Ab initio calculations of mid-mass nuclei

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Outline:

Progress
Ground state energies (& problems)
Spectra
Uncertainties

ESNT workshop
New developments in nuclear energy-density-functionals models

CEA Saclay, 28 November 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 (e.g. SRG machinery)

⬇

Limited applicability

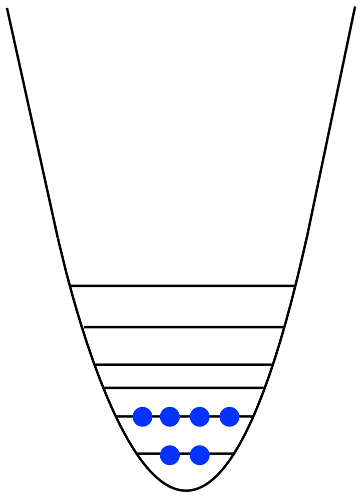
Controlled extrapolations

Test fundamental interactions

➡ Complementary to effective many-body methods

Different ab initio strategies

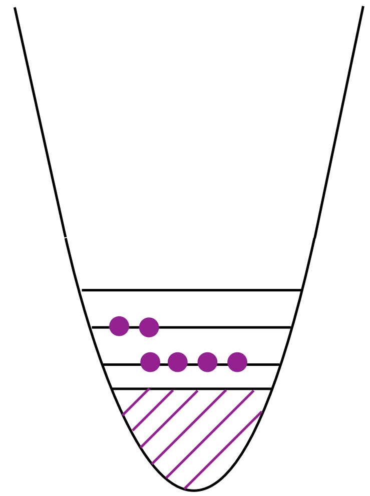
Light nuclei



Virtually exact

NCSM, GFMC, ...

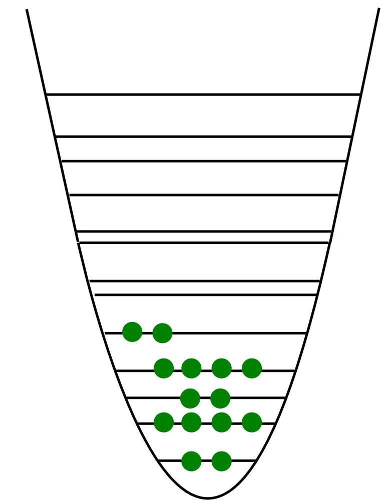
Medium-mass nuclei



Valence space

Microscopic SM

Mid/heavy nuclei



Based on expansion

GF, CC, IM-SRG, ...

Closed-shell

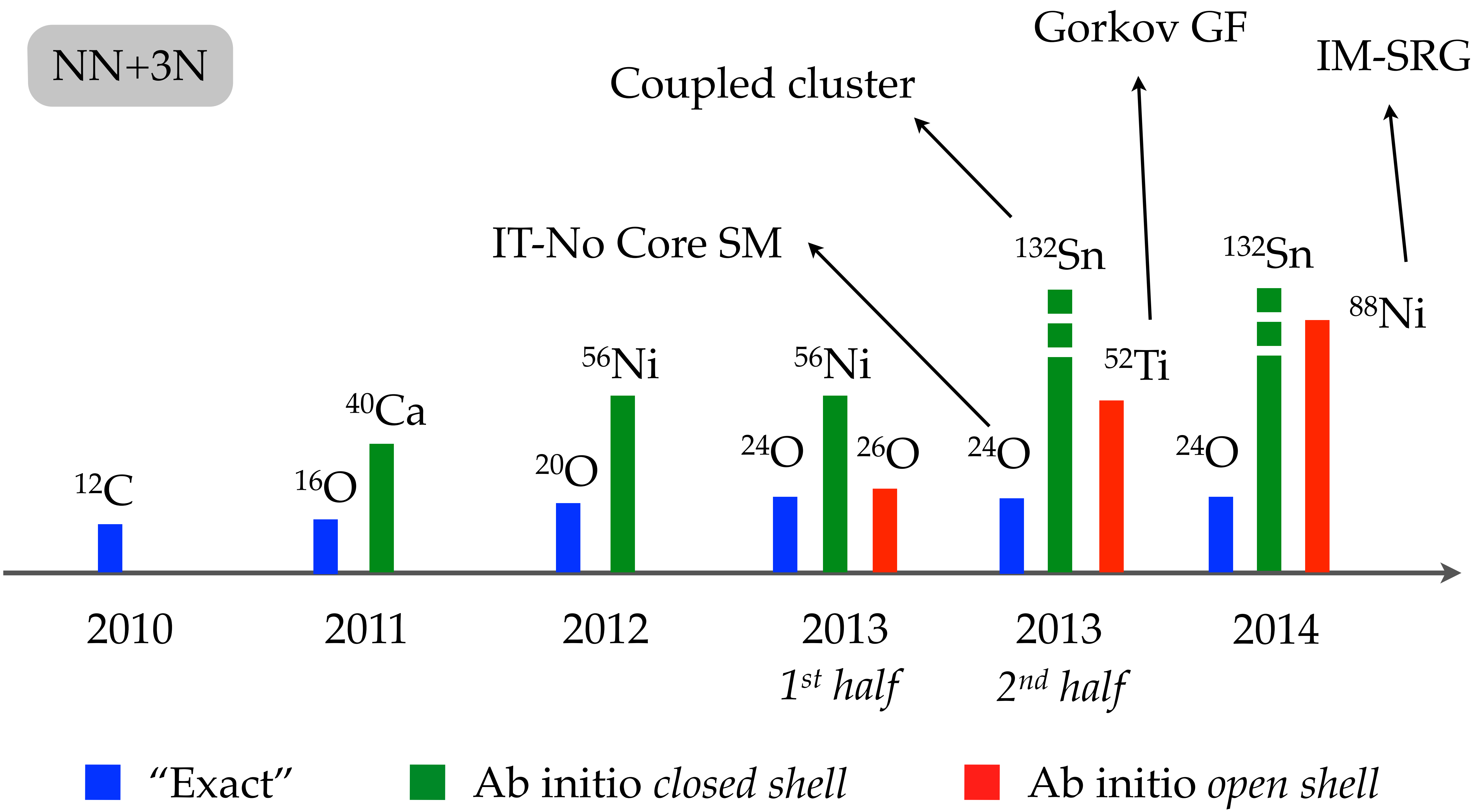
Open-shell

All methods (should be able to) take the same input Hamiltonian

➟ Alternative approach: lattice EFT

Current limits / reach of ab initio calculations

➟ Heavier system computed in the different types of ab initio



Traditional nuclear interactions

✪ Based on one-boson exchange models

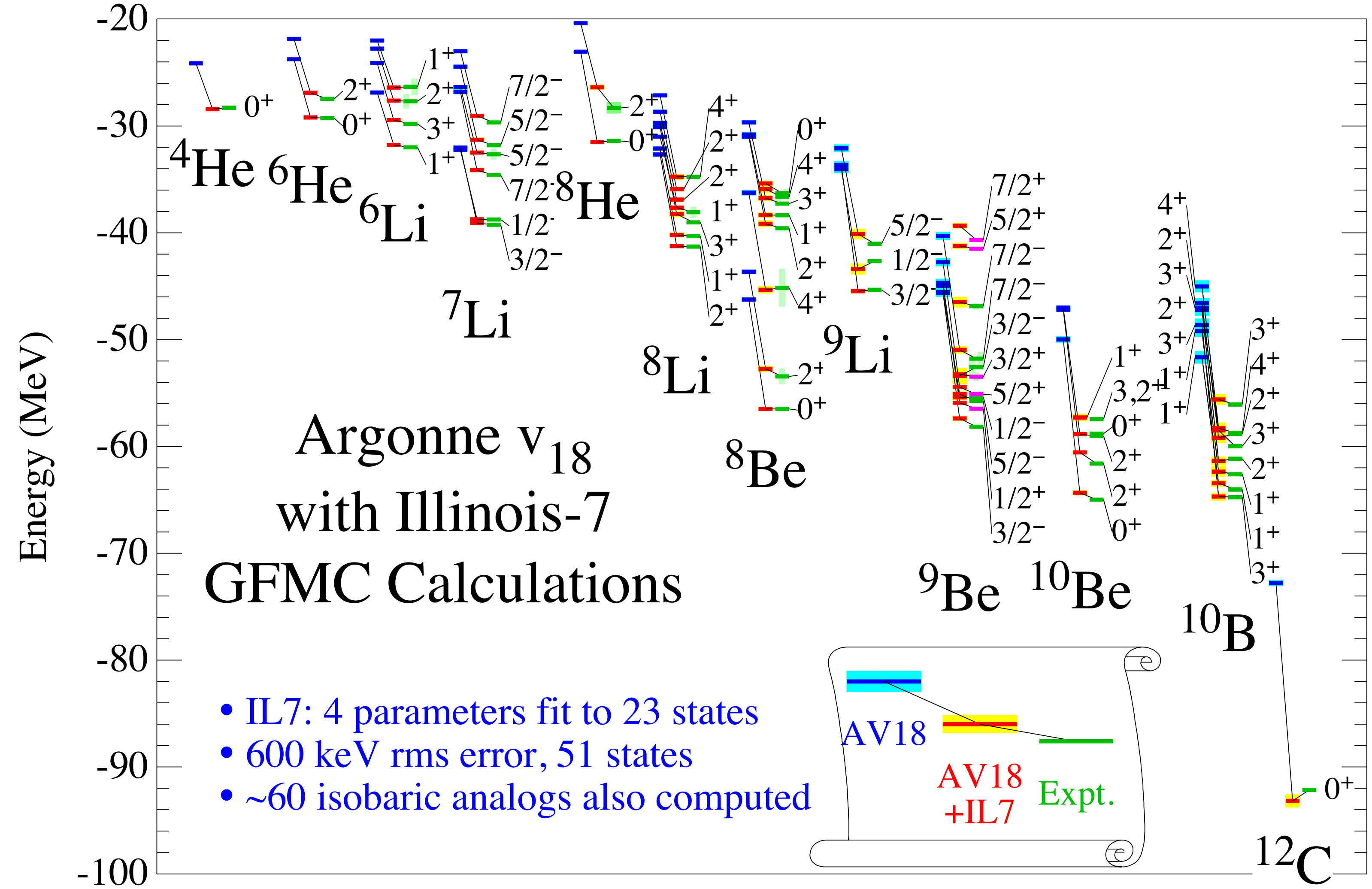
- ➟ Model with arbitrary number of parameters
- ➟ Feature a *hard core*
- ➟ Three-body forces mainly phenomenological

Not systematically improvable

Not consistent with NN

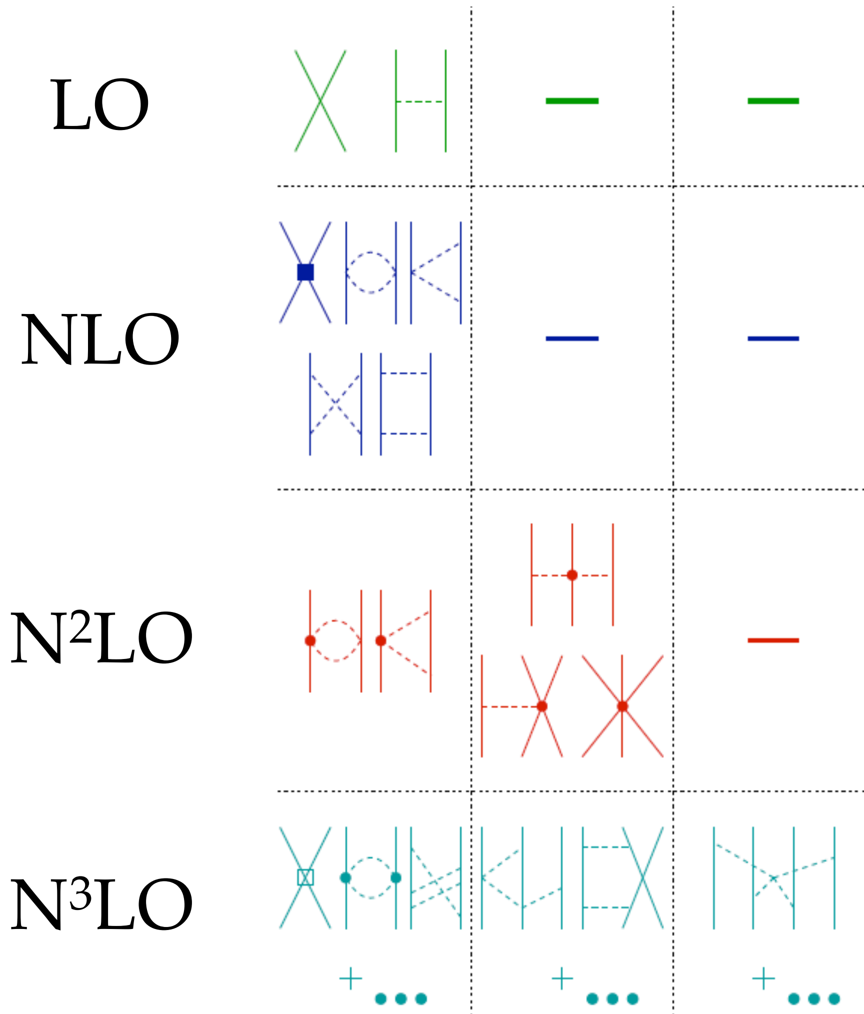
Limits severely many-body calculations

CD-Bonn
Av18
Reid
Nijmegen
…



[Pieper & Wiringa 2001]

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

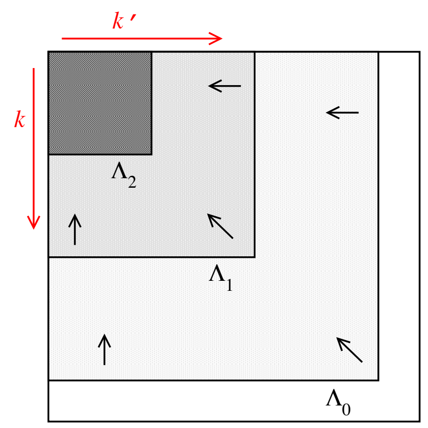
- ➟ Different orders in EFT
- ➟ Consistency of cutoffs?
- ➟ Order-by-order convergence unclear
- ➟ More fundamental problem: EFT power counting

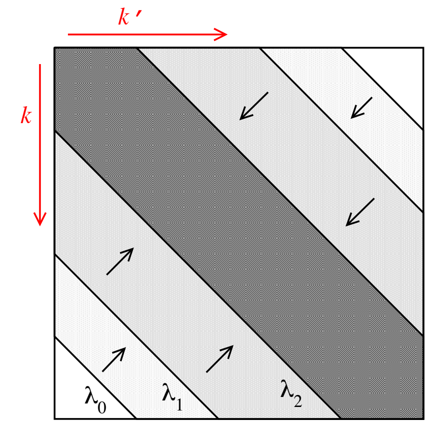
RG techniques for NN & 3N forces

✪ Renormalization group techniques for NN and 3N forces

➟ Lower the *resolution scale* of the original Hamiltonian

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

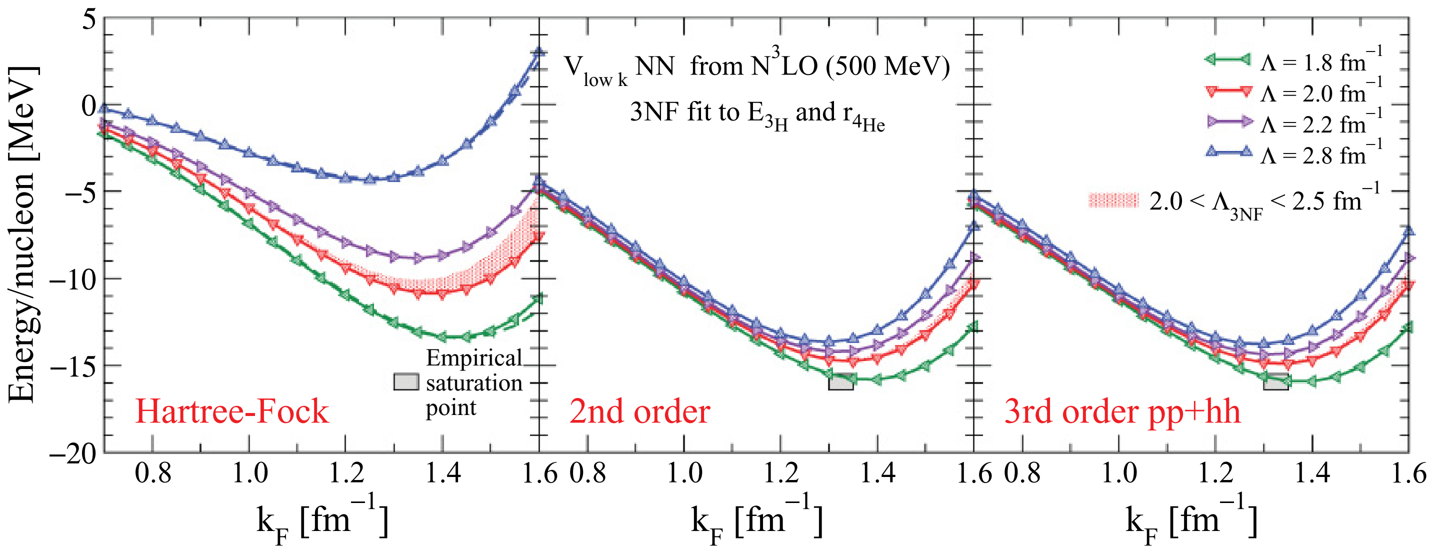




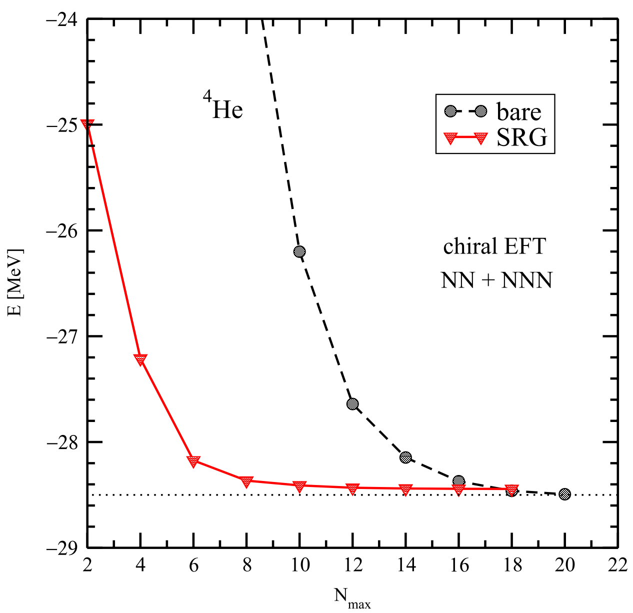
V_{SRG}

✪ 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 N³LO (500 MeV)
- ➟ SRG-evolved to 2.0 fm^{-1}

[Entem and Machleidt 2003]

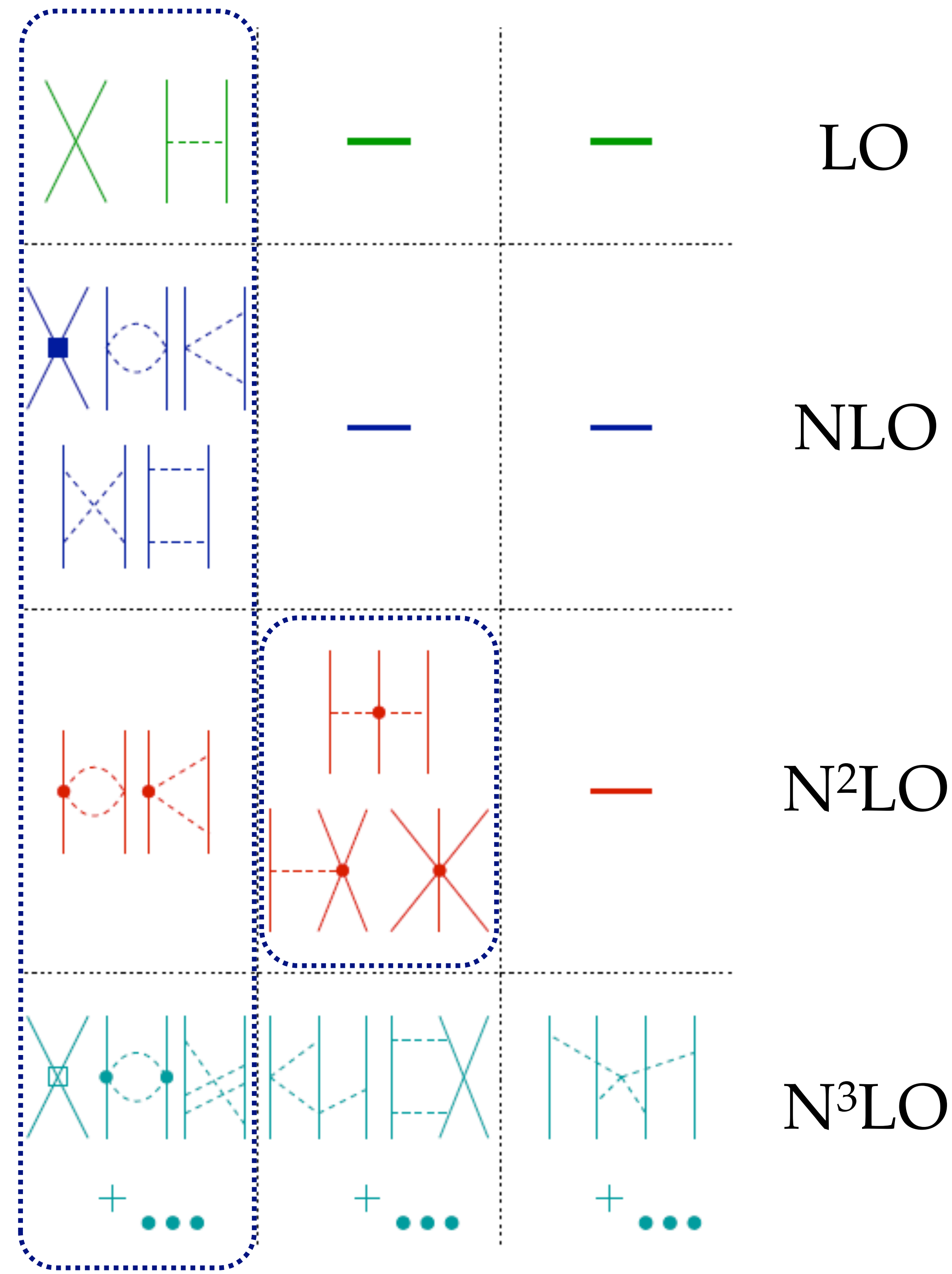
✪ 3N potential:

- ○ chiral N²LO (400 MeV)
- ➟ SRG-evolved to 2.0 fm^{-1}

[Navrátil 2007]

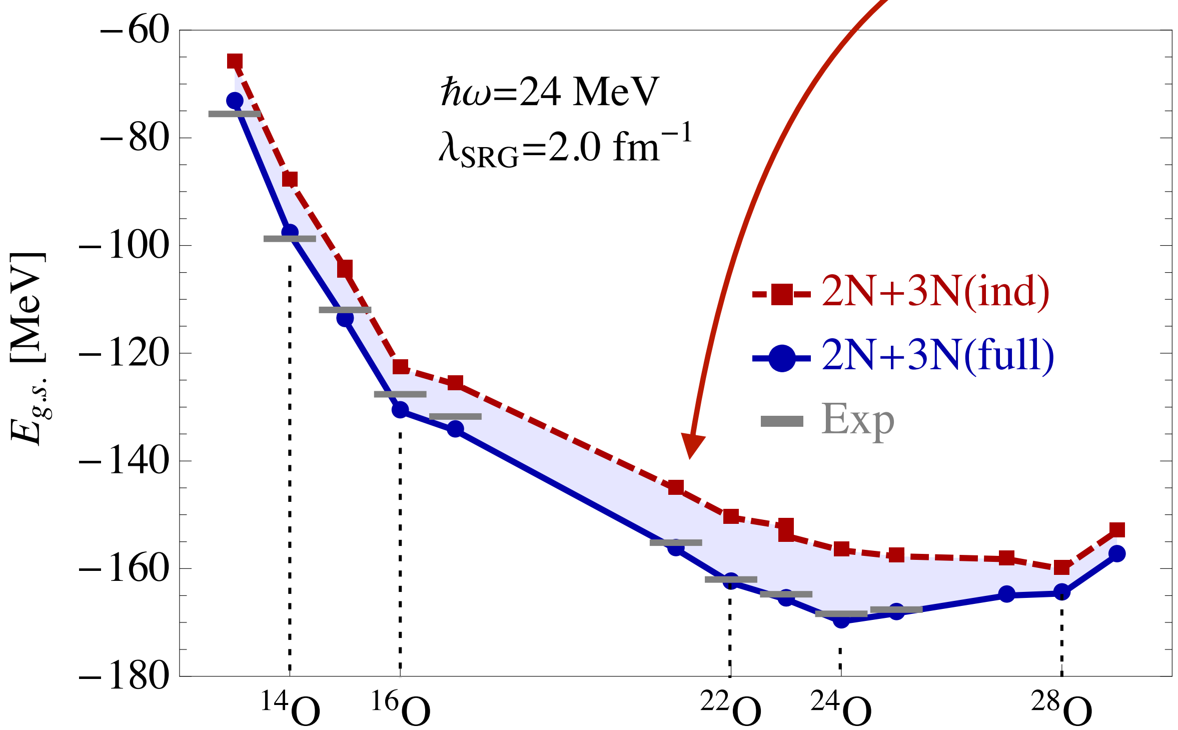
➟ Choice of cutoff to reduce induced 4N contributions

[Roth *et al*. 2012]

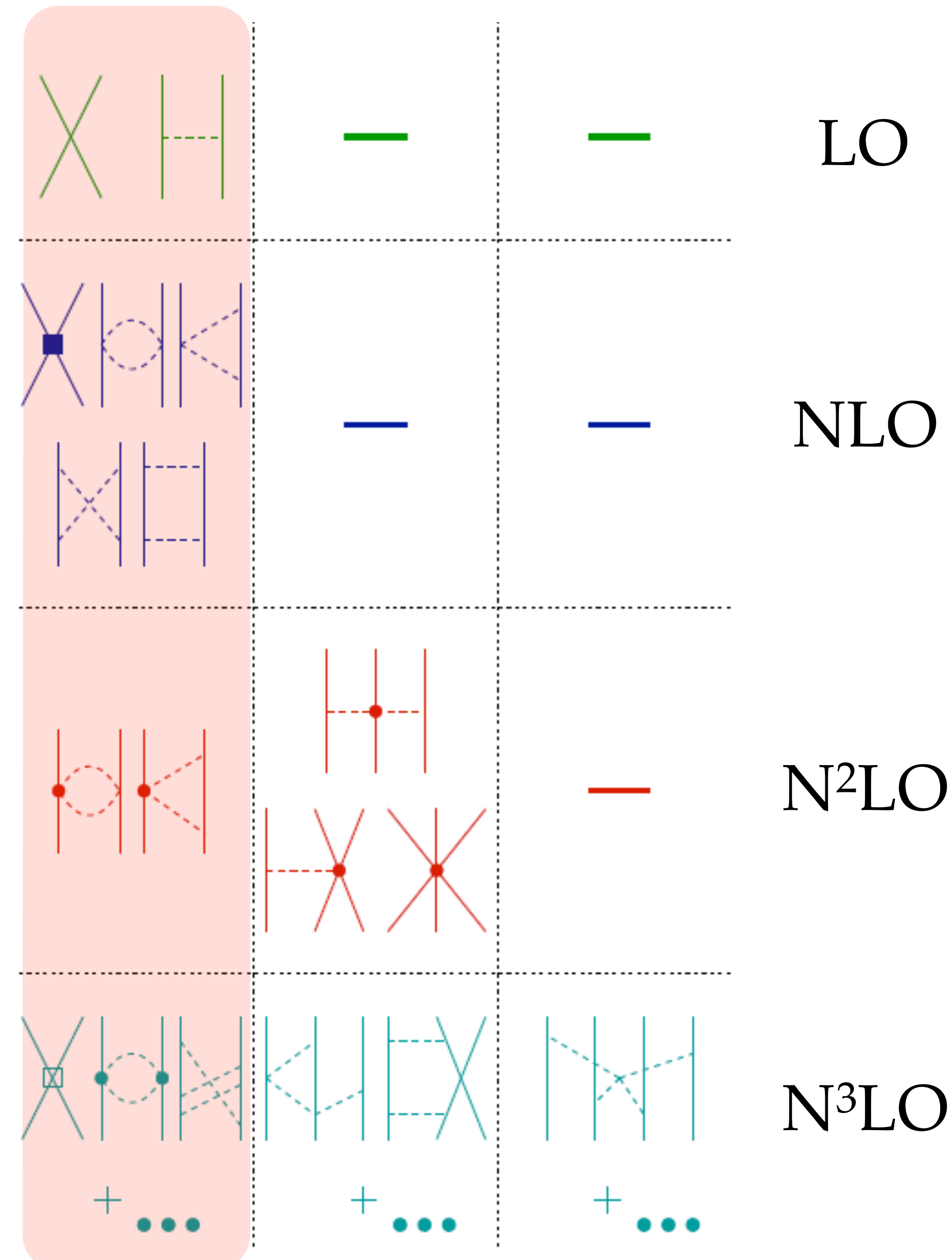


Chiral NN+3N in the oxygen chain

✪ Self-consistent Green's functions



[Cipollone, Barbieri & Navrátil 2013]



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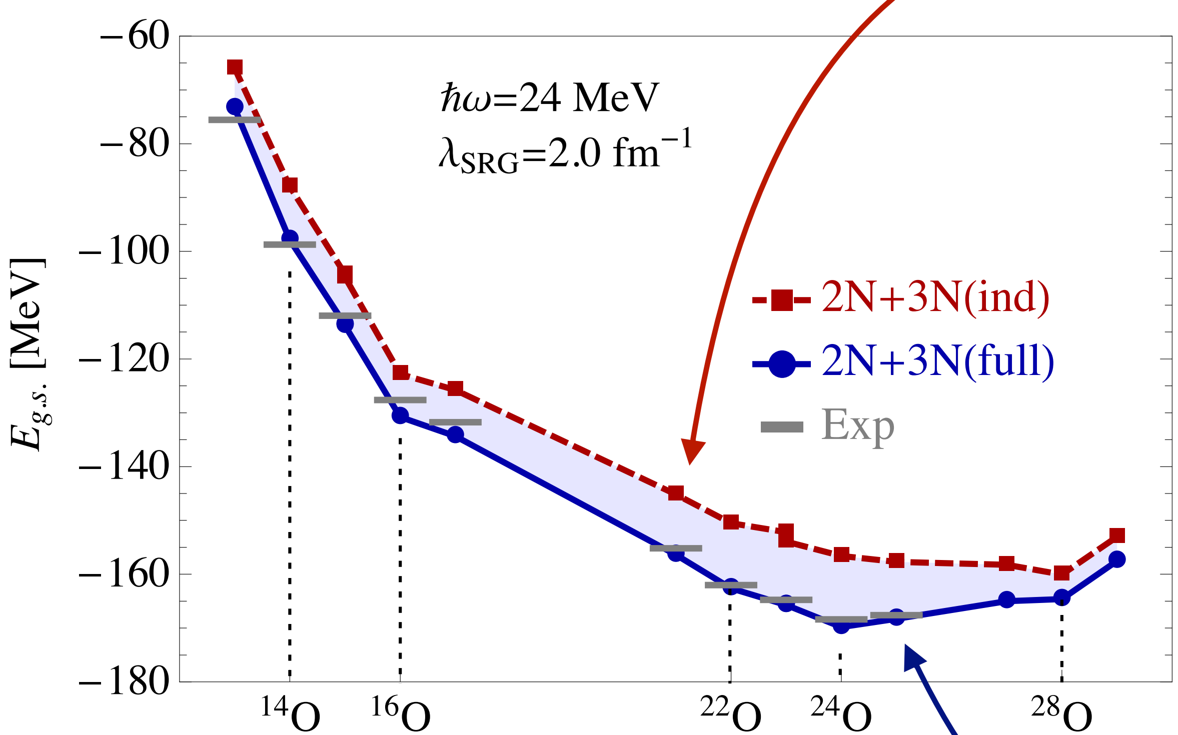
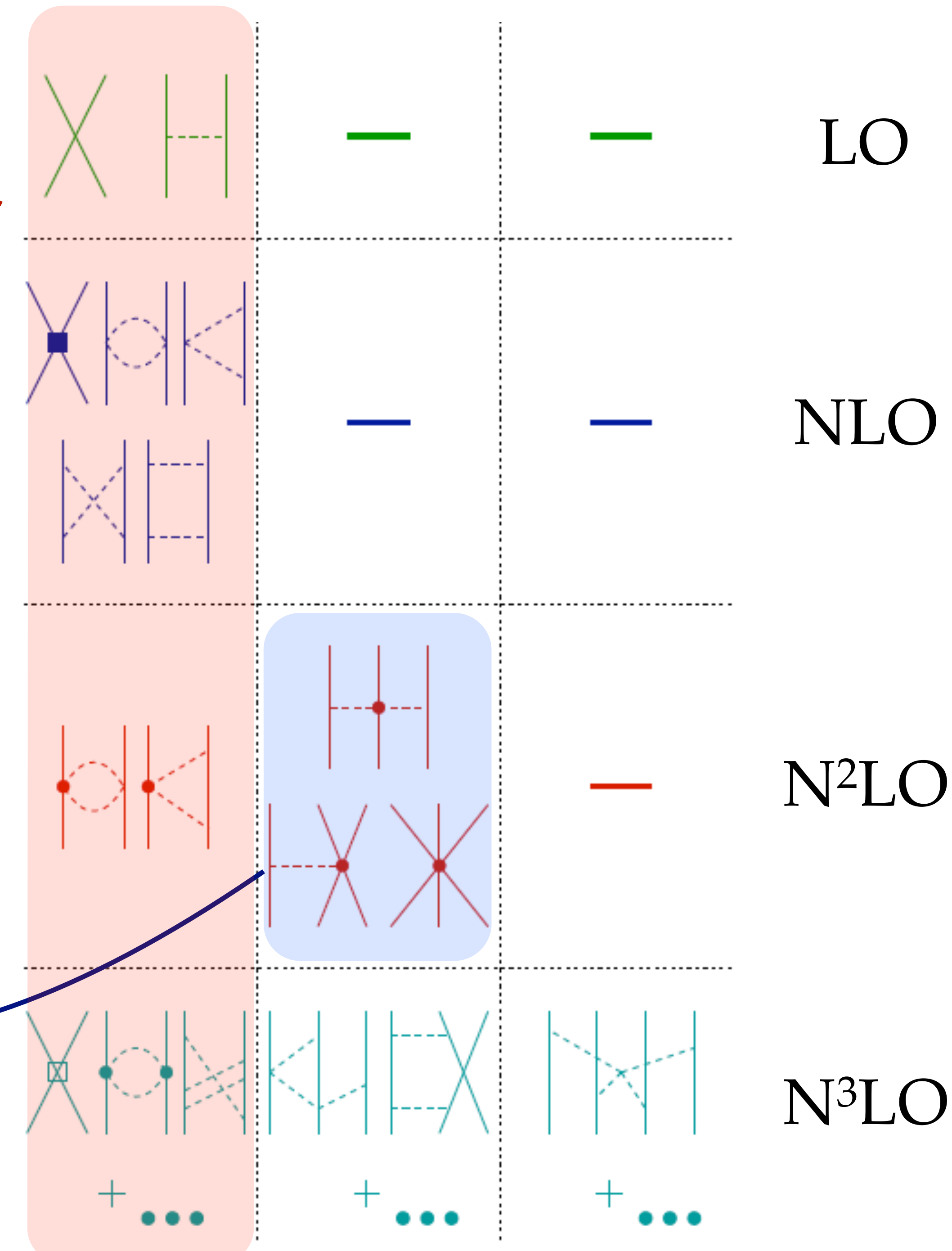




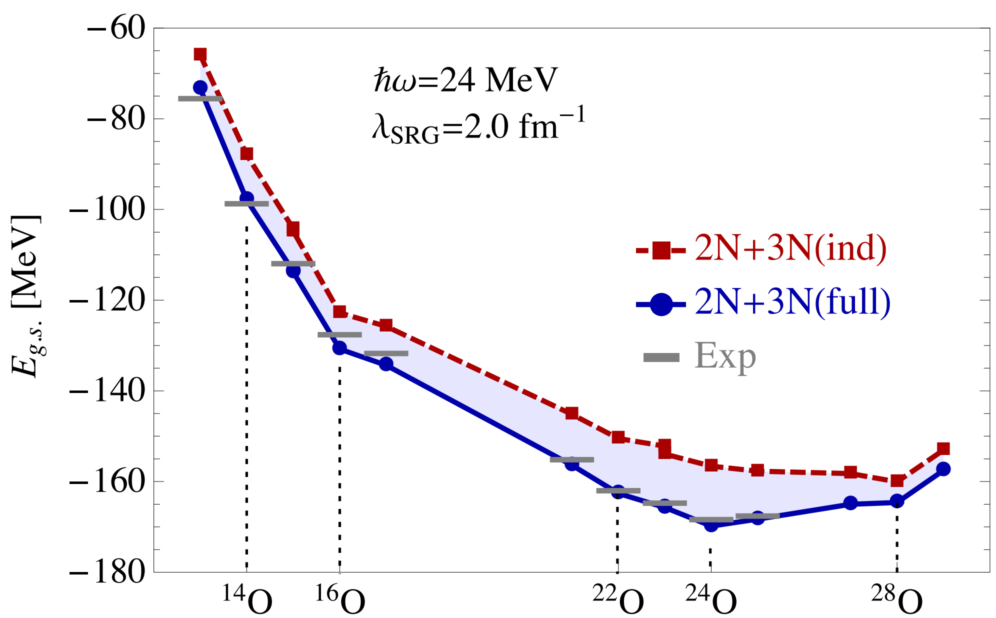
[Cipollone, Barbieri & Navrátil 2013]

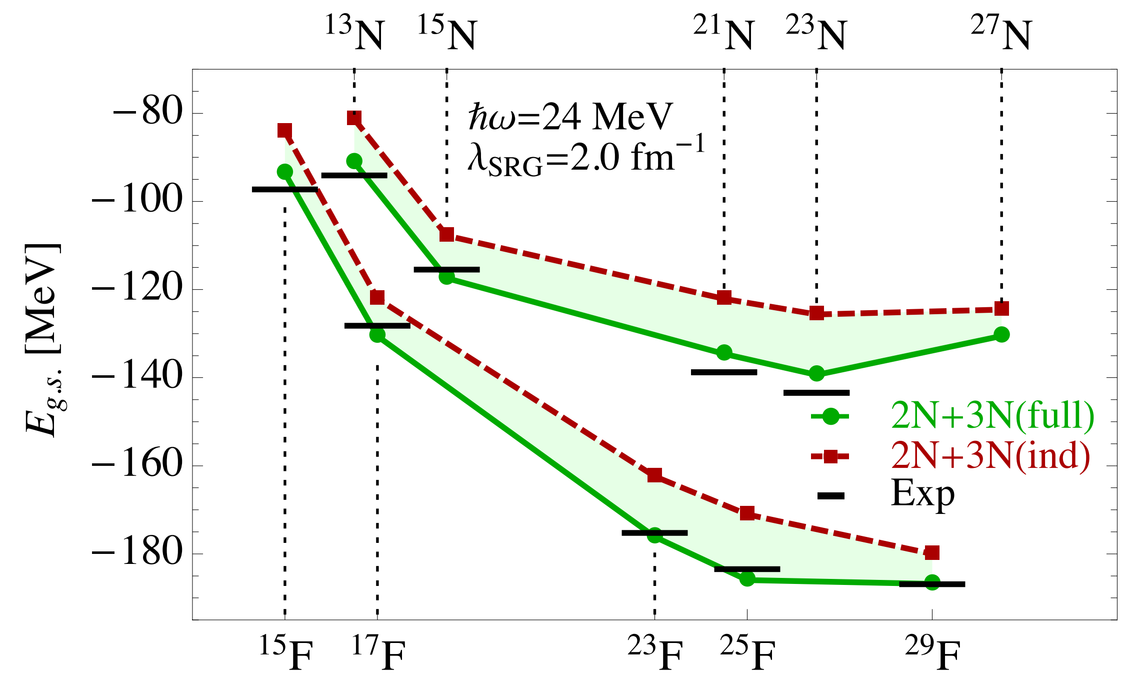
➟ Overall good agreement with data

➟ 3NF crucial for reproducing driplines

Chiral NN+3N in the oxygen chain (and nearby)

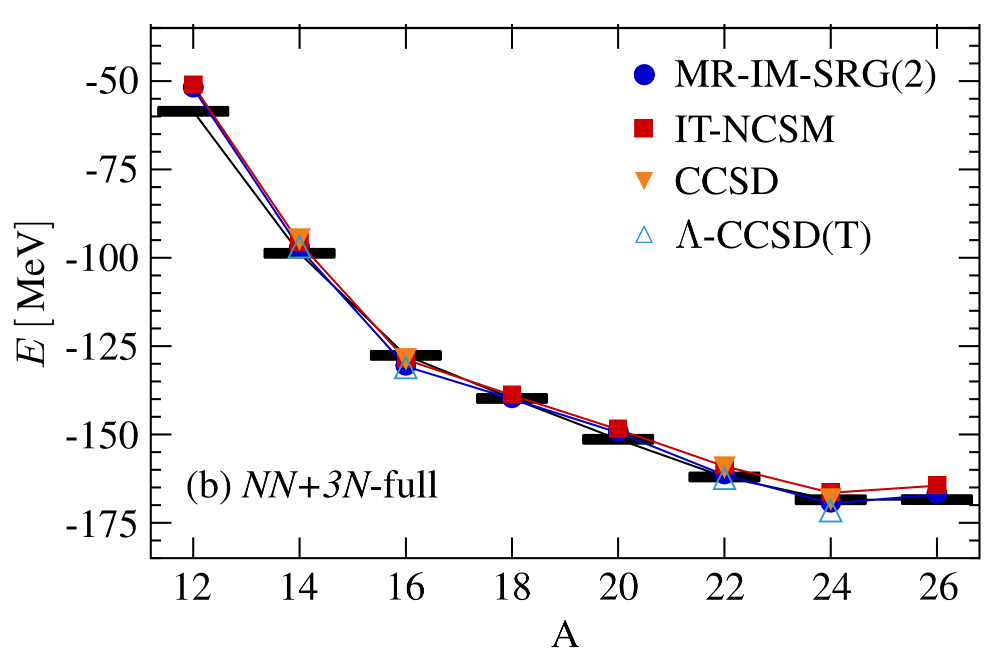
✪ Extend description to Z = 7 and 9 isotopic chains with GF method

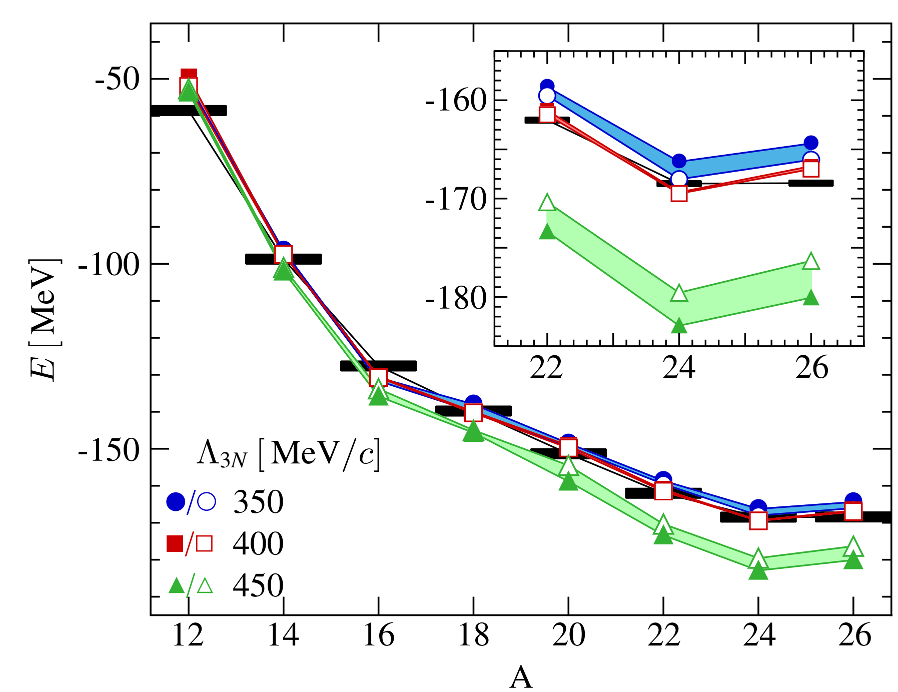




[Cipollone *et al.* 2013]

✪ Excellent agreement between different ab initio methods





[Hergert *et al.* 2013]

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

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

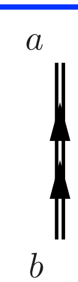
Breaks particle-number symmetry

- ➟ 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 $\Omega_0 = \sum_{A'} |c_{A'}|^2 \, \Omega_0^{A'} \approx E_0^A - \mu A$

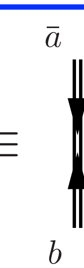
set of 4 Gorkov propagators

[Gorkov 1958]

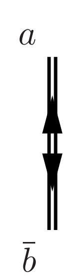
$$i\, G^{11}_{ab}(t,t') \equiv \langle \Psi_0 | T \left\{ a_a(t) a_b^\dagger(t') \right\} | \Psi_0 \rangle \quad \equiv$$



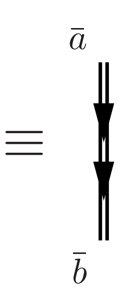
$$i\, G^{21}_{ab}(t,t') \equiv \langle \Psi_0 | T \left\{ \bar{a}_a^\dagger(t) a_b^\dagger(t') \right\} | \Psi_0 \rangle \quad \equiv$$



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



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

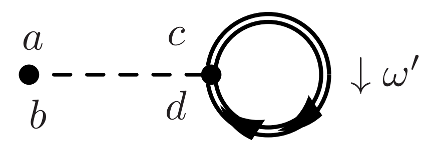


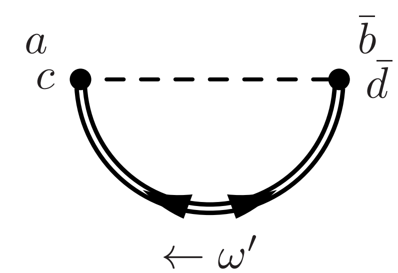
Gorkov equation & self-energy

✪ Many-body Schrödinger equation ⟶ Dyson / Gorkov equation

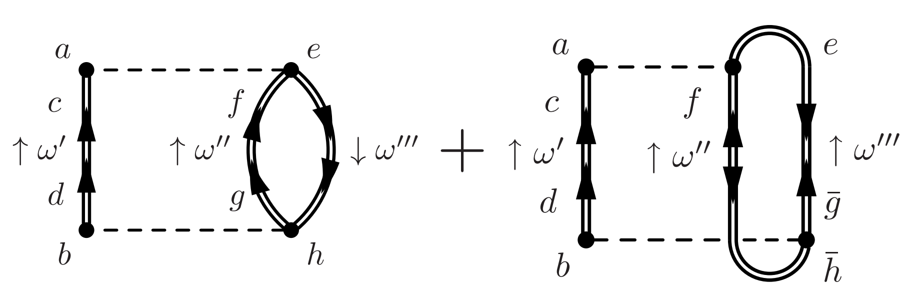
$$\mathbf{G}_{ab}(\omega) = \mathbf{G}^{(0)}_{ab}(\omega) + \sum_{cd} \mathbf{G}^{(0)}_{ac}(\omega)\, \mathbf{\Sigma}^{\star}_{cd}(\omega)\, \mathbf{G}_{db}(\omega)$$

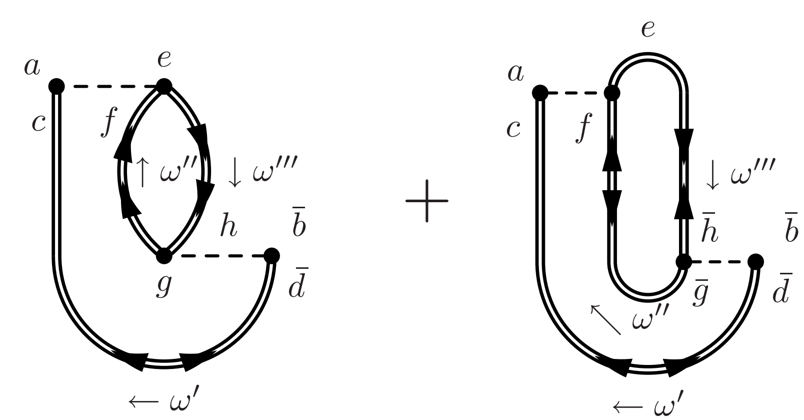
✪ 1st order ➟ energy-independent self-energy

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

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

✪ 2nd order ➟ energy-dependent self-energy

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

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

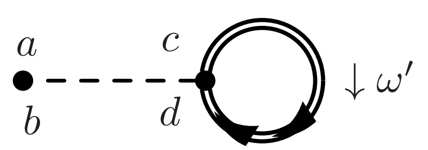
Gorkov equation & self-energy

✪ Gorkov equation ⟶ energy *dependent* eigenvalue problem

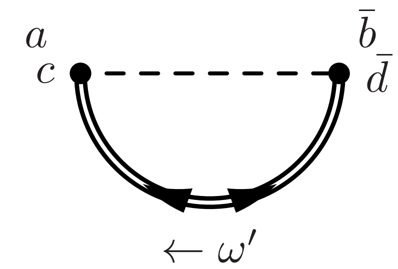
$$\sum_b \begin{pmatrix} t_{ab} - \mu_{ab} + \Sigma^{11}_{ab}(\omega) & \Sigma^{12}_{ab}(\omega) \\ \Sigma^{21}_{ab}(\omega) & -t_{ab} + \mu_{ab} + \Sigma^{22}_{ab}(\omega) \end{pmatrix} \Bigg|_{\omega_k} \begin{pmatrix} \mathcal{U}^k_b \\ \mathcal{V}^k_b \end{pmatrix} = \omega_k \begin{pmatrix} \mathcal{U}^k_a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

✪ 1st order ➟ energy-independent self-energy

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

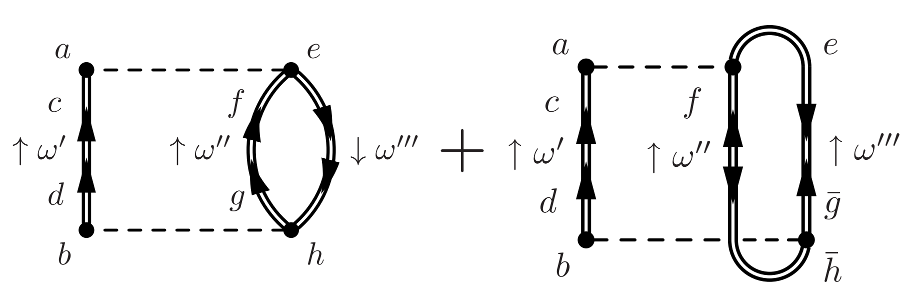


$\Sigma^{12\,(1)}_{ab} =$

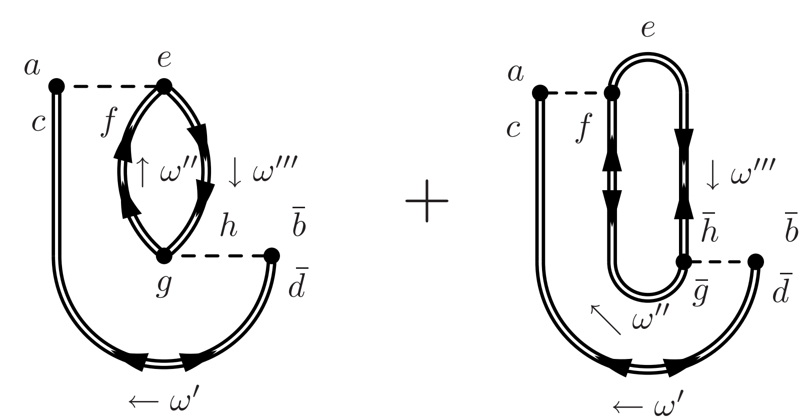


✪ 2nd order ➟ energy-dependent self-energy

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



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



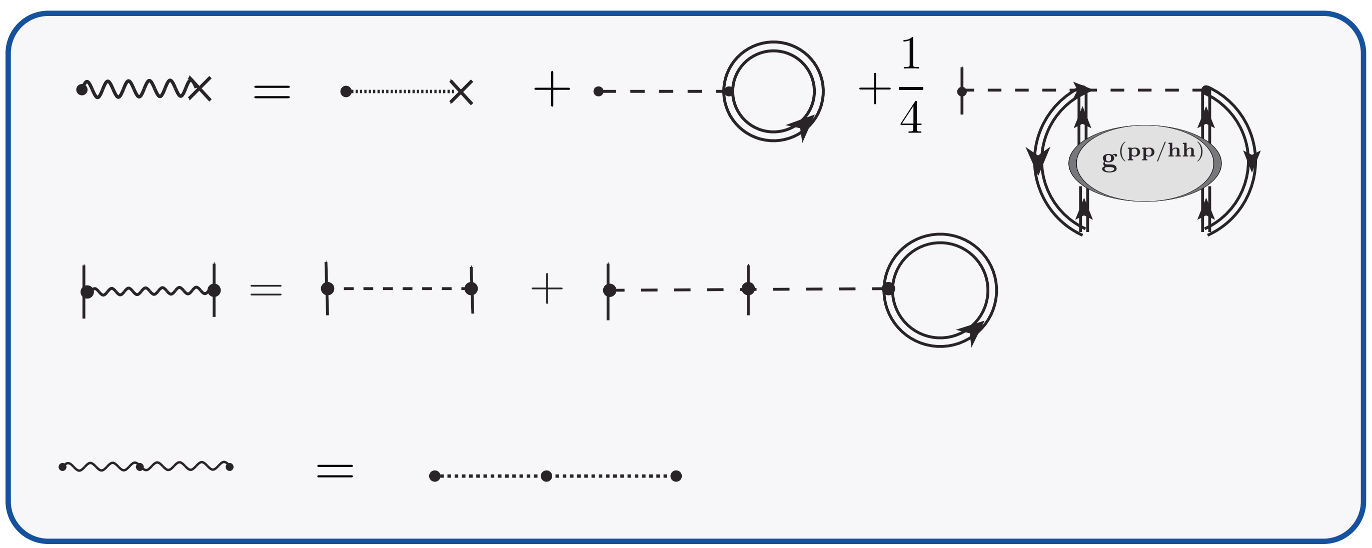
Three-body forces

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

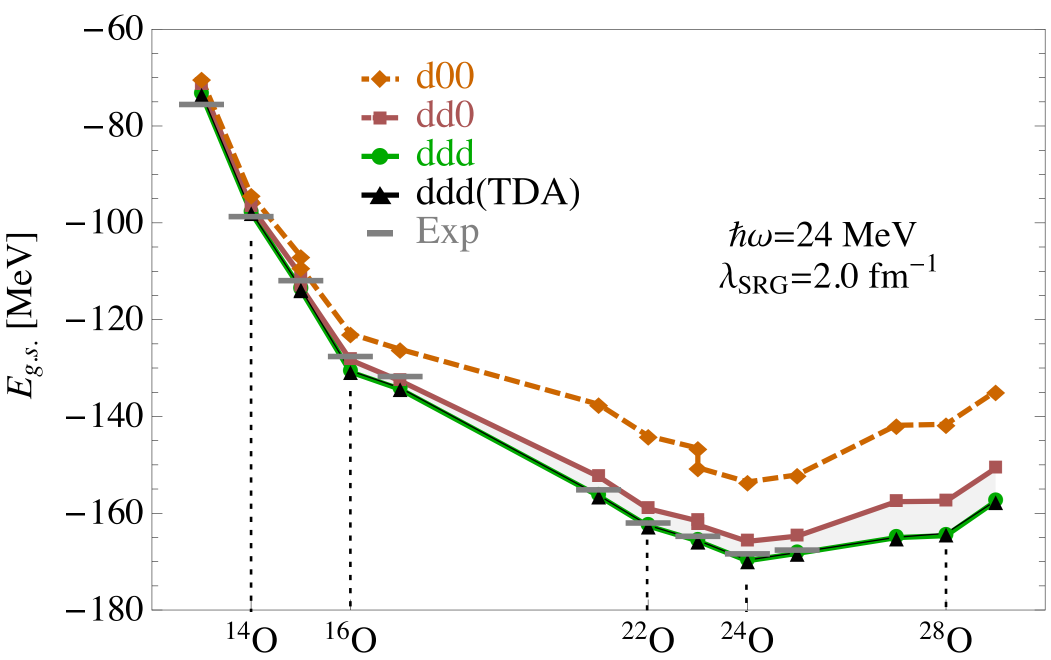
➟ Contractions with fully correlated density matrix

➟ Generalization of normal ordering

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

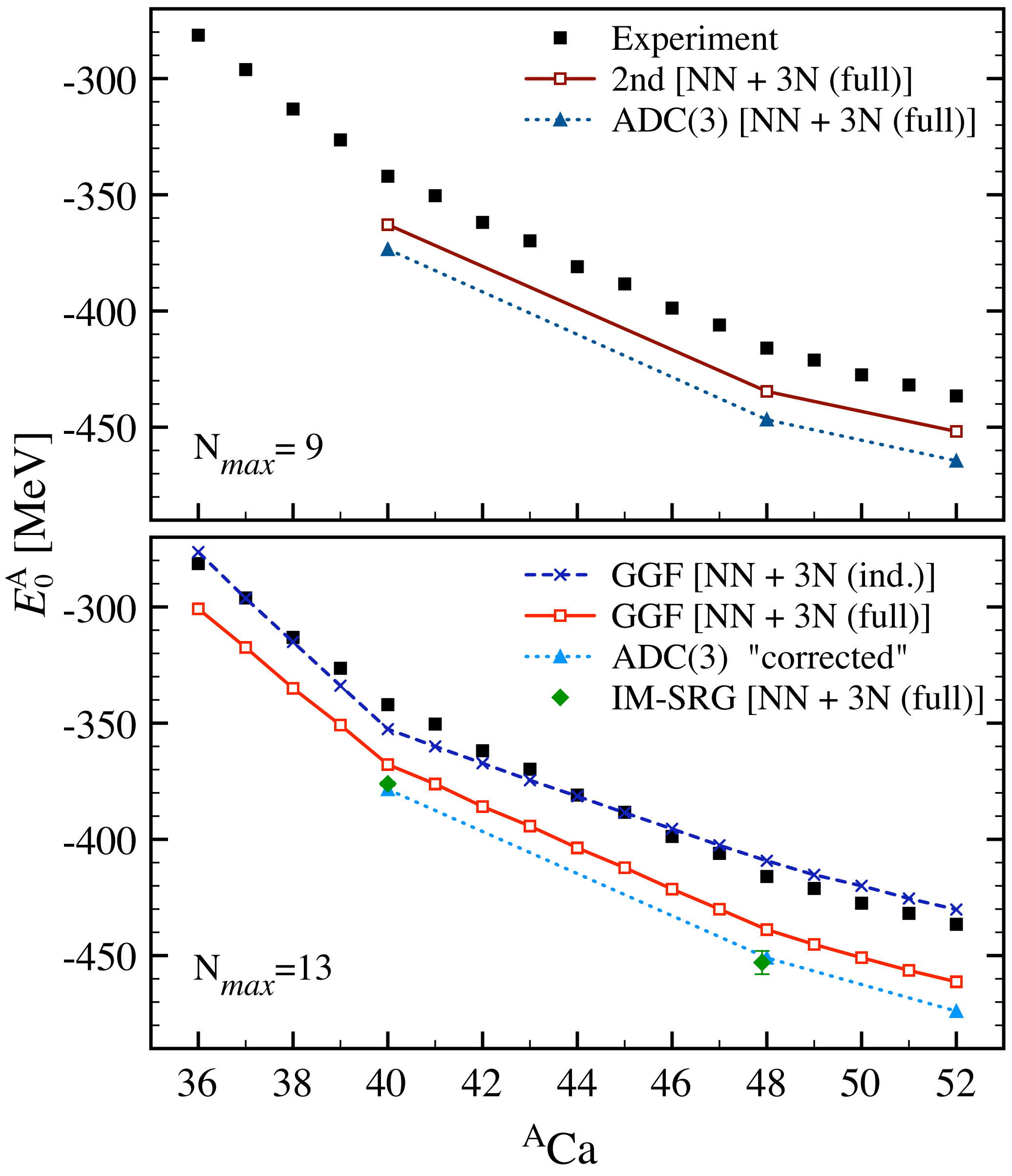


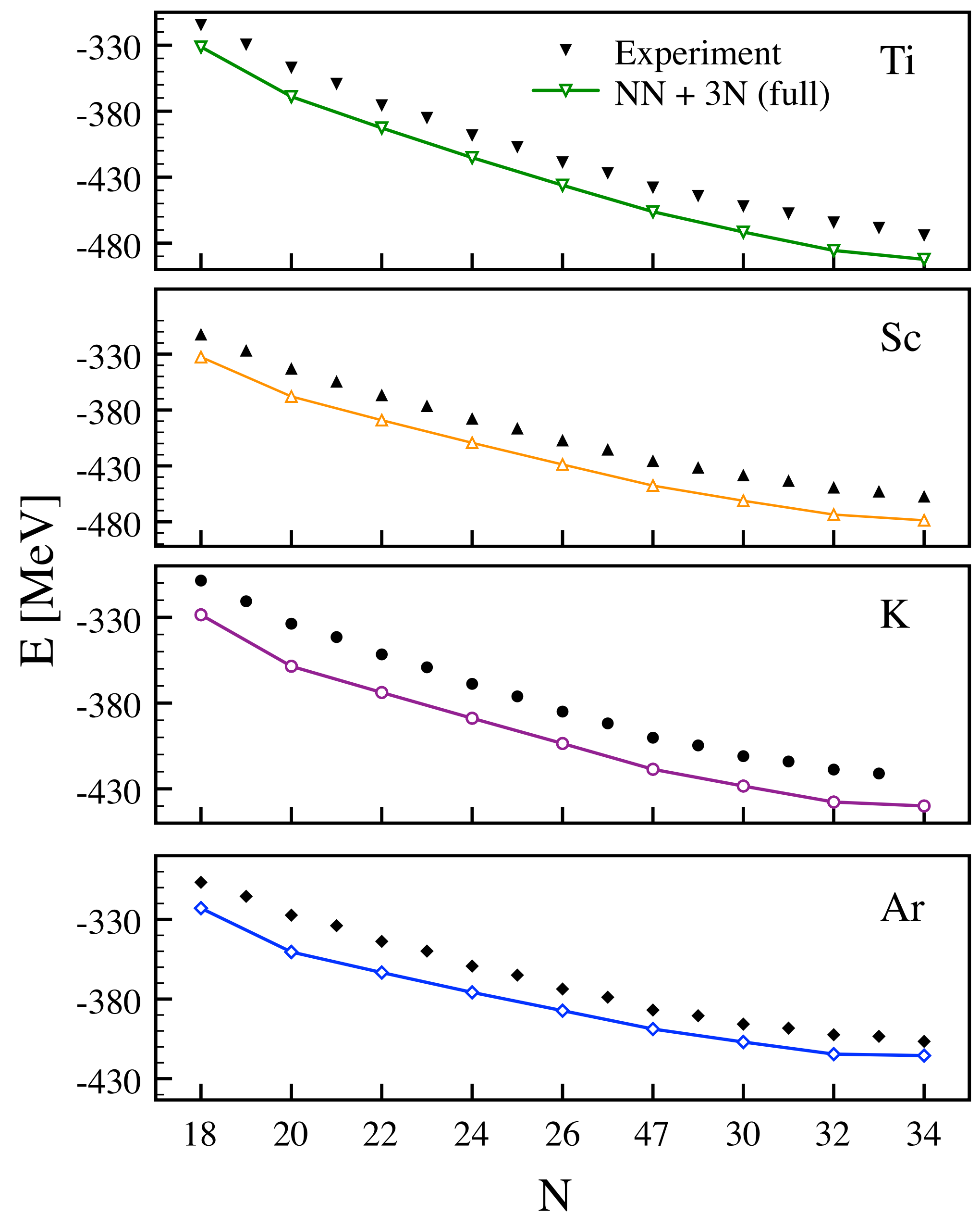
[Cipollone *et al.* 2013]



➟ Use of dressed propagators provides extra correlations

Binding energies around Ca



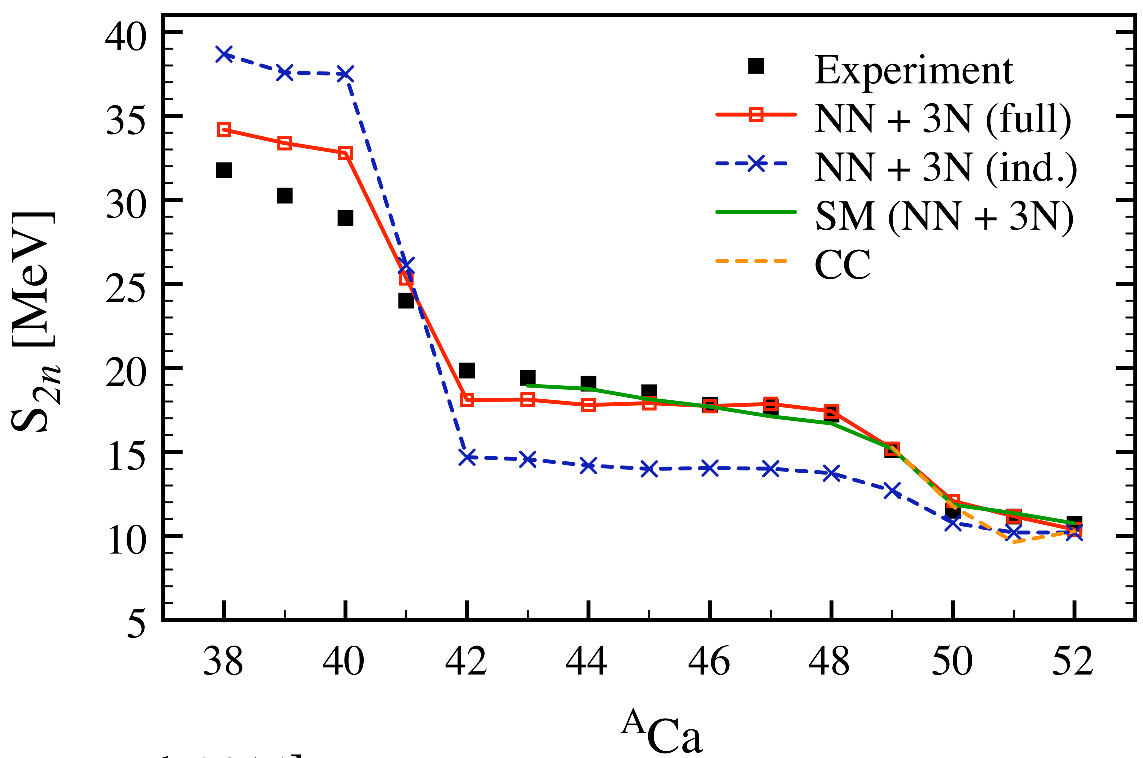


[Somà *et al.* 2014]

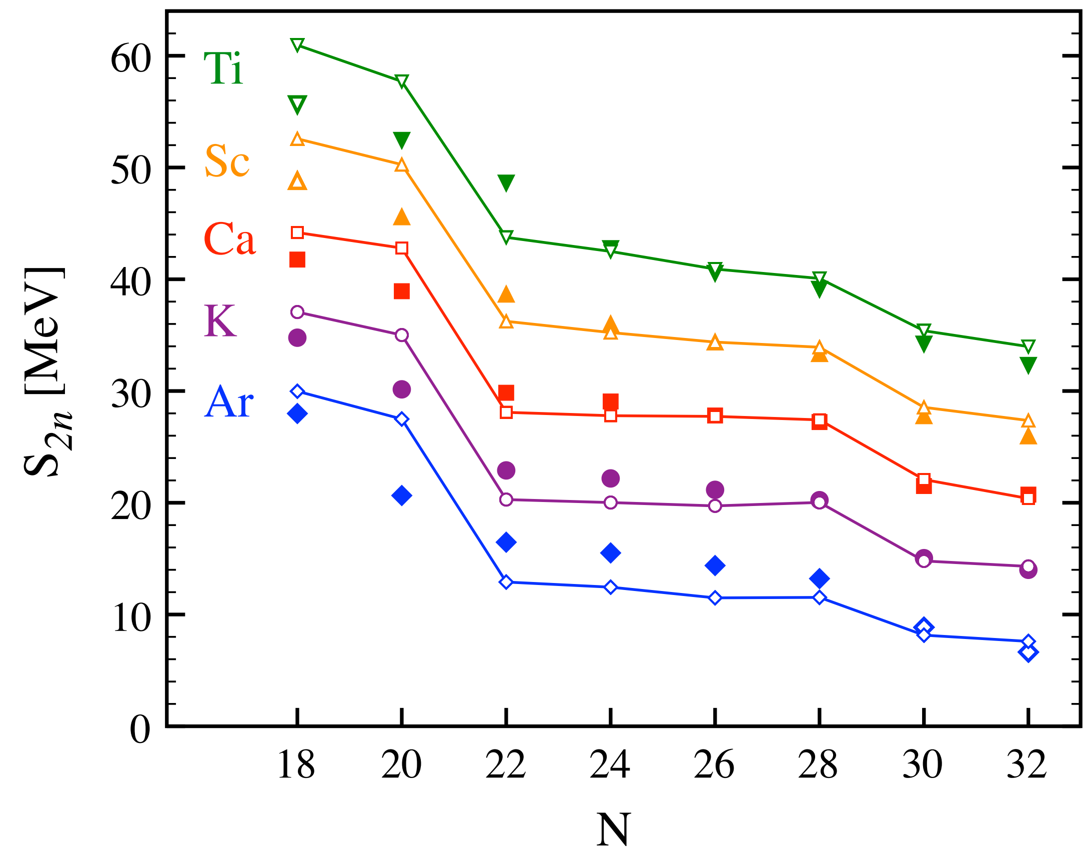
➟ NN + full 3N correct the trend of binding energies

➟ Systematic overbinding through all chains around Z=20

Two-neutron separation energies around Ca

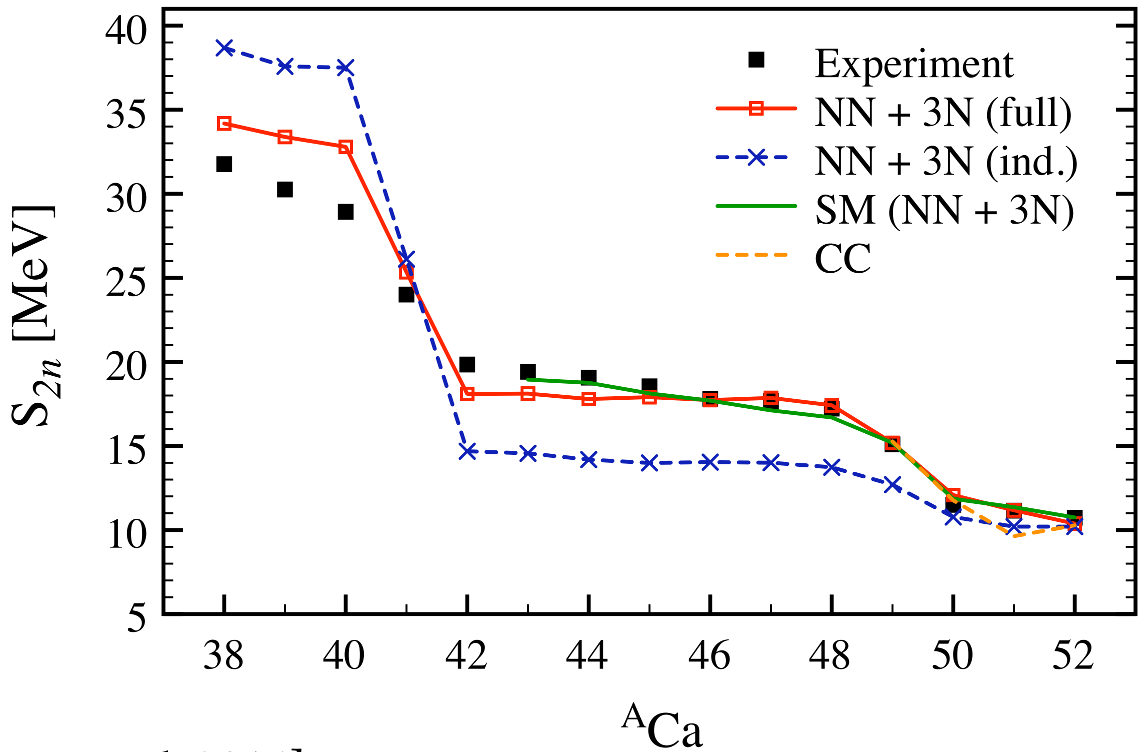


[Somà *et al.* 2014]

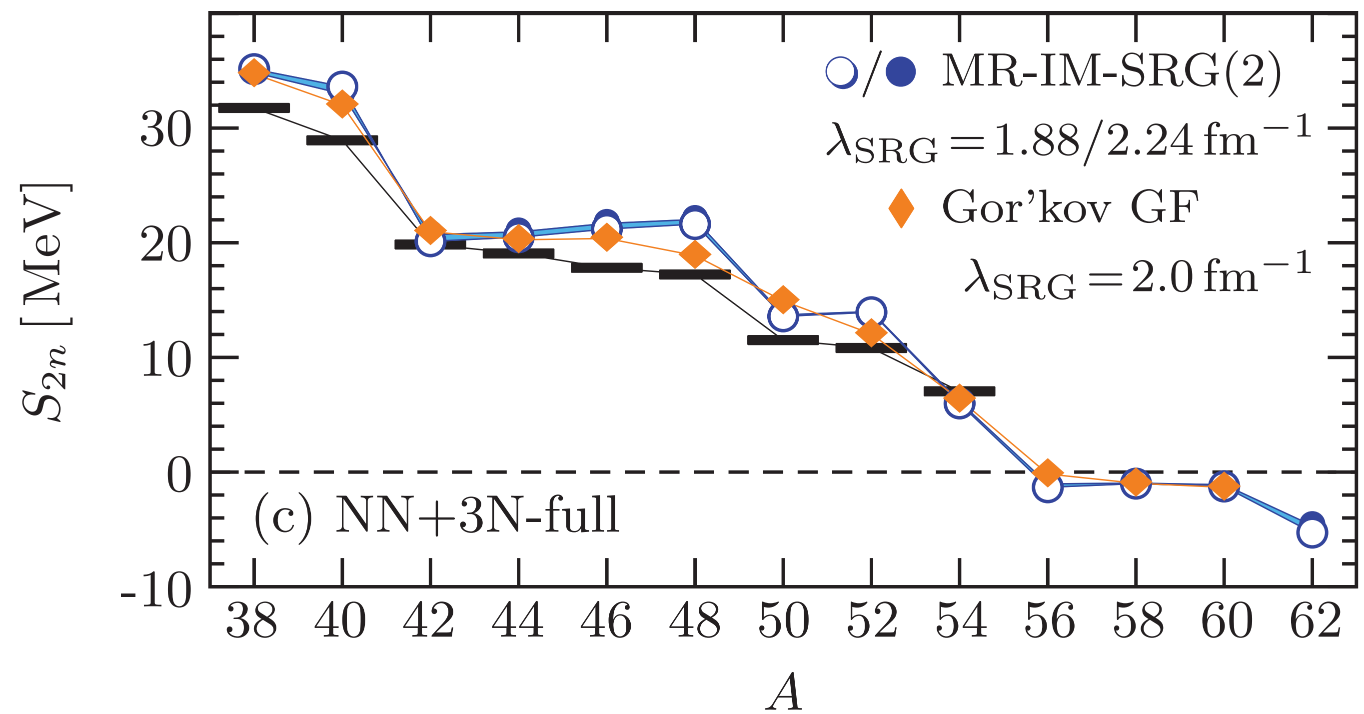


- ➟ S_{2n} well reproduced with chiral NN + 3N interactions
- ➟ Microscopic calculations extended to the whole Ca chain
- ➟ Neighbouring Z=18-22 chains computed within the same GGF framework
- ➟ Overestimation of N=20 gap traced back to spectrum too spread out

Two-neutron separation energies around Ca



[Somà *et al.* 2014]



[Hergert *et al.* 2014]

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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

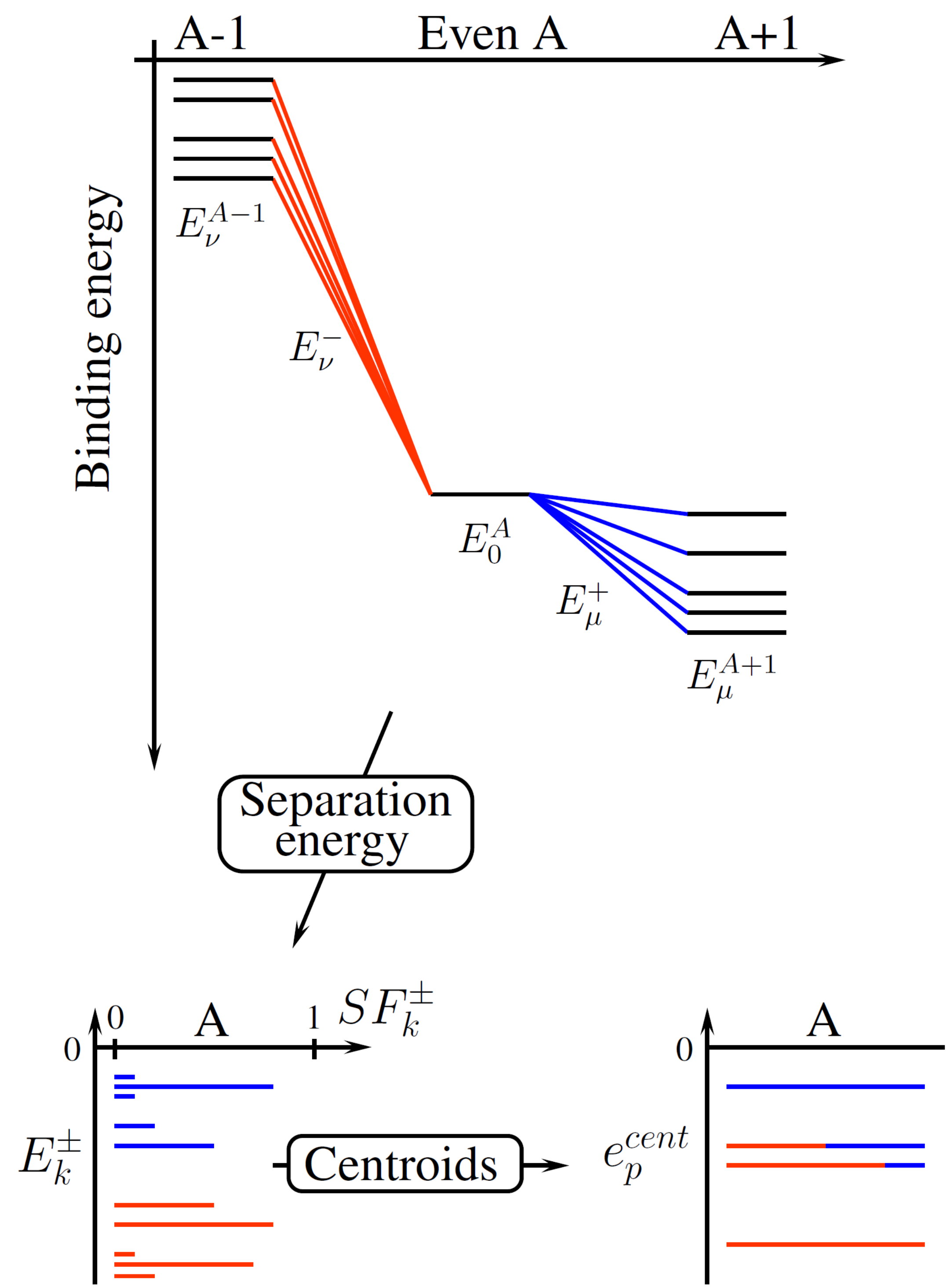
where $\begin{cases} \mathcal{U}^{k*}_a \equiv \langle \Psi_k | a^\dagger_a | \Psi_0 \rangle \\ \mathcal{V}^{k*}_a \equiv \langle \Psi_k | \bar{a}_a | \Psi_0 \rangle \end{cases}$

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

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

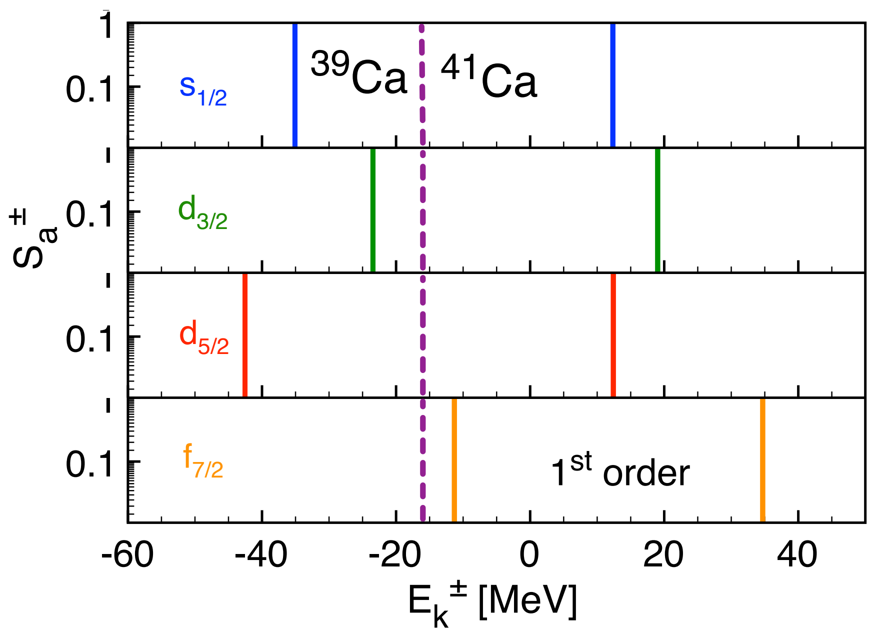
$$SF^-_k \equiv \sum_{a \in \mathcal{H}_1} \left| \langle \psi_k | a_a | \psi_0 \rangle \right|^2 = \sum_{a \in \mathcal{H}_1} \left| \mathcal{V}^k_a \right|^2$$



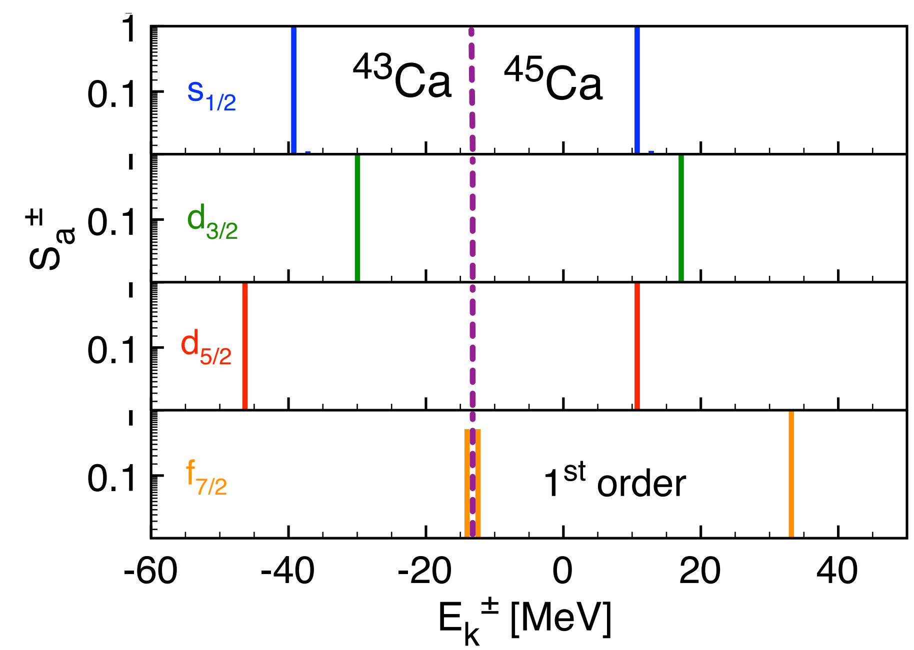
[figure from J. Sadoudi]

Spectral strength distribution

Dyson 1st order (HF)



Gorkov 1st order (HFB)

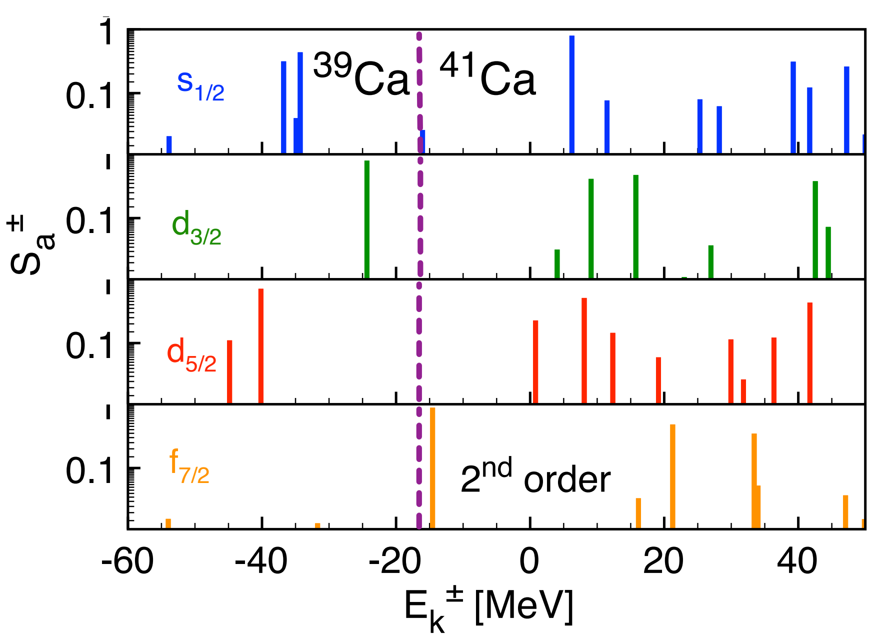


Fragmentation

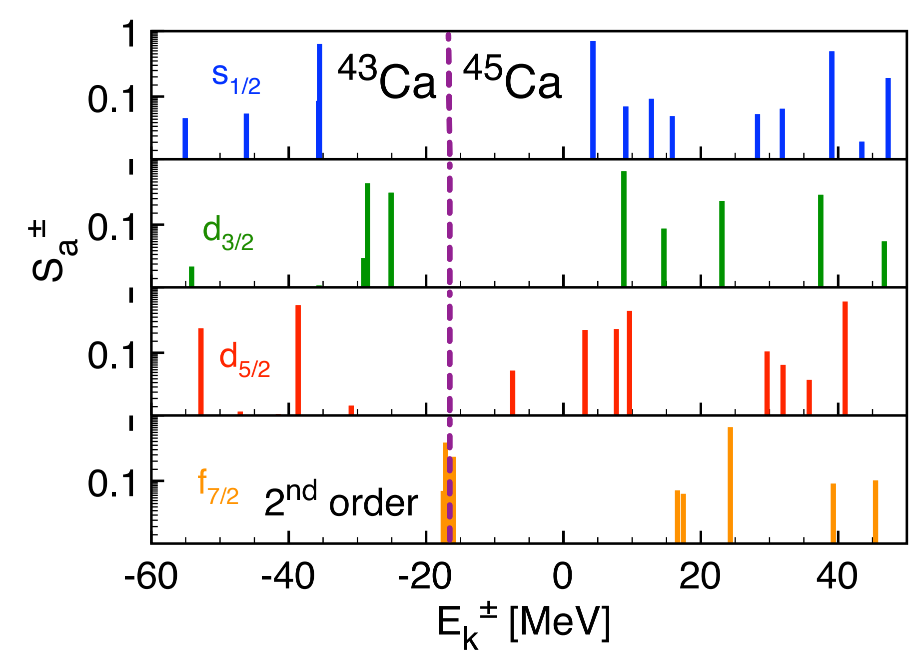
Static pairing →

↓ Dynamical fluctuations ↓

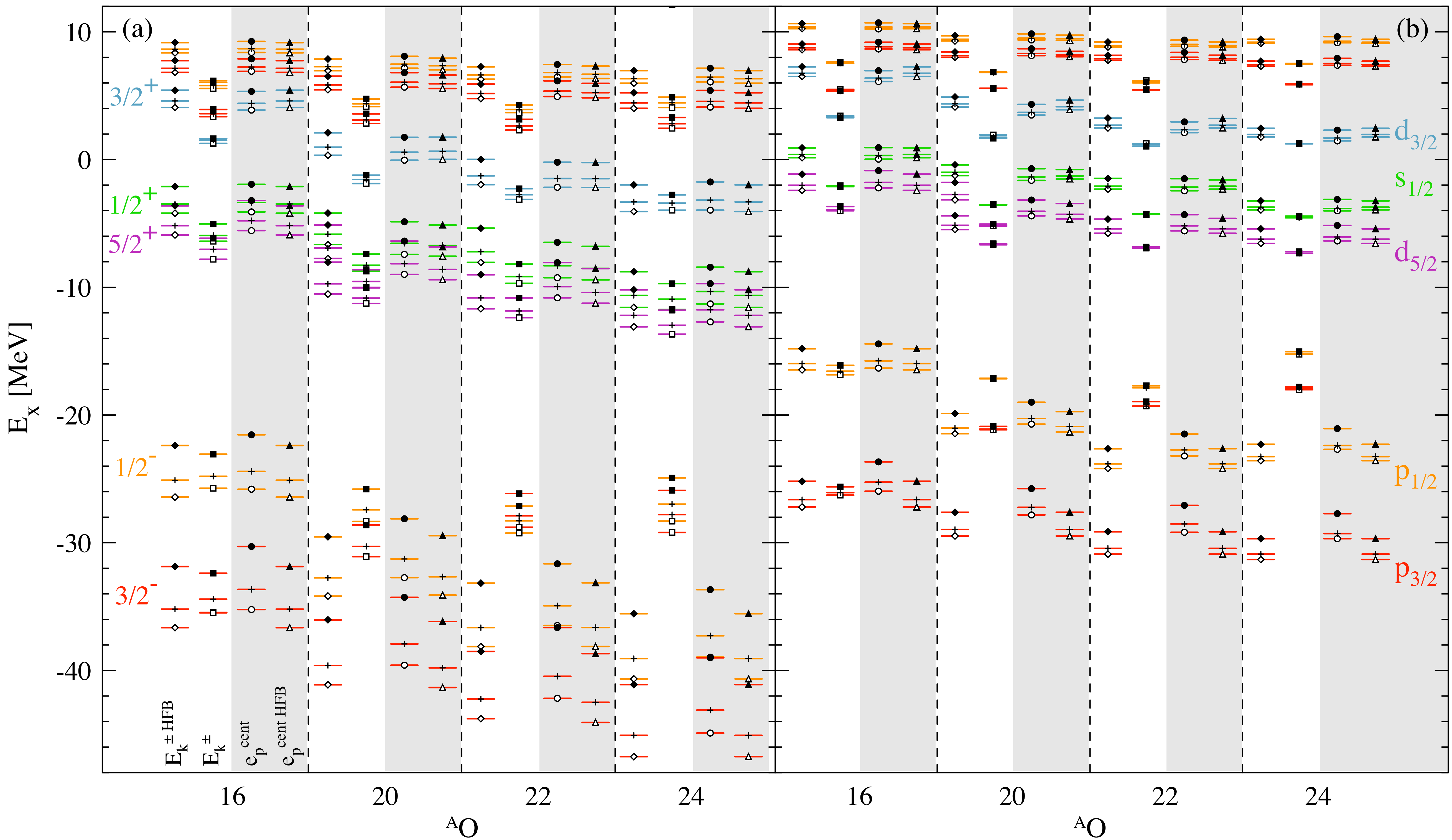
Dyson 2nd order



Gorkov 2nd order



Effective single-particle energies



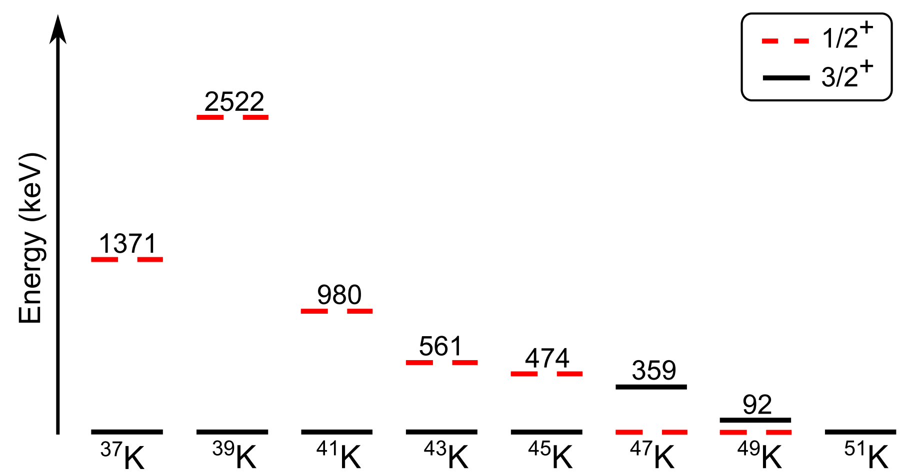
[Duguet, Hergert, Holt, Somà 2014]

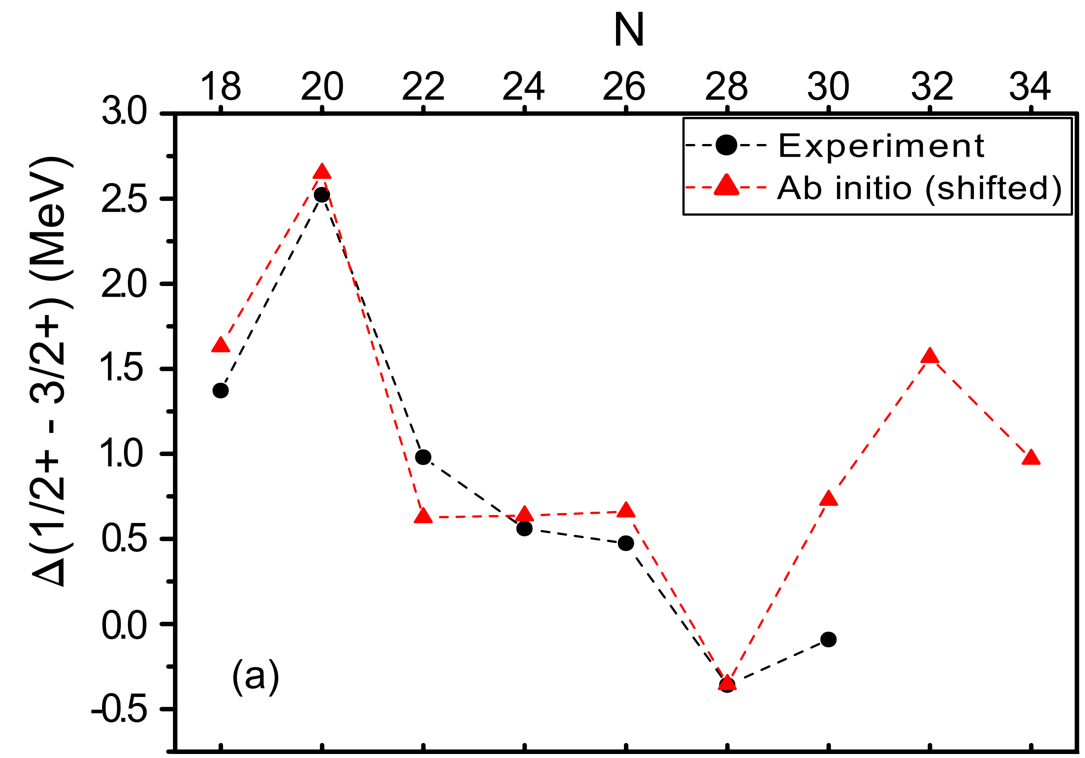
Potassium ground states (re)inversion

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

➟ Laser spectroscopy @ ISOLDE

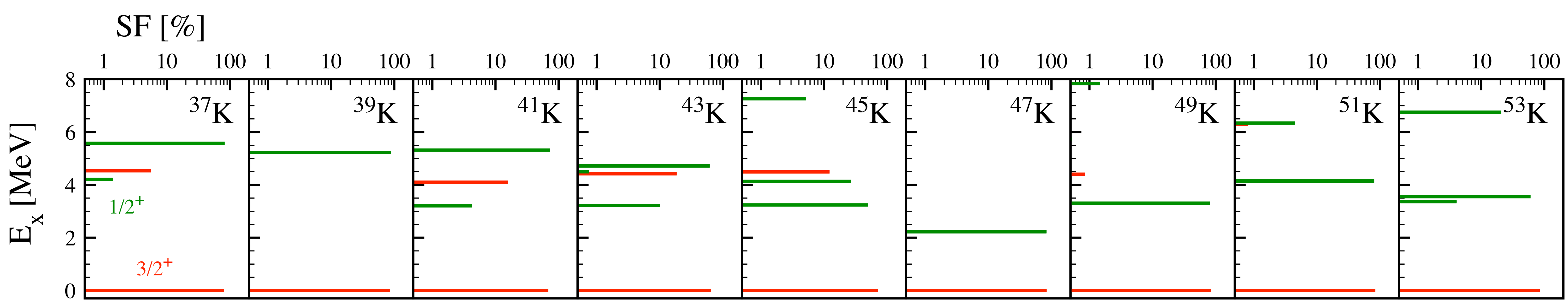
[Papuga, *et al.* 2013]





[Papuga, Somà *et al.* 2014]

➟ GGF calculations of K spectra



Error estimates in ab initio calculations

✪ Long-term goal: predictive calculations with quantified theoretical errors

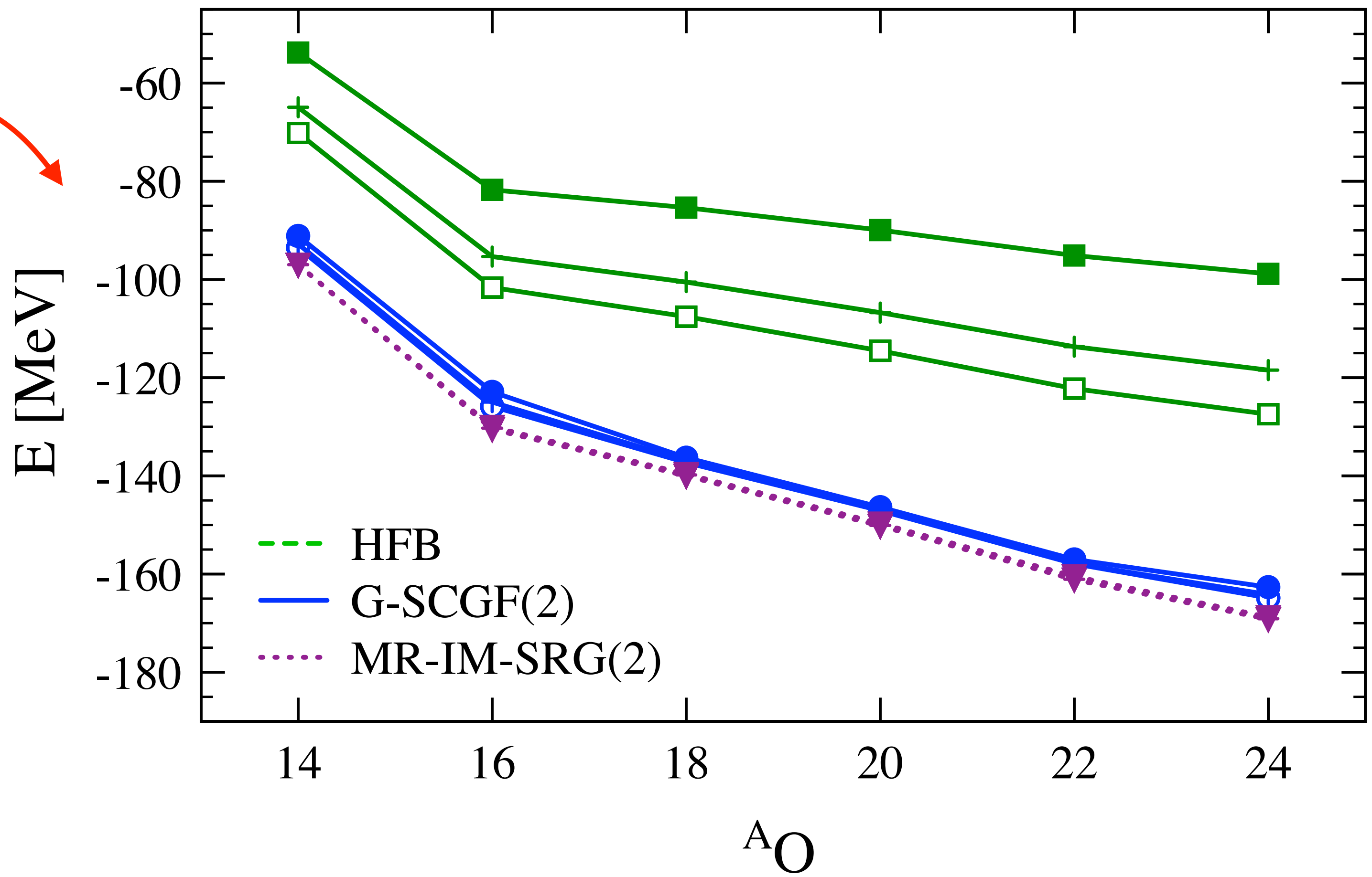
✪ Possible sources of error:

1) Hamiltonian

2) Many-body expansion

3) Model space truncation

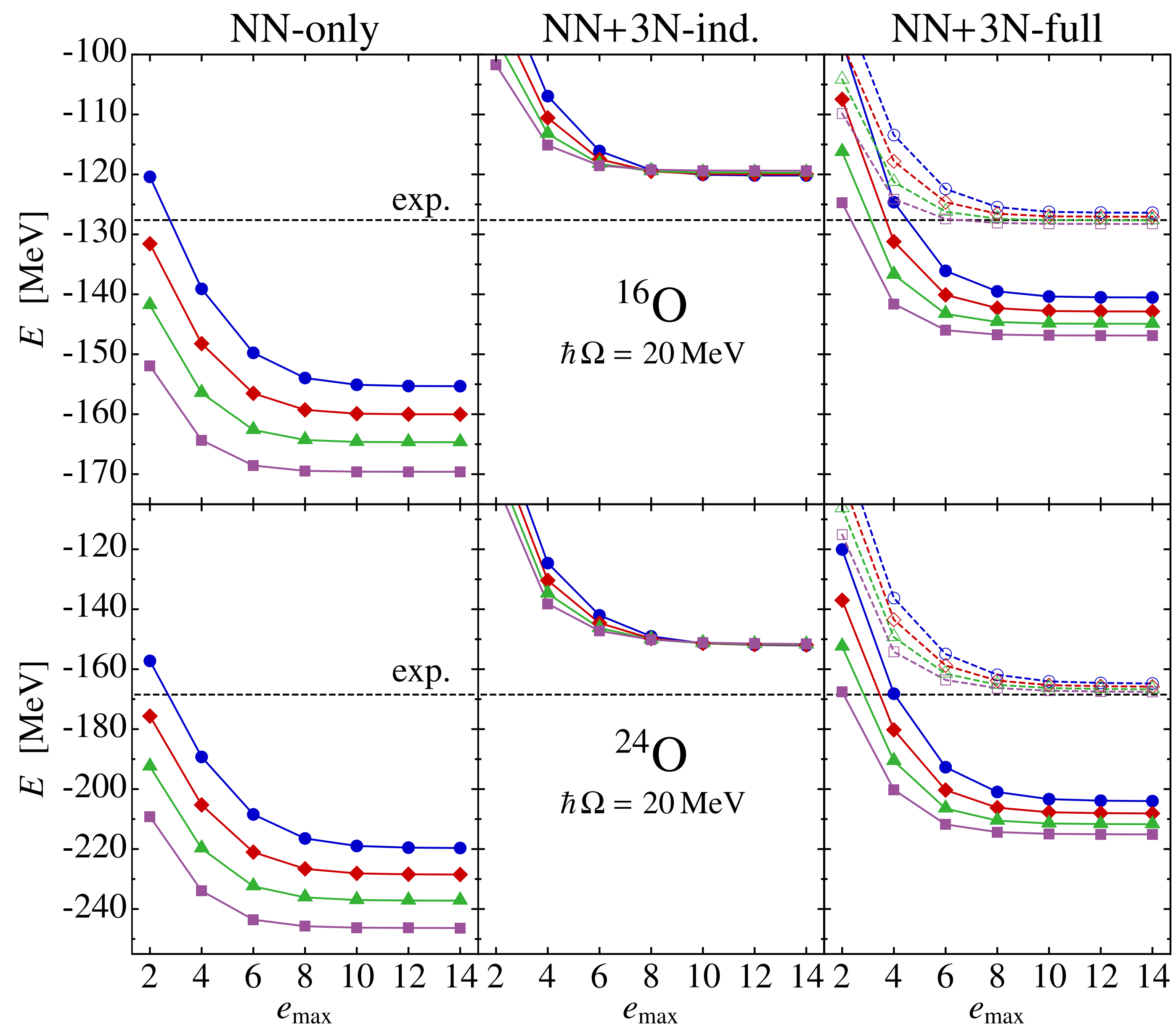
4) Numerical algorithms



Error estimates in ab initio calculations

- ✪ Long-term goal: predictive calculations with quantified theoretical errors
- ✪ Possible sources of error:

1) Hamiltonian → SRG
2) Many-body expansion
3) Model space truncation
4) Numerical algorithms



[Roth *et al.* 2012]

Ongoing developments

✪ Many-body methods

- ➠ Extension to doubly open-shell (i.e. allow for deformation)

  [Signoracci, Duguet, Hagen]

- ➠ Restoration of broken symmetries

  [Duguet 2014; Duguet, Barbieri & Somà]

- ➠ …

✪ Inter-nucleon interactions

- ➠ SRG including 4N forces

  [Calci *et al.*]

- ➠ Chiral N^{3}LO 3N forces

  [Hebeler, Krebs *et al.*]

- ➠ Separable representation of NN and 3N interactions

  [Lesinski]

- ➠ …

Conclusions

✪ Ab initio approaches in a good shape

➟ Agreement between different methods up to medium masses

➟ Benchmarks for more effective approaches?

✪ Many-body interactions (& SRG) promising, but more problematic

➟ Chiral EFT
- issue of Deltas and order-by-order convergence
- issue of power counting

➟ SRG
- issue of induced many-body operators
- issue of induced many-body operators

Is the ab initio route viable at all?

➟ First attempts towards a chiral-inspired *effective interaction*

[Ekström, Forssén, Hagen, *et al.*]