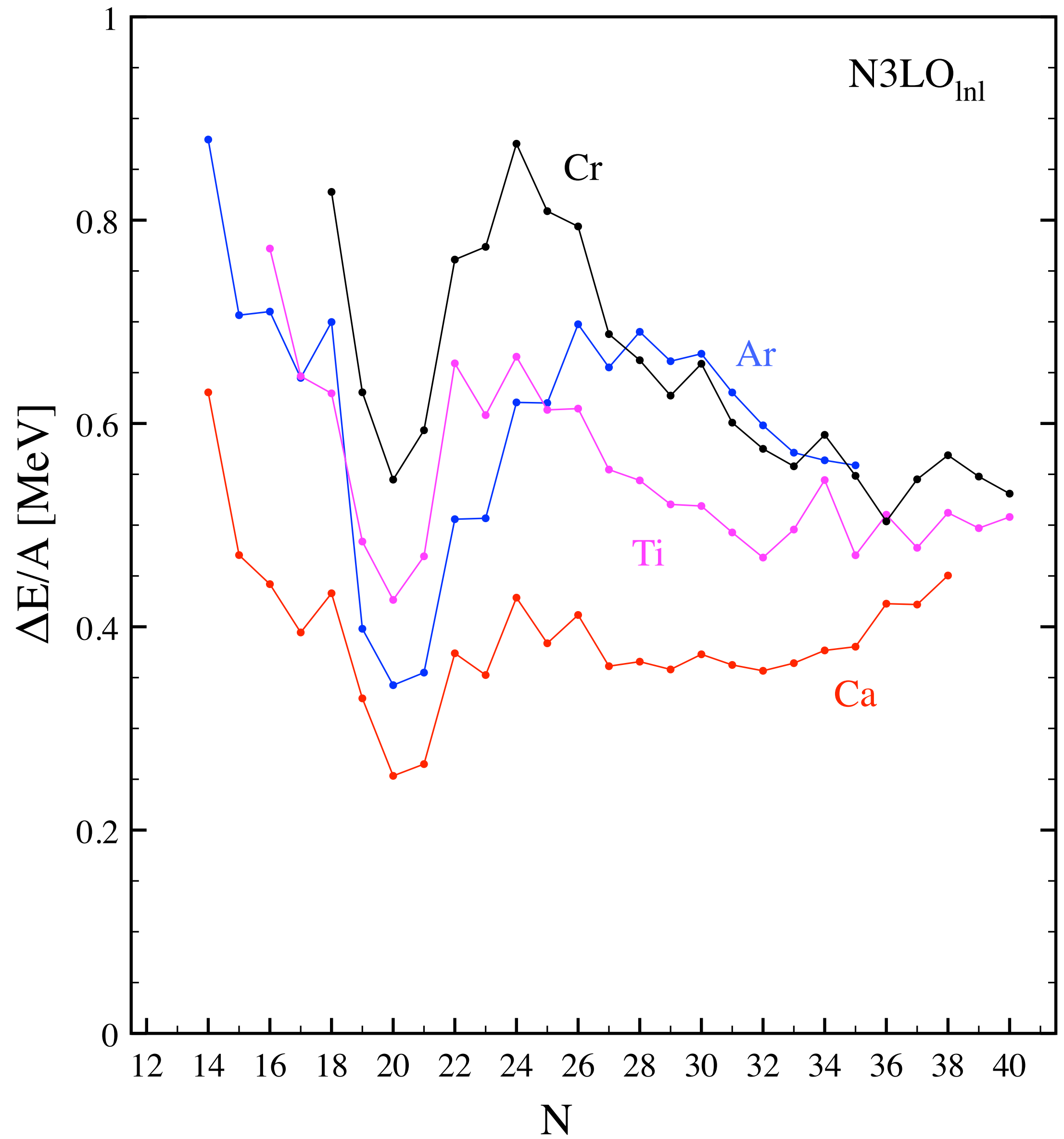

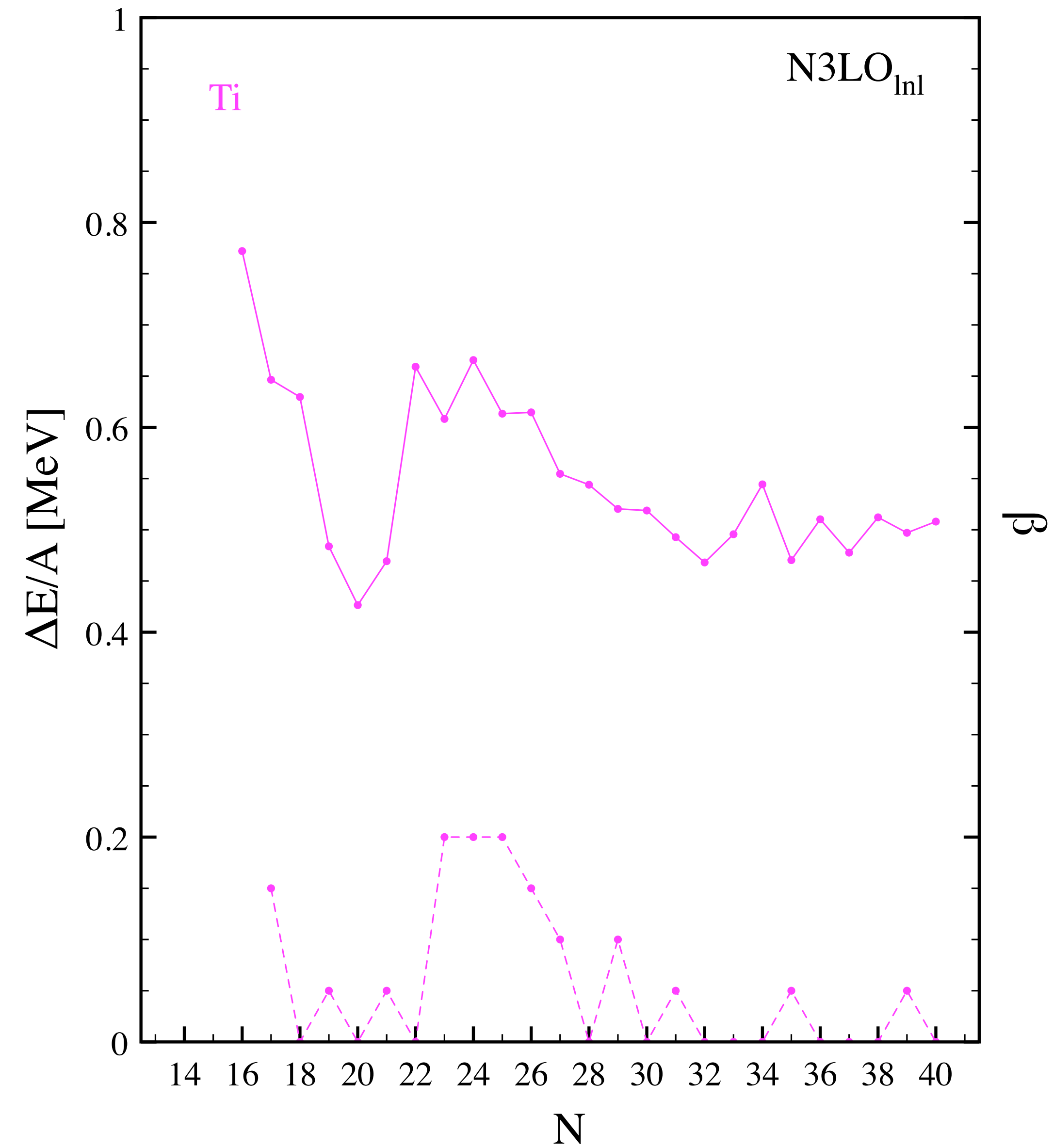

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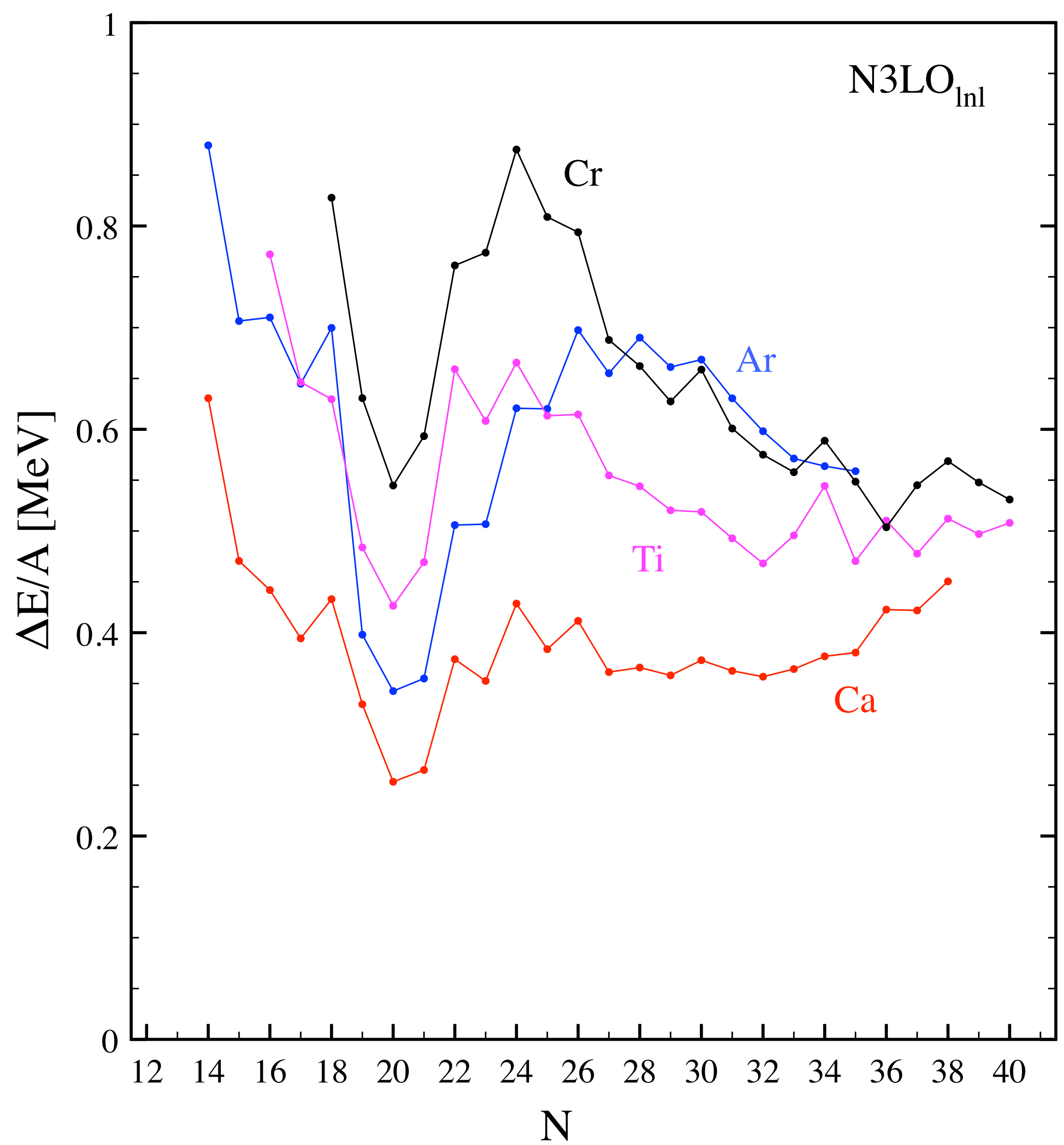
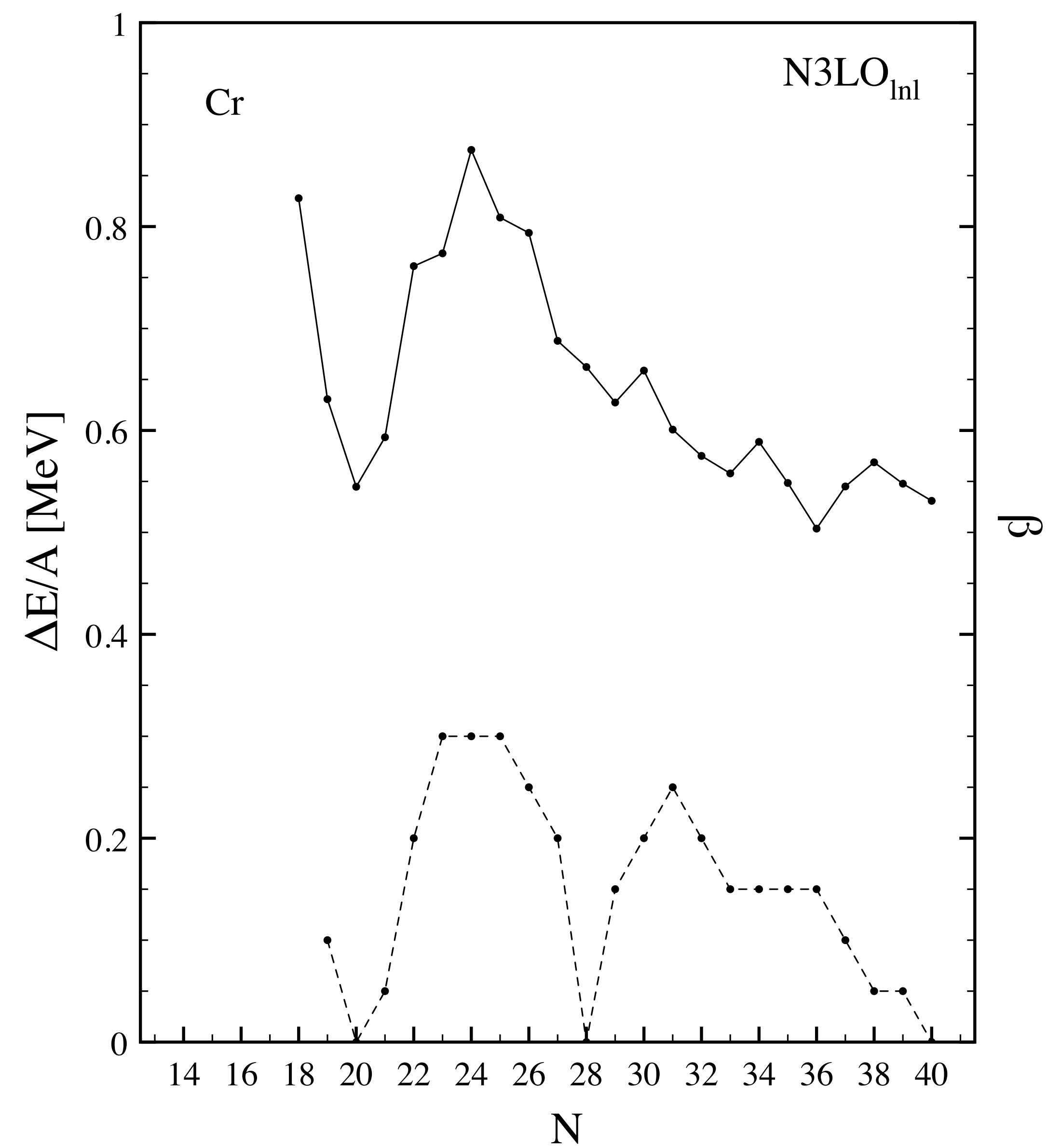
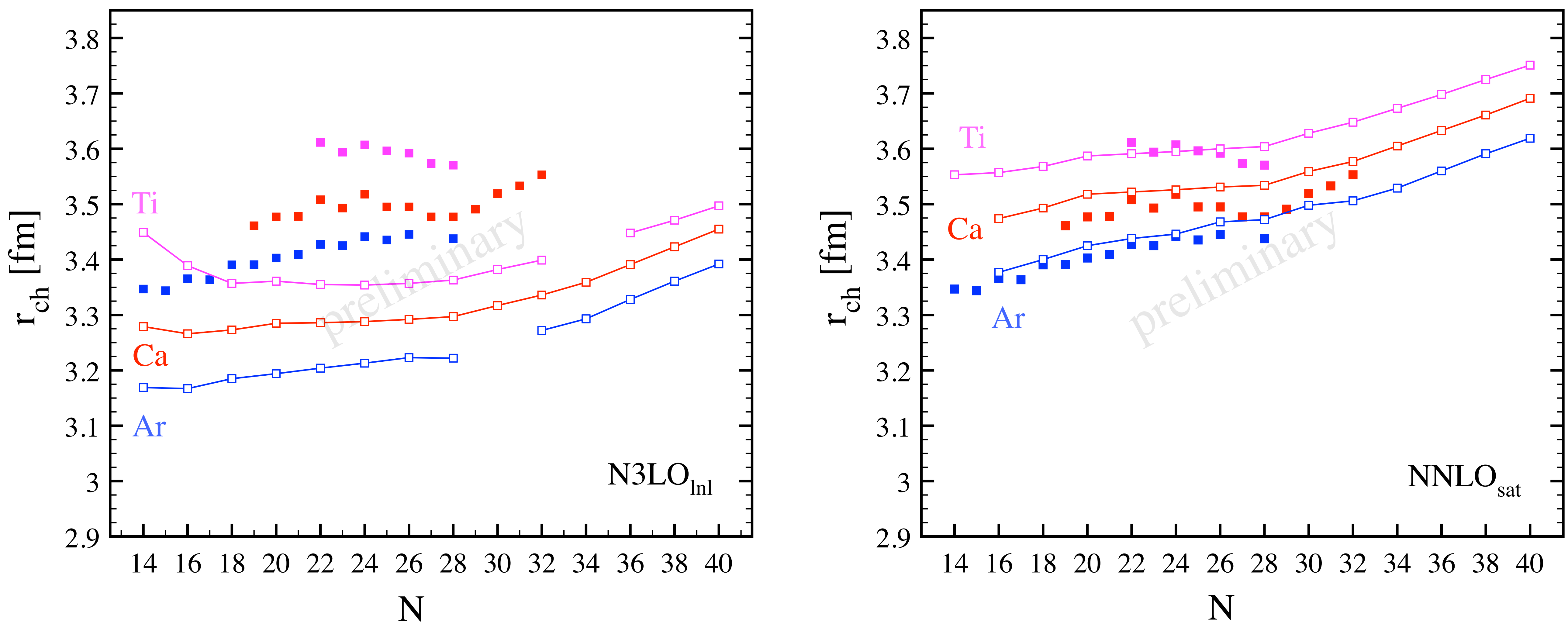




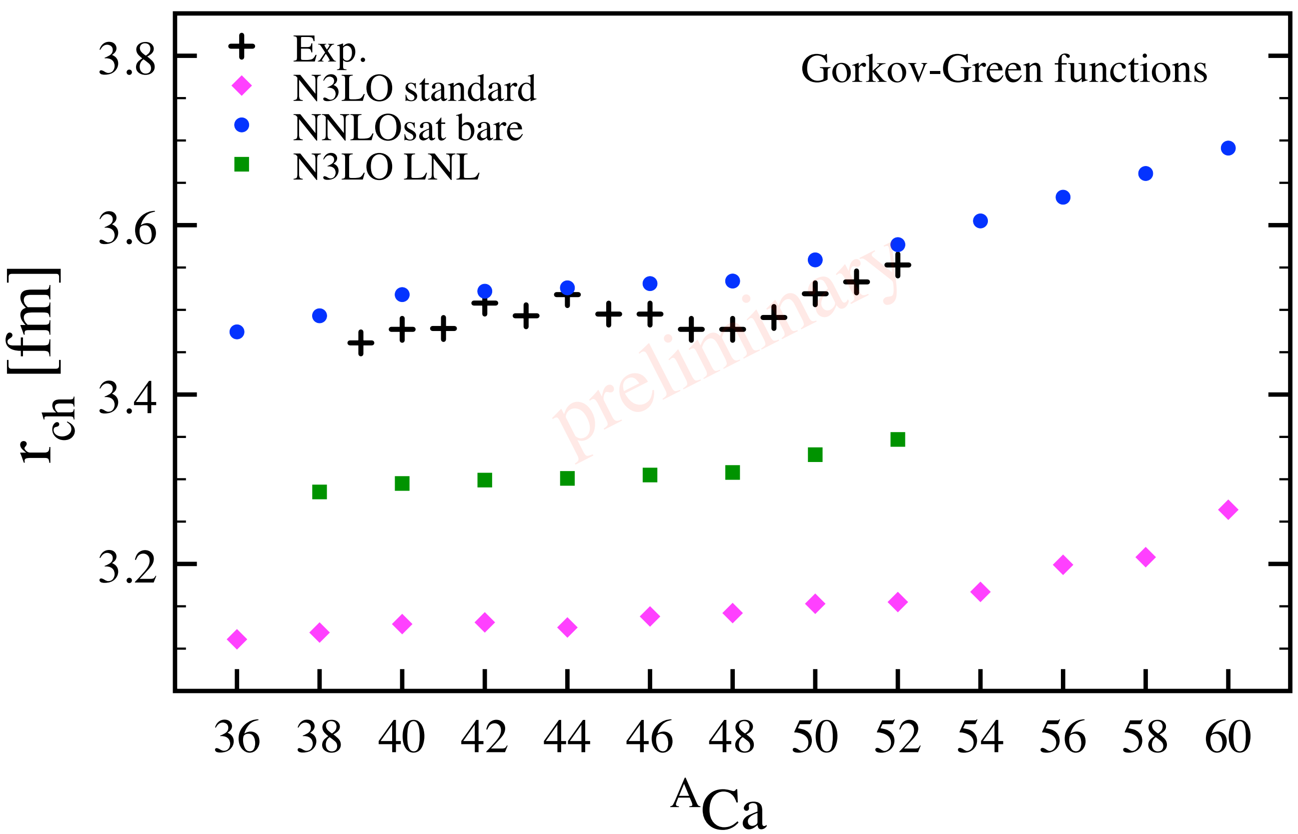
Charge radii

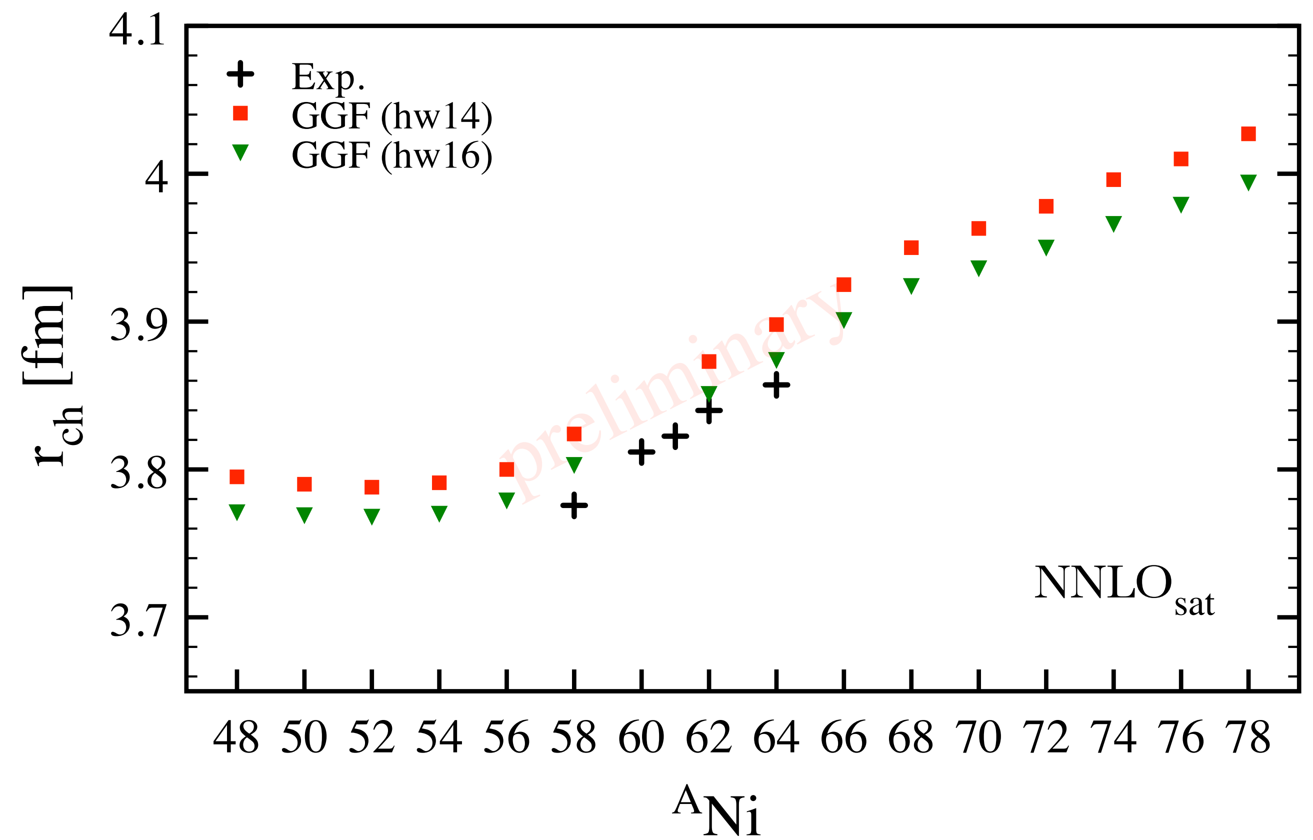
- **Charge radii along argon, calcium and titanium chains**



Charge radii

⦿ **Charge radii along calcium and nickel chains**





○ Large sensitivity on the employed nuclear Hamiltonian

○ Correlation with spectrum and/or saturation properties?

○ Do we need to include radii in the fit?

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Spectral representation

$$G_{ab}(z) = \sum_{\mu} \frac{\langle \Psi_0^A | a_a \mid \Psi_\mu^{A+1} \rangle \langle \Psi_\mu^{A+1} \mid a_b^\dagger | \Psi_0^A \rangle}{z - E_\mu^+ + i\eta} + \sum_{\nu} \frac{\langle \Psi_0^A | a_b^\dagger \mid \Psi_\nu^{A-1} \rangle \langle \Psi_\nu^{A-1} \mid a_a | \Psi_0^A \rangle}{z - E_\nu^- - i\eta}$$

Spectral representation

Spectroscopic probabilities matrices

$$S_\mu^{+ab} \equiv \langle \Psi_0^{\mathrm{A}} | a_a | \Psi_\mu^{\mathrm{A}+1} \rangle \langle \Psi_\mu^{\mathrm{A}+1} | a_b^\dagger | \Psi_0^{\mathrm{A}} \rangle$$
$$S_\nu^{-ab} \equiv \langle \Psi_0^{\mathrm{A}} | a_a^\dagger | \Psi_\nu^{\mathrm{A}\text{-}1} \rangle \langle \Psi_\nu^{\mathrm{A}\text{-}1} | a_b | \Psi_0^{\mathrm{A}} \rangle$$

Spectroscopic factors

$$SF_\mu^+ \equiv \mathrm{Tr}_{\mathcal{H}_1}\left[\mathbf{S}_\mu^+\right] = \sum_{a \in \mathcal{H}_1} \left|U_\mu^a\right|^2$$
$$SF_\nu^- \equiv \mathrm{Tr}_{\mathcal{H}_1}\left[\mathbf{S}_\nu^-\right] = \sum_{a \in \mathcal{H}_1} \left|V_\nu^a\right|^2$$

$$G_{ab}(z) = \sum_\mu \frac{\langle \Psi_0^A | a_a \mid \Psi_\mu^{A+1} \rangle \langle \Psi_\mu^{A+1} \mid a_b^\dagger | \Psi_0^A \rangle}{z - E_\mu^+ + i\eta} + \sum_\nu \frac{\langle \Psi_0^A | a_b^\dagger \mid \Psi_\nu^{A-1} \rangle \langle \Psi_\nu^{A-1} \mid a_a | \Psi_0^A \rangle}{z - E_\nu^- - i\eta}$$

Eigenstates of A+1

Eigenstates of A-1

One-nucleon addition separation energies

$$E_\mu^+ \equiv E_\mu^{A+1} - E_0^A$$

One-nucleon removal separation energies

$$E_\nu^- \equiv E_0^A - E_\nu^{A-1}$$

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One-nucleon removal separation energies

$$E_\nu^- \equiv E_0^A - E_\nu^{A-1}$$

Combining numerator and denominator result in the spectral function

Spectral function

$$\mathbf{S}(z) \equiv \sum_{\mu \in \mathcal{H}_{A+1}} \mathbf{S}_\mu^+ \; \delta(z - E_\mu^+) + \sum_{\nu \in \mathcal{H}_{A-1}} \mathbf{S}_\nu^- \; \delta(z - E_\nu^-)$$

Spectral strength distribution

$$\begin{aligned}\mathcal{S}(z) &\equiv \mathrm{Tr}_{\mathcal{H}_1}[\mathbf{S}(z)] \\ &= \sum_{\mu \in \mathcal{H}_{A+1}} SF_\mu^+ \, \delta(z - E_\mu^+) + \sum_{\nu \in \mathcal{H}_{A-1}} SF_\nu^- \, \delta(z - E_\nu^-)\end{aligned}$$

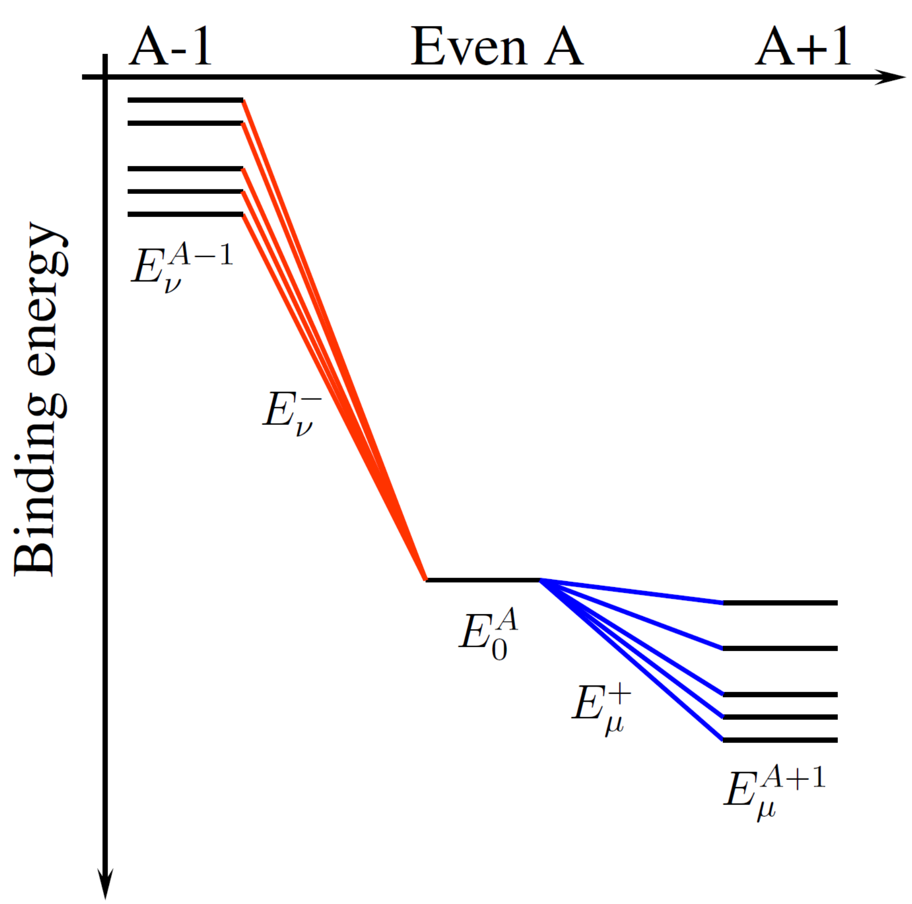
Spectral representation

$$\boxed{G_{ab}(z) = \sum_{\mu} \frac{U_a^{\mu} (U_b^{\mu})^*}{z - E_{\mu}^{+} + i\eta} + \sum_{\nu} \frac{(V_a^{\nu})^* V_b^{\nu}}{z - E_{\nu}^{-} - i\eta}}$$

Separation energies

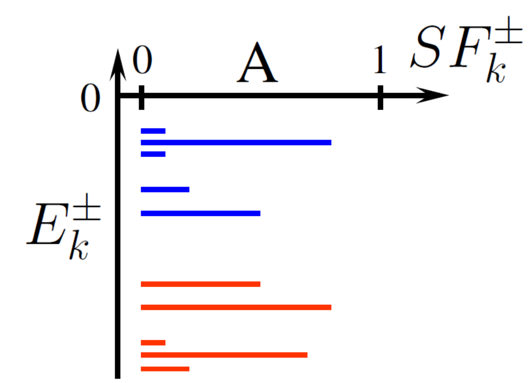
$$E_{\mu}^{+} \equiv E_{\mu}^{A+1} - E_0^{A}$$

$$E_{\nu}^{-} \equiv E_0^{A} - E_{\nu}^{A-1}$$



Spectral strength distribution

$$\mathcal{S}(z) = \sum_{\mu \in \mathcal{H}_{A+1}} SF_{\mu}^{+} \, \delta(z - E_{\mu}^{+}) + \sum_{\nu \in \mathcal{H}_{A-1}} SF_{\nu}^{-} \, \delta(z - E_{\nu}^{-})$$



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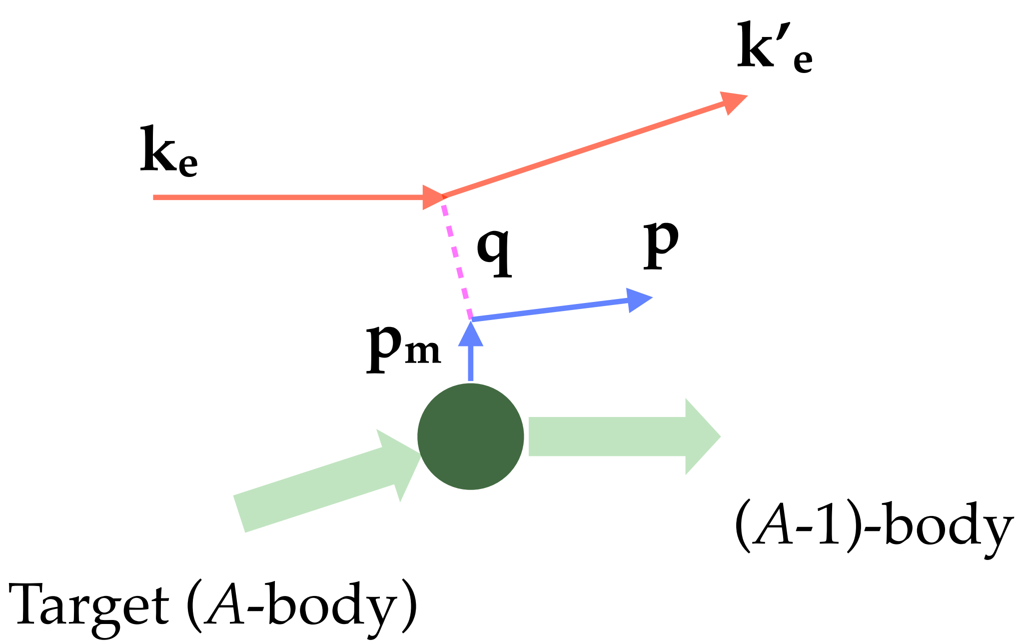
Spectral strength in experiments

⦿ Clean connection to (*e,e′p*) experiments



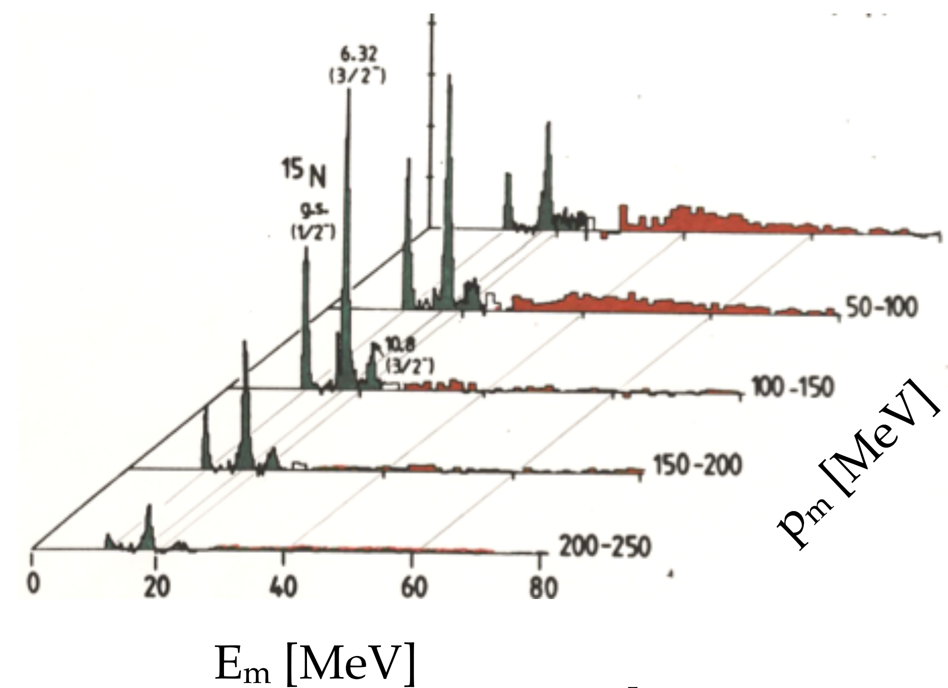
○ Measuring **q** and **p** gives information on $\mathbf{p_m}$

○ Similarly for missing energy E_m

○ Spectral strength distribution ↔ $P(p_m, E_m)$

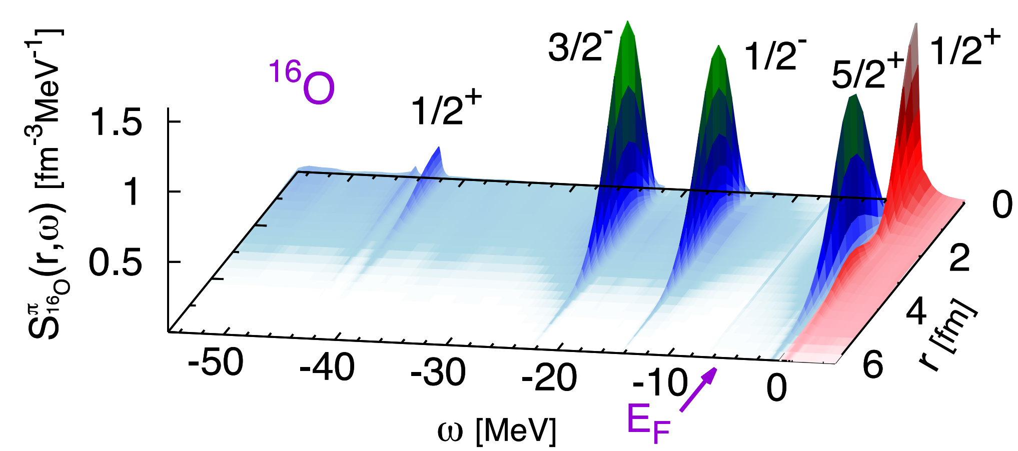
⦿ Spectroscopy via knockout / transfer exp.

Results from (e,e′p) on ^{16}O (ALS in Saclay)



[Mougey *et al.* 1980]

SCGF calculations

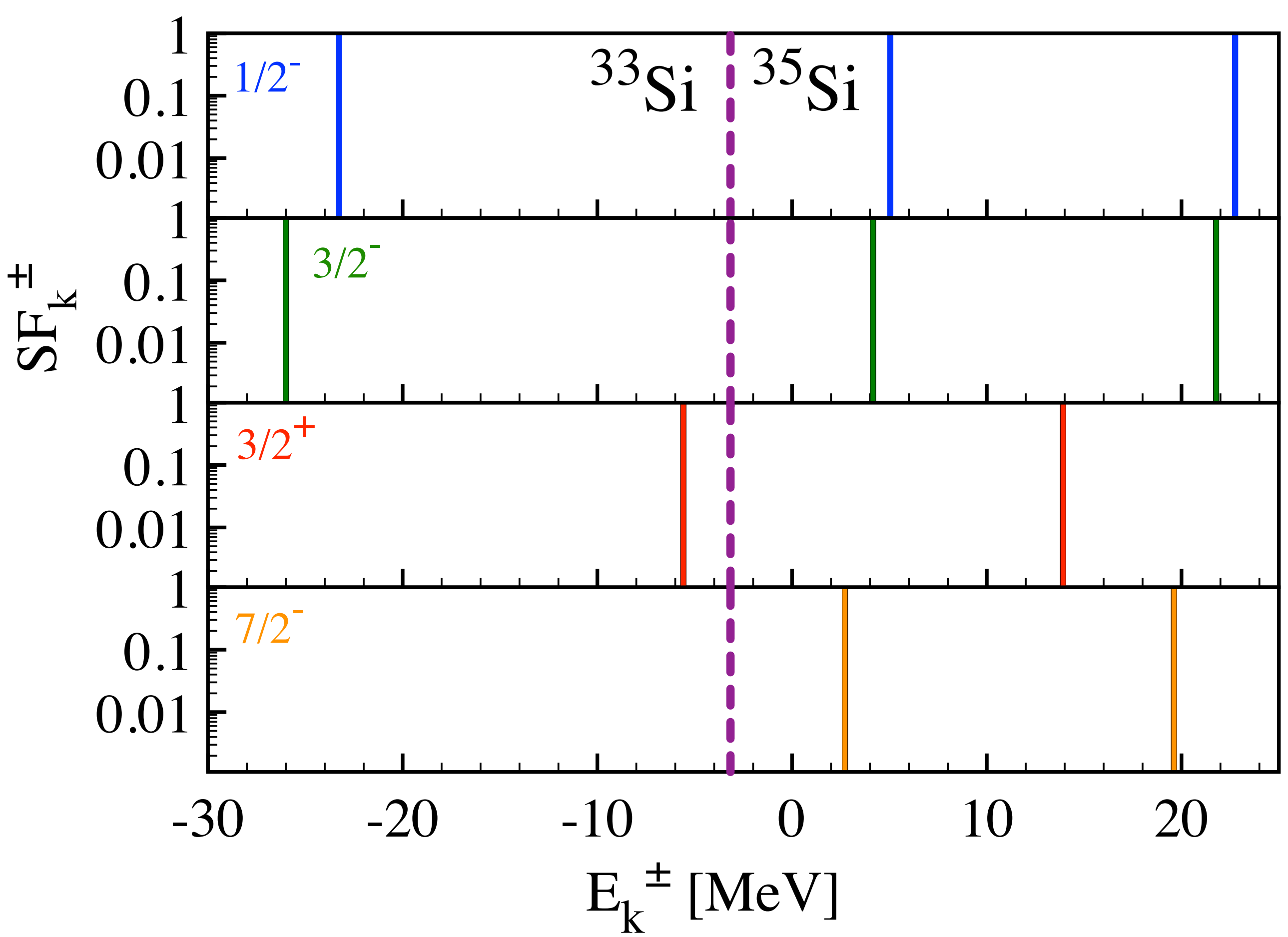


[Cipollone *et al.* 2015]

Spectral strength distribution

- ^{34}Si neutron addition & removal strength

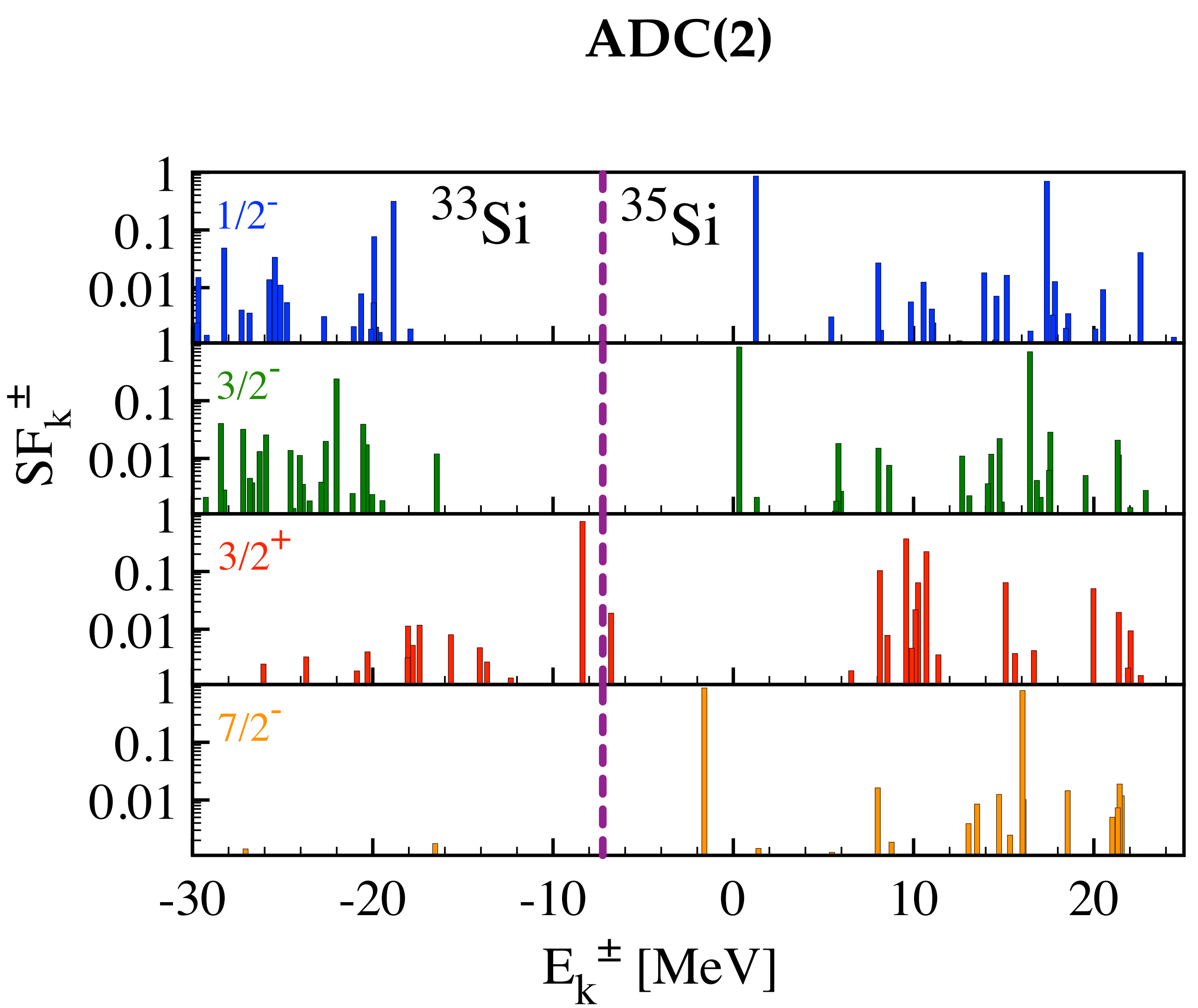
ADC(1)



- Independent-particle picture

Spectral strength distribution

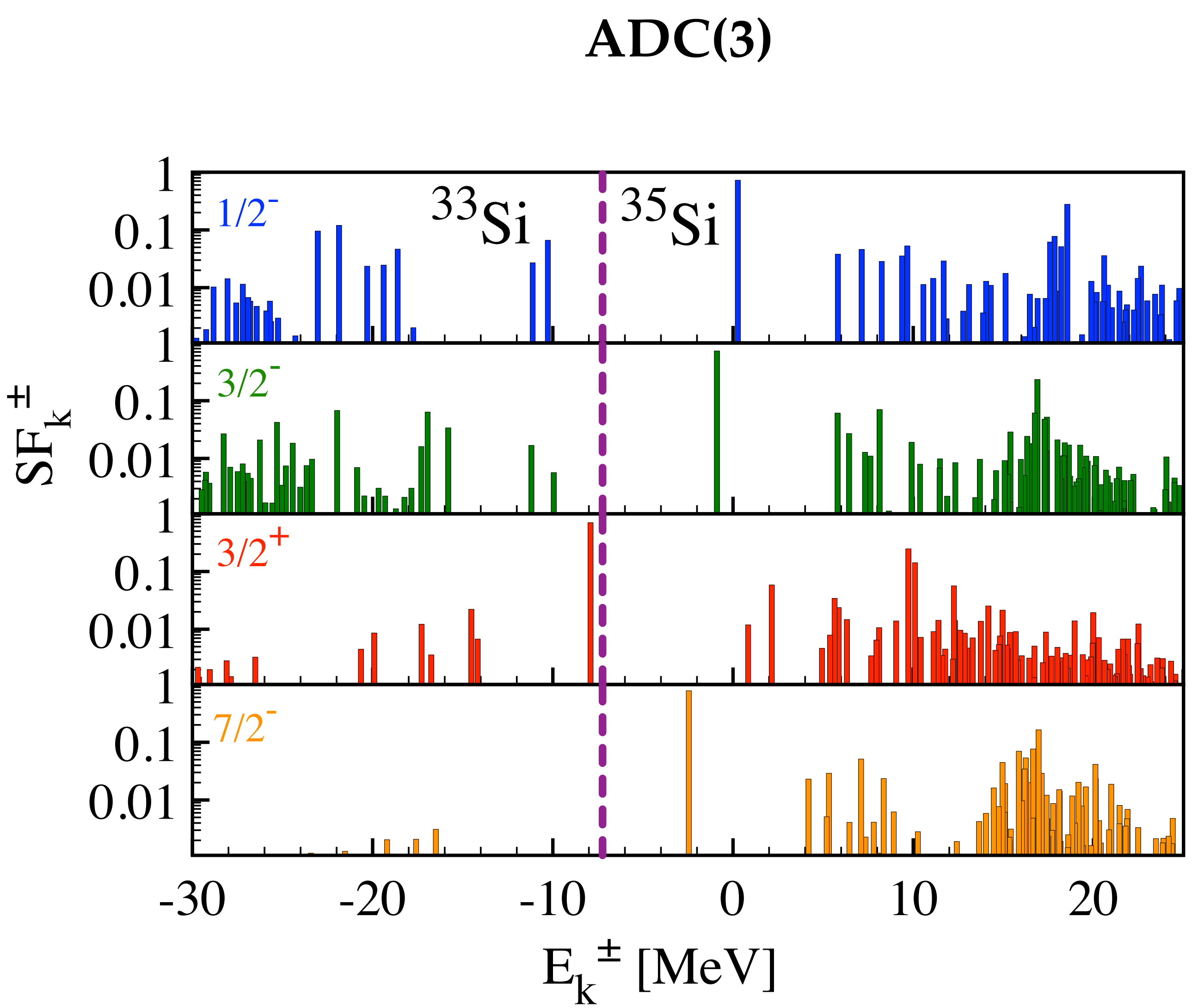
- ^{34}Si neutron addition & removal strength



- Second-order dynamical correlations fragment IP peaks

Spectral strength distribution

⦿ ^{34}Si neutron addition & removal strength



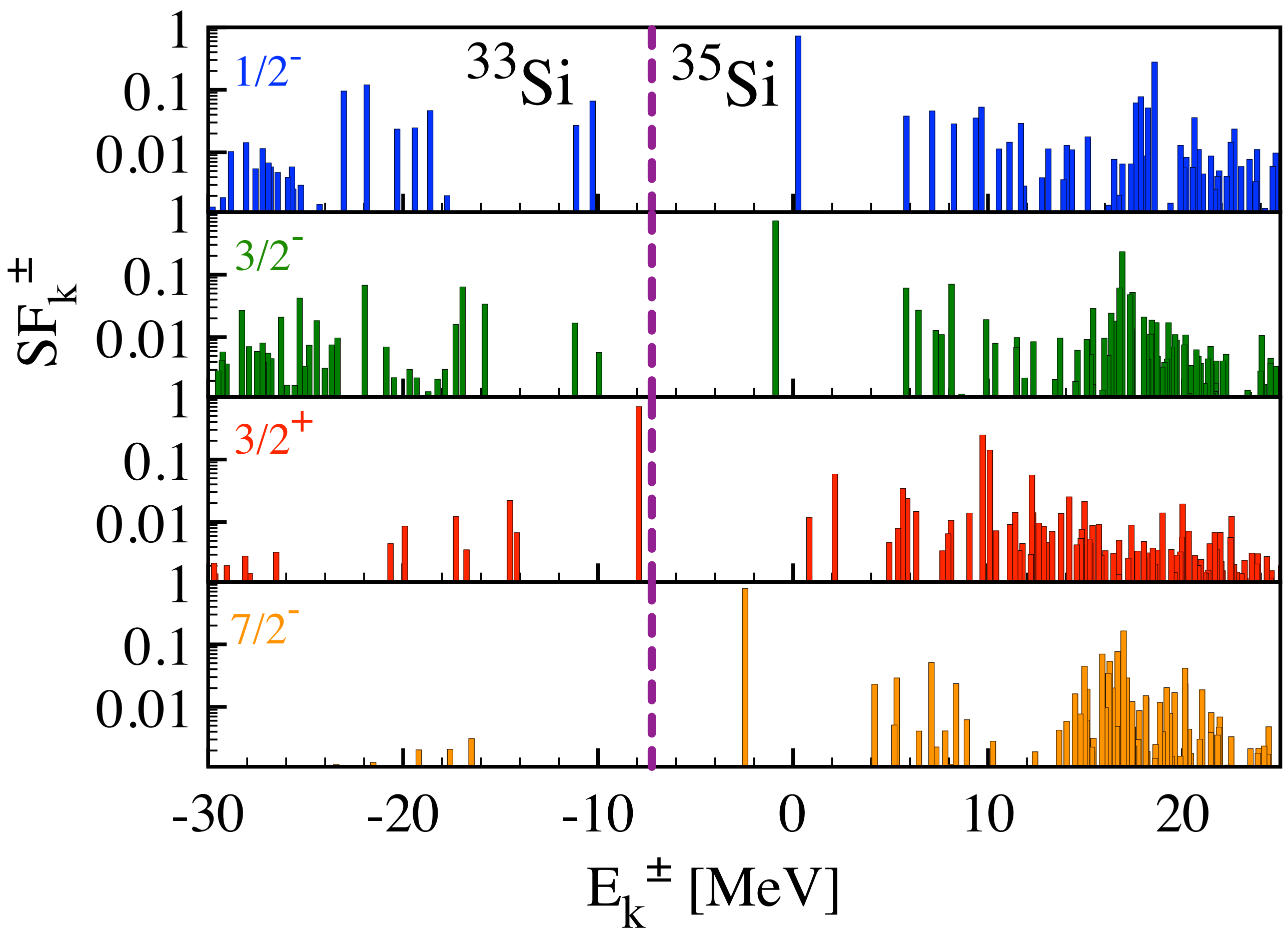
○ Third-order compresses the spectrum (main peaks)

○ Further fragmentation is generated

Spectral strength distribution

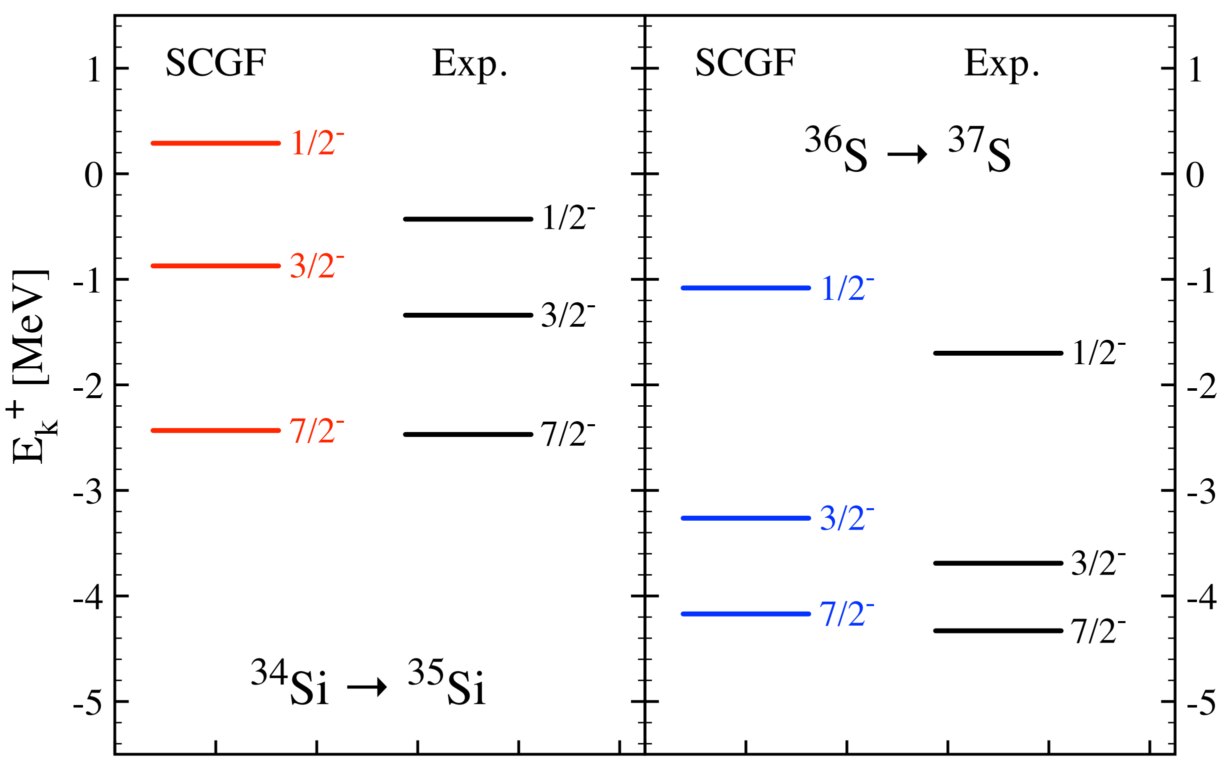
⦿ ^{34}Si neutron addition & removal strength

ADC(3)



One-neutron addition

Exp. data: [Thorn *et al.* 1984] [Eckle *et al.* 1989] [Burgunder *et al.* 2014]



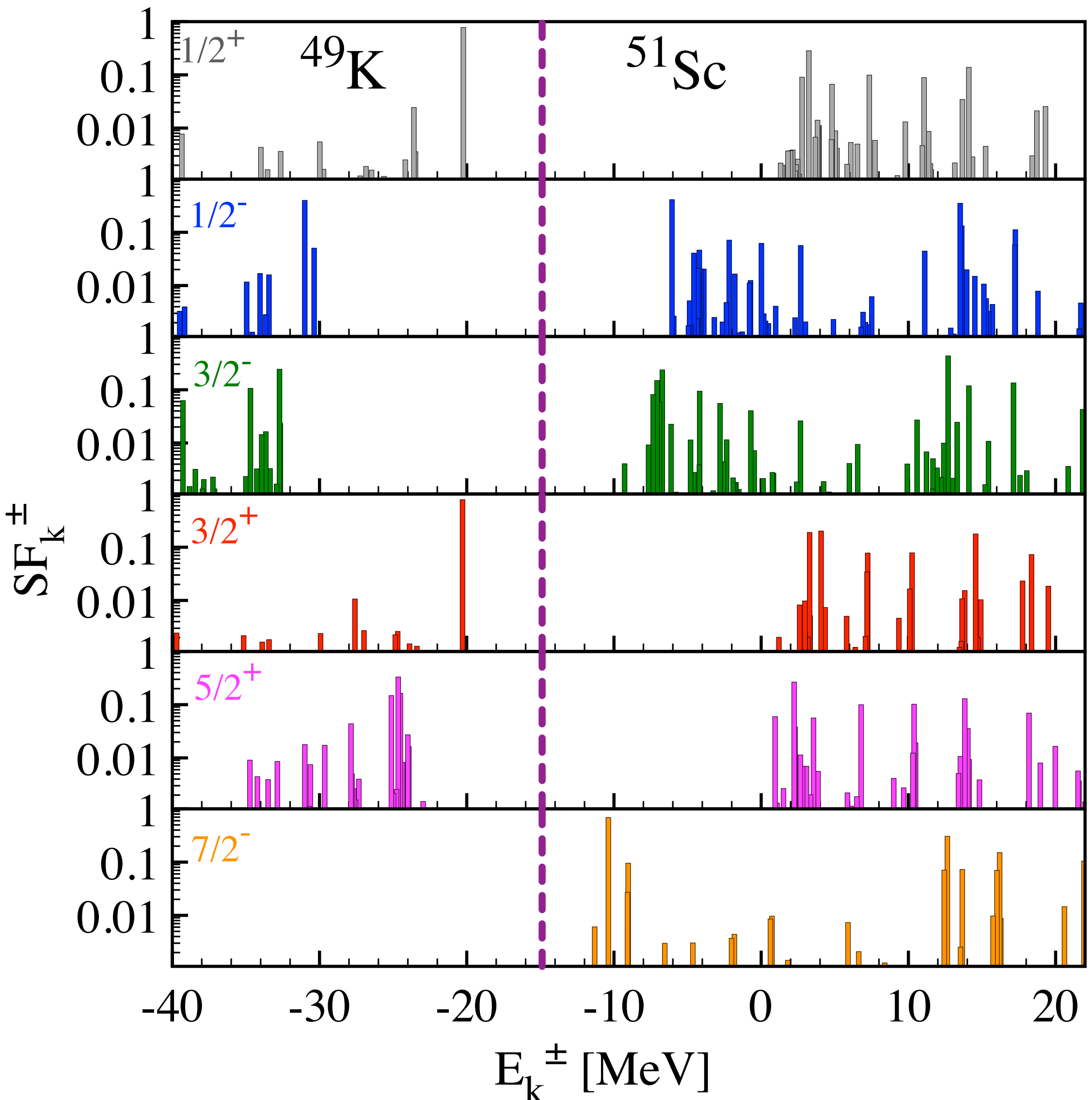
Reduction of $E_{1/2^-}$ - $E_{3/2^-}$ spin-orbit splitting (unique in the nuclear chart) well reproduced

○ Third-order correlations compress the spectrum

○ Further fragmentation is generated

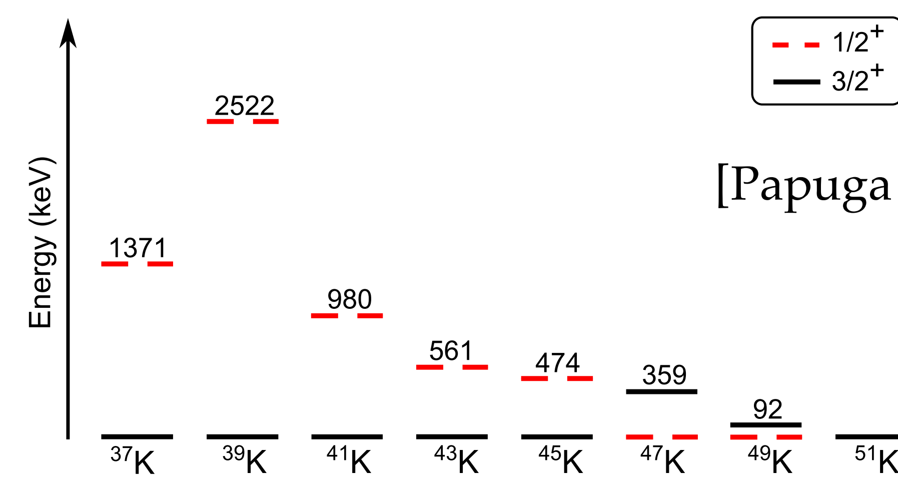
K spectra

➪ **K spectra show interesting g.s. spin inversion and re-inversion**

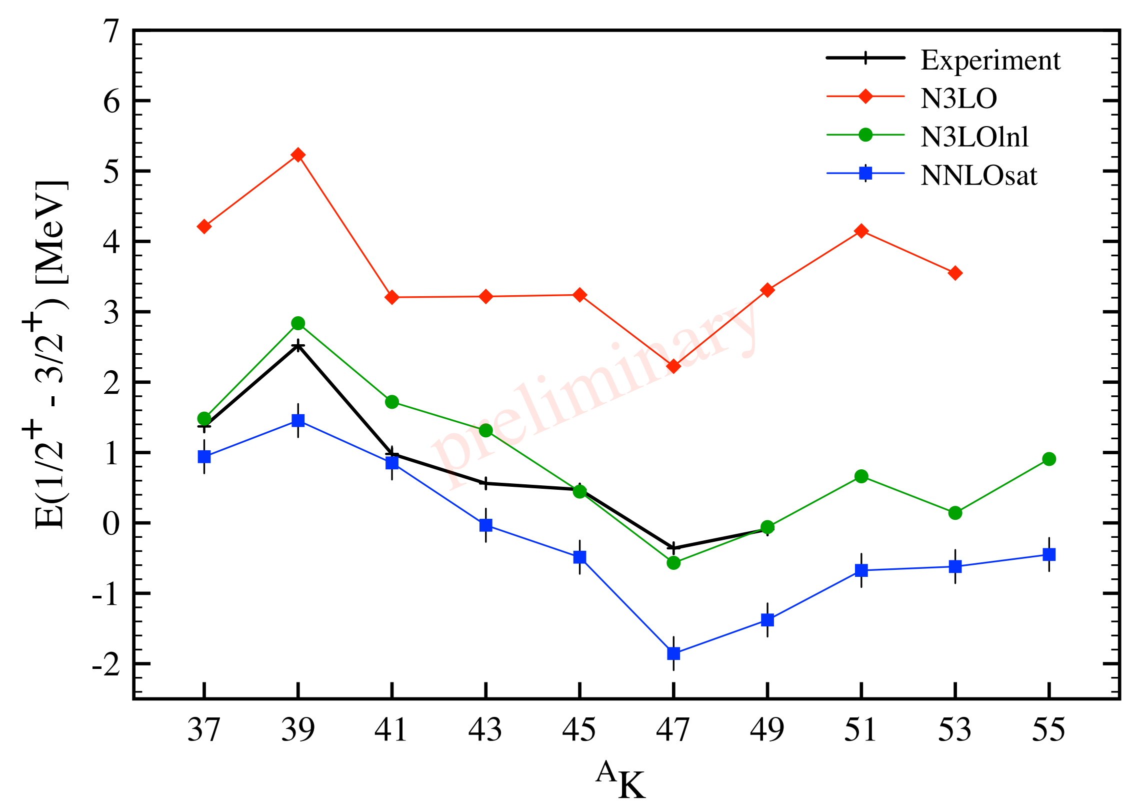


One-proton addition
and removal from ^{50}Ca

Laser spectroscopy COLLAPS @ ISOLDE

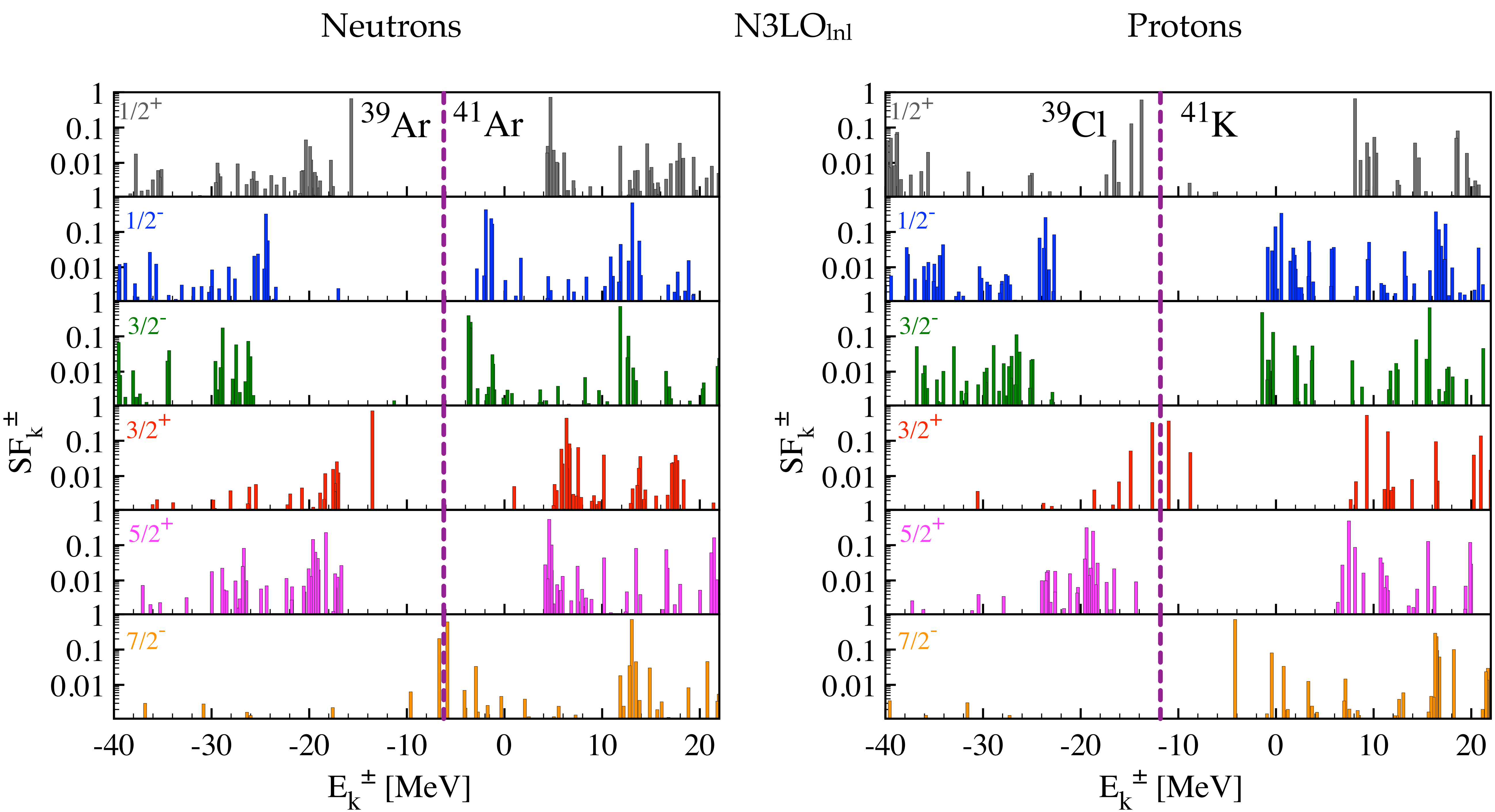


[Papuga *et al.* 2013]



Spectral function of ^{40}Ar

- Relevant for neutrino-nucleus scattering (e.g. DUNE)



Spectral function of ^{40}Ar

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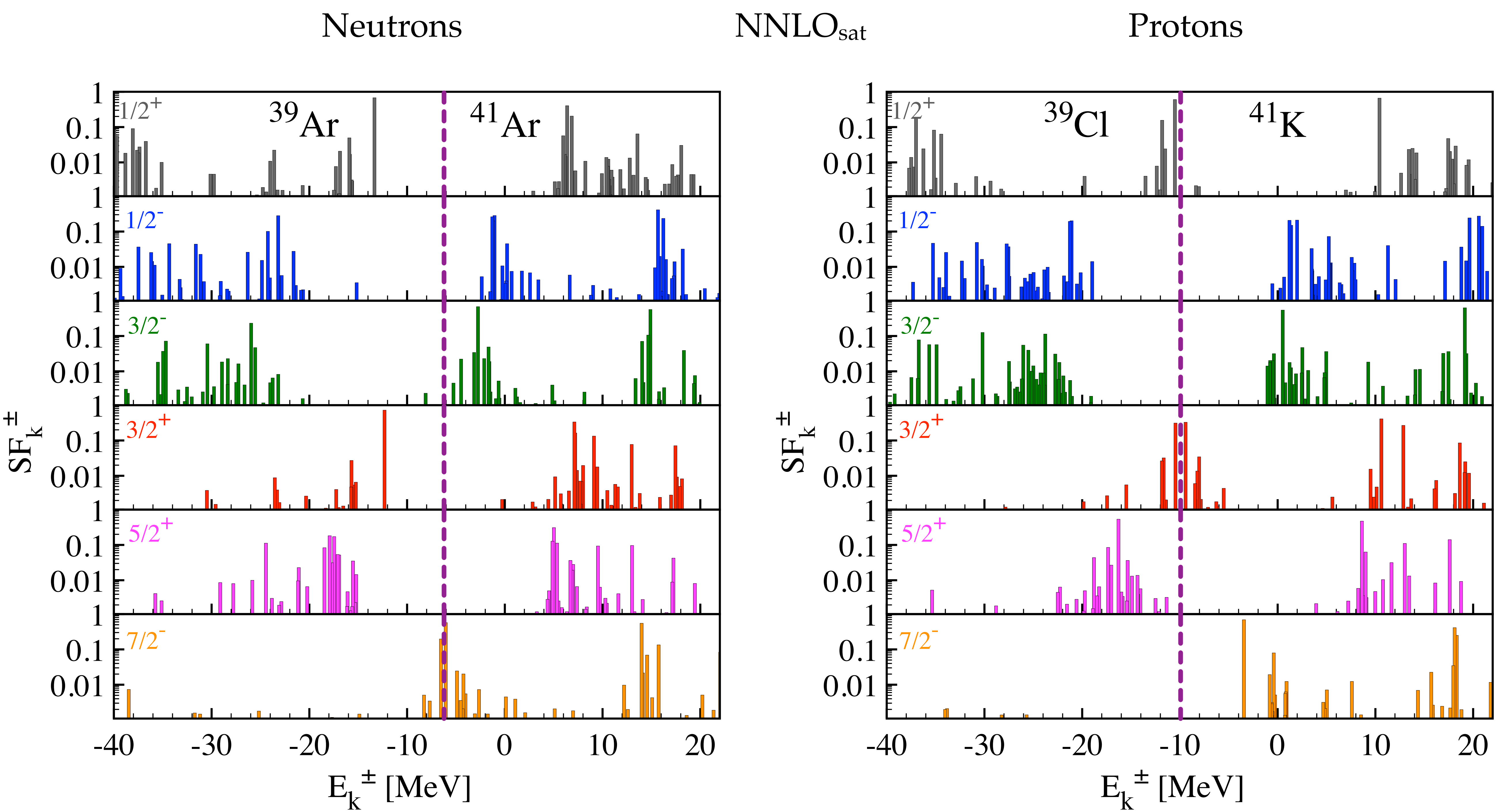
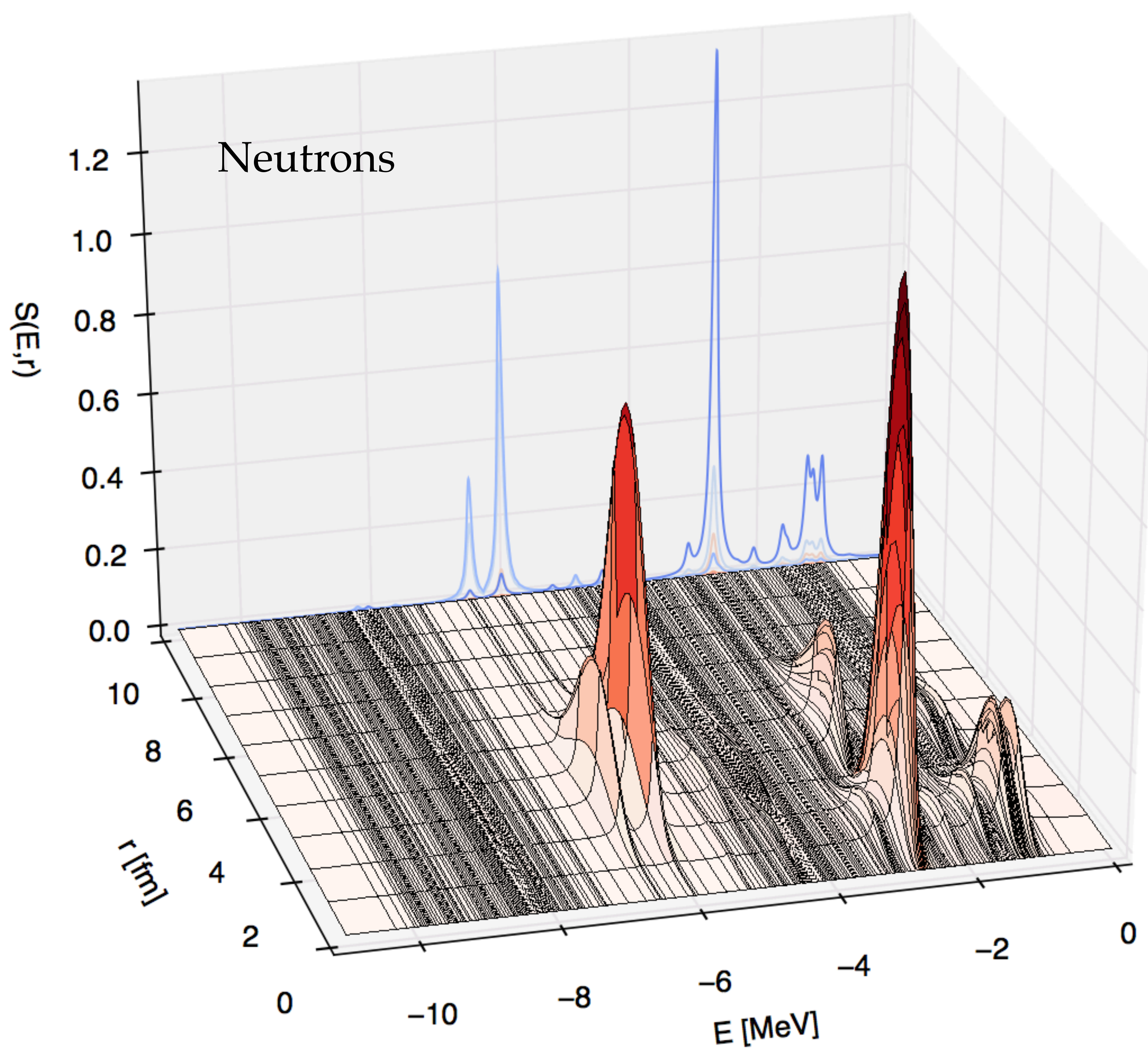


Spectral function of ^{40}Ar

- ADC(2) truncation, $\mathrm{NNLO_{sat}}$ interaction



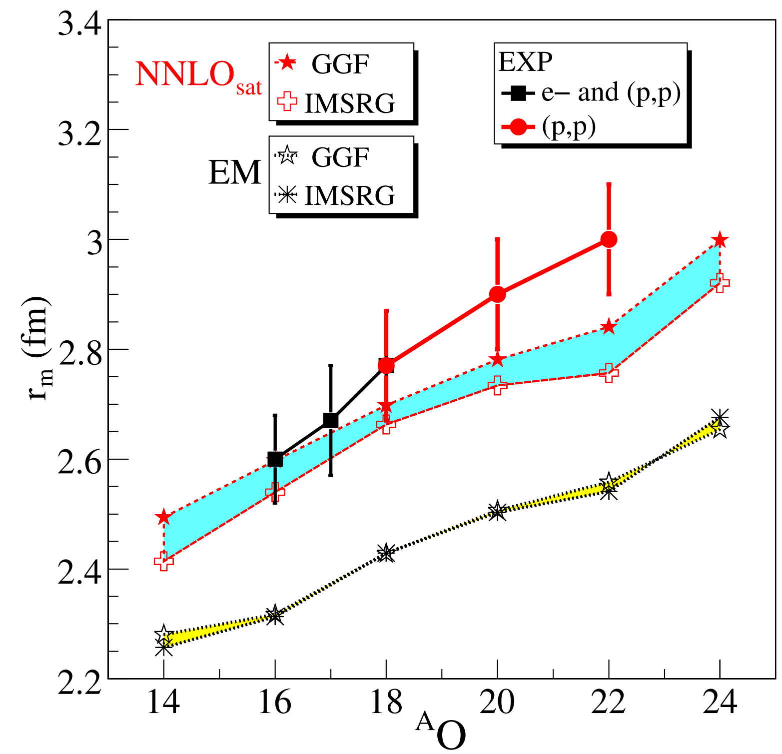
Conclusions

⊙ **Many-body formalism well grounded**

- Closed- & open-shell nuclei, g.s. observables & spectroscopy, …
- Two-body propagators to be implemented to access spectroscopy of even-even systems

⊙ **At present, interactions constitute main source of uncertainty**

- ChEFT is undergoing intense development, facing fundamental & practical issues
- Pragmatic choices lead to successful applications
- Different observables needed to test interactions



⊙ **Extension of ab initio simulations to heavy nuclei**

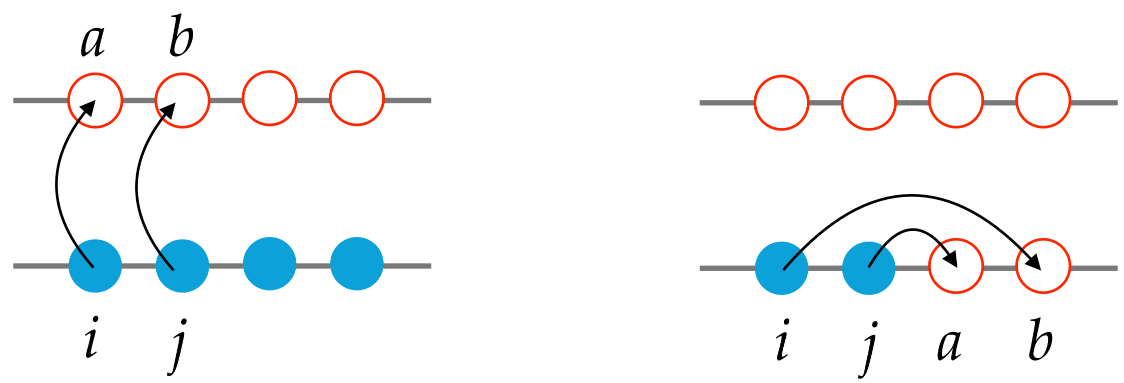
- Computational challenges: 3NF, higher-order tensors, …
- Formal challenges: extension to doubly open-shell, symmetry restoration

Appendix

Doubly open-shell nuclei

- Approximate/truncated methods capture correlations via an expansion in **ph excitations**
- Open-shell nuclei are **(near-)degenerate** with respect to ph excitations

closed-shell



open-shell

- Solution: multi-determinantal or **symmetry-breaking** reference state
    - Symmetry-breaking solution allows to **lift the degeneracy**

Pairing correlations
↕
Superfluidity
↕
Breaking of U(1)

Quadrupole correlations
↕
Deformation
↕
Breaking of SU(2)

Singly open-shells

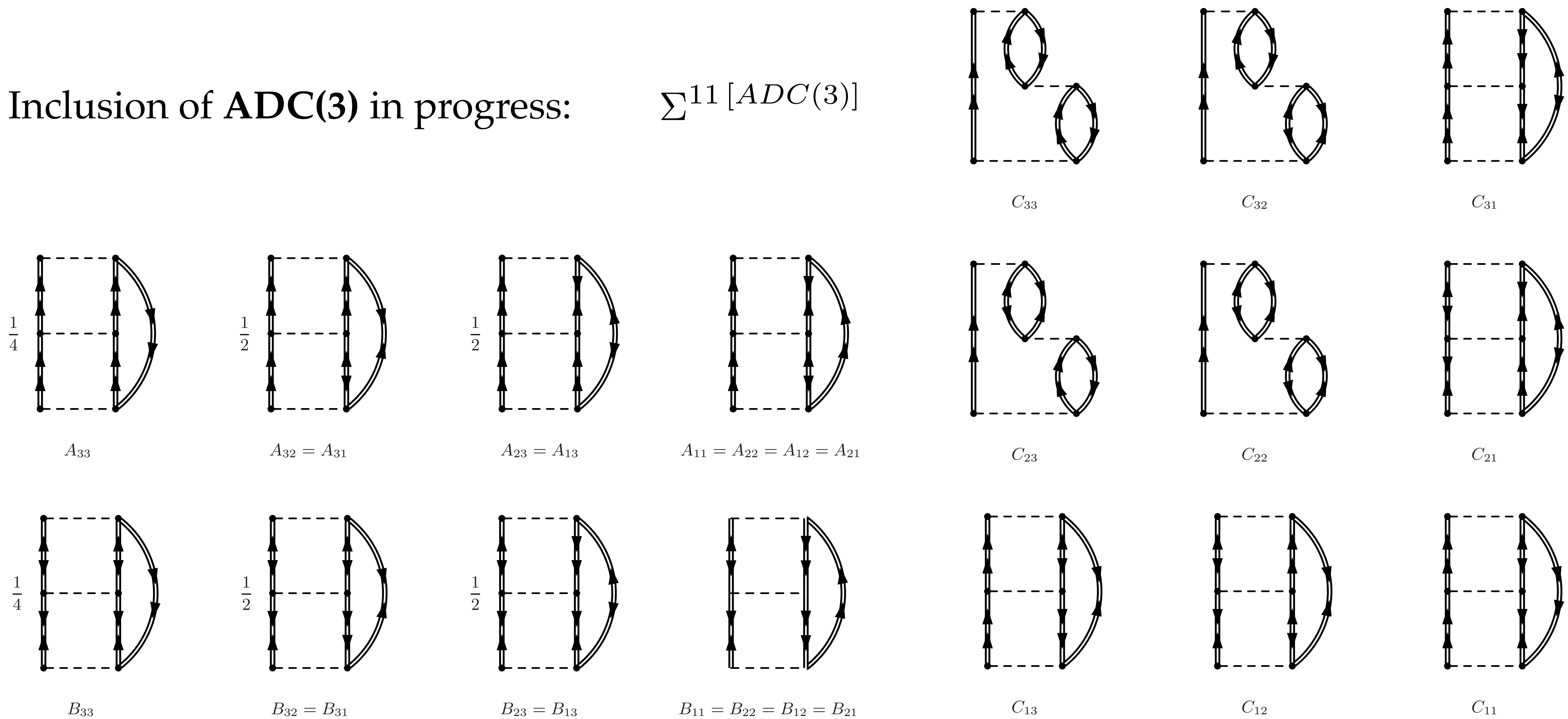
Doubly open-shells

Developed and implemented

To be developed and implemented

Gorkov-Green's functions

Inclusion of **ADC(3)** in progress: $\Sigma^{11\,[ADC(3)]}$



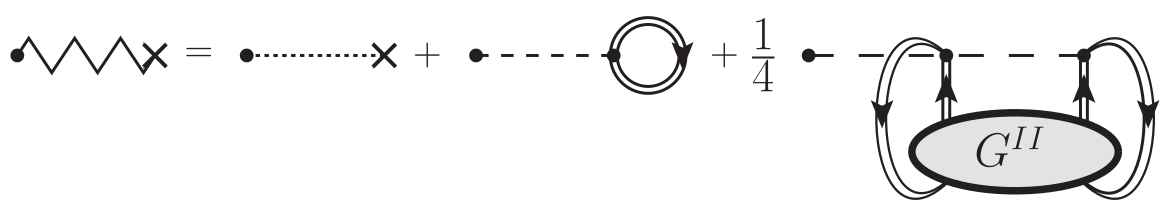
[Barbieri, Duguet & Somà *in prep.*]

ADC(n) diagrams	***n*=1**	**2**	**3**
Dyson	1	1	2
Gorkov	2	4	34

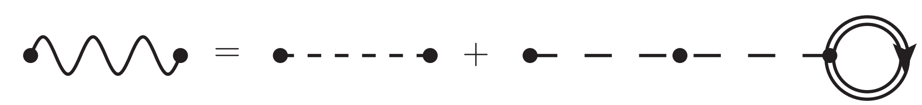
Three-body forces

- Hamiltonians for A-nucleon systems contain in principle up to A-body operators
  - At least **three-body forces** need to be included in realistic ab initio calculations
- Diagrammatic expansion can be simplified by exploiting the concept of **effective interactions**
  - Generalisation of normal ordering (fully correlated density matrices)

effective 1-body

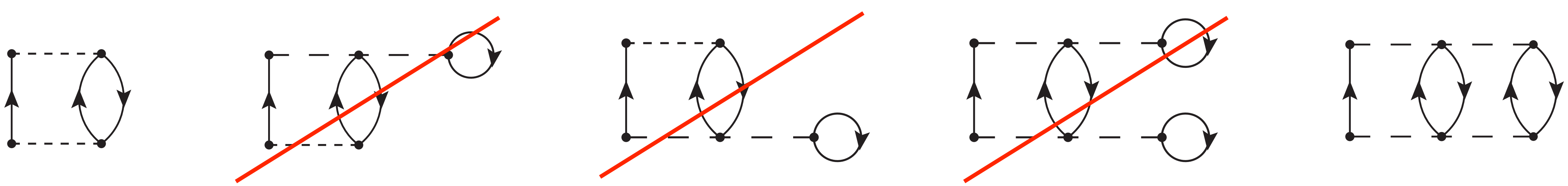


effective 2-body



[Carbone, Cipollone, Barbieri, Rios, Polls 2013]

- One introduces **interaction-irreducible** diagrams

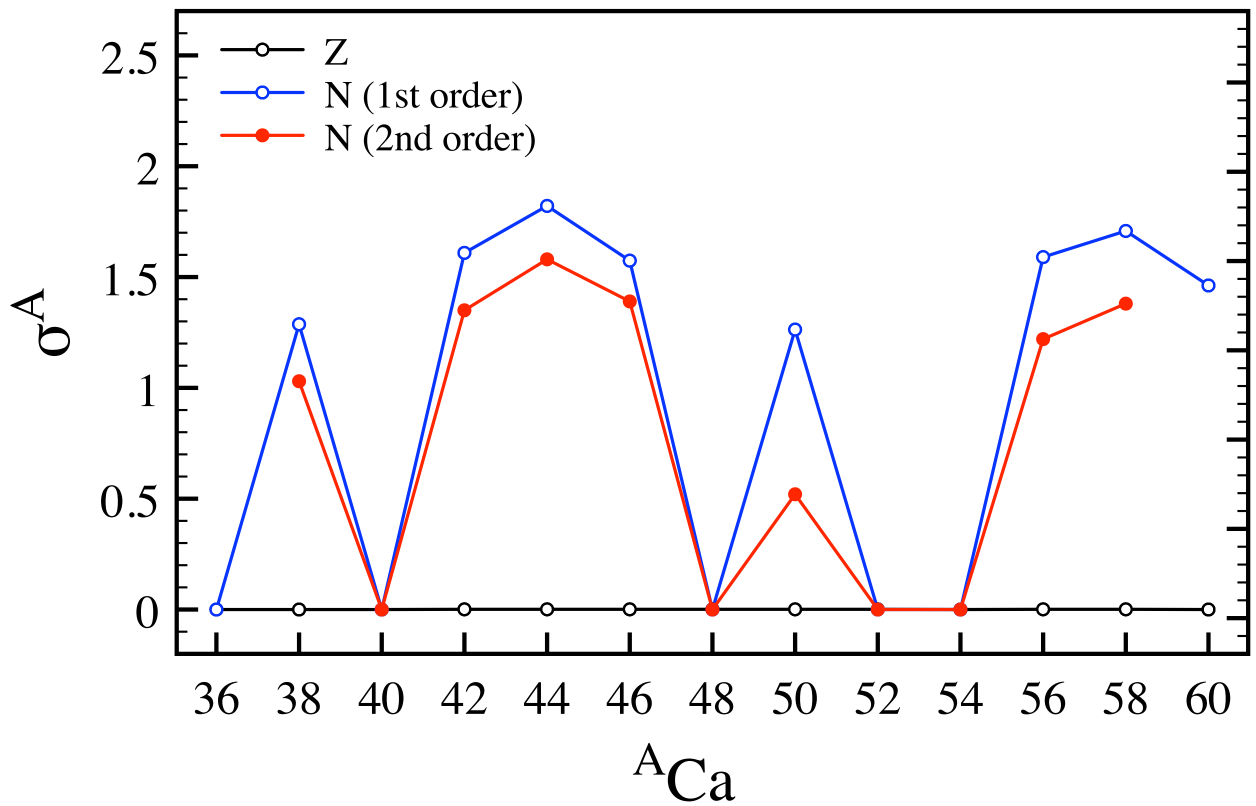


- Galitskii-Migdal-Koltun sum rule needs to be modified to account for 3N term W

$$E_0^N = \frac{1}{2\pi}\int_{-\infty}^{\epsilon_F^-} d\omega \sum_{\alpha\beta}(T_{\alpha\beta}+\omega\delta_{\alpha\beta})\,\mathrm{Im}\,G_{\beta\alpha}(\omega) - \frac{1}{2}\langle\Psi_0^N|\hat{W}|\Psi_0^N\rangle$$

Symmetry breaking and restoration

- Variance in particle number as an indicator of symmetry breaking



$$\sigma_A = \sqrt{\langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2}$$

➟ Only concerns neutron number

➟ Decreases as many-body order increases

- Eventually, symmetries need to be restored

- Only recently the formalism was developed for MBPT and CC

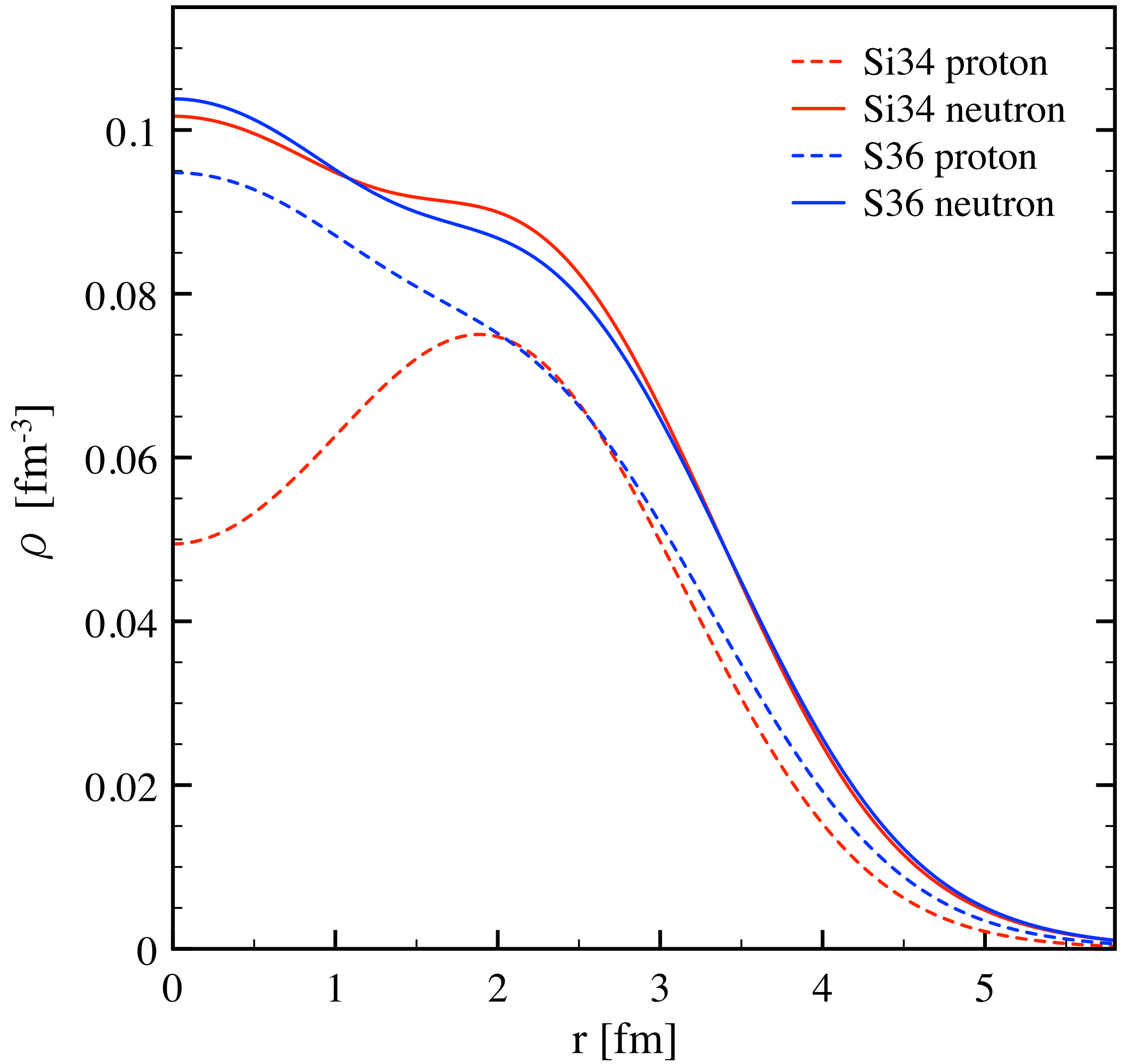
  - Case of **SU(2)** [Duguet 2014]

  - Case of **U(1)** [Duguet & Signoracci 2016]

- Symmetry-restored Gorkov GF formalism still to be developed

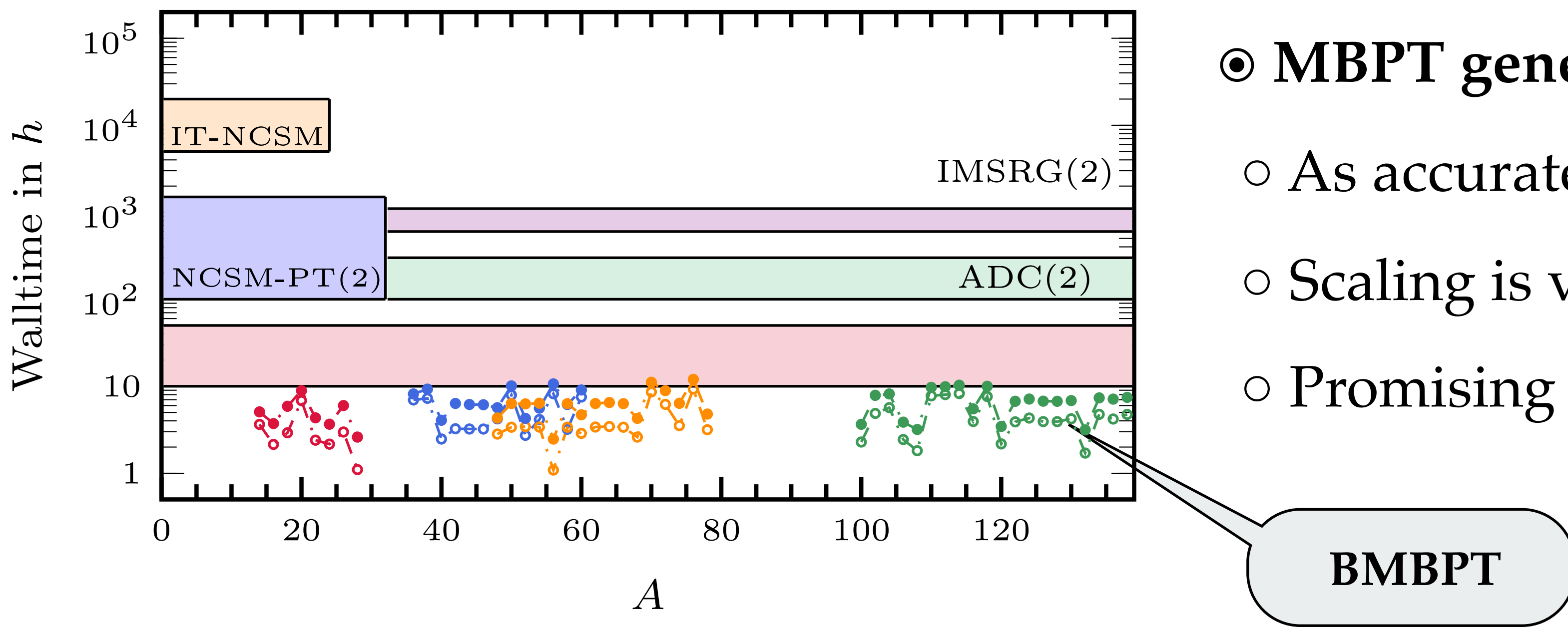
Point-nucleon densities

- **Point-proton** density of ^{34}Si displays a marked depletion in the centre
- **Point-neutron** distributions little affected by removal/addition of two protons
- Bubble structure can be quantified by the **depletion factor** $F \equiv \frac{\rho_{\max} - \rho_c}{\rho_{\max}}$ ➟ $F_p(^{34}\mathrm{Si}) = 0.34$



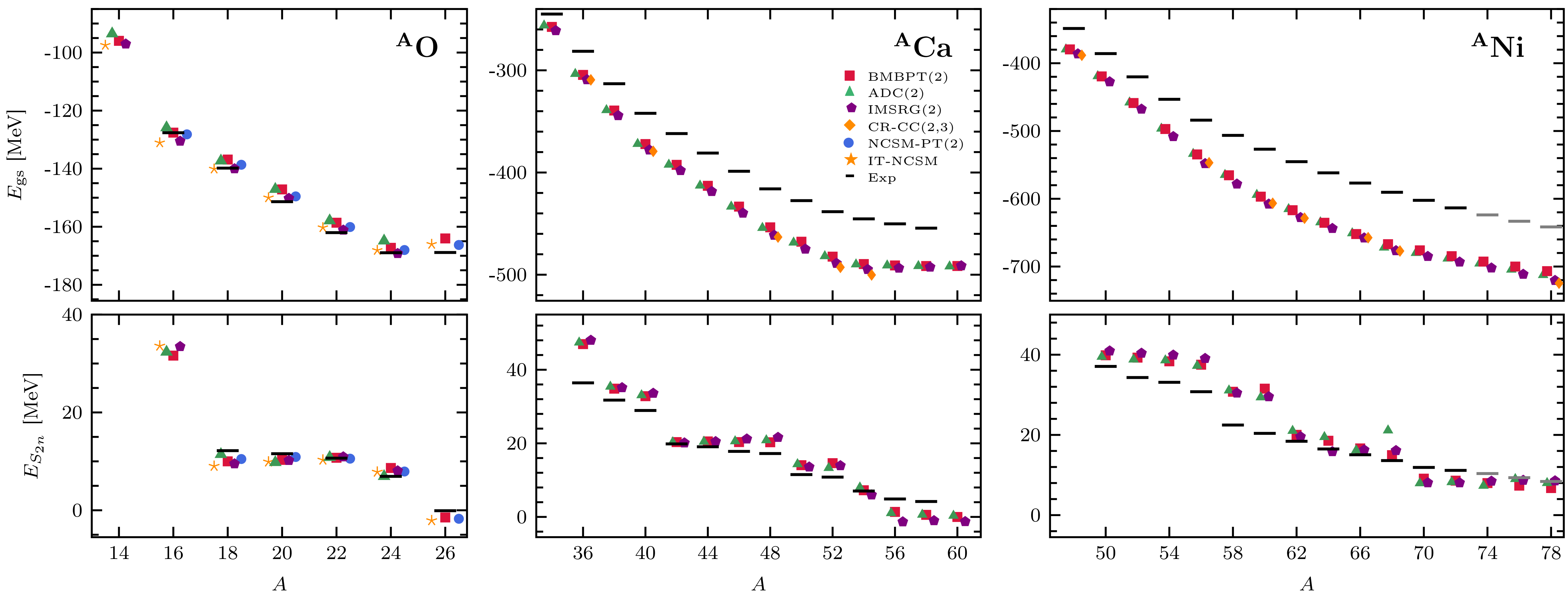
➟ Going from proton to (observable) charge density will smear out depletion

Bogolyubov many-body perturbation theory



- **MBPT generalised to open-shell nuclei**
  - As accurate as non-perturbative methods for soft H
  - Scaling is very favourable
  - Promising tool for diagnostic

[Tichai, Arthuis, *et al.* (in preparation)]



Odd-even systems

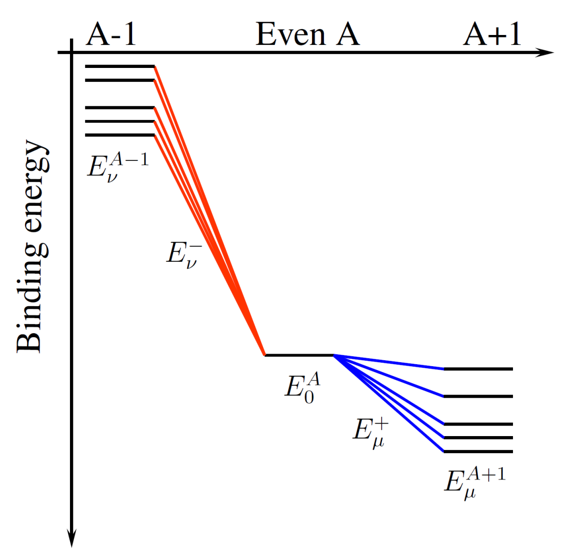
⦿ Current implementation targets $J^\pi = 0^+$ states

➟ Equations simplify: j-coupled scheme, block-diagonal structure, ...

⦿ Different possibilities to compute odd-even g.s. energies:

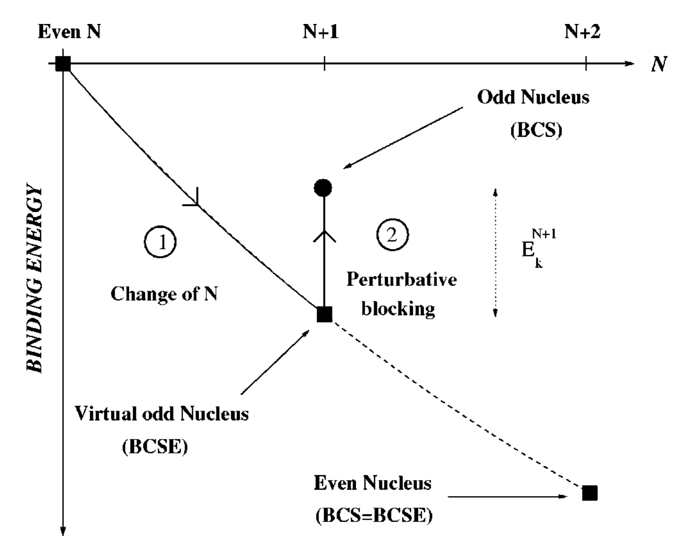
① From separation energies

➟ Either from A-1 or A+1



② From fully-paired even number-parity state

➟ "Fake" odd-A plus correction

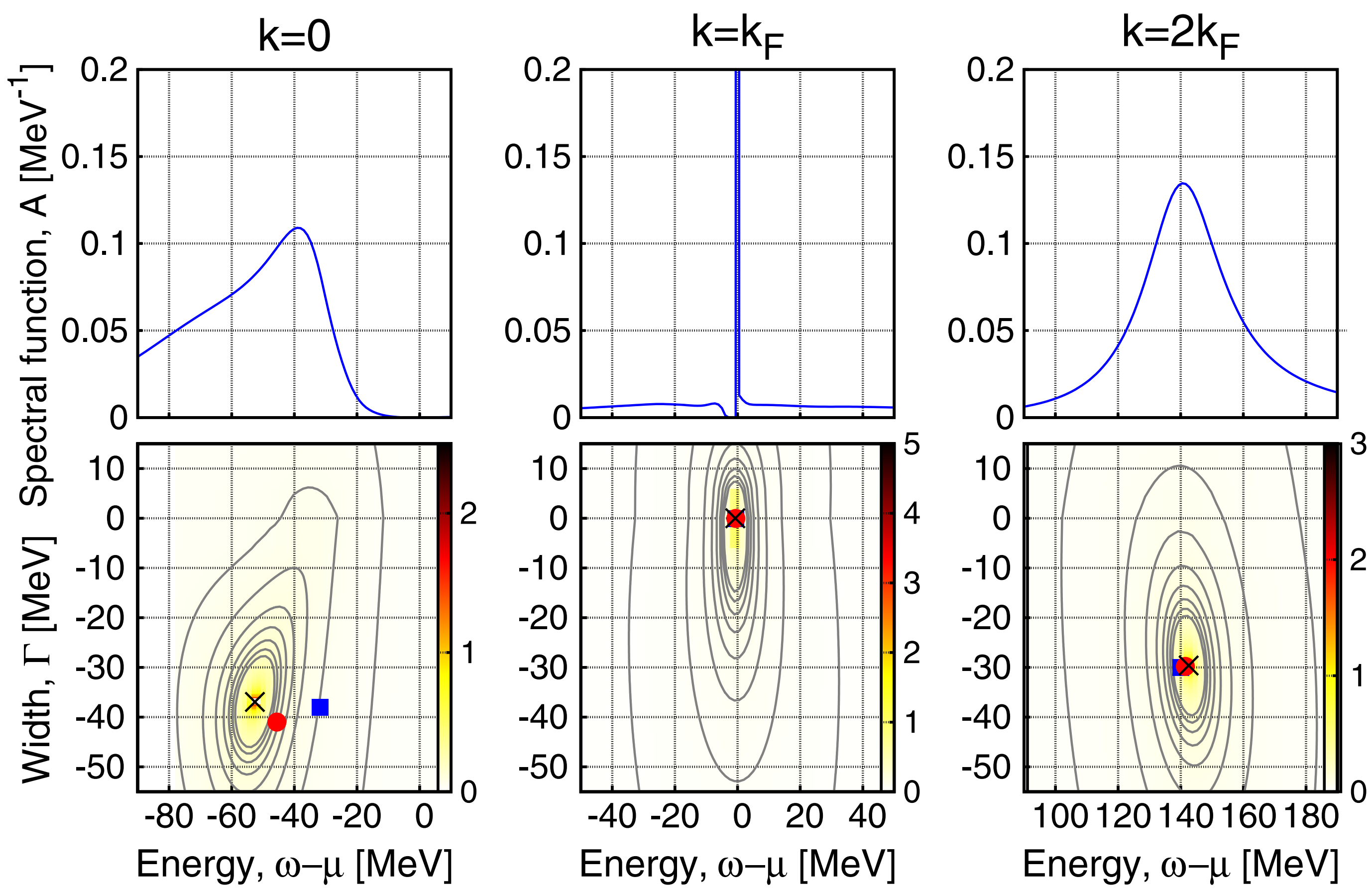


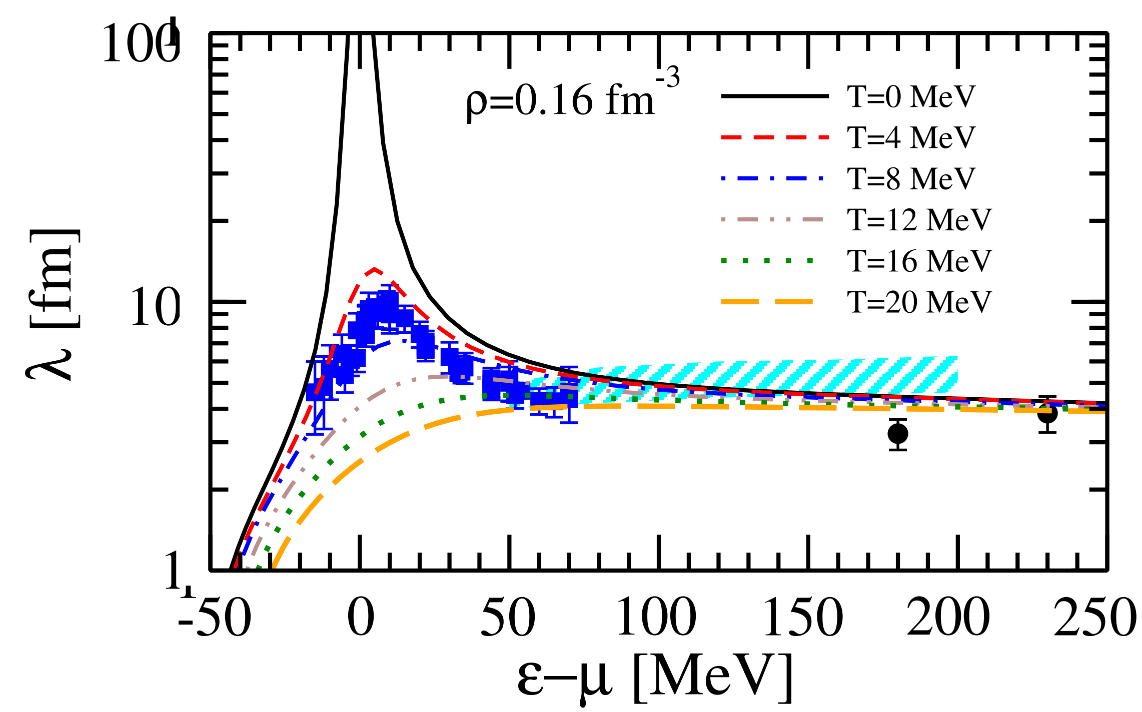
[Duguet *et al.* 2001]

Two methods agree within 2-300 keV

Fragmentation of single-particle strength in infinite matter

- **Spectral function depicts correlations**
  - Broad peak signals depart from mean-field/independent particle picture
  - Well-defined (long-lived) quasiparticles at the Fermi surface
  - Long mean free path for E < E_F





[Rios, Somà 2012]