Chiral forces along mid-mass isotope chains

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with

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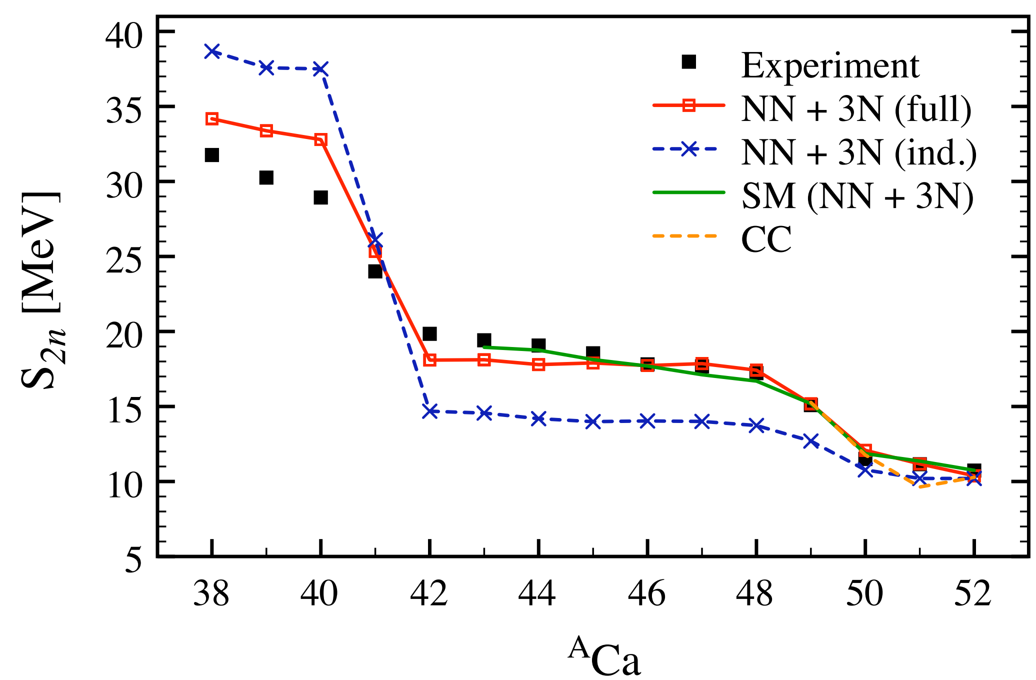


ICNT workshop
Physics of exotic nuclei: theoretical advances and challenges

RIKEN, 9 June 2014

Ab initio nuclear structure

Ab initio many-body theories

- Inter-nucleon interactions as input
- Solve A-body Schrödinger eq.
- Thorough assessment of errors

Recent progress is impressive:

➟ New models available (χ-EFT based)

➟ New techniques available (open-shells)

➟ On the way (cf. SRG machinery)

Limited applicability

Controlled extrapolations

Test fundamental interactions

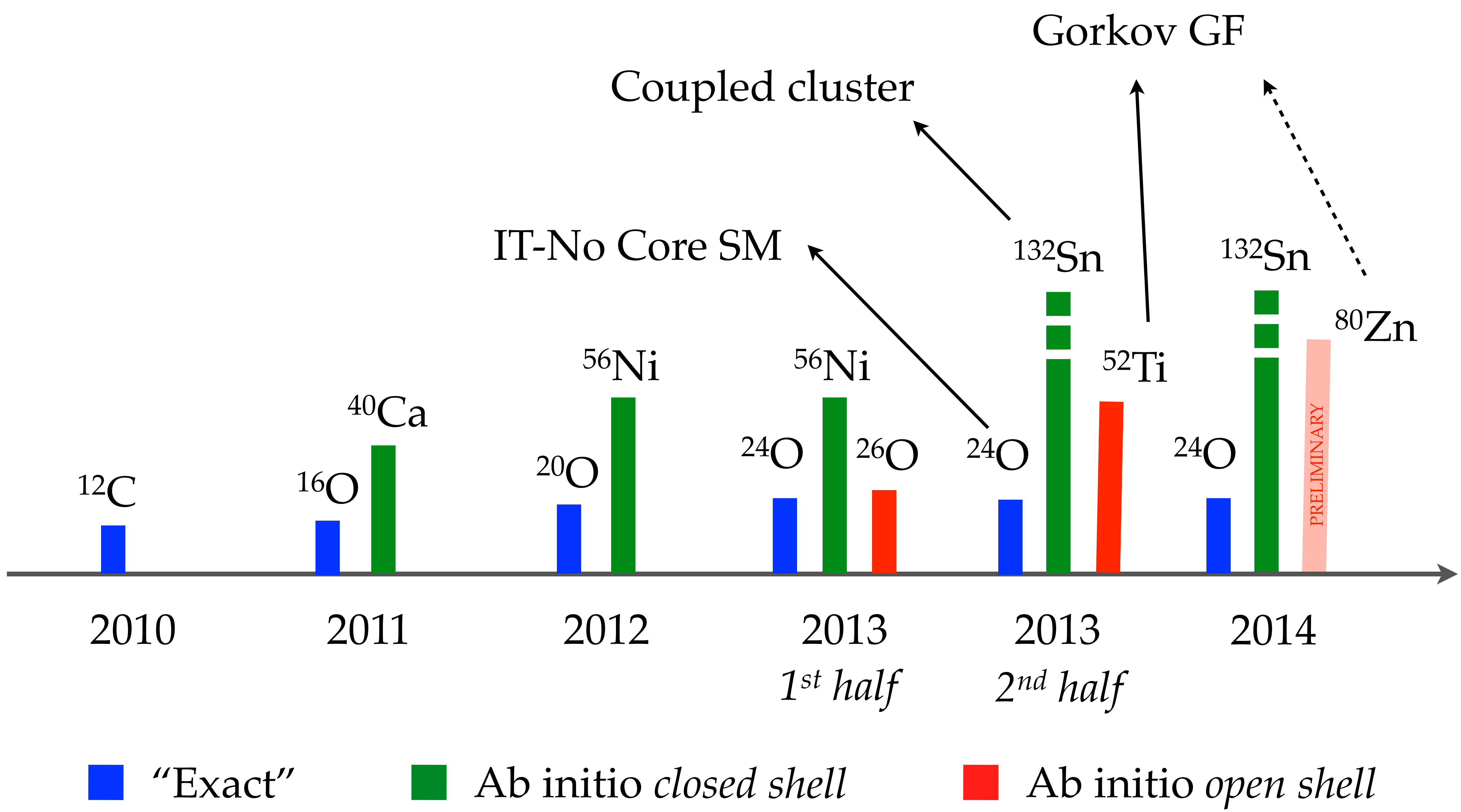
Complementary to effective many-body methods

Crucial for exotic nuclei!

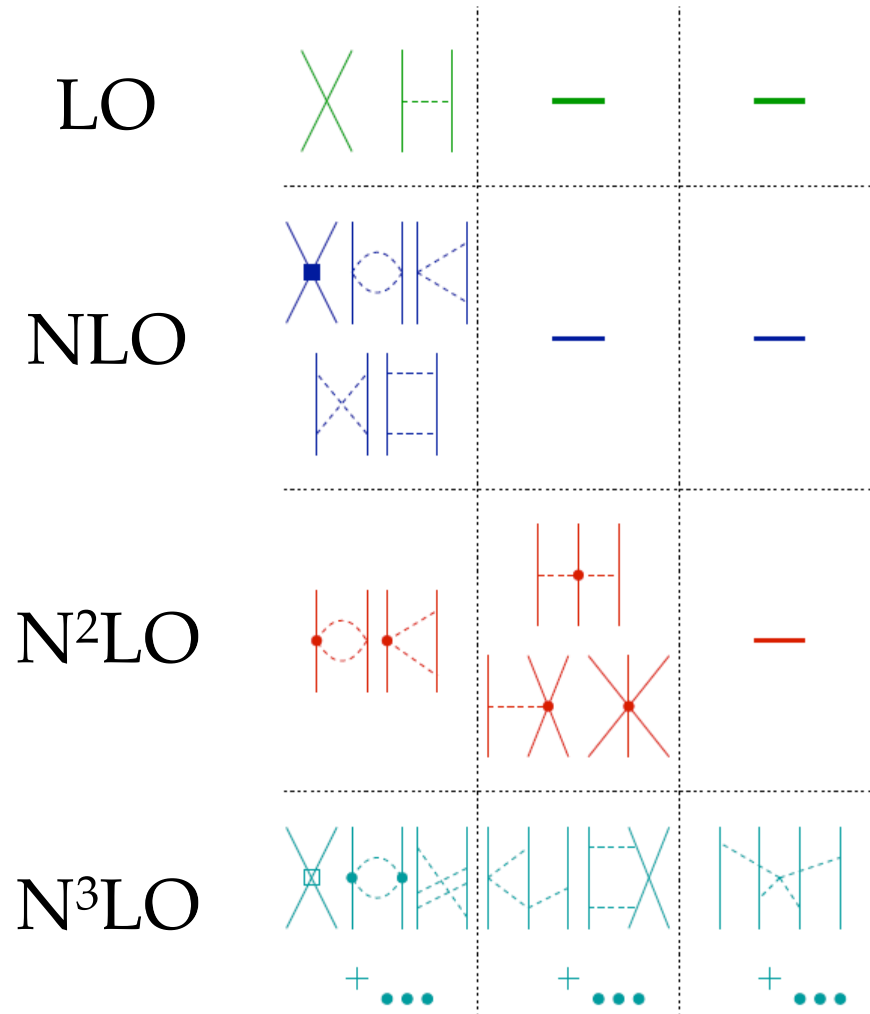
Current limits / reach of ab initio calculations

➟ Heavier system computed in the different types of ab initio

NN+3N



Chiral EFT & inter-nucleon interactions



- ✪ Separation of scales
- ✪ Expansion in powers of momenta
- ✪ Long-range physics explicit
  +
  Short-range couplings
- ✪ Consistent many-body forces
- ✪ Systematic, provides error estimates

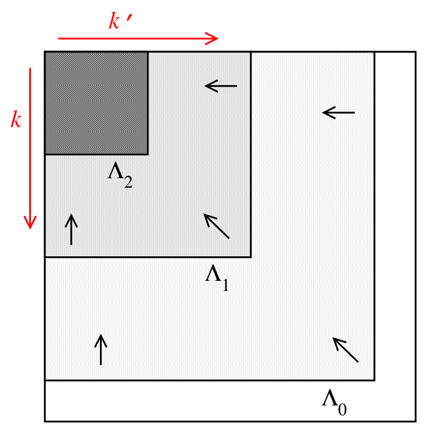
✪ Very promising, but yet not completely satisfactory

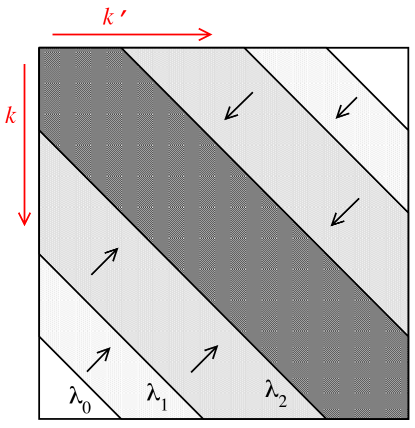
- ➟ Different orders in EFT
- ➟ Consistency of cutoffs?
- ➟ Order-by-order convergence unclear
- ➟ More fundamental problem: EFT power counting

RG techniques for NN & 3N forces

- Renormalization group techniques for NN and 3N forces
  - ➡ Lower the *resolution scale* of the original Hamiltonian

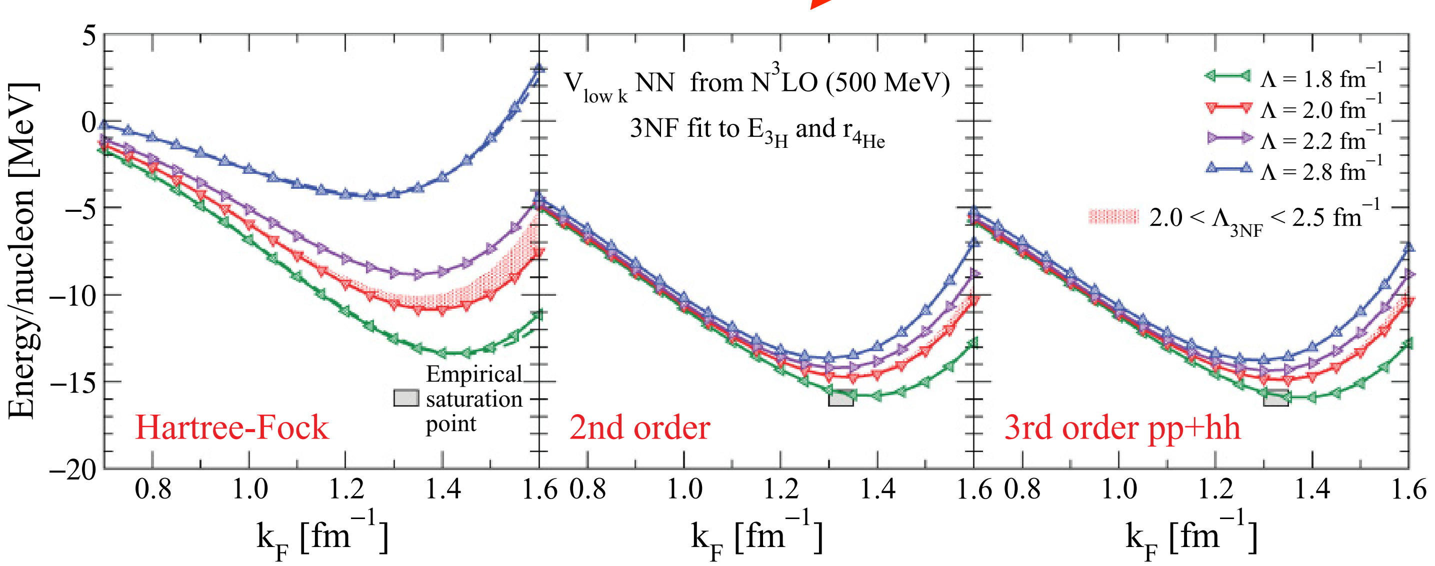
$V_{\text{low-k}}$



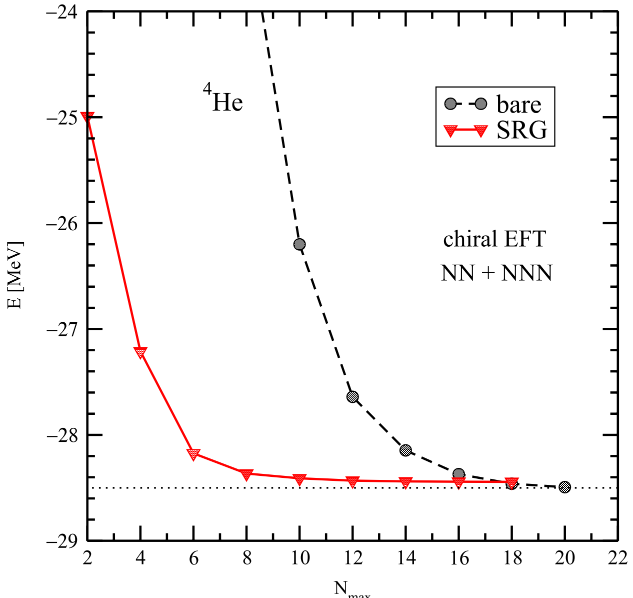


V_{SRG}

- Improved convergence of many-body calculations
  - ➡ Smaller many-body truncations & smaller model spaces needed



[Hebeler *et al.* 2011]



[Jurgenson, Navratil & Furnstahl 2013]

Choice of NN+3N potential

✪ NN potential:

○ chiral N^{3}LO (500 MeV)

➟ SRG-evolved to 2.0 fm^{-1}

[Entem and Machleidt 2003]

✪ 3N potential:

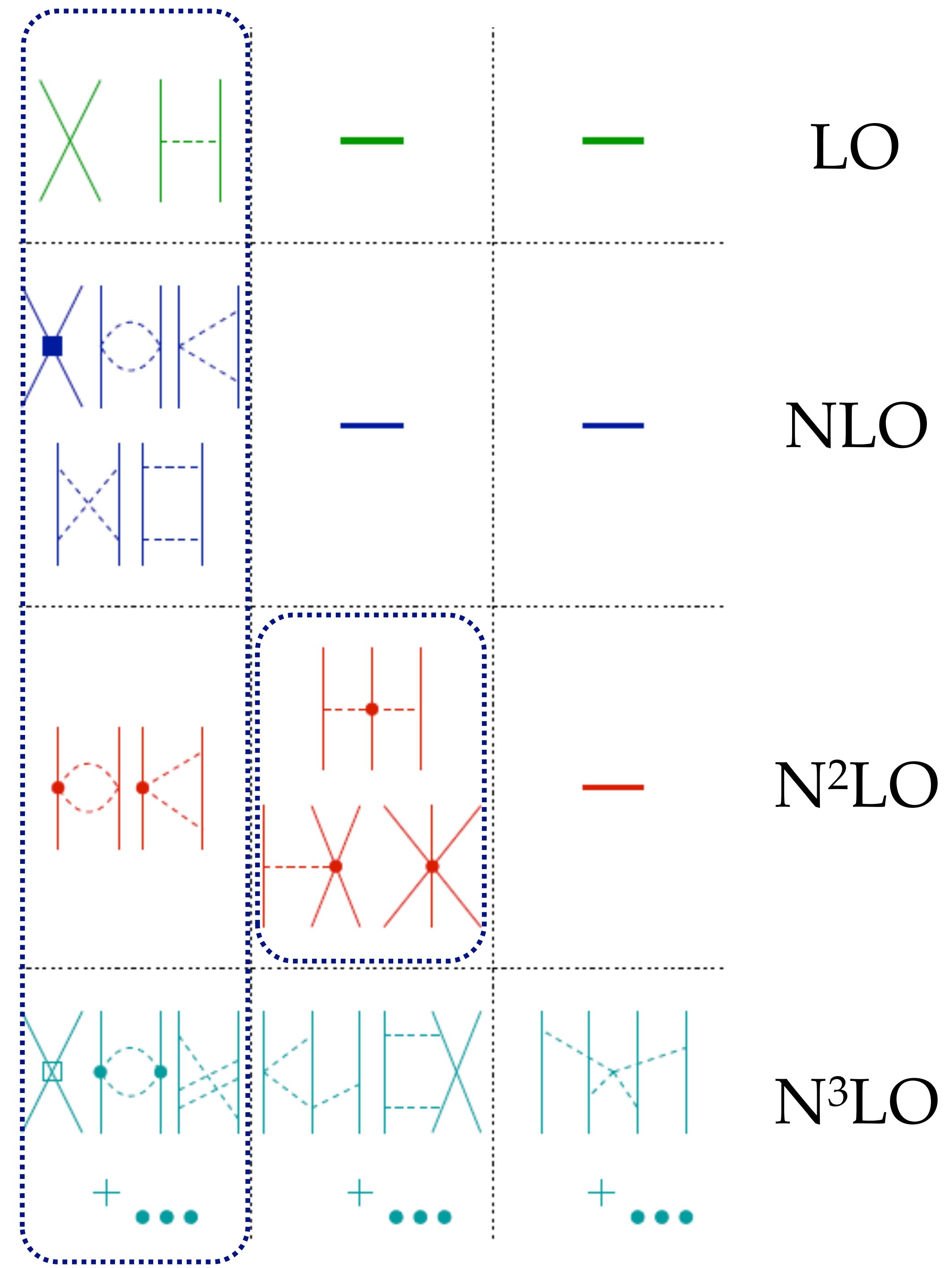
○ chiral N^{2}LO (400 MeV)

➟ SRG-evolved to 2.0 fm^{-1}

[Navrátil 2007]

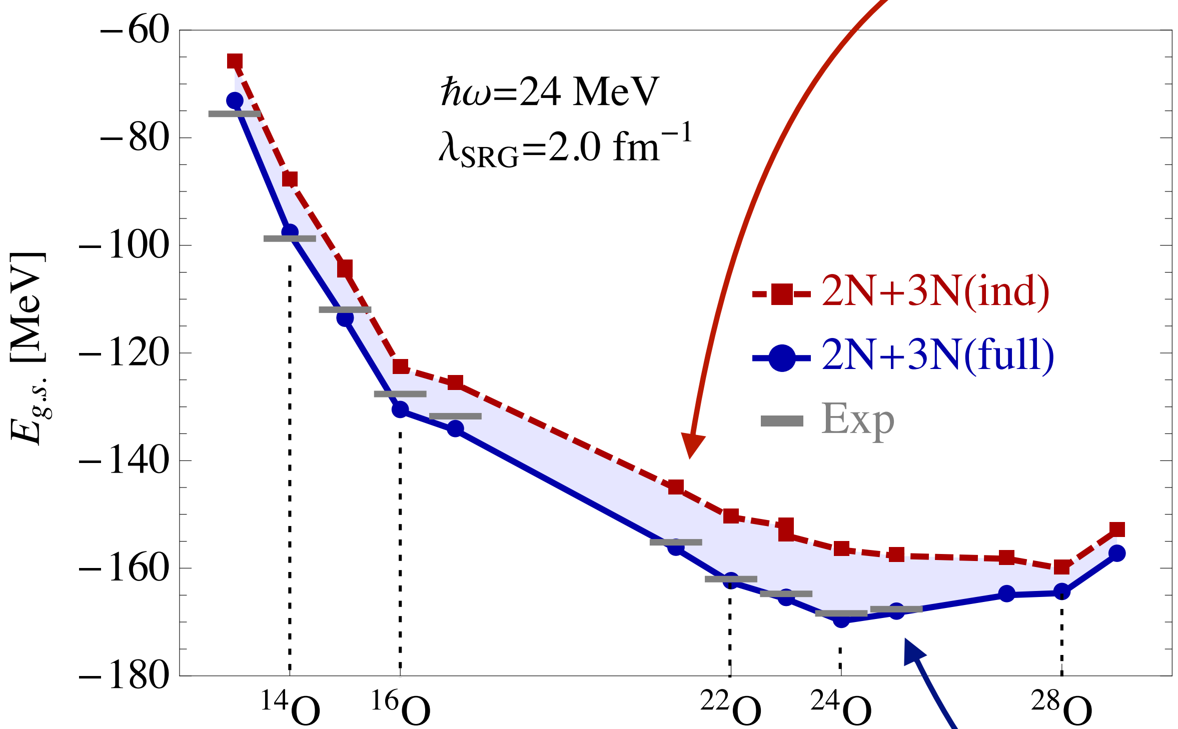
➟ Choice of cutoff to reduce induced 4N contributions

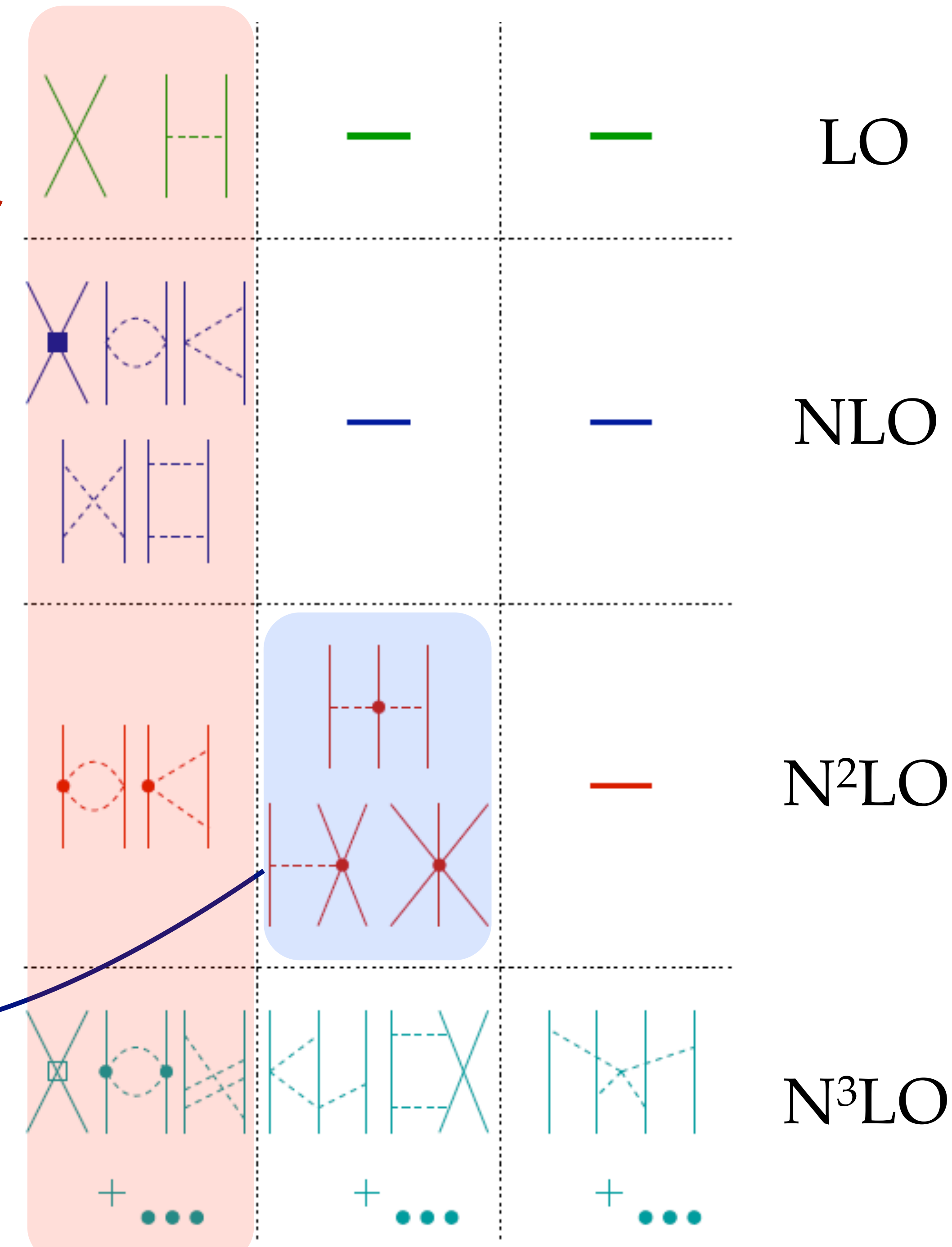
[Roth *et al*. 2012]



Chiral NN+3N in the oxygen chain

✪ Self-consistent Green's functions





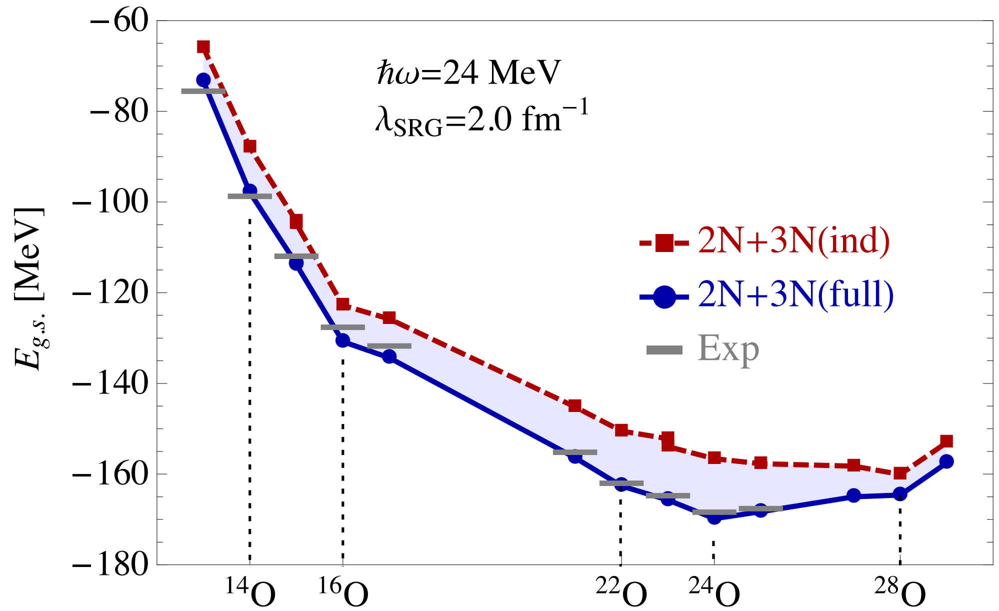
[Cipollone, Barbieri & Navrátil 2013]

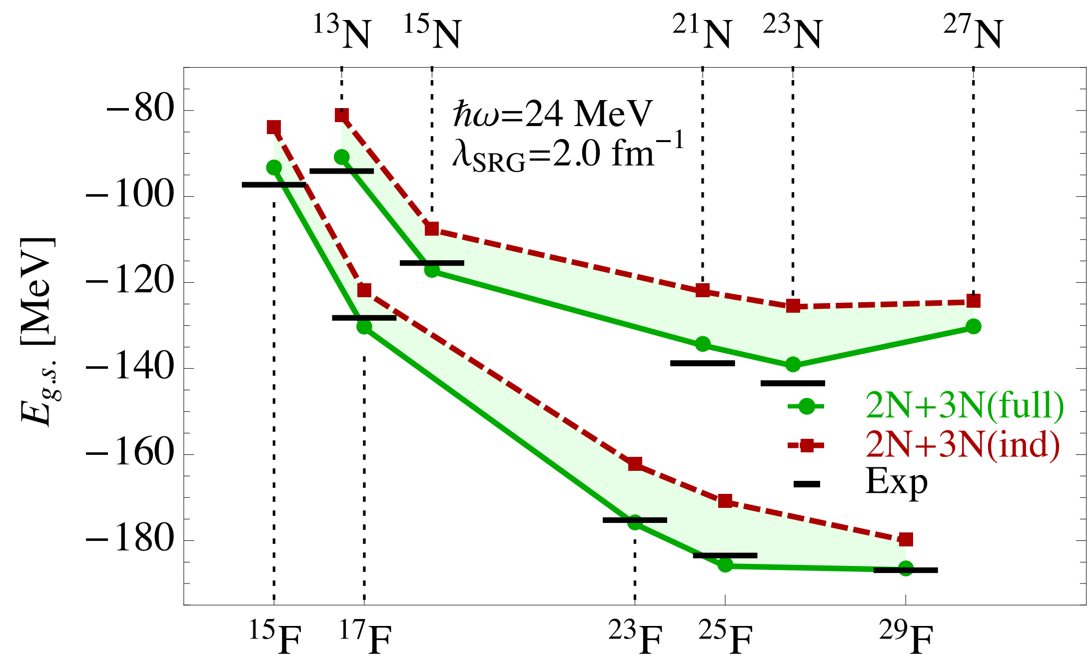
➟ Overall good agreement with data

➟ 3NF crucial for reproducing driplines

Around oxygen

✪ Consistent description of Z = 7, 8, 9 isotopic chains with GF method



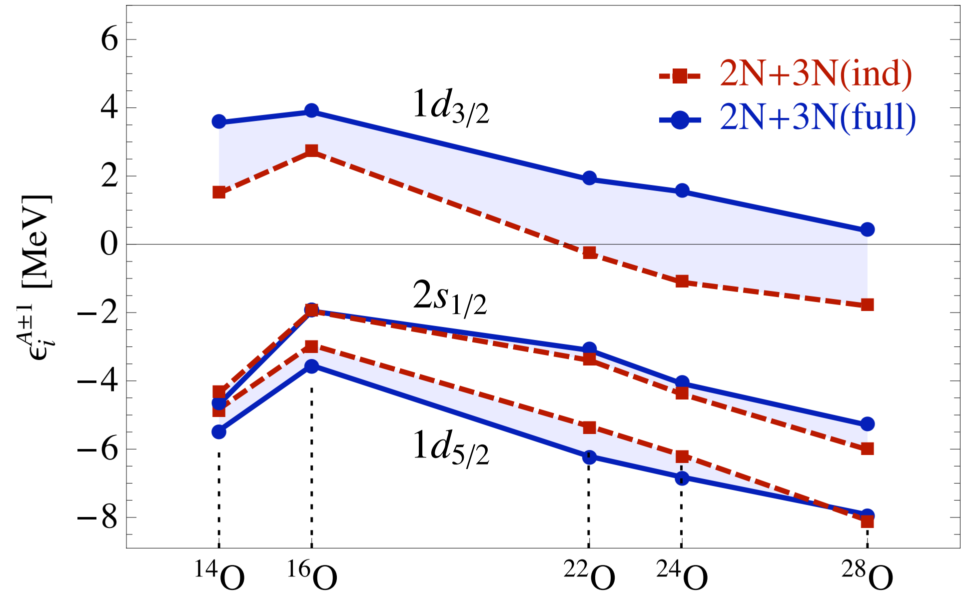


[Cipollone, Barbieri & Navrátil 2013]

➟ $d_{3/2}$ raised by genuine 3NF

➟ Ab initio confirmation of microscopic SM

[Otsuka *et al.* 2010, see also Hergert *et al.* 2013]



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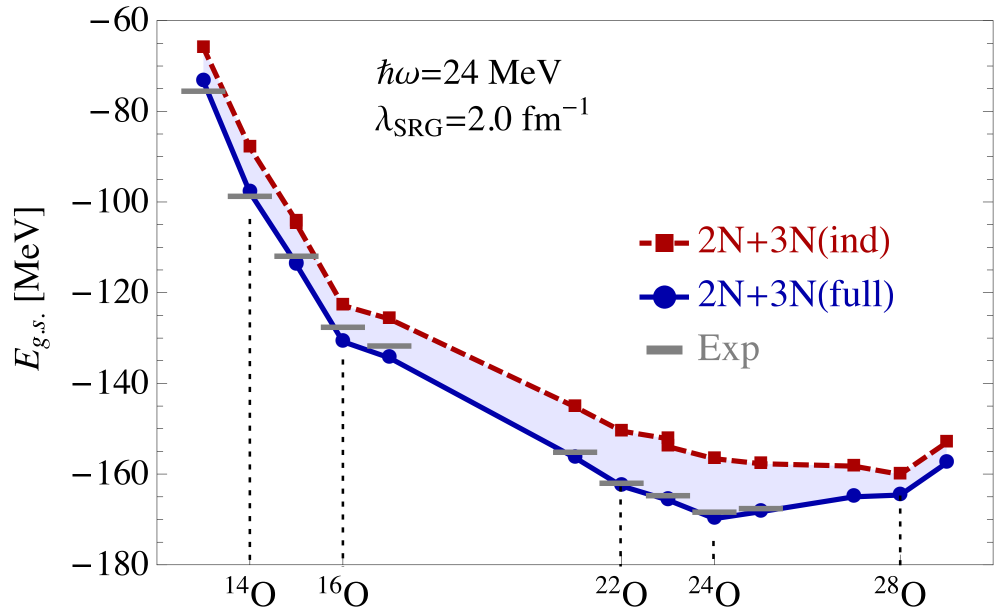
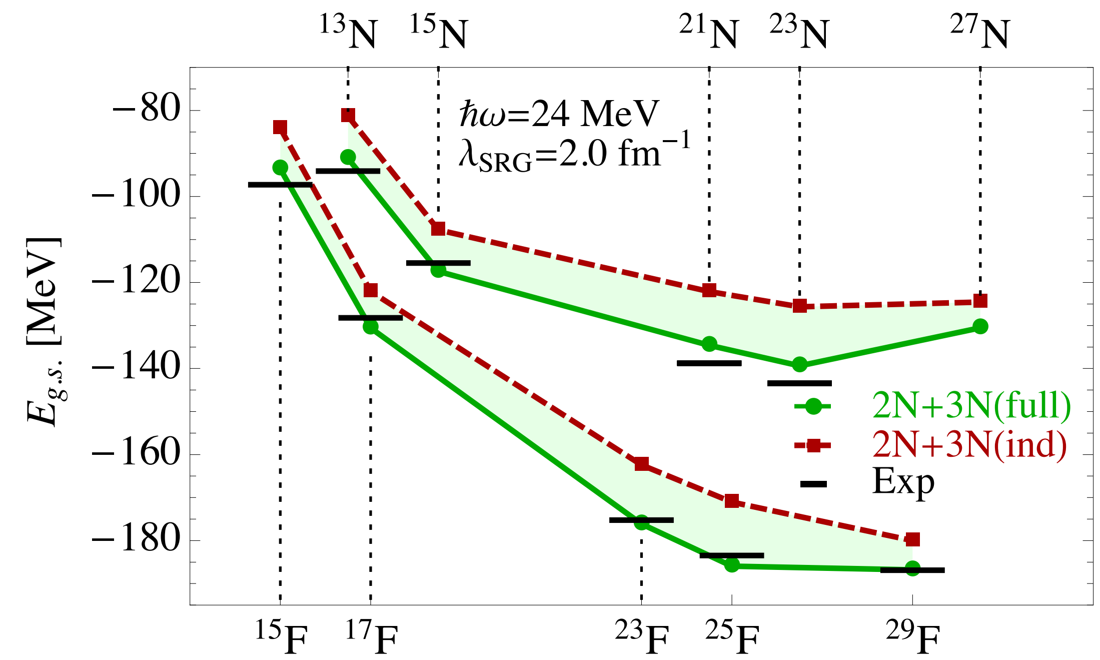
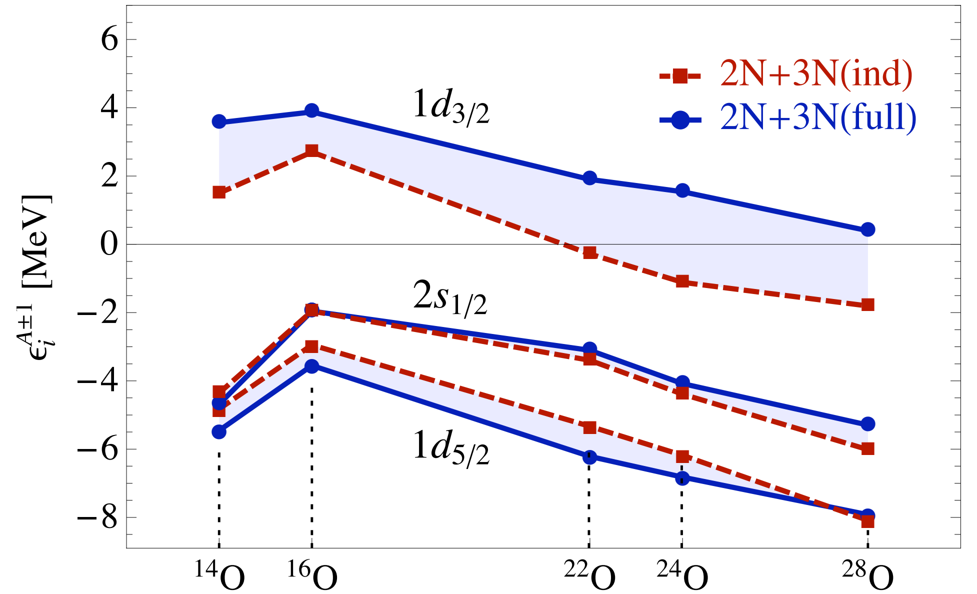




[Cipollone, Barbieri & Navrátil 2013]



But: radii underestimated

- ~5-15% discrepancy with experiment
- 3NF do not impact radii significantly

Ab initio *open-shell:* Gorkov-Green's functions

✪ Self-consistent Green's functions

- ➟ Many-body truncation in the self-energy expansion (cf. CC, IM-SRG, ...)
- ➟ Access to *A±1* systems via spectral function
- ➟ Natural connection to scattering (e.g. optical potentials)

✪ Gorkov scheme

- ➟ Goes beyond standard expansion schemes limited to doubly closed-shell
  - ○ Formulate the expansion scheme around a Bogoliubov vacuum
  - ○ Single-reference method (cf. MR in quantum chemistry or IM-SRG)
  - ○ Exploit breaking (and restoration) of U(1) symmetry
- ➟ From few tens to hundreds of medium-mass open-shell nuclei
  - ○ *Formalism* VS, Duguet & Barbieri, PRC 84 064317 (2011)
  - ○ *Proof of principle* VS, Barbieri & Duguet, PRC 87 011303 (2013)
  - ○ *Technical aspects* VS, Barbieri & Duguet, PRC 89 024323 (2014)
  - ○ *NN+3N* VS, Cipollone, Barbieri, Navrátil & Duguet, PRC 89 061301 (2014)

Gorkov framework

✪ Expand around an auxiliary many-body state

$$|\Psi_0\rangle \equiv \sum_{A}^{\text{even}} c_A \, |\psi_0^A\rangle$$

Breaks particle-number symmetry

➟ Introduce a "grand-canonical" potential $\Omega = H - \mu A$

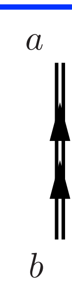
➟ $|\Psi_0\rangle$ minimizes $\Omega_0 = \langle \Psi_0 | \Omega | \Psi_0 \rangle$ under the constraint $A = \langle \Psi_0 | A | \Psi_0 \rangle$

➟ Observables of the A-body system $\Omega_0 = \sum_{A'} |c_{A'}|^2 \, \Omega_0^{A'} \approx E_0^A - \mu A$

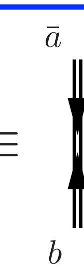
set of 4 Gorkov propagators

[Gorkov 1958]

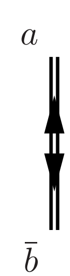
$$i\, G^{11}_{ab}(t,t') \equiv \langle \Psi_0 | T \left\{ a_a(t) a_b^\dagger(t') \right\} | \Psi_0 \rangle \quad \equiv$$



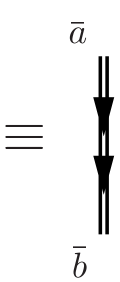
$$i\, G^{21}_{ab}(t,t') \equiv \langle \Psi_0 | T \left\{ \bar{a}_a^\dagger(t) a_b^\dagger(t') \right\} | \Psi_0 \rangle \quad \equiv$$



$$i\, G^{12}_{ab}(t,t') \equiv \langle \Psi_0 | T \left\{ a_a(t) \bar{a}_b(t') \right\} | \Psi_0 \rangle \quad \equiv$$



$$i\, G^{22}_{ab}(t,t') \equiv \langle \Psi_0 | T \left\{ \bar{a}_a^\dagger(t) \bar{a}_b(t') \right\} | \Psi_0 \rangle \quad \equiv$$



Inside the Green's function

✪ Separation energy spectrum

$$G^{11}_{ab}(\omega) = \sum_k \left\{ \frac{\mathcal{U}^k_a \, \mathcal{U}^{k*}_b}{\omega - \omega_k + i\eta} + \frac{\bar{\mathcal{V}}^{k*}_a \, \bar{\mathcal{V}}^k_b}{\omega + \omega_k - i\eta} \right\}$$

Lehmann representation

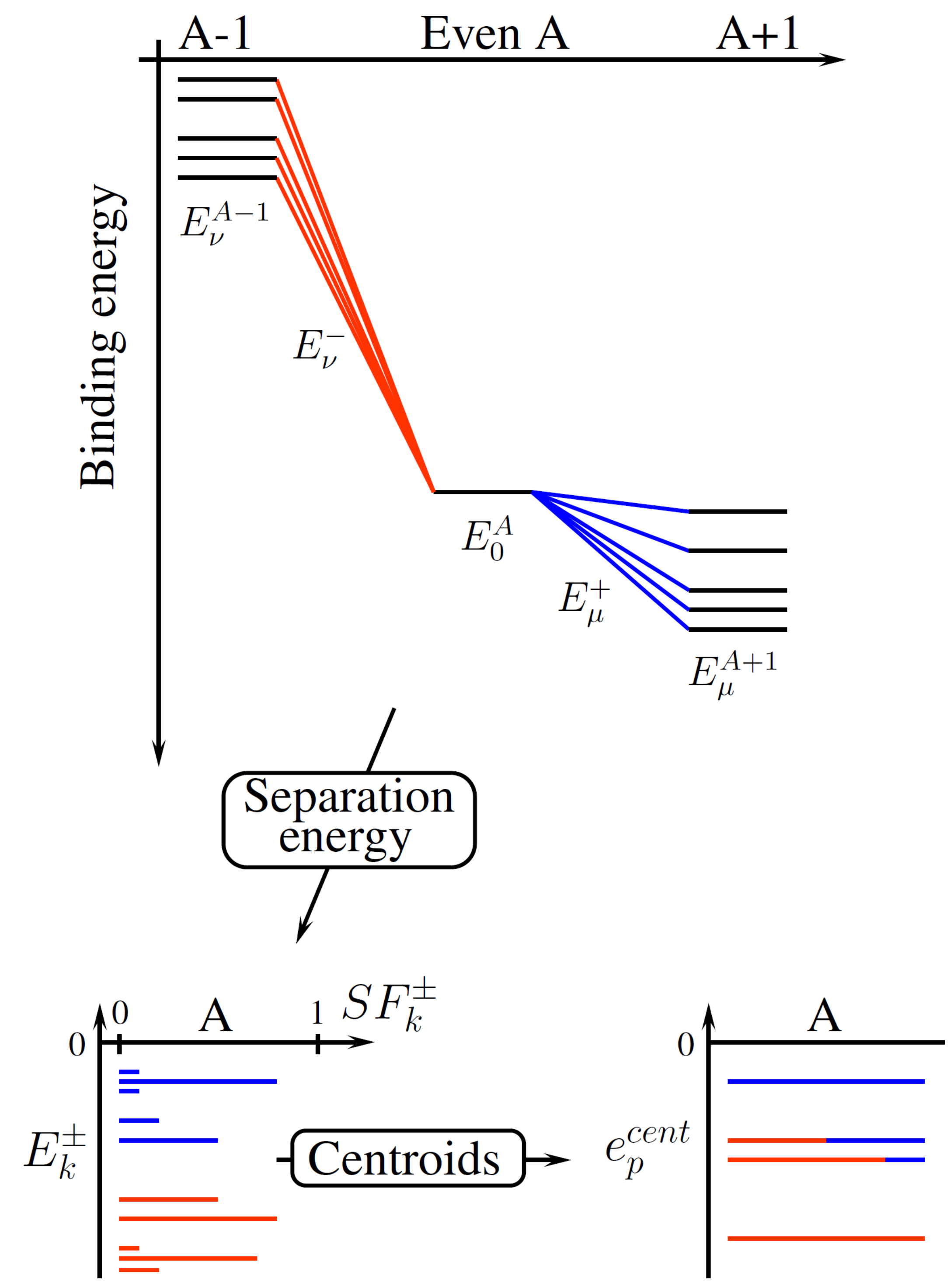
where $\begin{cases} \mathcal{U}^{k*}_a \equiv \langle \Psi_k | a^\dagger_a | \Psi_0 \rangle \\ \mathcal{V}^{k*}_a \equiv \langle \Psi_k | \bar{a}_a | \Psi_0 \rangle \end{cases}$

and $\begin{cases} E^{+\,(A)}_k \equiv E^{A+1}_k - E^A_0 \equiv \mu + \omega_k \\ E^{-\,(A)}_k \equiv E^A_0 - E^{A-1}_k \equiv \mu - \omega_k \end{cases}$

✪ Spectroscopic factors

$$SF^+_k \equiv \sum_{a \in \mathcal{H}_1} \left| \langle \psi_k | a^\dagger_a | \psi_0 \rangle \right|^2 = \sum_{a \in \mathcal{H}_1} \left| \mathcal{U}^k_a \right|^2$$

$$SF^-_k \equiv \sum_{a \in \mathcal{H}_1} \left| \langle \psi_k | a_a | \psi_0 \rangle \right|^2 = \sum_{a \in \mathcal{H}_1} \left| \mathcal{V}^k_a \right|^2$$



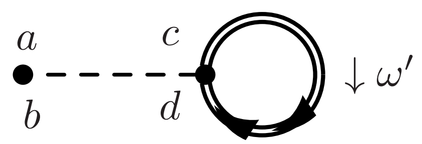
[figure from J. Sadoudi]

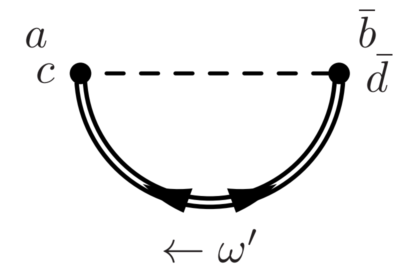
Gorkov equation & self-energy

✪ Gorkov equation $\longrightarrow$ energy *dependent* eigenvalue problem

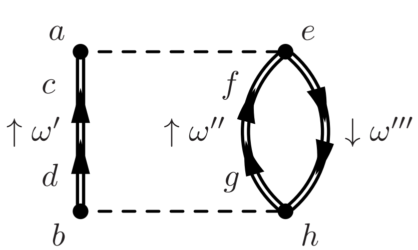
$$\boxed{\sum_b \begin{pmatrix} t_{ab} - \mu_{ab} + \Sigma^{11}_{ab}(\omega) & \Sigma^{12}_{ab}(\omega) \\ \Sigma^{21}_{ab}(\omega) & -t_{ab} + \mu_{ab} + \Sigma^{22}_{ab}(\omega) \end{pmatrix}\Bigg|_{\omega_k} \begin{pmatrix} \mathcal{U}^k_b \\ \mathcal{V}^k_b \end{pmatrix} = \omega_k \begin{pmatrix} \mathcal{U}^k_a \\ \mathcal{V}^k_a \end{pmatrix}}$$

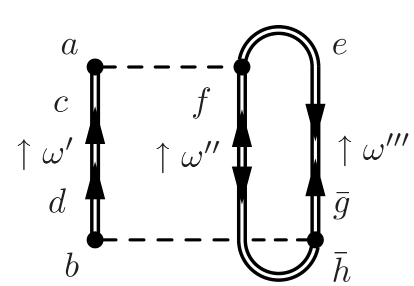
✪ 1st order ➟ energy-independent self-energy

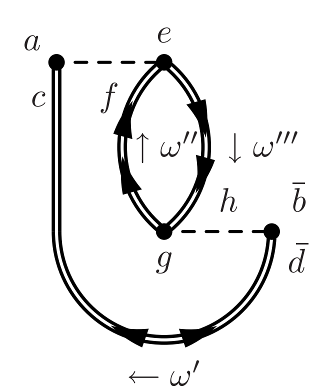
$\Sigma^{11\,(1)}_{ab} =$ 

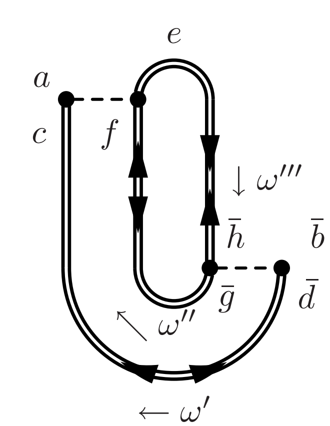
$\Sigma^{12\,(1)}_{ab} =$ 

✪ 2nd order ➟ energy-dependent self-energy

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

$+$ 

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

$+$ 

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[Schirmer & Angonoa 1989]

energy *independent* eigenvalue problem

$\propto N_b^3$

typically ~10^6-10^7

$$\boxed{\begin{pmatrix} T-\mu+\Lambda & \tilde{h} & \mathcal{C} & -\mathcal{D}^\dagger \\ \tilde{h}^\dagger & -T+\mu-\Lambda & -\mathcal{D}^\dagger & \mathcal{C} \\ \mathcal{C}^\dagger & -\mathcal{D} & E & 0 \\ -\mathcal{D} & \mathcal{C}^\dagger & 0 & -E \end{pmatrix} \begin{pmatrix} \mathcal{U}^k \\ \mathcal{V}^k \\ \mathcal{W}_k \\ \mathcal{Z}_k \end{pmatrix} = \omega_k \begin{pmatrix} \mathcal{U}^k \\ \mathcal{V}^k \\ \mathcal{W}_k \\ \mathcal{Z}_k \end{pmatrix}}$$

Krylov space eigenvalue problem

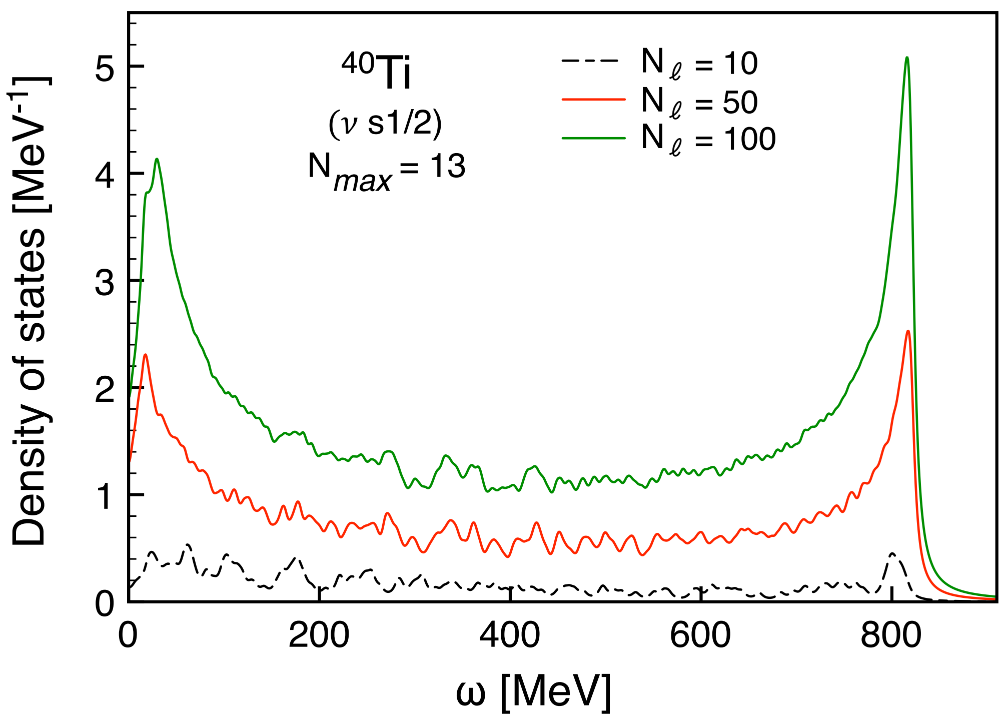
$\propto N_{\mathrm{Lanczos}}$

typically ~10^2-10^3

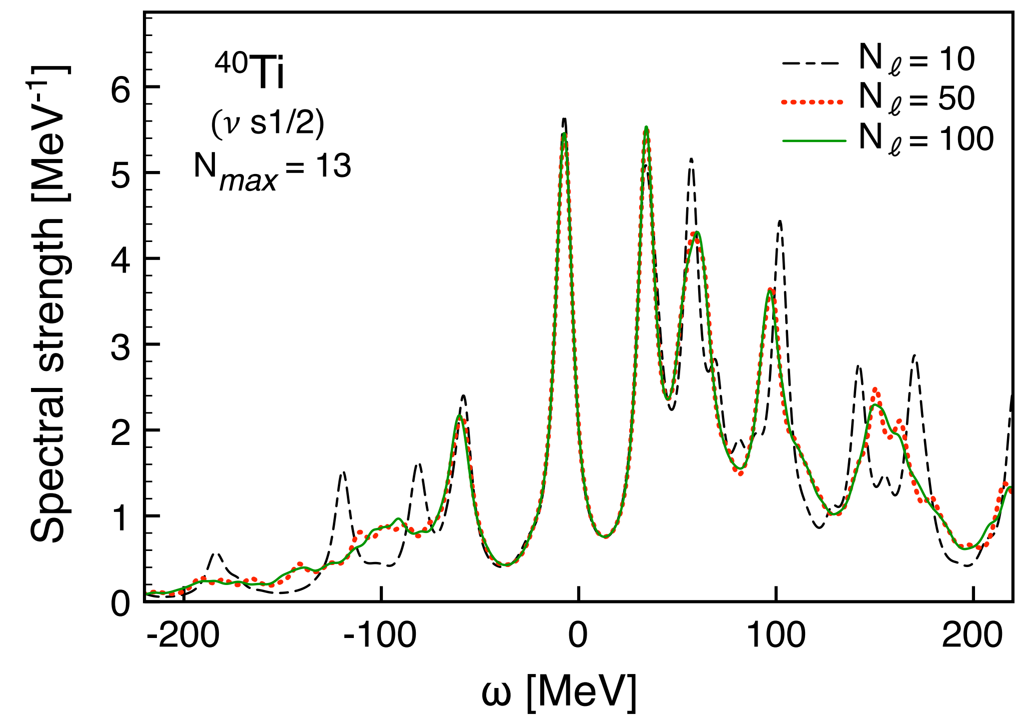
$$\boxed{\begin{pmatrix} T-\mu+\Lambda & \tilde{h} & \mathcal{C} & -\mathcal{D}^\dagger \\ \tilde{h}^\dagger & -T+\mu-\Lambda & -\mathcal{D}^\dagger & \mathcal{C} \\ \mathcal{C}^\dagger & -\mathcal{D} & E & 0 \\ -\mathcal{D} & \mathcal{C}^\dagger & 0 & -E \end{pmatrix} \begin{pmatrix} \mathcal{U}^k \\ \mathcal{V}^k \\ \mathcal{W}_k \\ \mathcal{Z}_k \end{pmatrix} = \omega_k \begin{pmatrix} \mathcal{U}^k \\ \mathcal{V}^k \\ \mathcal{W}_k \\ \mathcal{Z}_k \end{pmatrix}}$$

Testing Krylov projection & model space truncation

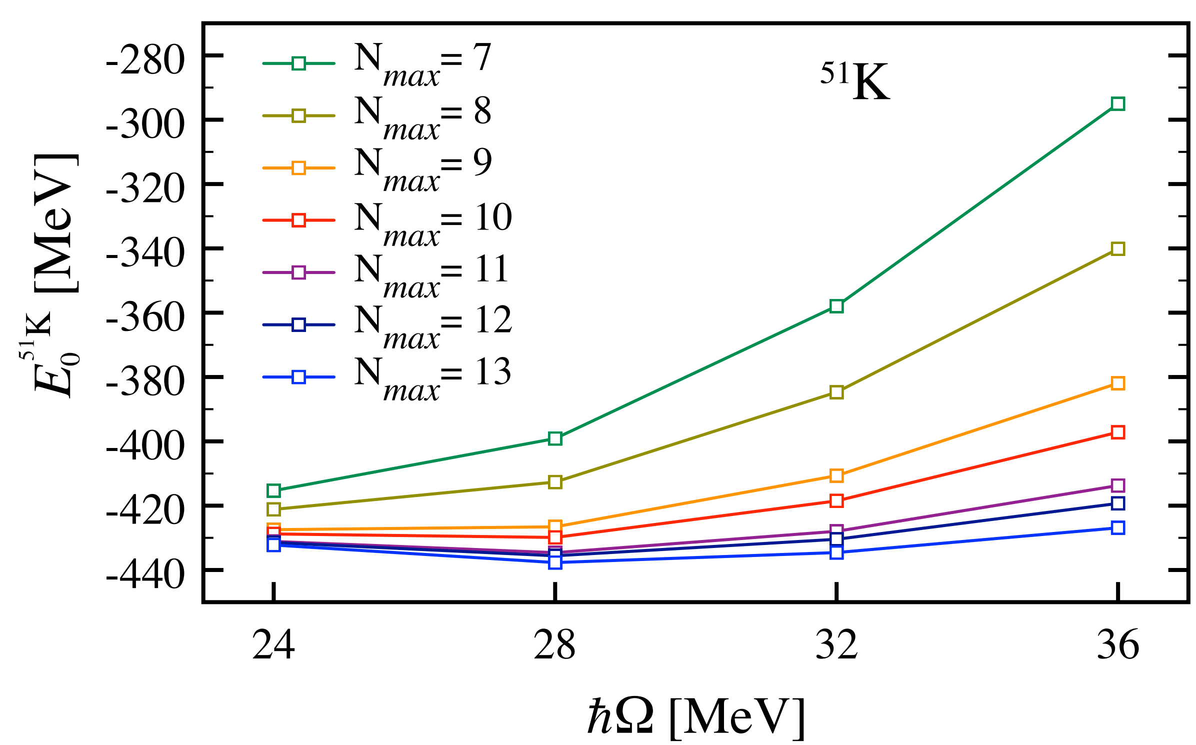
Density of states



Spectral strength



Krylov projection well under control



Error from model space truncation around 1 MeV

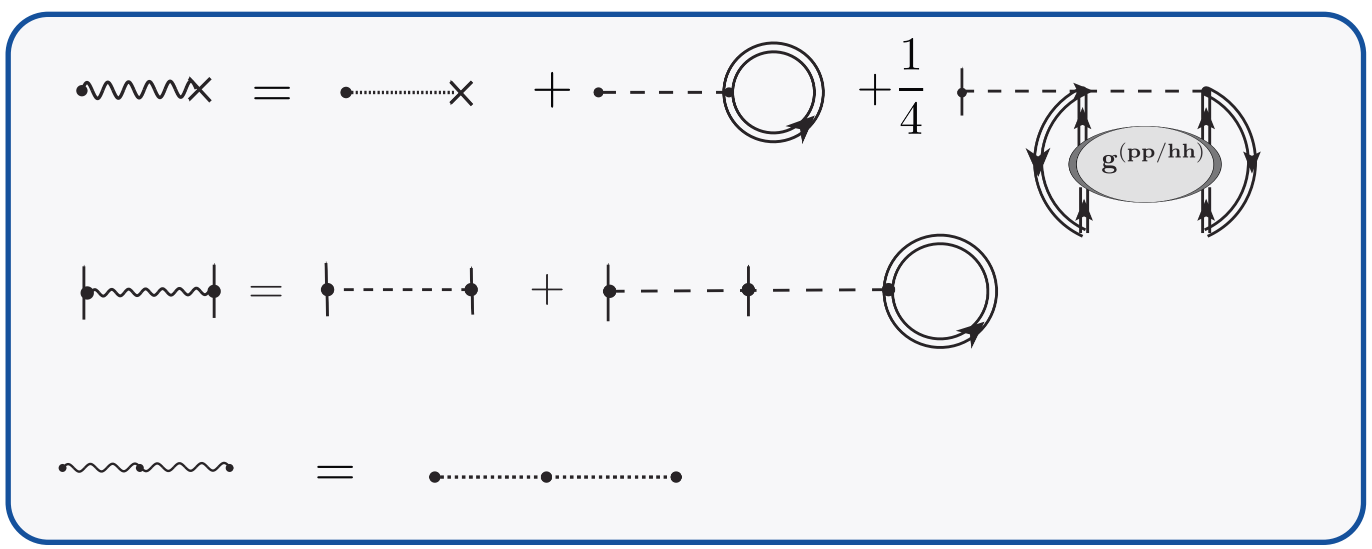
Three-body forces

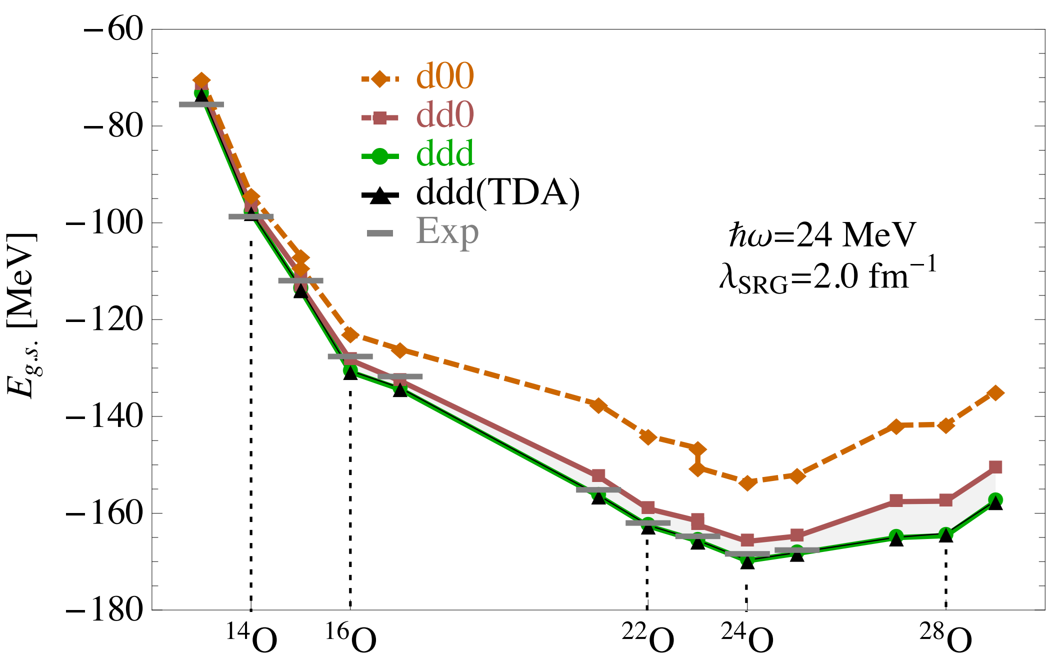
✪ One- and two-body forces derived from the 3N part of the Hamiltonian

➟ Contractions with fully correlated density matrix

➟ Generalization of normal ordering

✪ Galitskii-Koltun sum rule modified to account for 3N piece

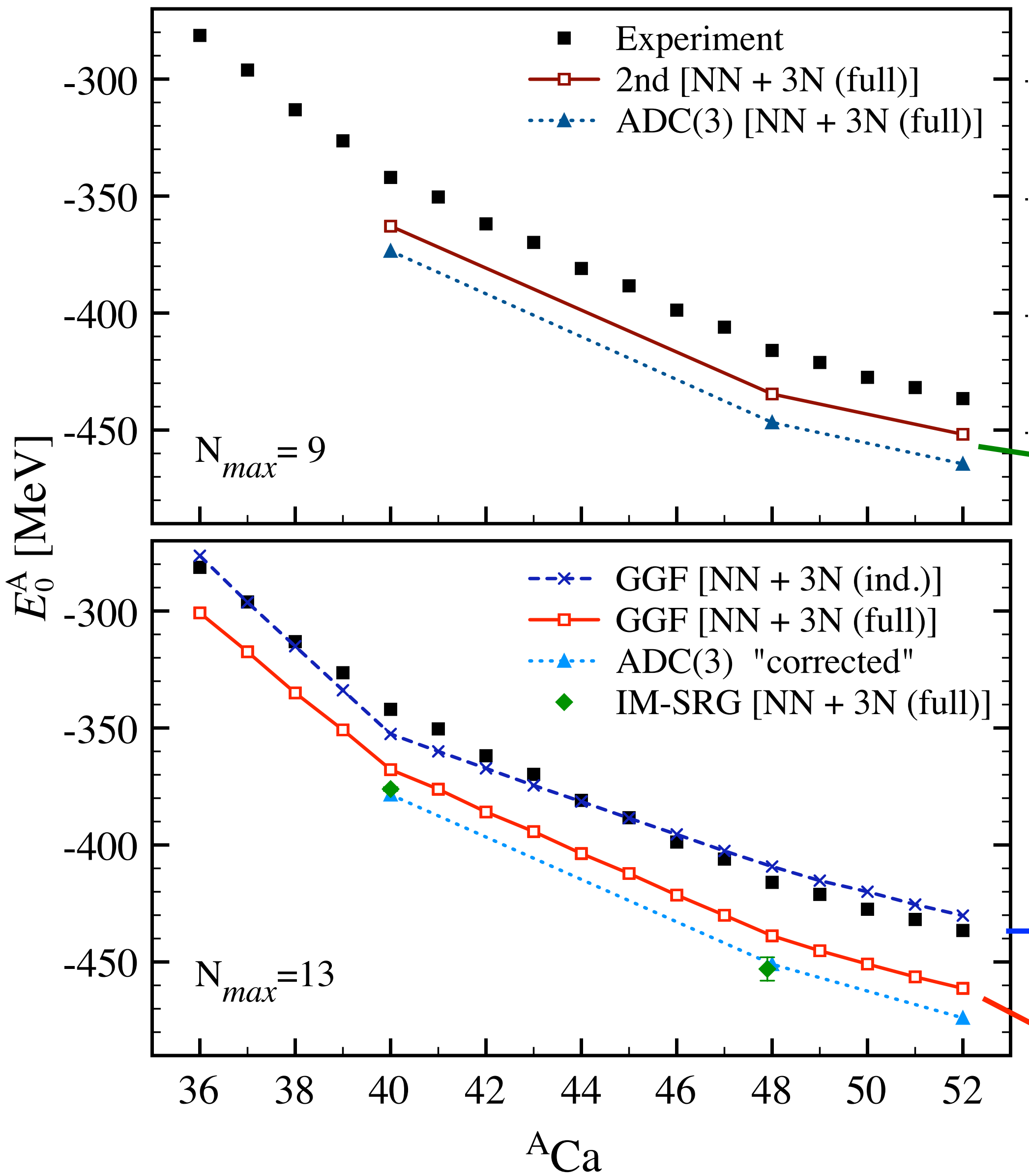




[Cipollone *et al.* 2013]

➟ Use of dressed propagators provides extra correlations

Binding energies around Ca

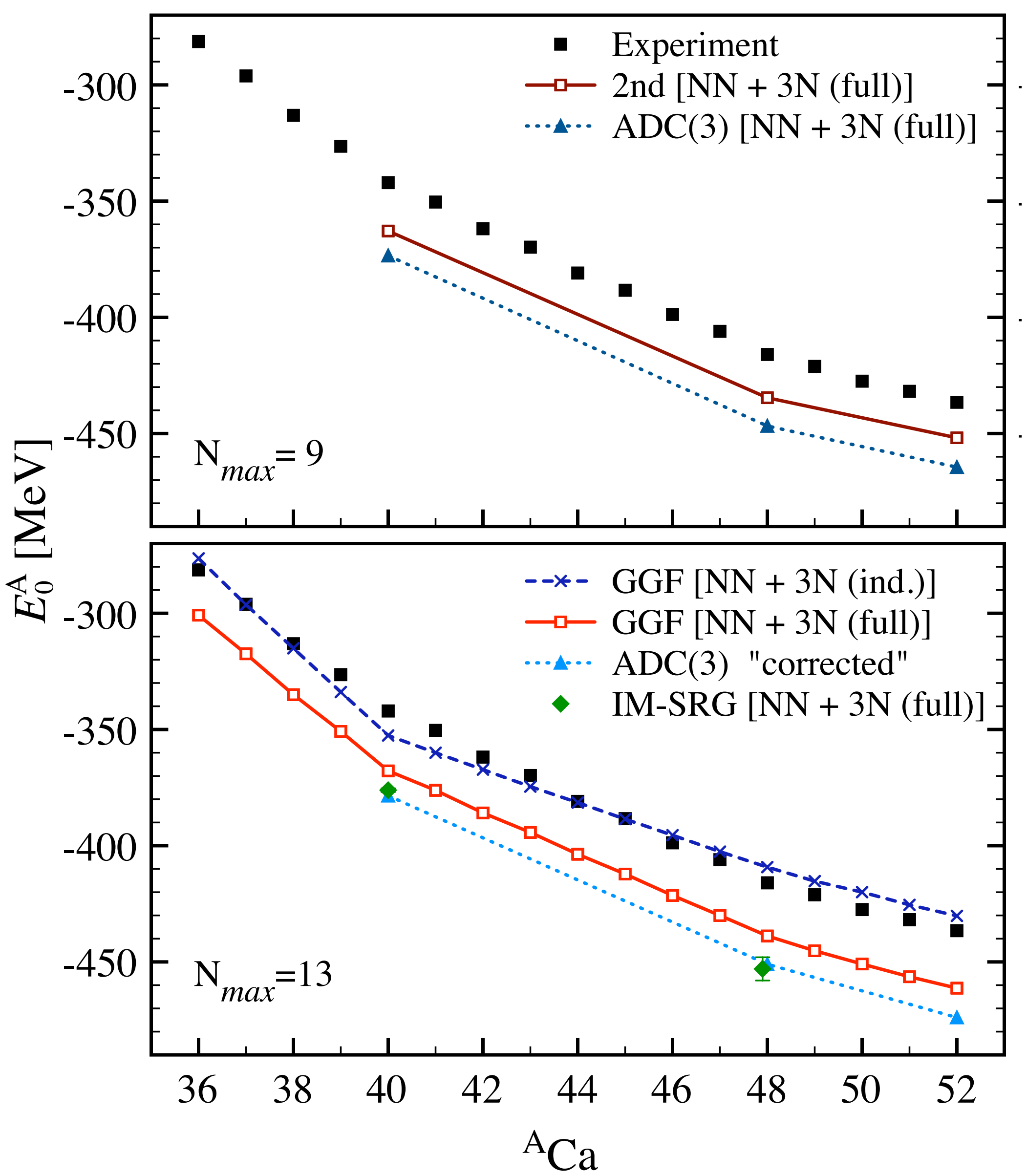


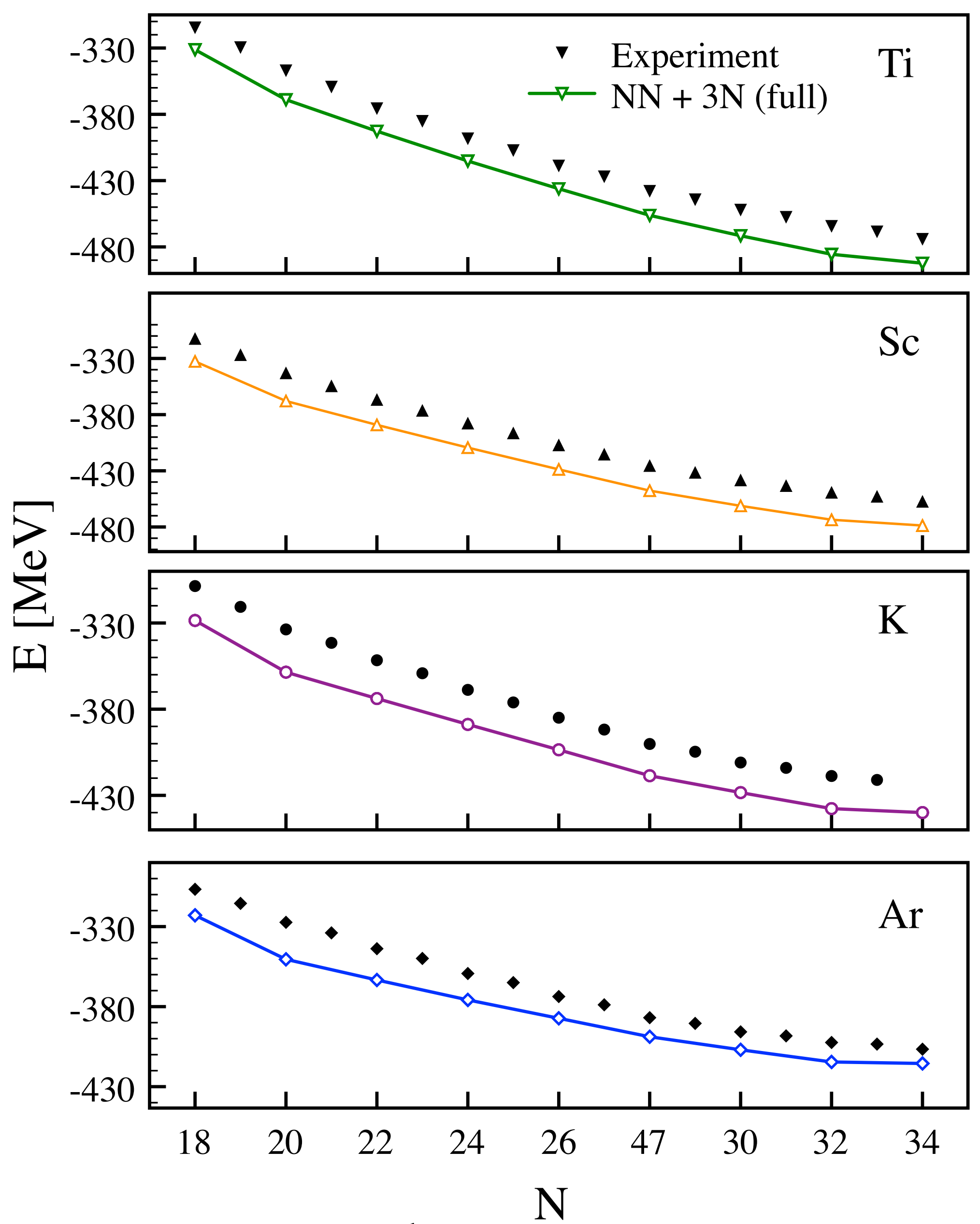
Estimate of the many-body truncation error

Original 3NF correct for trend

Systematic overbinding

Binding energies around Ca



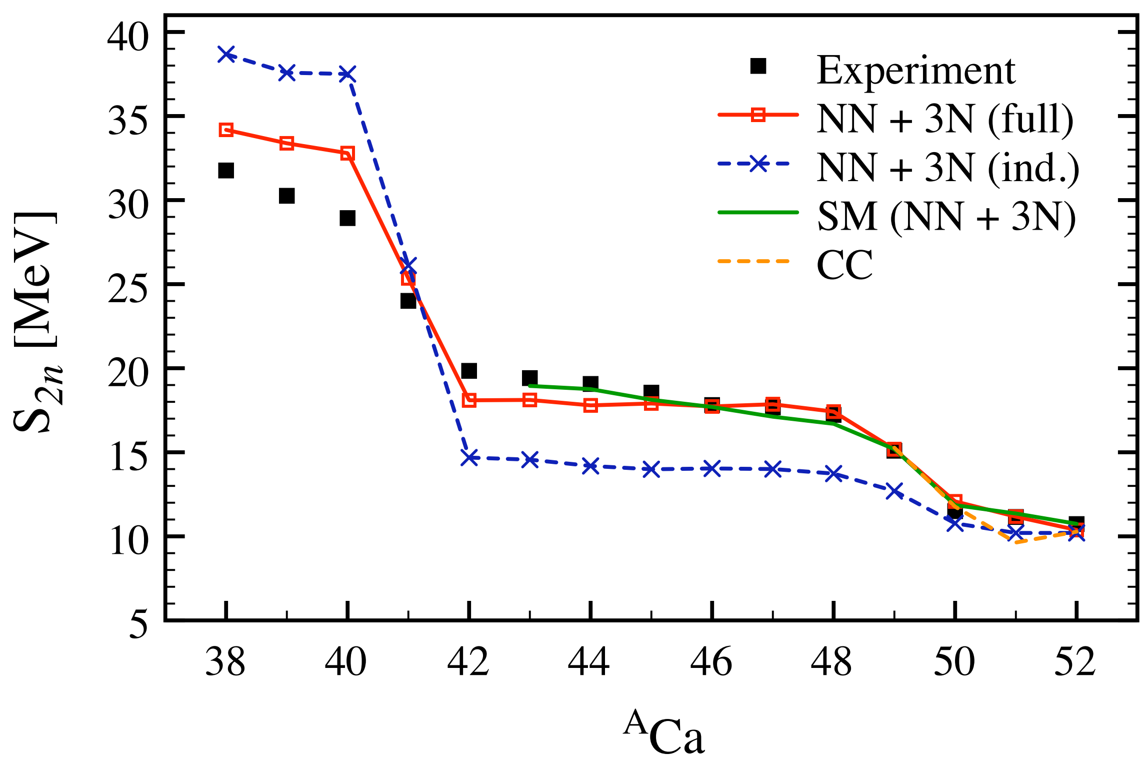


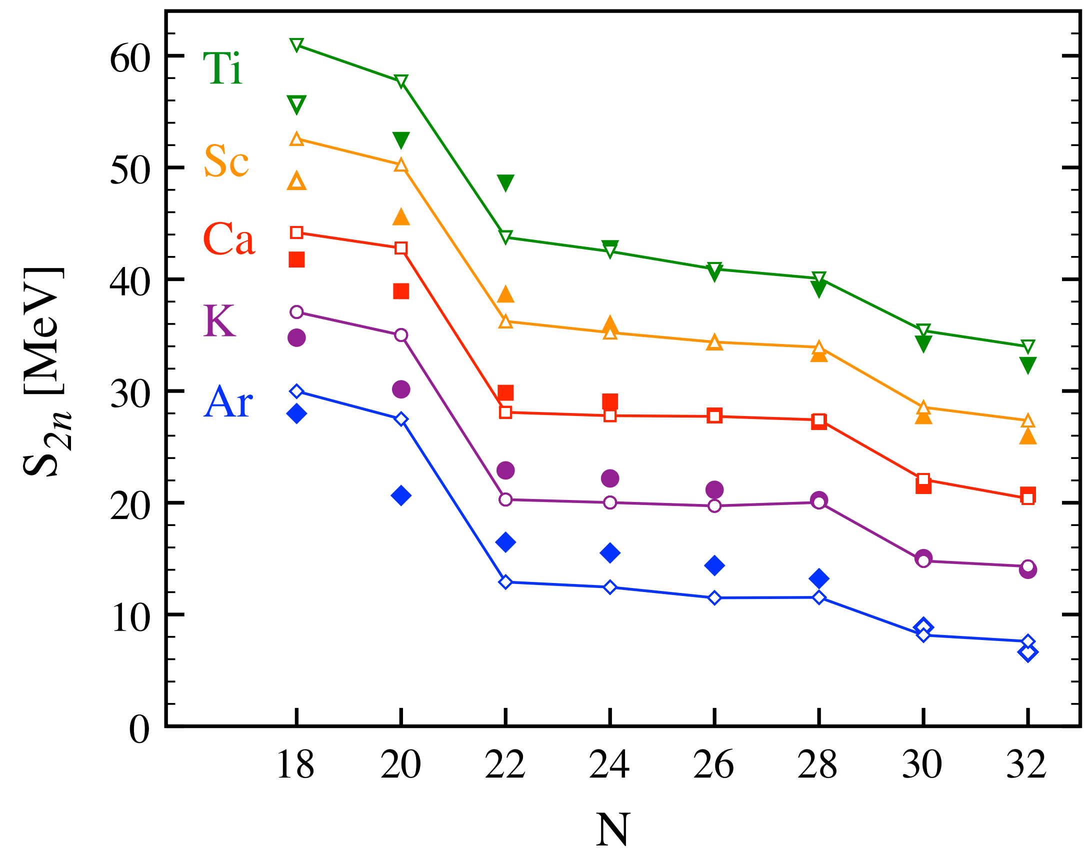
➟ Results confirmed within different many-body approaches

➟ NN + full 3N correct the trend of binding energies

➟ Systematic overbinding through all chains around Z=20

Two-neutron separation energies around Ca





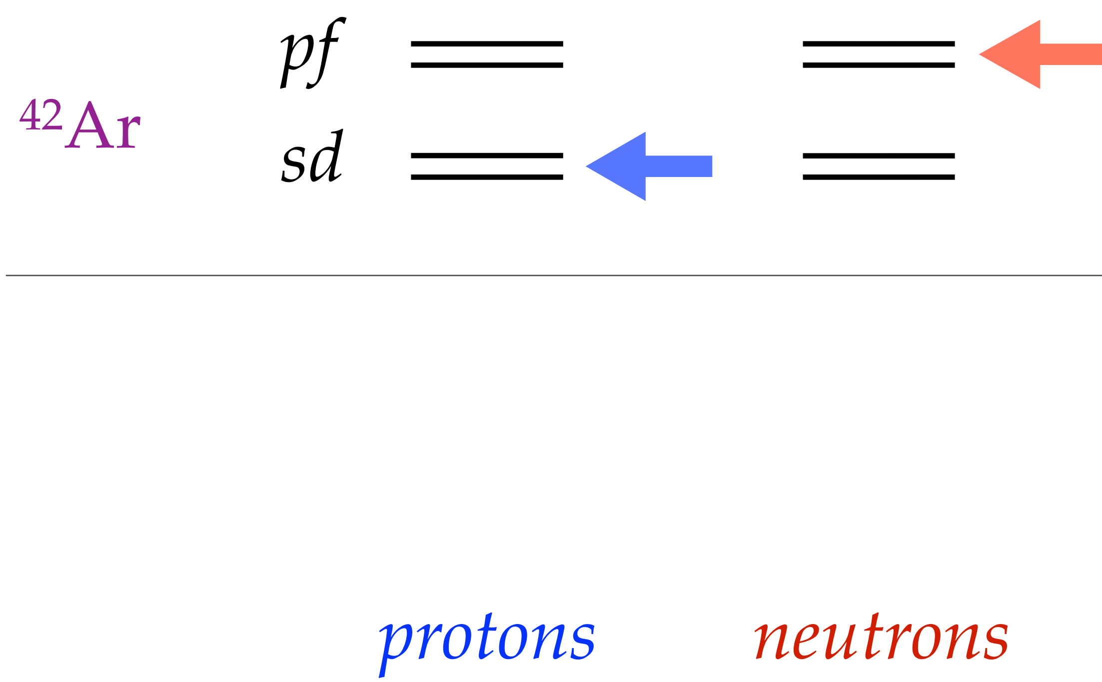
➟ S_{2n} well reproduced with chiral NN + 3N interactions

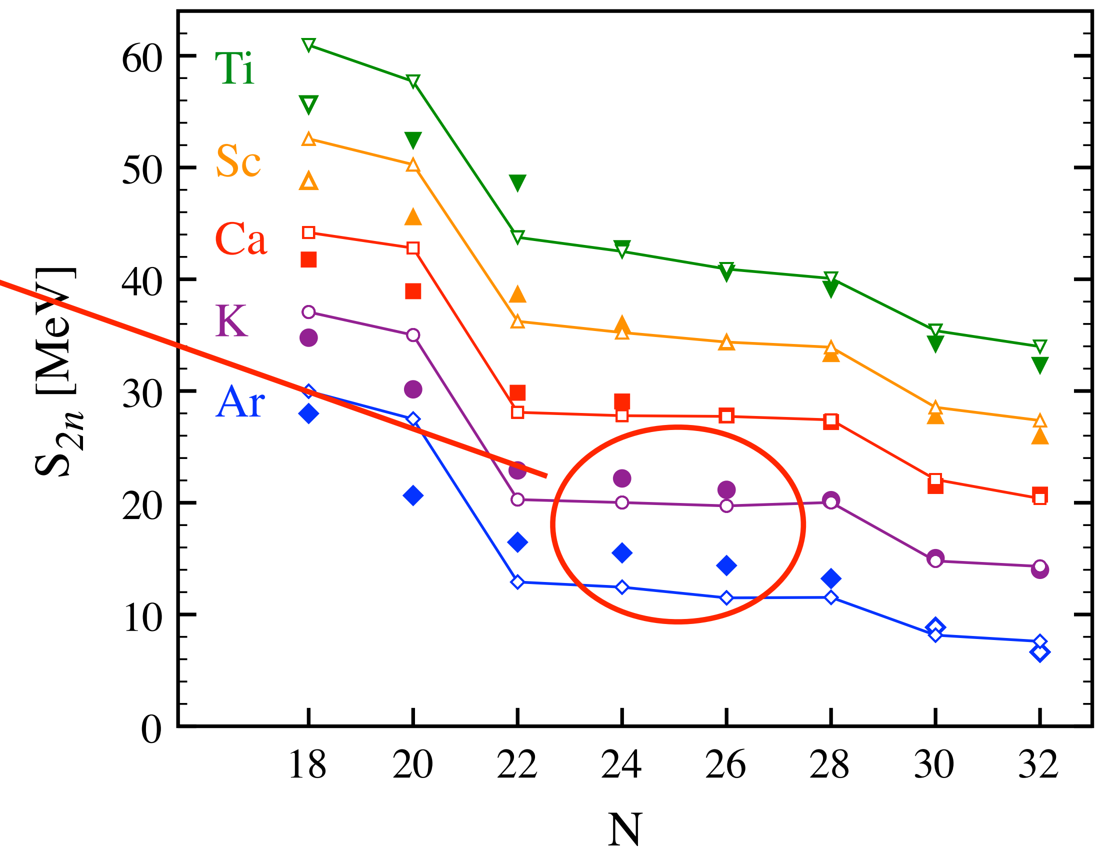
➟ Microscopic calculations extended to the whole Ca chain

➟ Neighbouring Z=18-22 chains computed within the same GGF framework

➟ Overestimation of N=20 gap traced back to spectrum too spread out

Two-neutron separation energies around Ca





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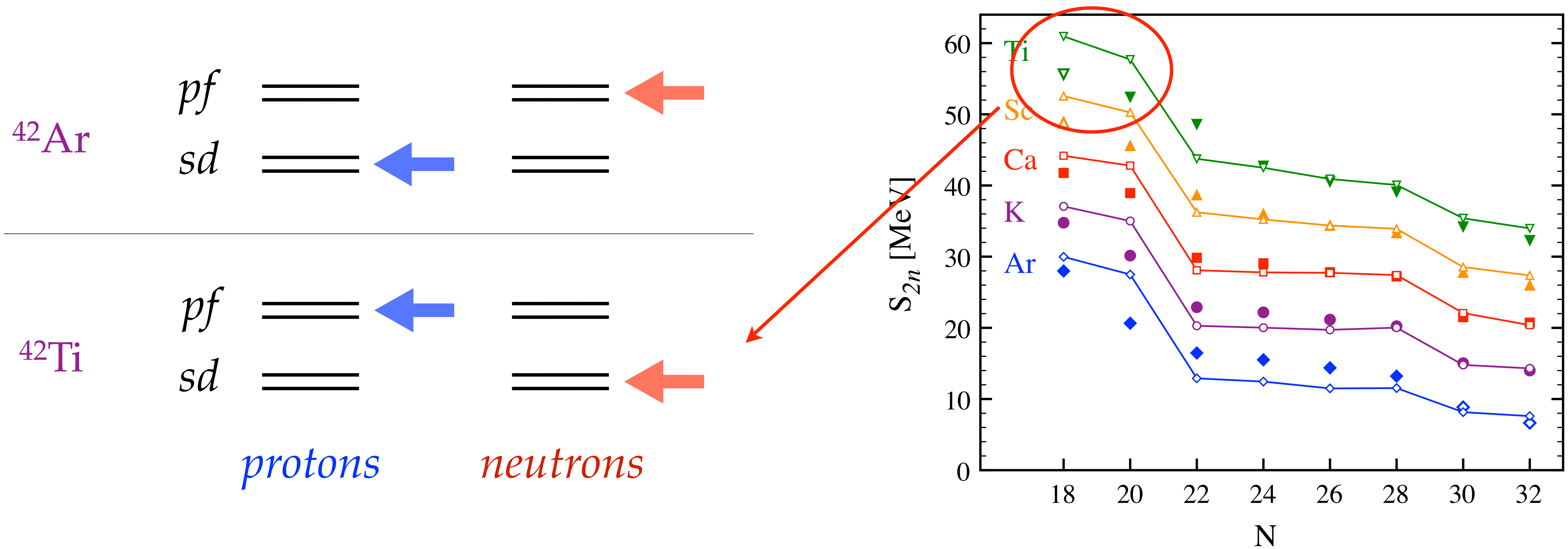

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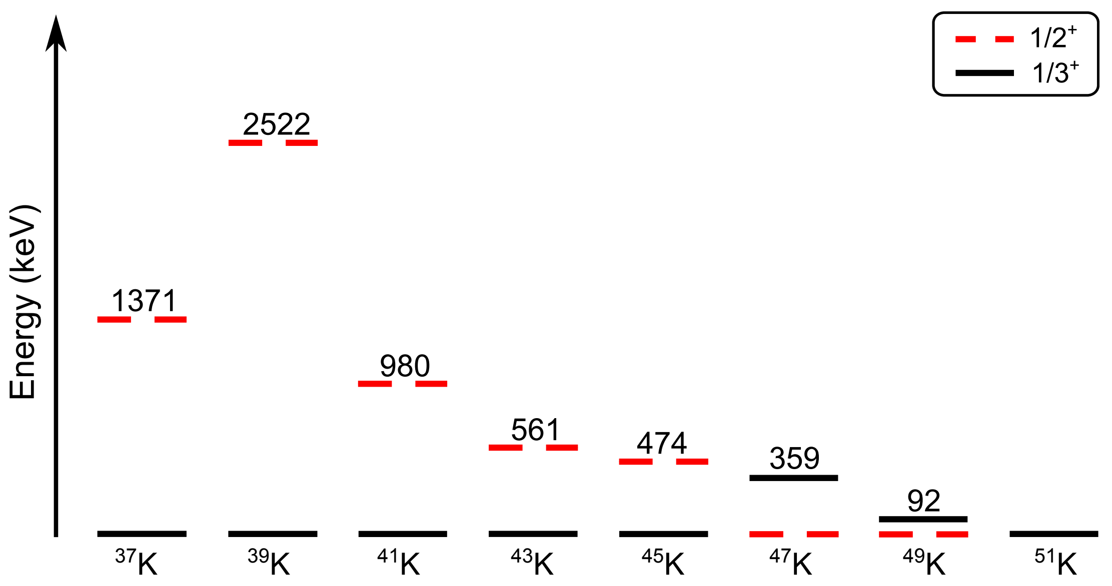
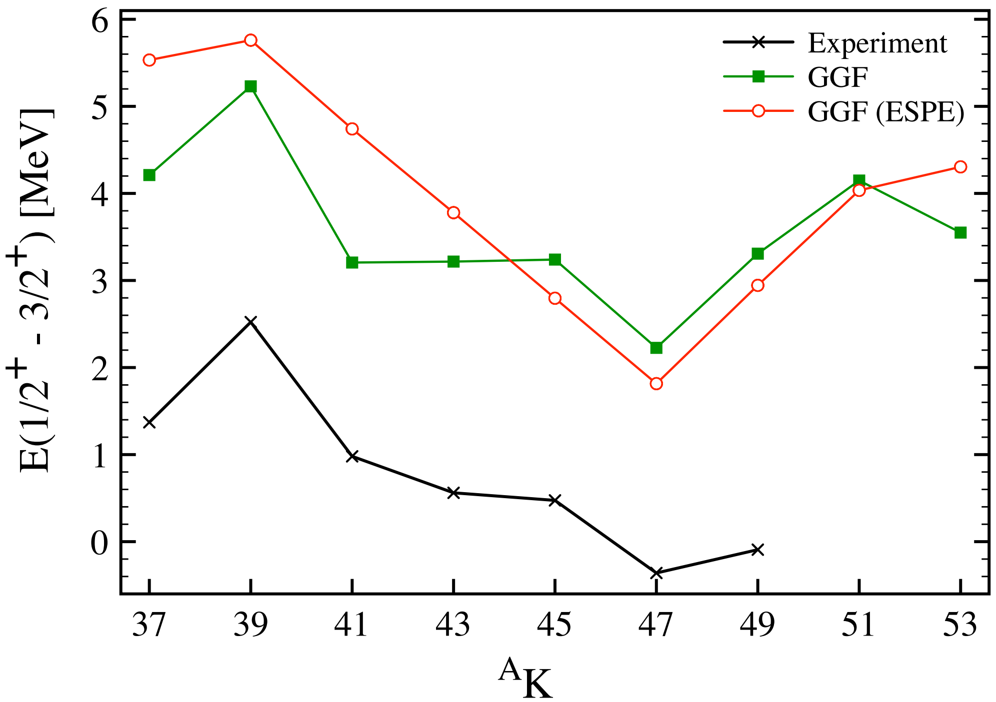
Potassium ground states (re)inversion

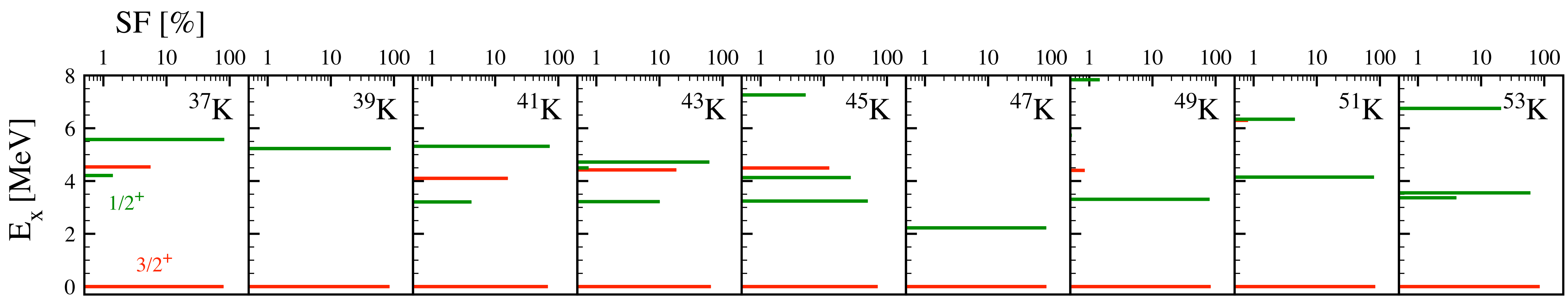
✪ Ground-state spin inversion & re-inversion recently established

➟ Laser spectroscopy experiment @ ISOLDE





[Papuga, Somà *et al.* in preparation]



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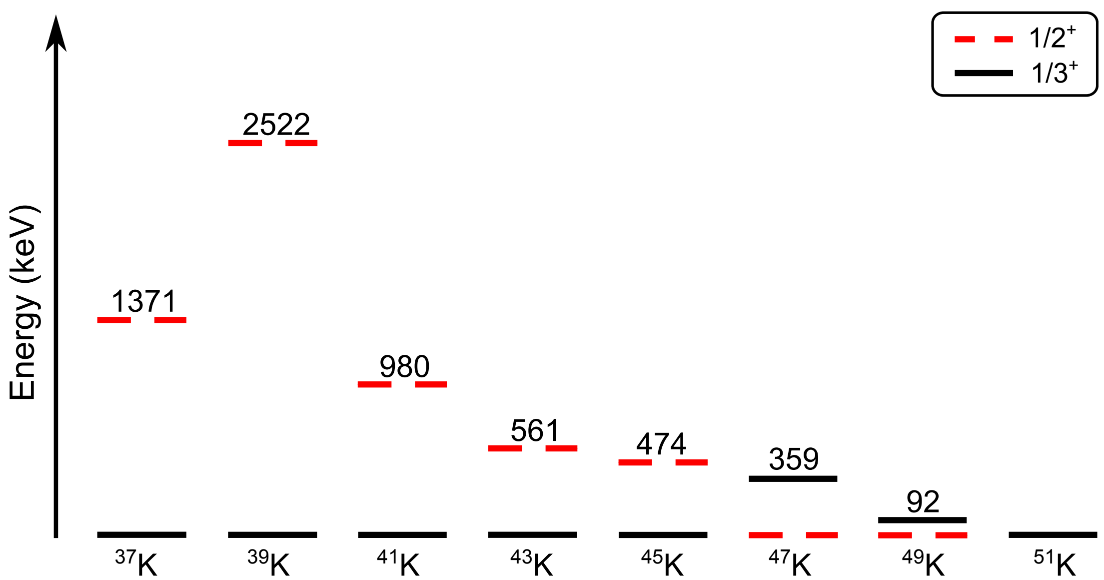
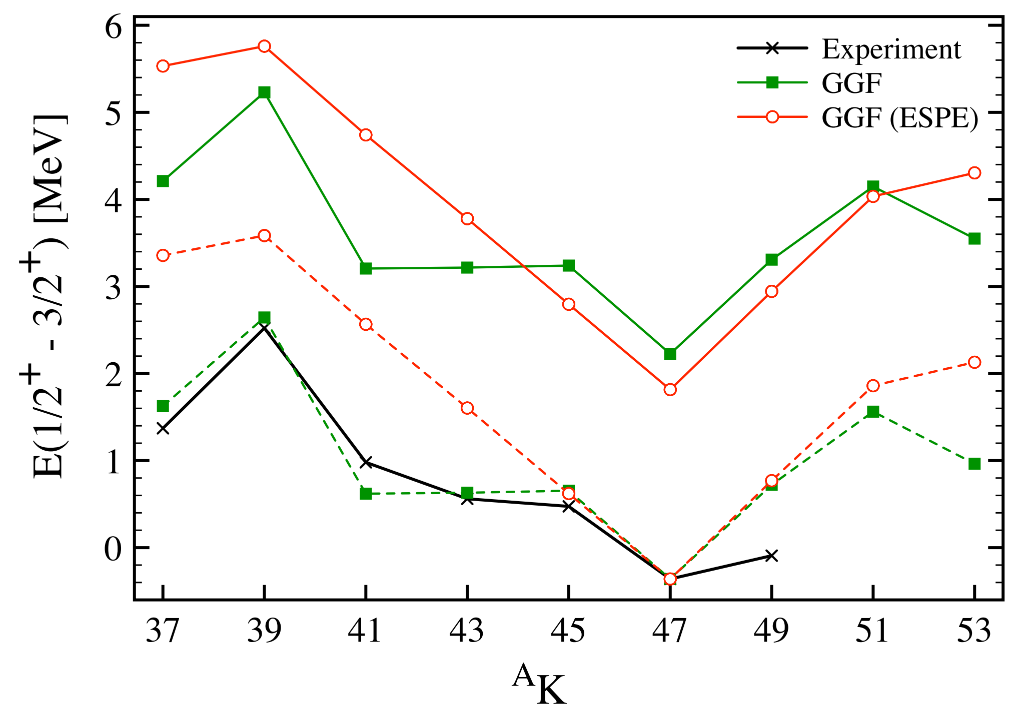
➟ Laser spectroscopy experiment @ ISOLDE





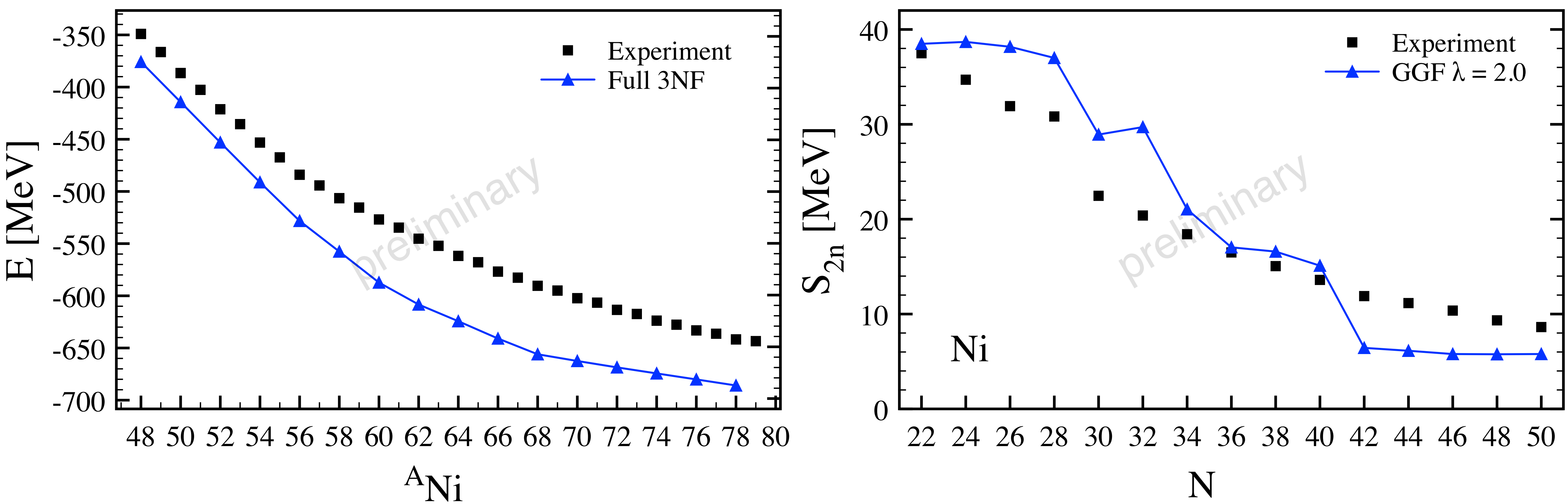
[Papuga, Somà *et al.* in preparation]

➟ Underlying mechanism emerges qualitatively

➟ Relative trend well reproduced

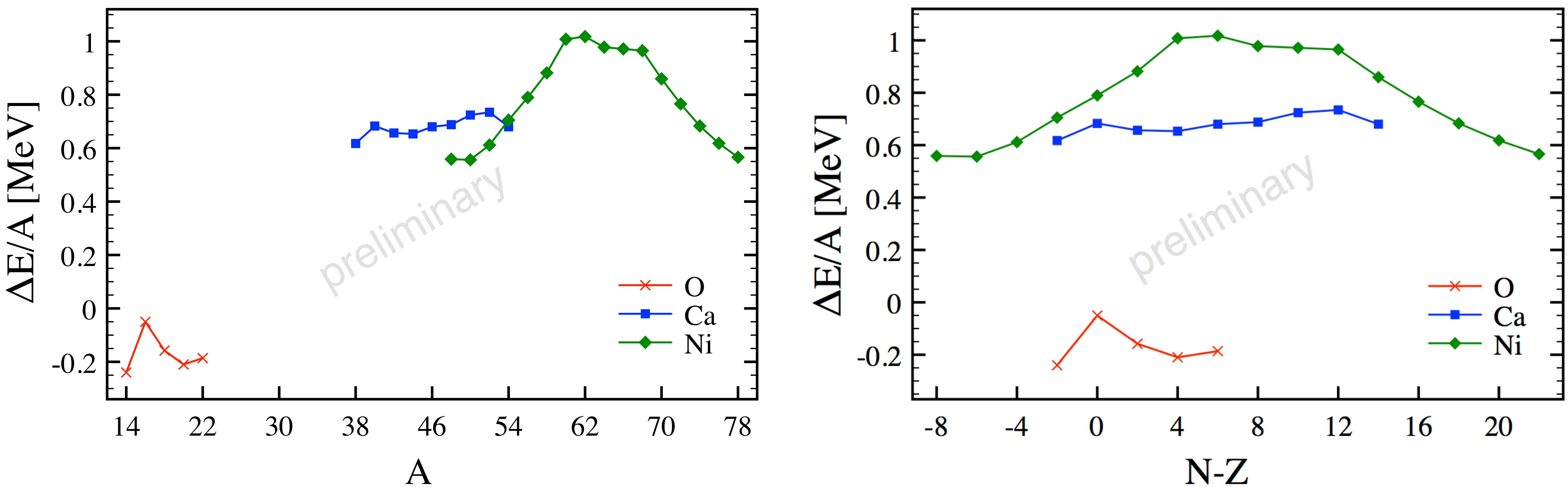
Towards heavier systems

➟ Overbinding & overestimation of major shell gaps confirmed in Ni chain



[Somà *et al.*, in preparation]

Chiral potentials and overbinding in nuclei



[Somà *et al.*, in preparation]

➟ Overbinding seems to increase with mass number

➟ Confirmed by different ab initio methods (see Binder *et al.* 2013)

➟ Saturation at too high density in nuclear matter?

Need consistent calculations

Conclusions

✪ Ab initio calculations can now challenge NN & 3N interactions in medium-mass nuclei

✪ Gorkov-Green's functions

➟ Access open-shell nuclei from an ab initio standpoint

➟ Simultaneous description of g.s. energies and spectral strength

Chiral potentials in the mid-mass region:

➟ Three-body forces necessary to reproduce trends

➟ Current chiral forces systematically overbind mid-mass systems

Related to overestimation of magic gaps

Next developments:

➟ Third-order corrections - ADC(3)

➟ Better treatment of the continuum

➟ Extension to scattering