

Towards many-body calculations on the basis of a consistent chiral power counting



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ESNT Program

Effective field theory and the many-body problem

SPhN, 16 May 2014

with T. Duguet, B. Long, M. Pavón Valderrama, U. van Kolck

Plan:

Intro & status of ab initio

Success & issues of chiral potentials

Gorkov-GF technique

Consistent power counting & many-body calculations

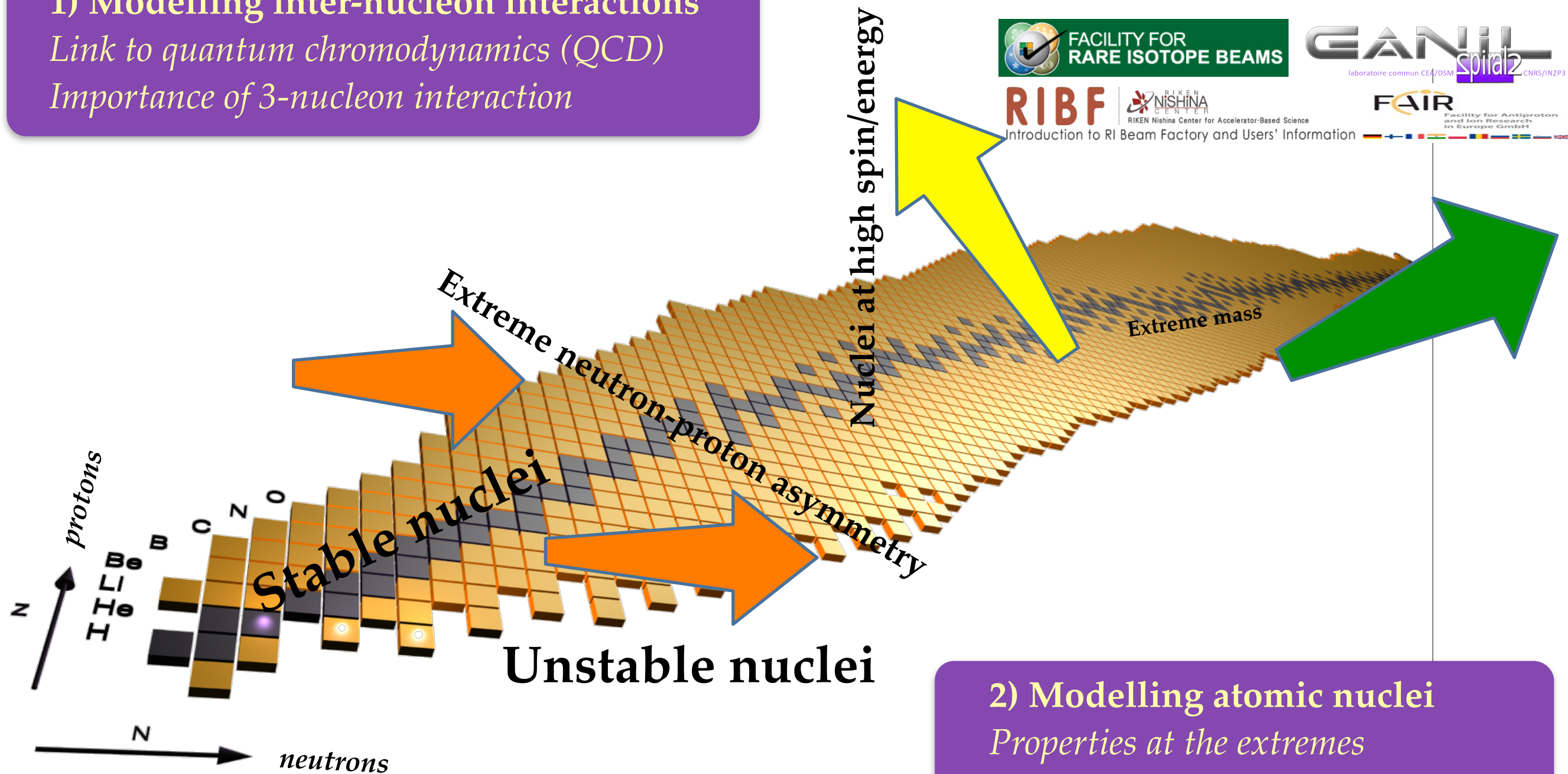
Low-energy nuclear physics: state of the art

1) Modelling inter-nucleon interactions

Link to quantum chromodynamics (QCD)

Importance of 3-nucleon interaction

Large-scale experimental facilities



2) Modelling atomic nuclei

Properties at the extremes

Reliable and consistent systematics

Ab initio vs effective many-body theories

Ab initio many-body theories

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



Limited applicability
Controlled extrapolations
Test fundamental interactions

Effective many-body theories

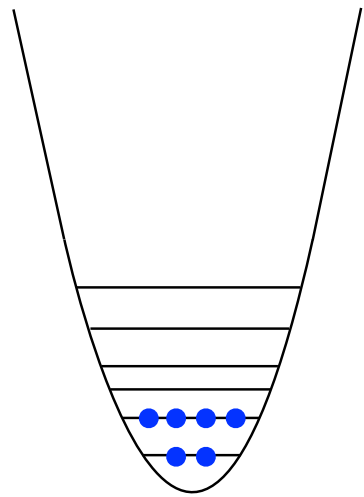
- ⇒ Based on effective interactions
- ⇒ Solve *simpler* many-body problem
- ⇒ Partial assessment of errors



Extended reach
Uncontrolled extrapolations
Aim at reproduction of data

Different ab initio philosophies

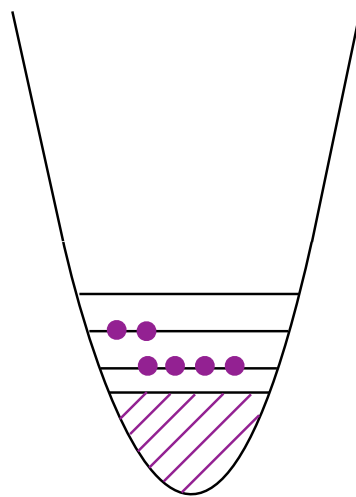
Light nuclei



“Exact”

NCSM, GFMC,

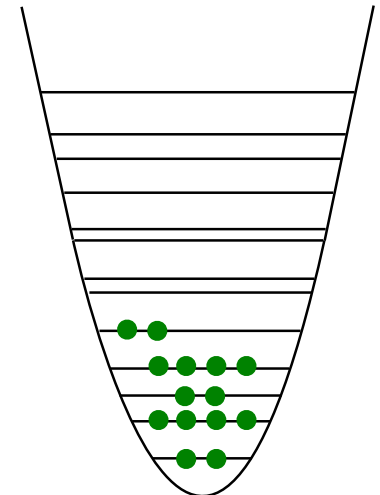
Medium-mass nuclei



Valence space

Microscopic SM

Medium-mass nuclei



Based on expansion

GF, CC, IM-SRG,

All methods (should be able to) take
the same input NN+3N interactions

Closed-shell

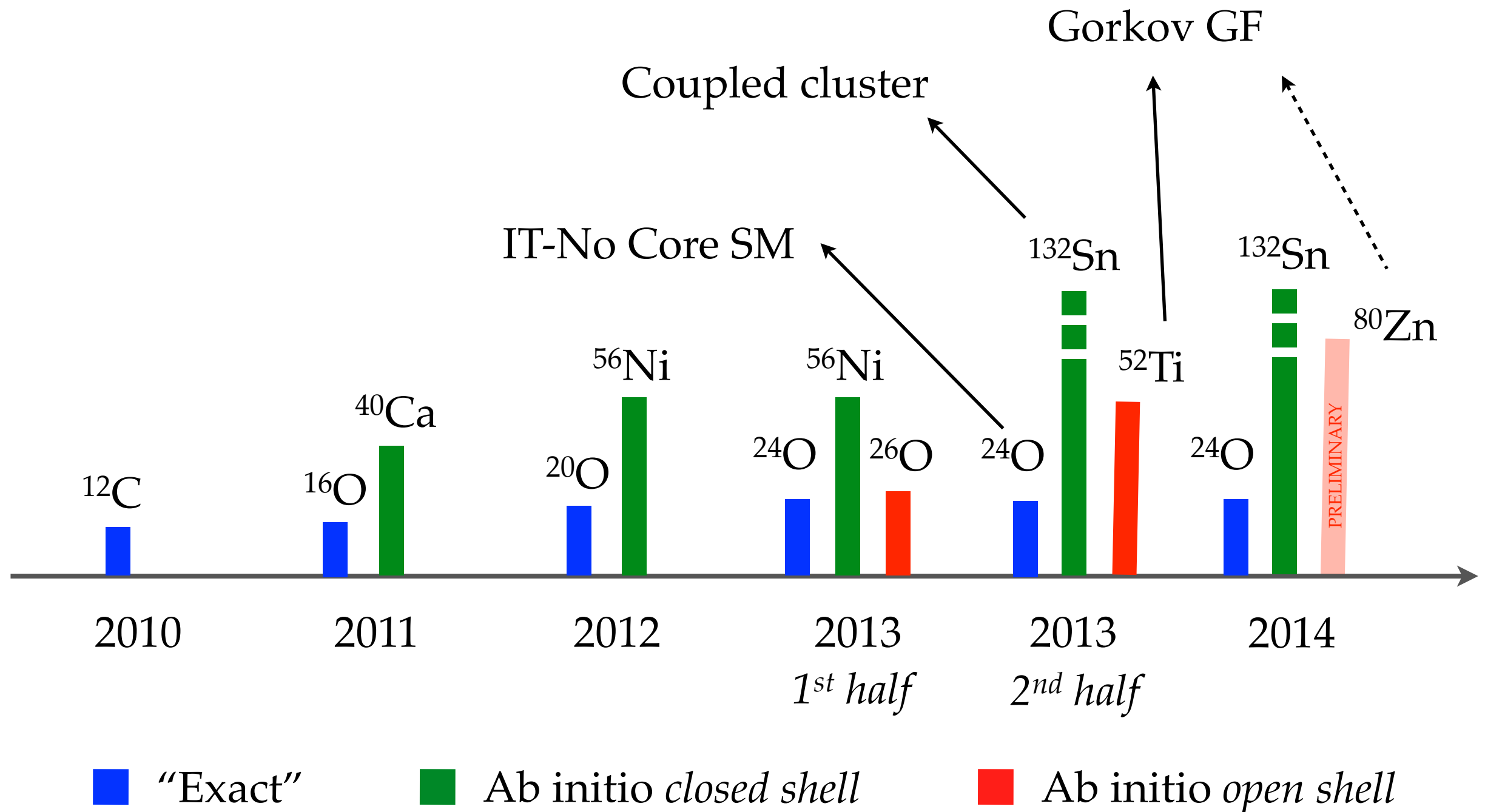
Open-shell

⇒ Alternative approach: lattice EFT

Current limits / reach of ab initio calculations

➡ Heavier system computed in the different types of ab initio

NN+3N



Traditional nuclear interactions

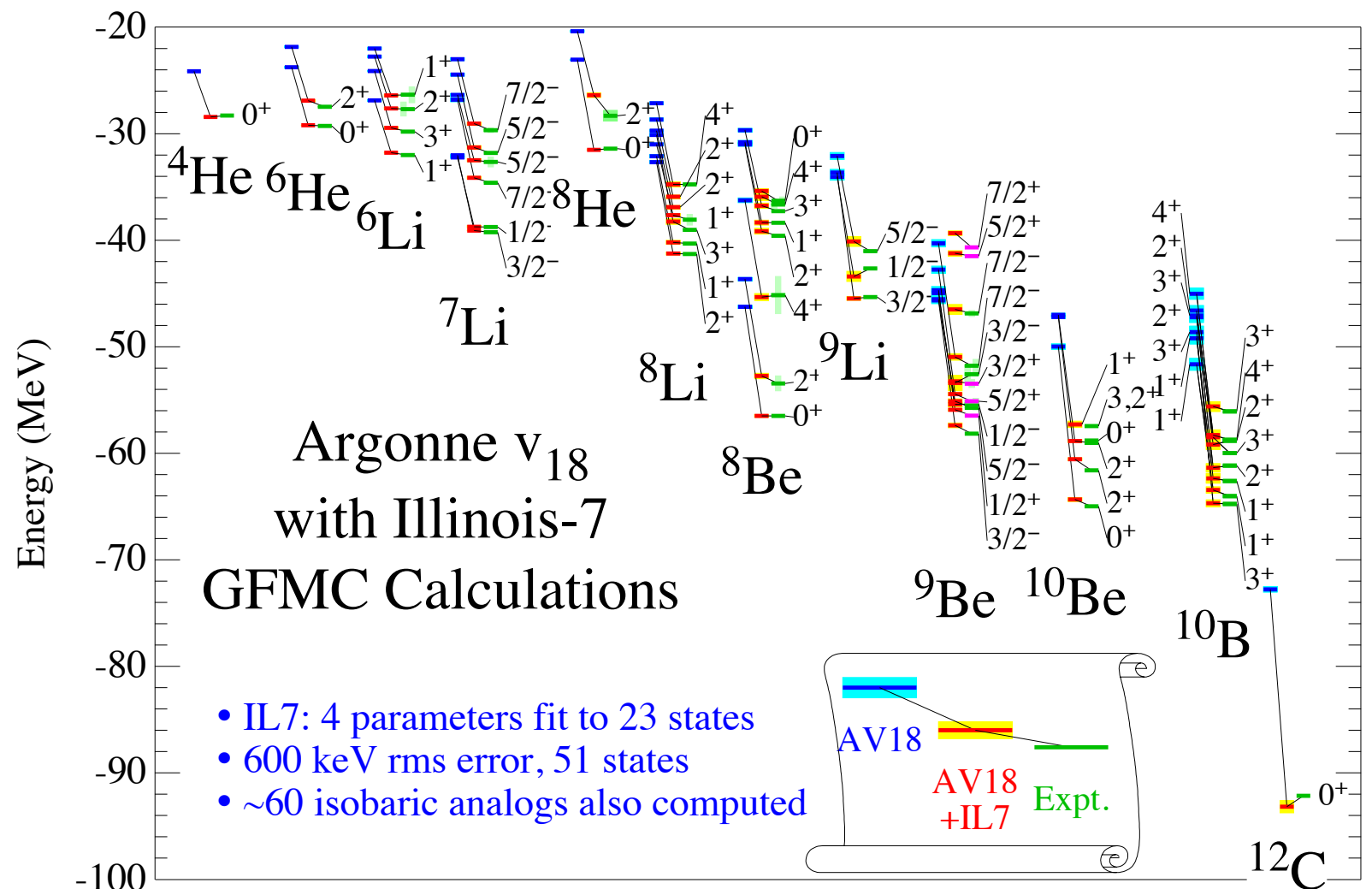
- ★ Based on one-boson exchange models
 - ⇒ Model with arbitrary number of parameters
 - ⇒ Feature a *hard core*
 - ⇒ Three-body forces mainly phenomenological

Not systematically
improvable

Not consistent
with NN

Limits severely many-body calculations

CD-Bonn
Av18
Reid
Nijmegen
...

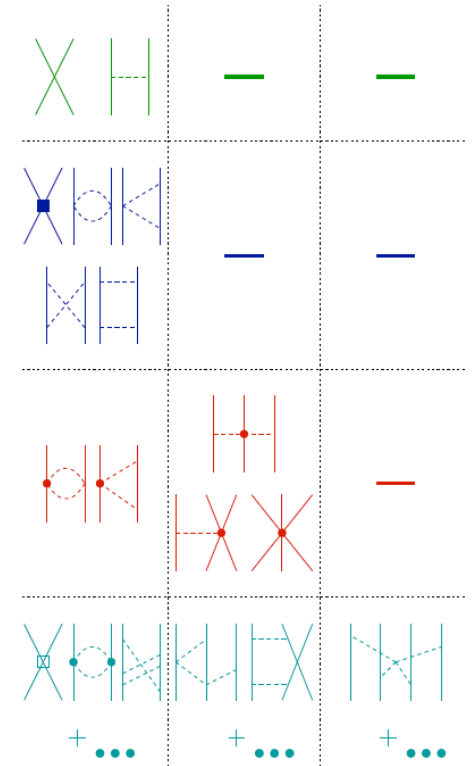


[Pieper & Wiringa 2001]

The modern approach: EFT & SRG

★ Chiral “effective field theory”

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



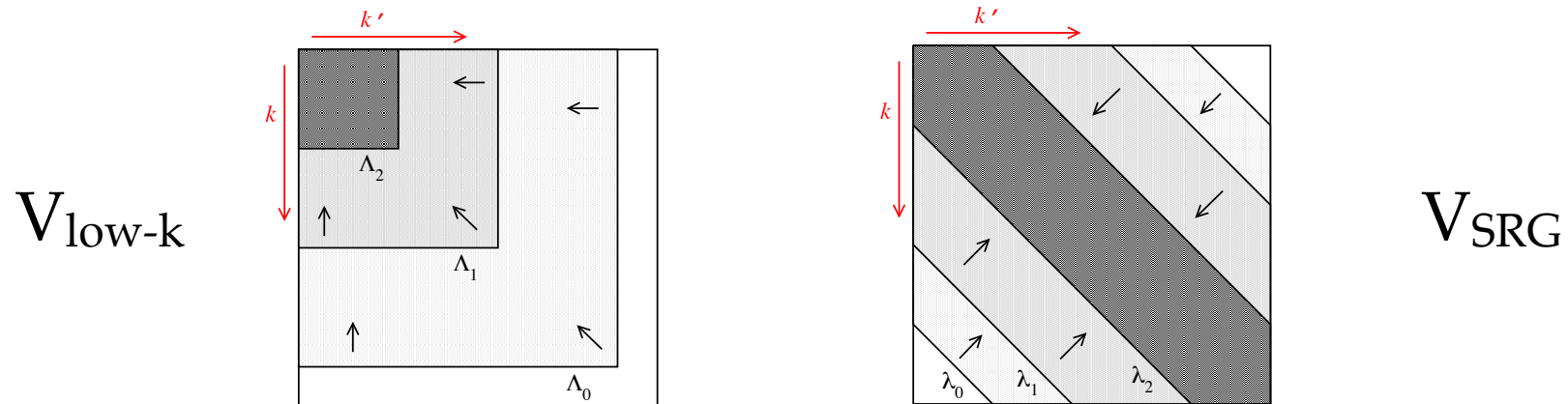
★ Renormalization group techniques for NN and 3N forces

- ⇒ Lowers the resolution scale of the original Hamiltonian
- ⇒ Improves convergence of many-body calculations
- ⇒ Contains diagnosis tools for missing many-body forces

RG techniques for NN & 3N forces

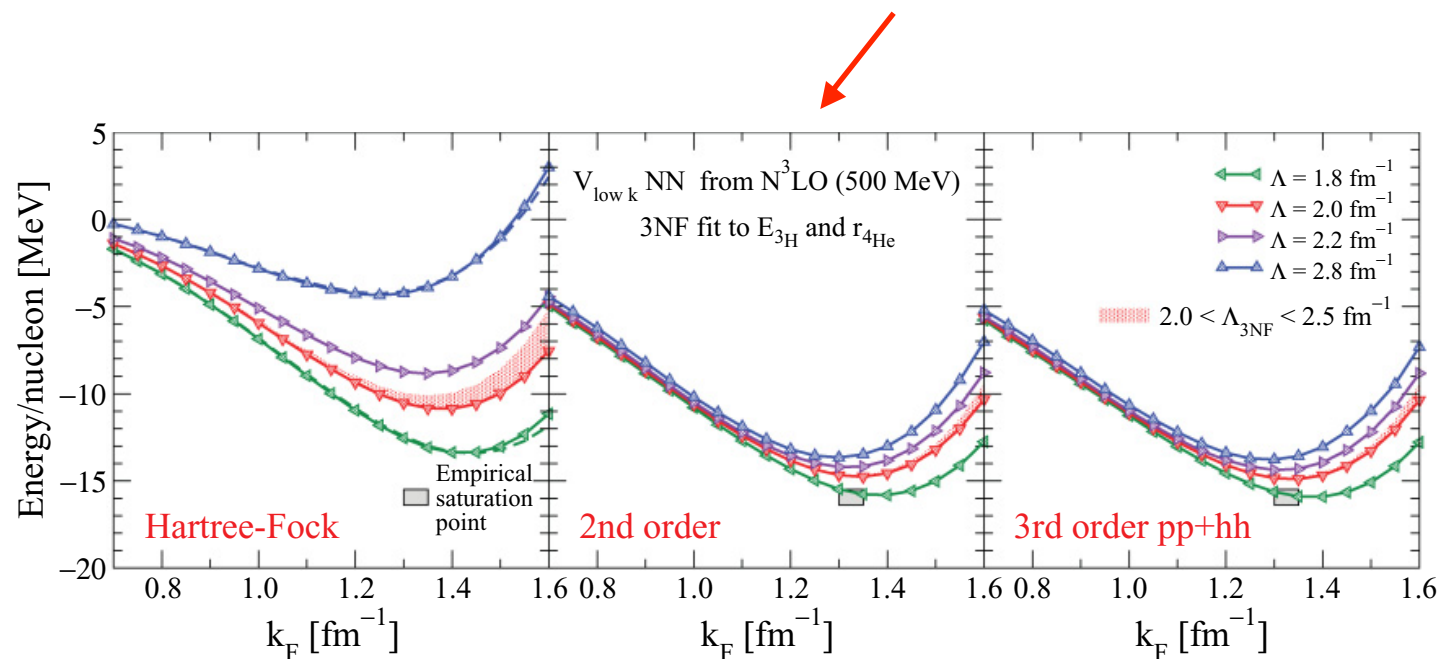
★ Renormalization group techniques for NN and 3N forces

⇒ Lower the *resolution scale* of the original Hamiltonian

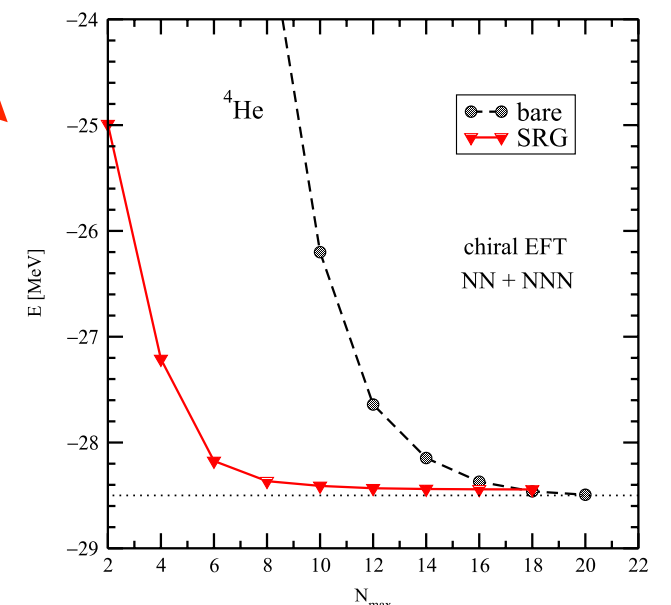


★ Improved convergence of many-body calculations

⇒ Smaller many-body truncations & smaller model spaces needed



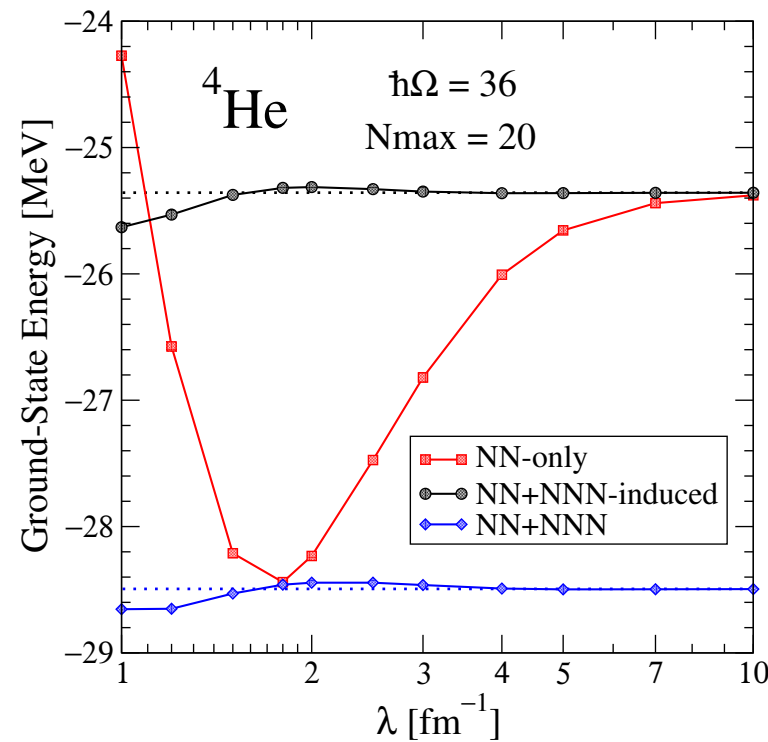
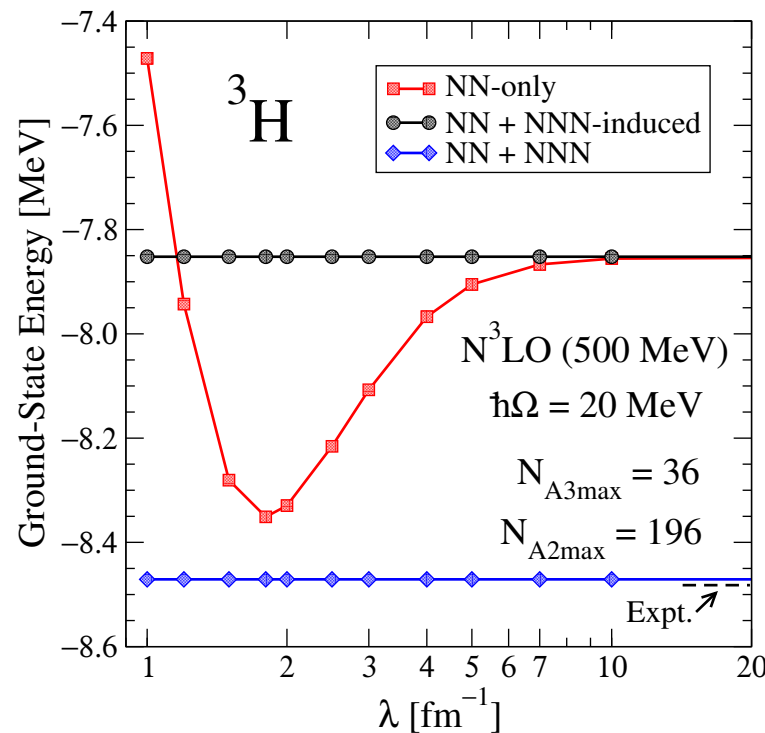
[Hebeler *et al.* 2011]



[Jurgenson, Navratil & Furnstahl 2013]

RG techniques for NN & 3N forces

★ But... (additional) many-body forces are generated

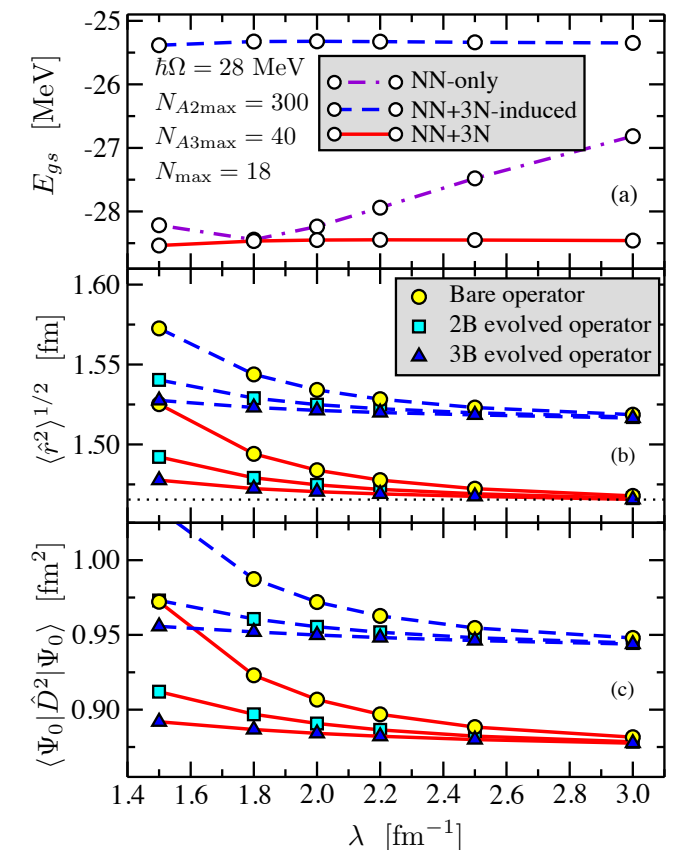


[Jurgenson *et al.* 2011]



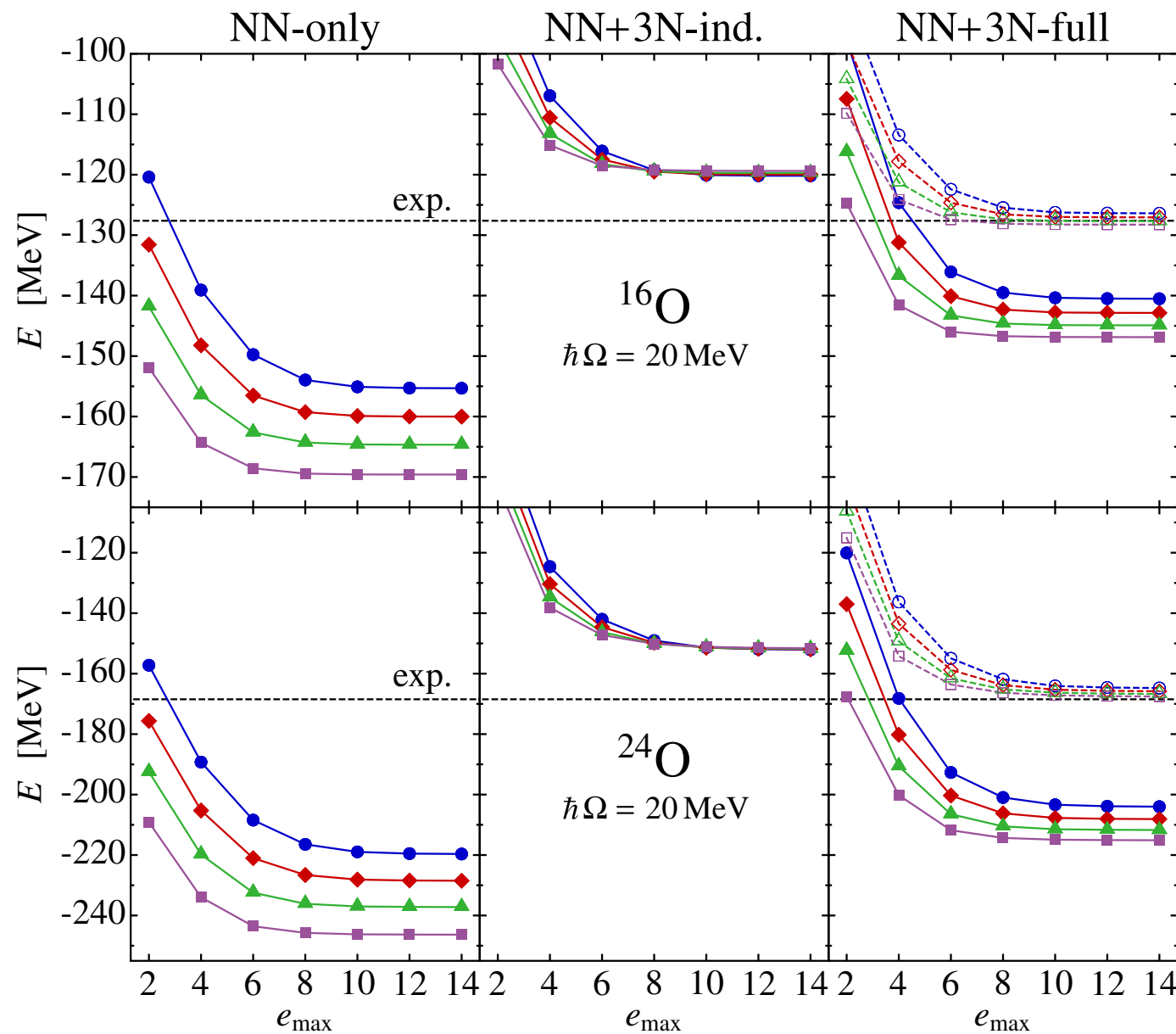
In fact, all operators have induced many-body terms!

[Schuster *et al.* 2014]



RG techniques for NN & 3N forces

★ SRG invariance becomes problematic in heavier systems



[Roth *et al.* 2012]

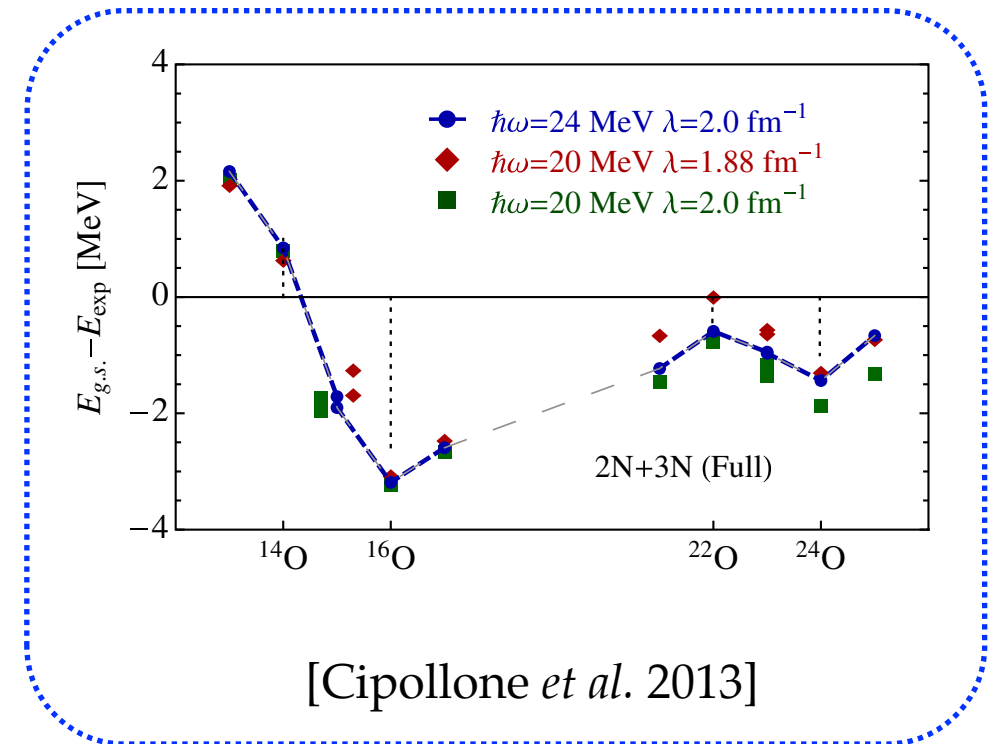


FIG. 4 (color online). CCSD ground-state energies for ^{16}O and ^{24}O as a function of e_{max} for the three types of Hamiltonians (see column headings) using the NO2B approximation for a range of flow parameters: $\alpha = 0.04 \text{ fm}^4$ (\bullet), 0.05 fm^4 (\blacklozenge), 0.0625 fm^4 (\blacktriangle), and 0.08 fm^4 (\blacksquare). The filled symbols for the $NN + 3N$ -full Hamiltonian are for the standard chiral $3N$ interaction with cutoff 500 MeV, the open symbols for a modified $3N$ interaction with cutoff 400 MeV (see text).

Current *standards* for NN+3N potential

①

★ NN potential:

○ chiral **N³LO** (500 MeV)

⇒ SRG-evolved to 2.0 fm^{-1}

[Entem and Machleidt 2003]

★ 3N potential:

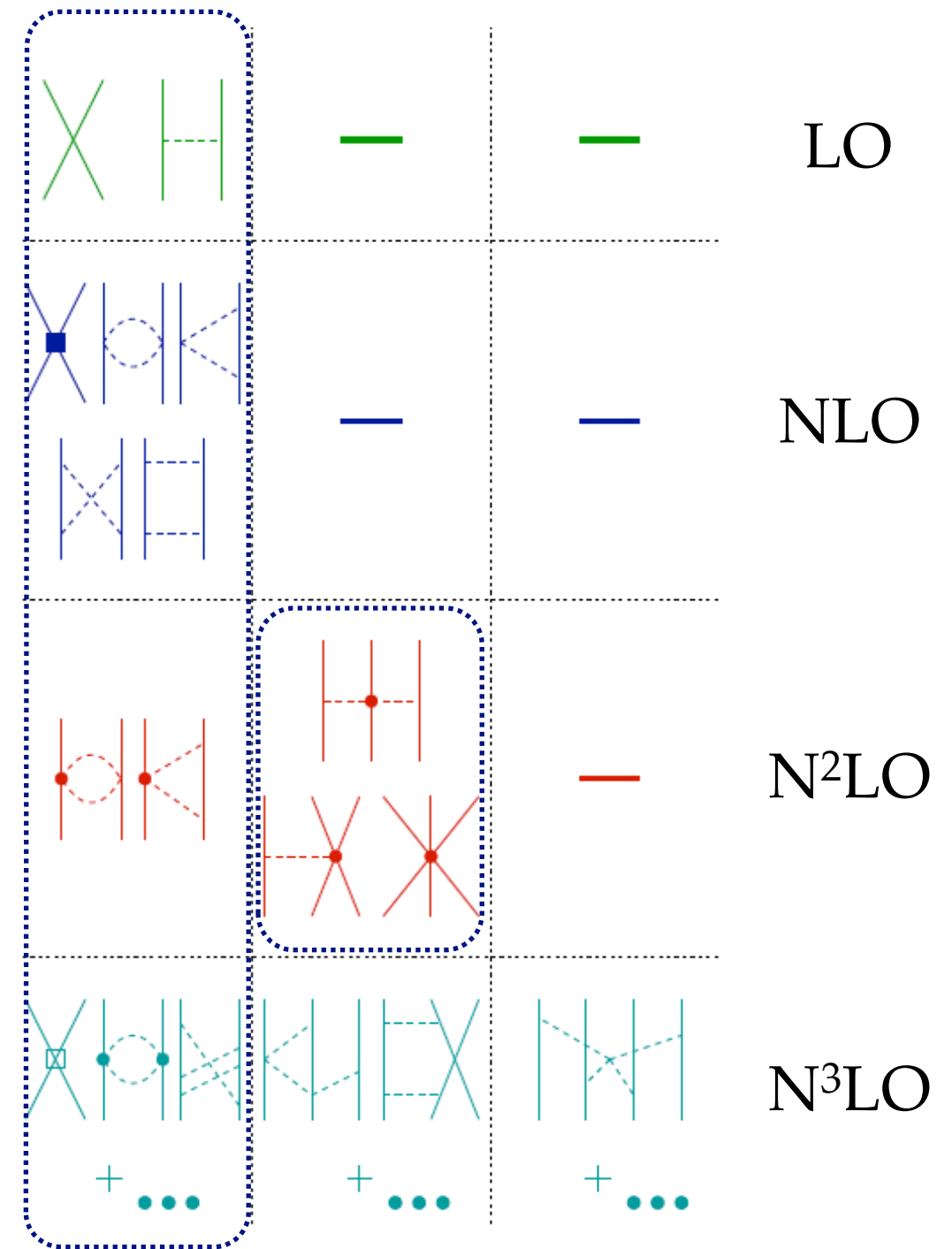
○ chiral **N²LO** (400 MeV)

⇒ SRG-evolved to 2.0 fm^{-1}

[Navrátil 2007]

⇒ Modified cutoff to reduce induced 4N contributions

[Roth *et al.* 2012]



Current *standards* for NN+3N potential

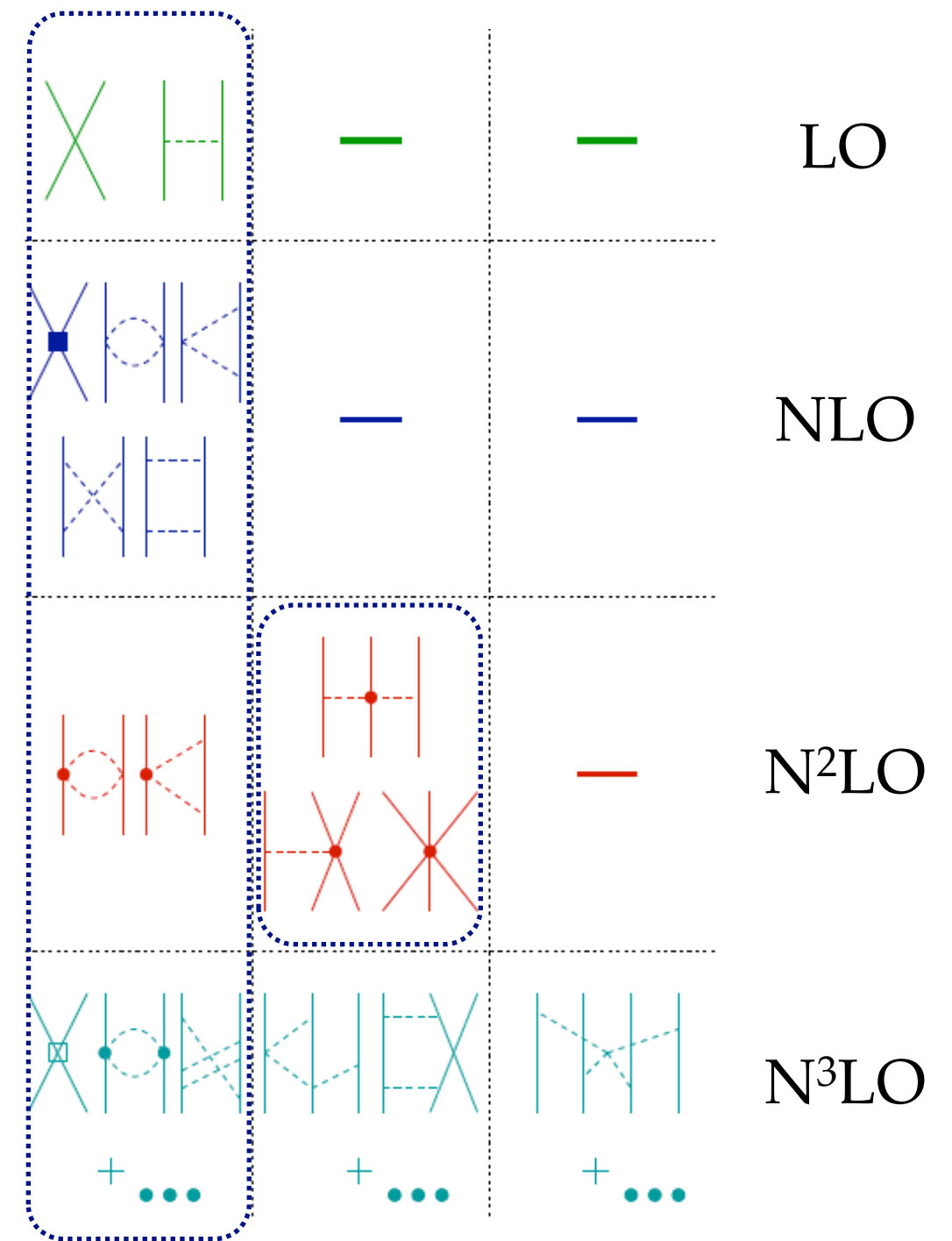
②

★ NN, 3N & 4N up to **N³LO**

⇒ various cutoff combinations

⇒ local & non-local versions

[Epelbaum *et al.*]



Current *standards* for NN+3N potential

③

★ N^2LO_{opt}

○ NN+3N (500 MeV)

⇒ optimised fit to NN phase shifts

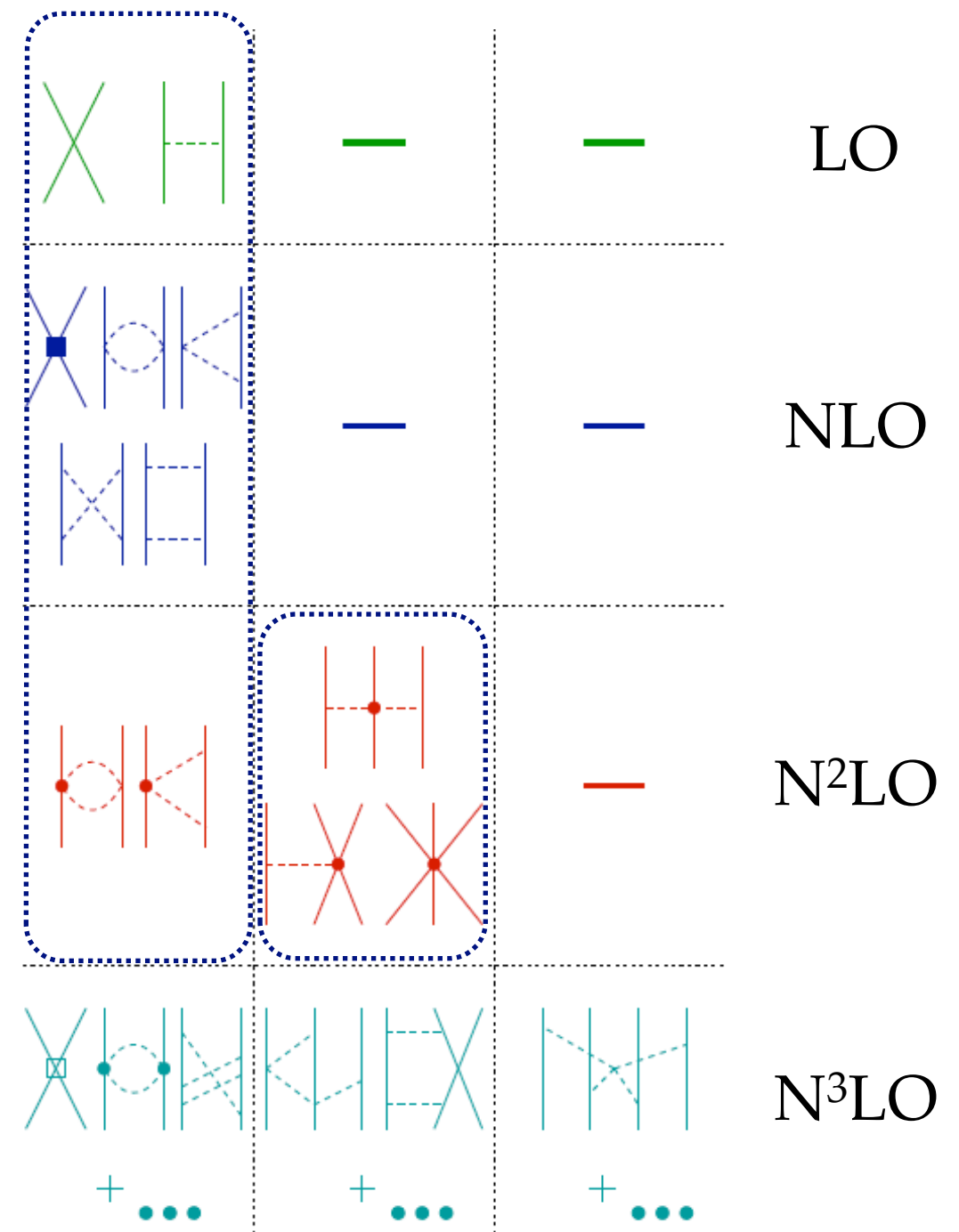
[Ekström *et al.* 2013]

★ $N^\times LO_{\text{opt}}$ 2.0

○ NN+3N (various cutoffs)

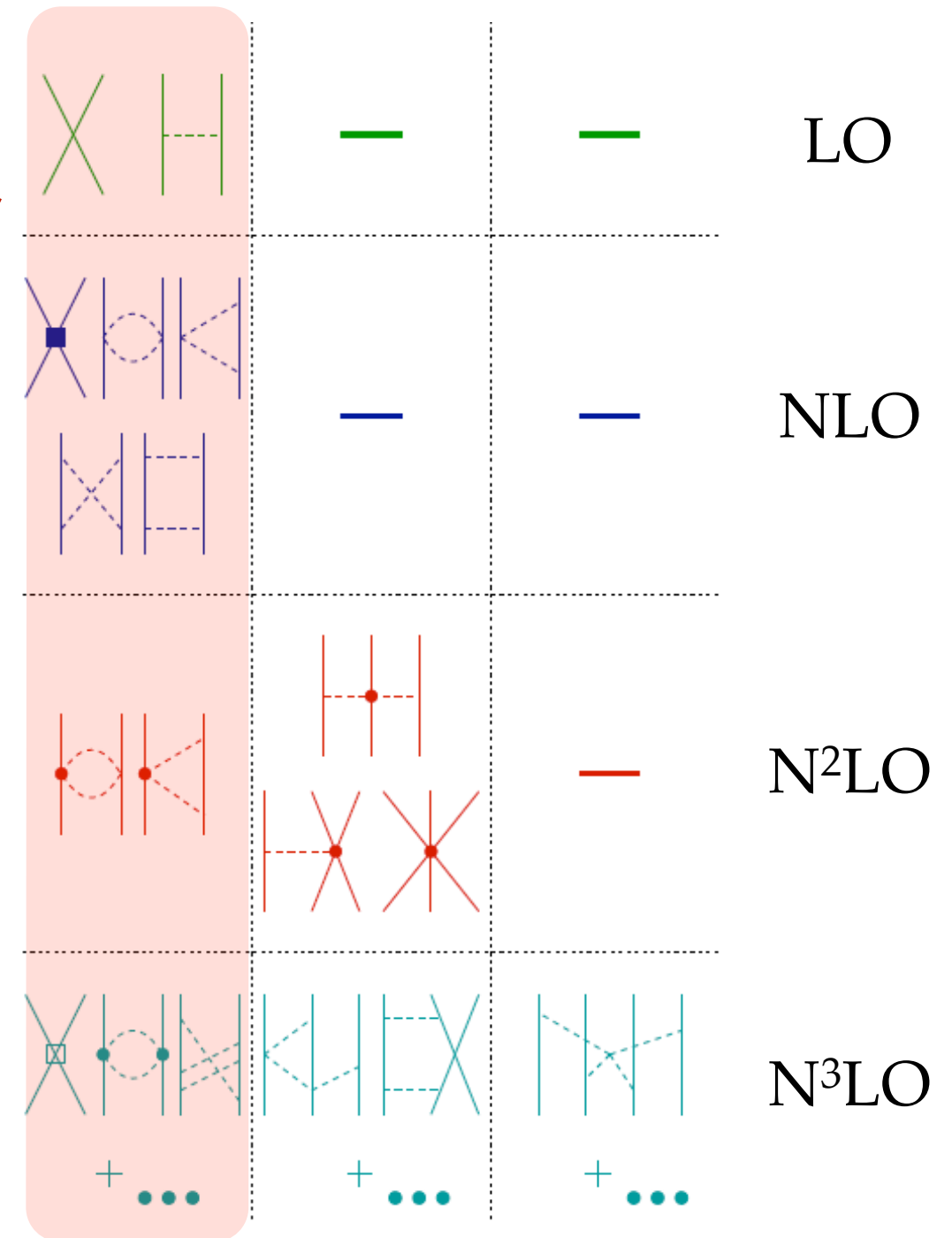
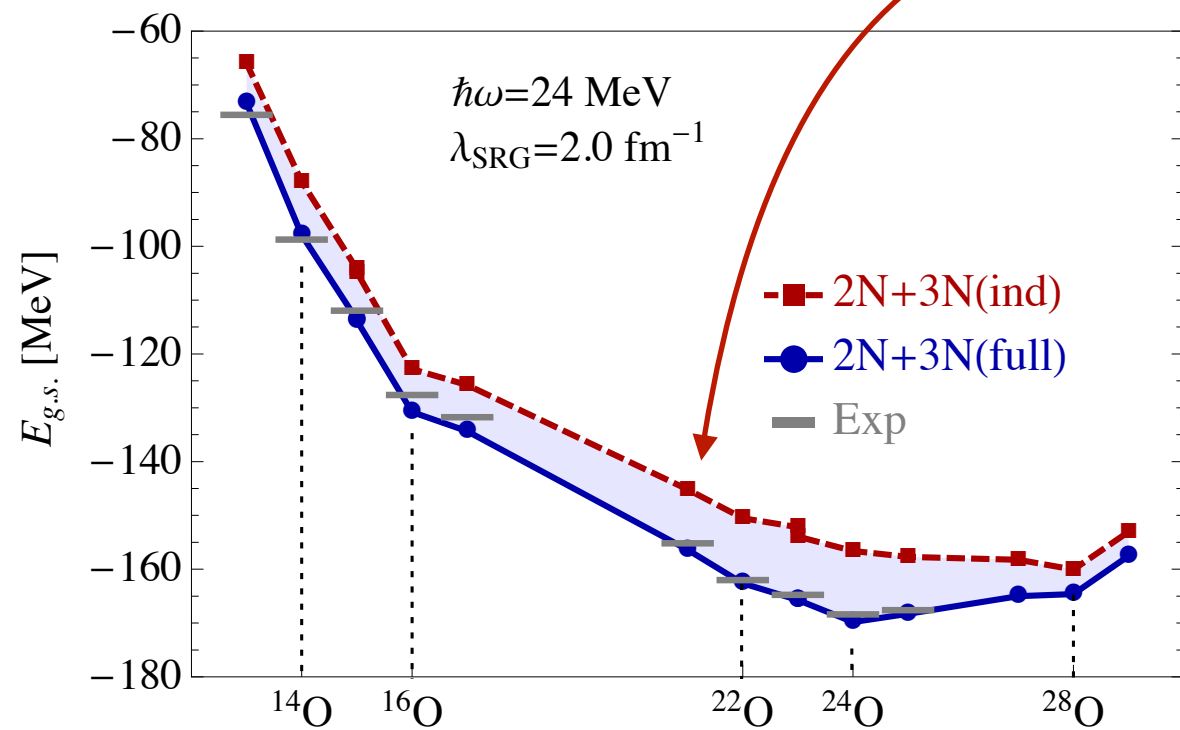
⇒ optimised fit to NN phase shifts
and / or medium-mass nuclei

[Ekström *et al.*, in preparation]



Chiral NN+3N in the oxygen chain

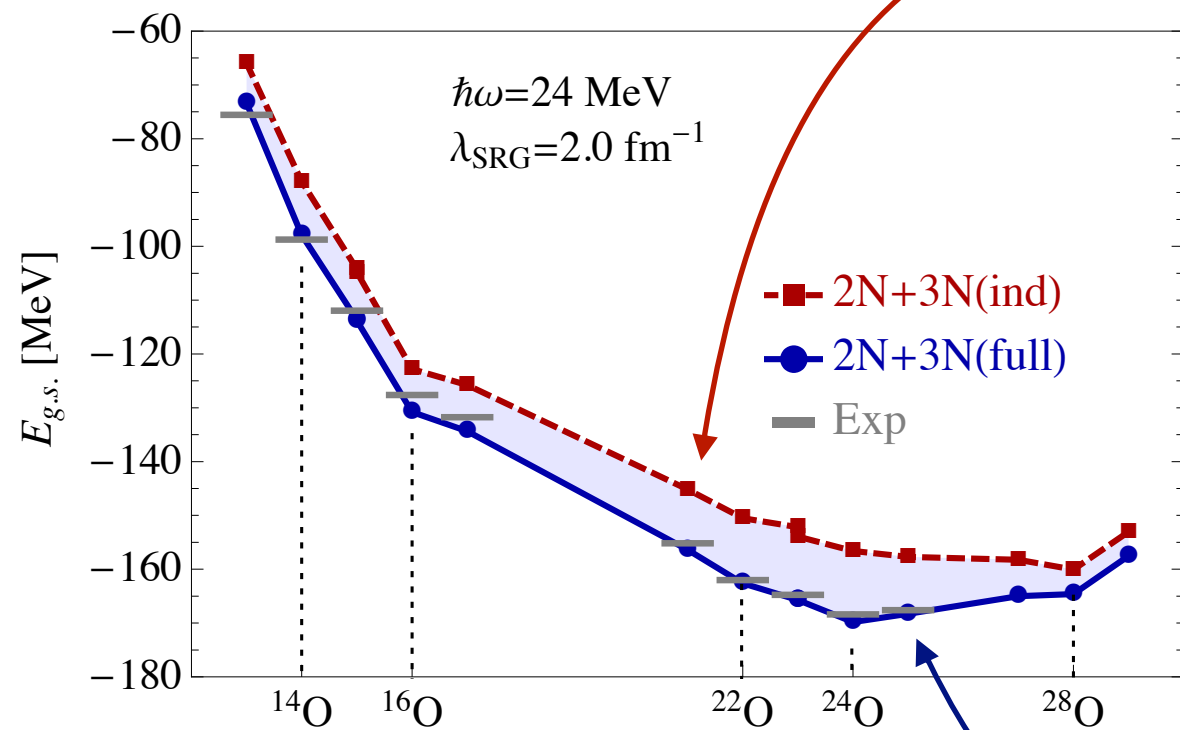
★ Self-consistent Green's functions



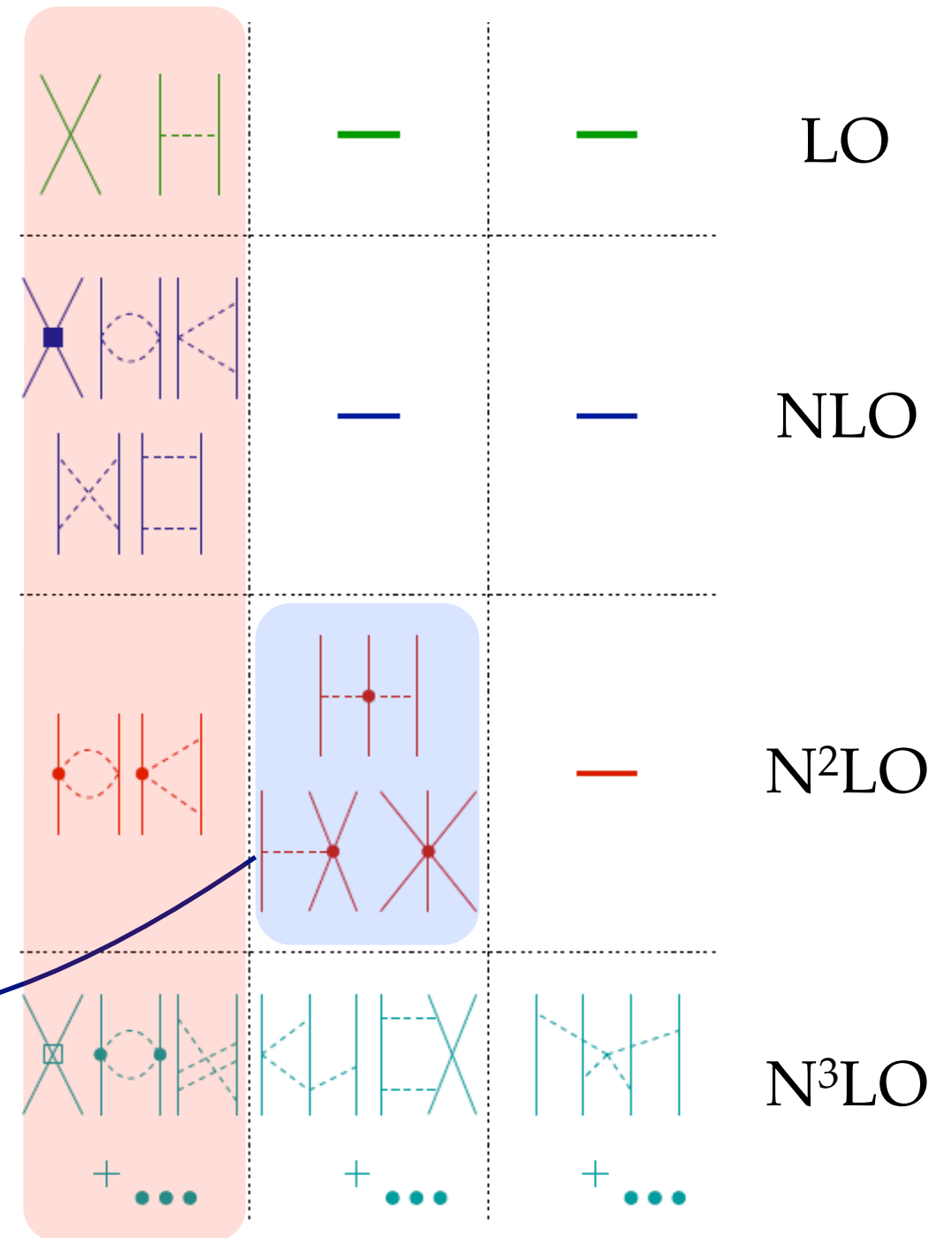
[Cipollone, Barbieri & Navrátil 2013]

Chiral NN+3N in the oxygen chain

★ Self-consistent Green's functions



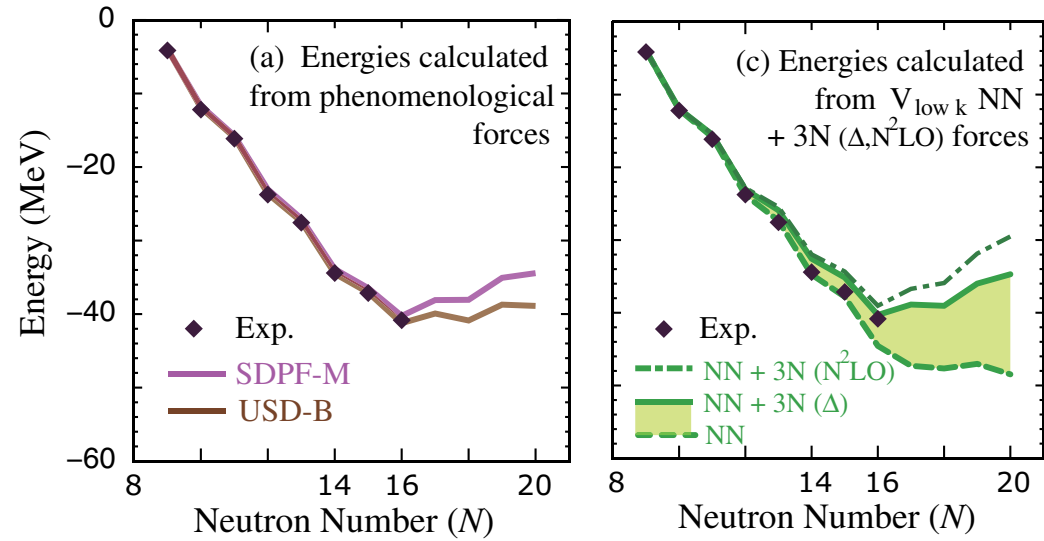
[Cipollone, Barbieri & Navrátil 2013]



- ➡ Overall good agreement with data
- ➡ 3NF crucial for reproducing driplines

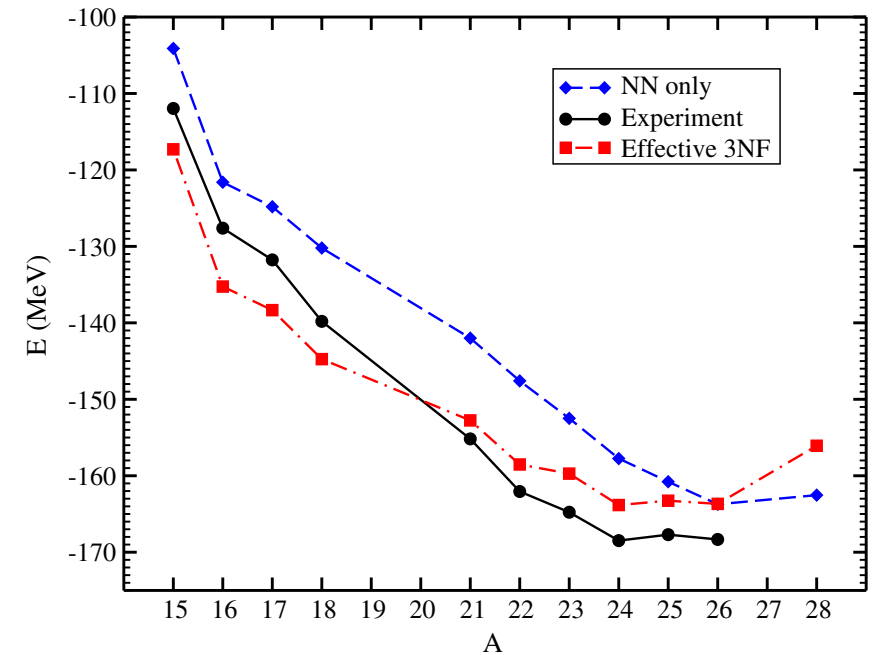
Chiral NN+3N in the oxygen chain

★ Shell Model (NN + 3N)



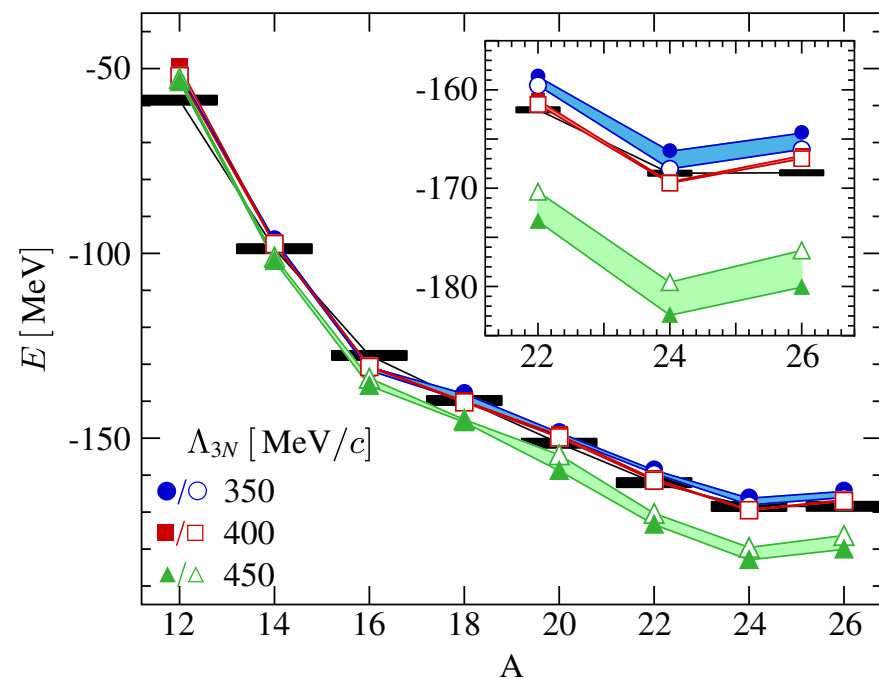
[Otsuka *et al.* 2010]

★ CC (NN + effective 3N)



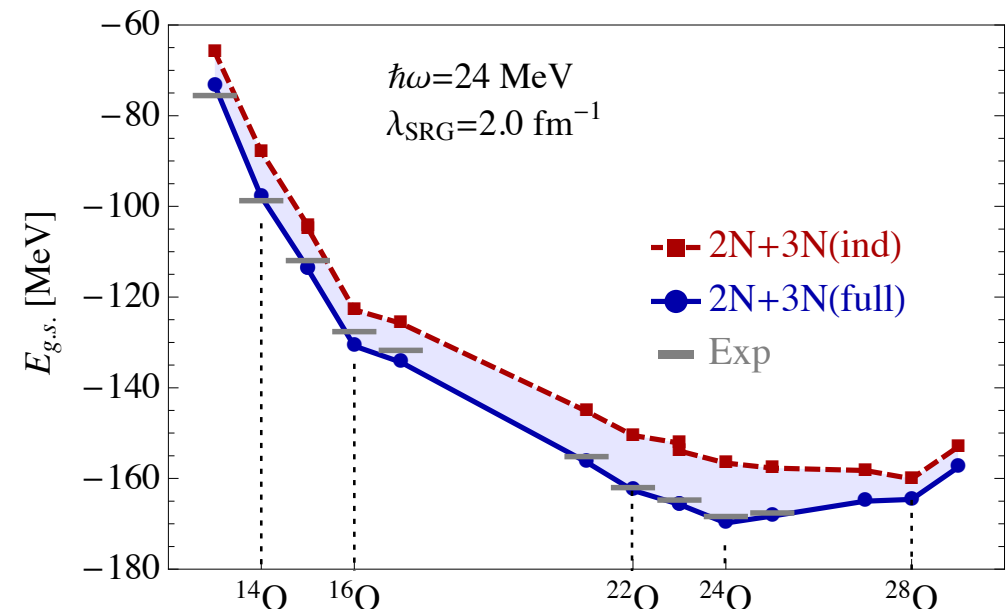
[Hagen *et al.* 2012]

★ IM-SRG (NN + 3N)



[Hergert *et al.* 2013]

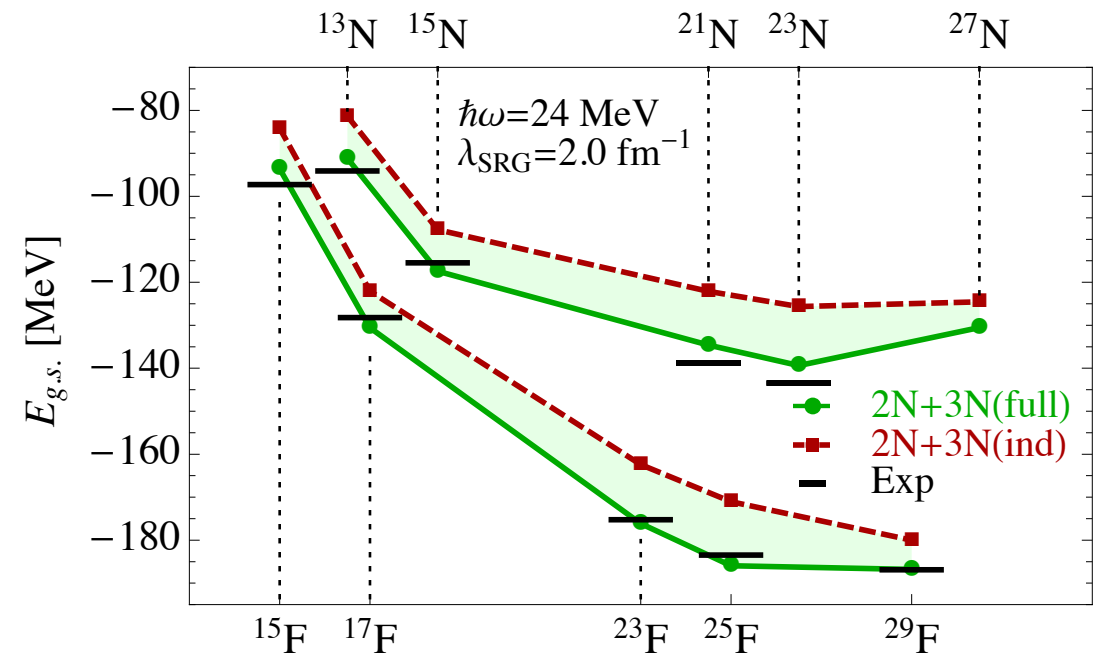
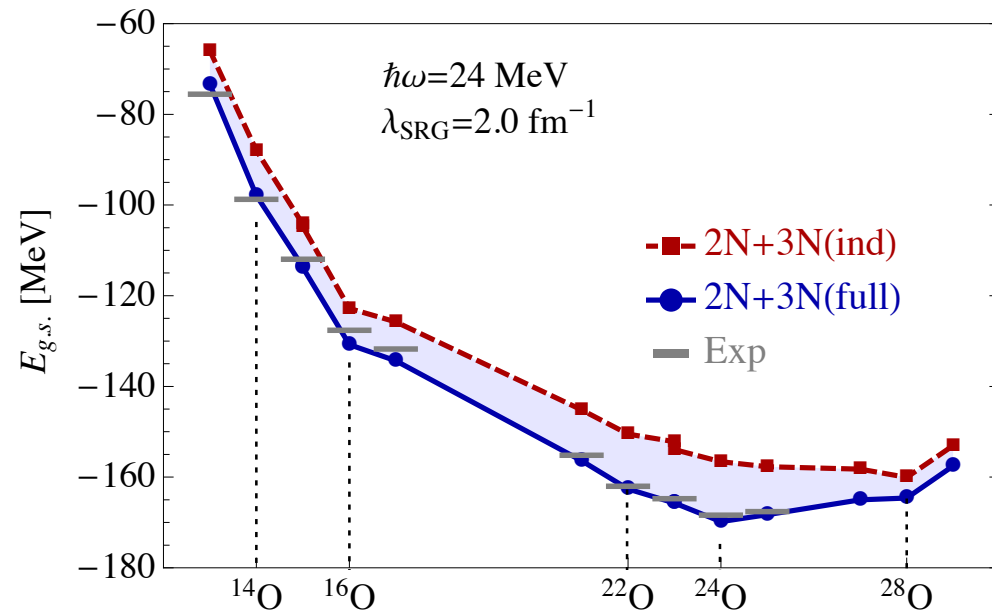
★ SCGF (NN + 3N)



[Cipollone *et al.* 2013]

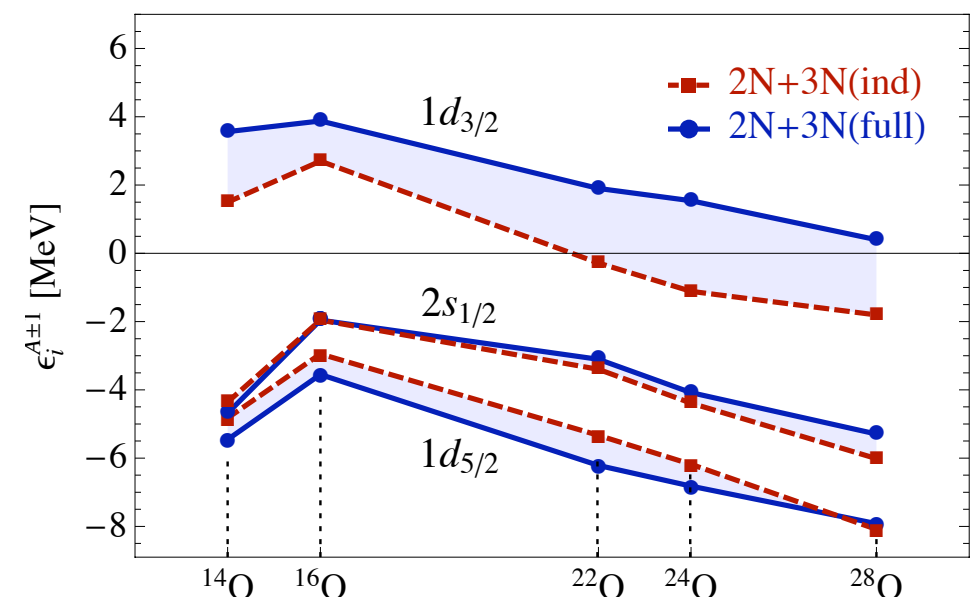
Around oxygen

★ Consistent description of $Z = 7, 8, 9$ isotopic chains with **GF method**

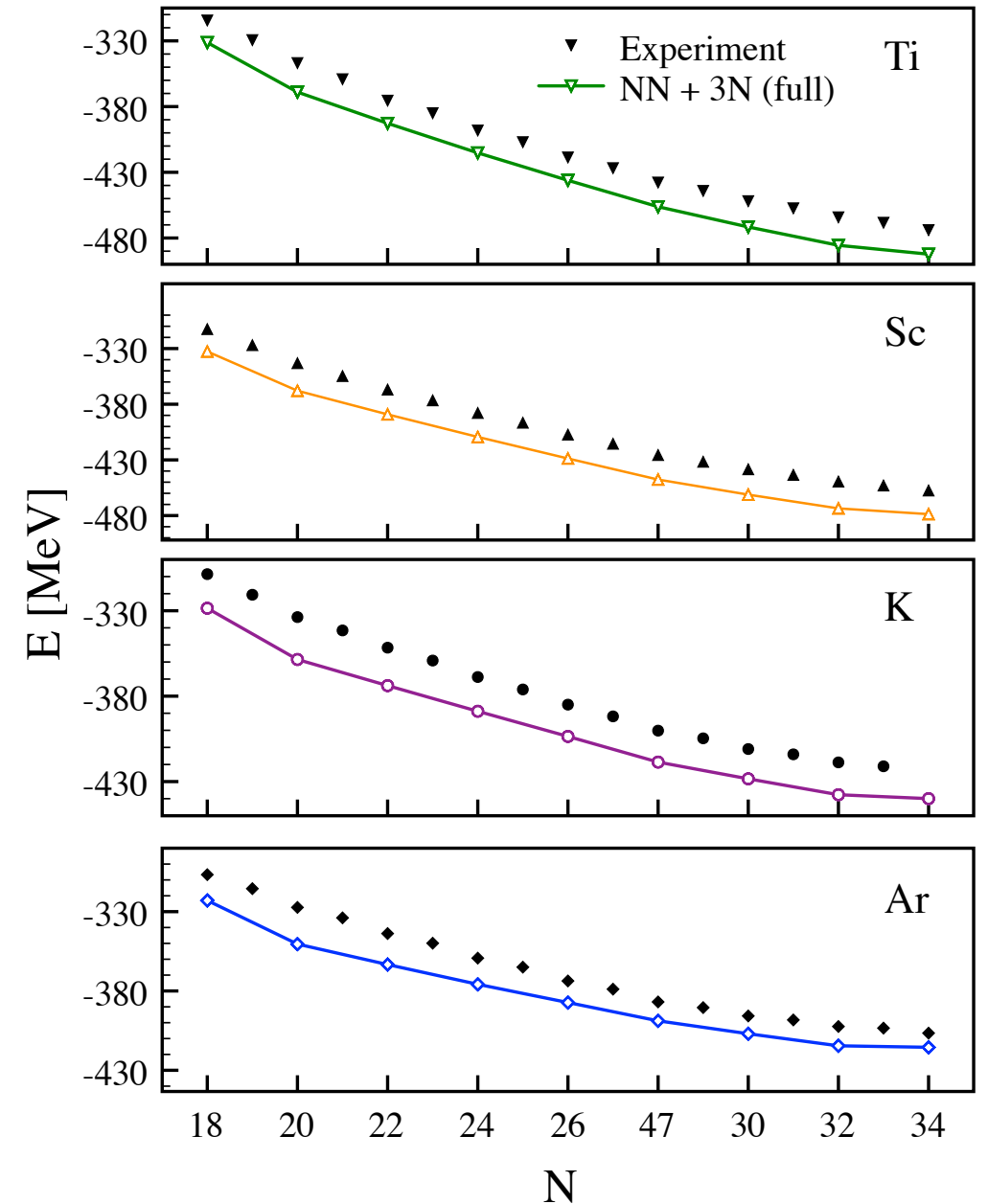
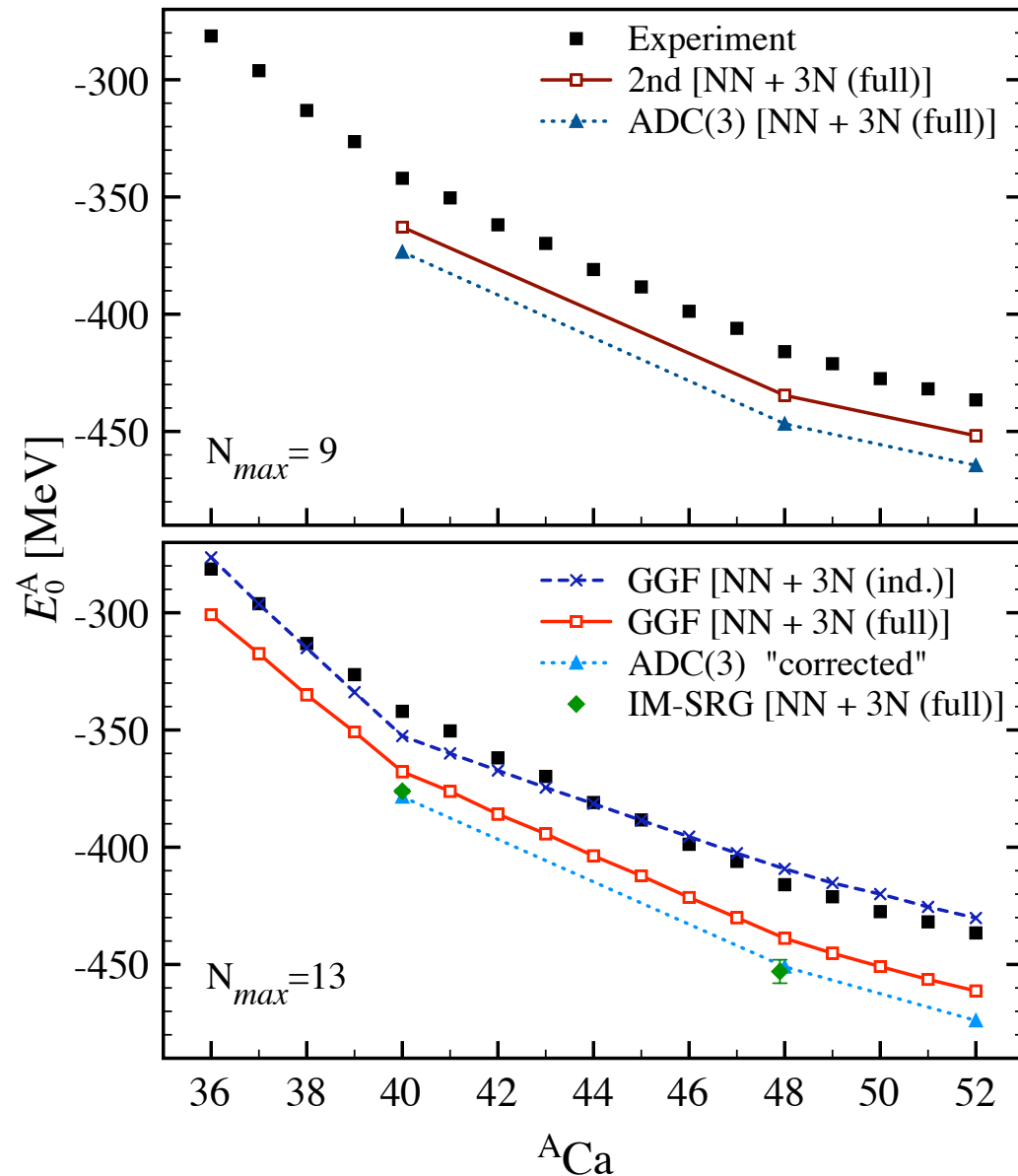


[Cipollone, Barbieri & Navrátil 2013]

- ⇒ Overall good agreement with data
- ⇒ 3NF crucial for reproducing driplines
- ⇒ $d_{3/2}$ raised by genuine 3NF

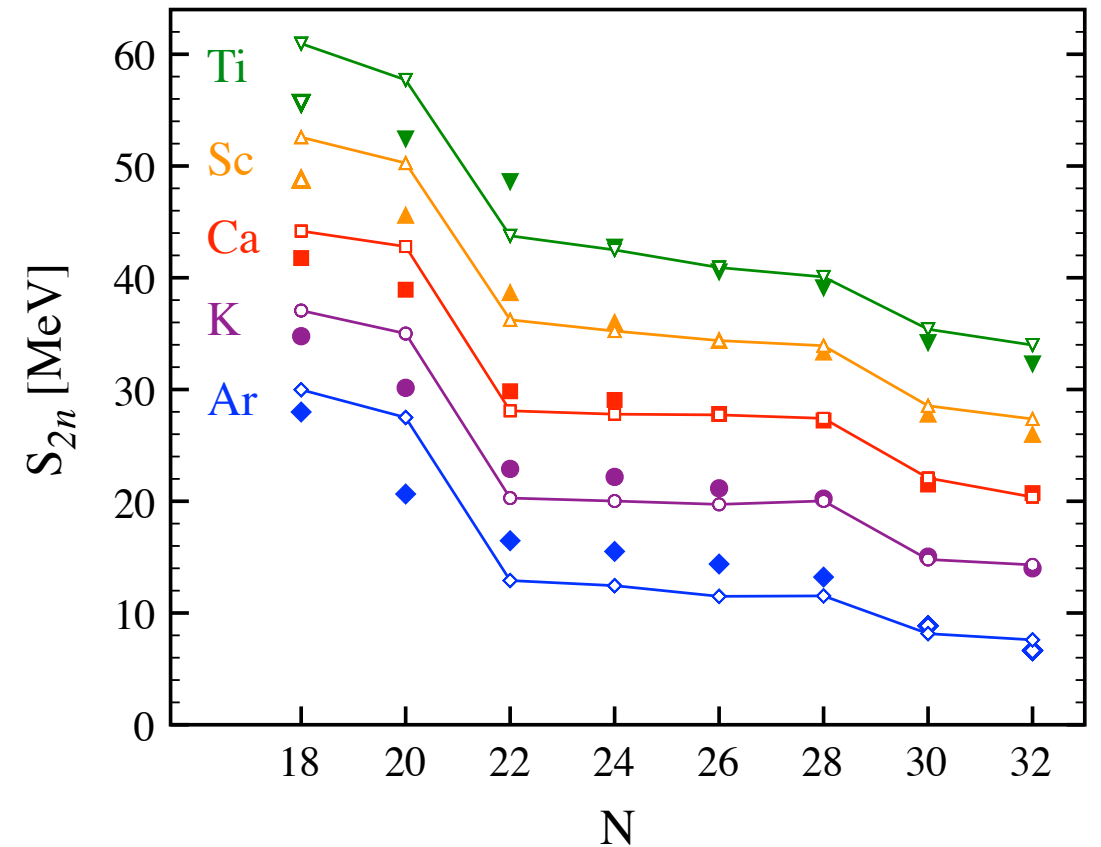
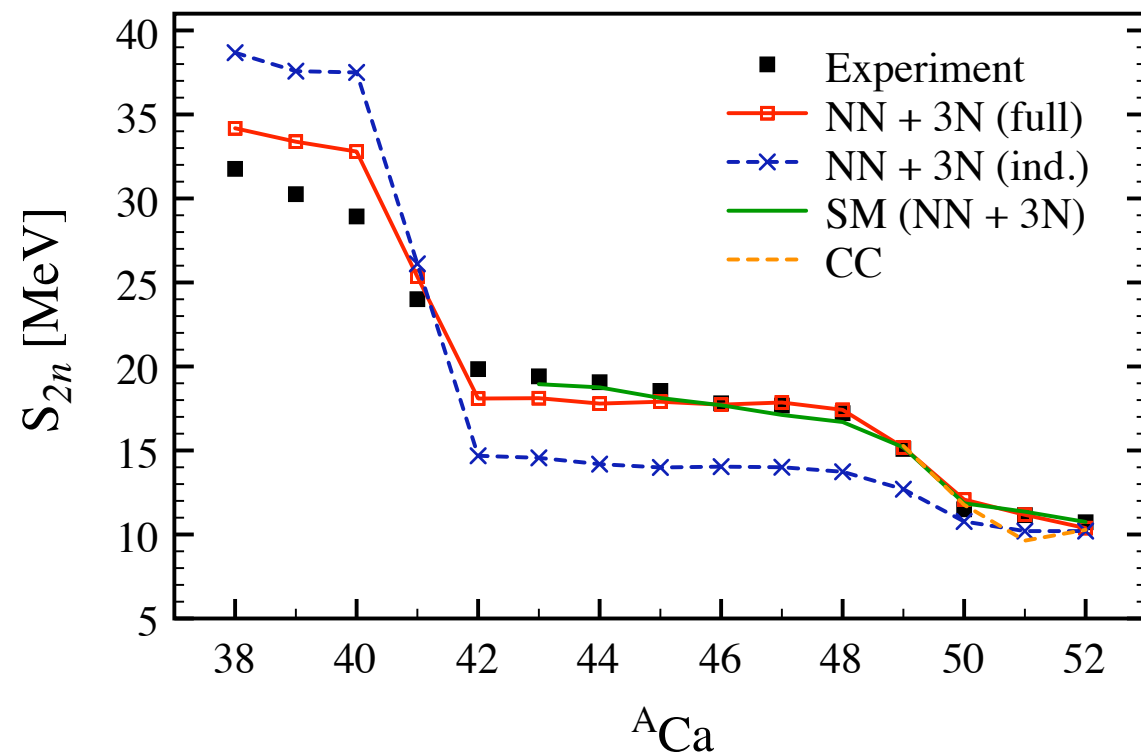


Binding energies around Ca



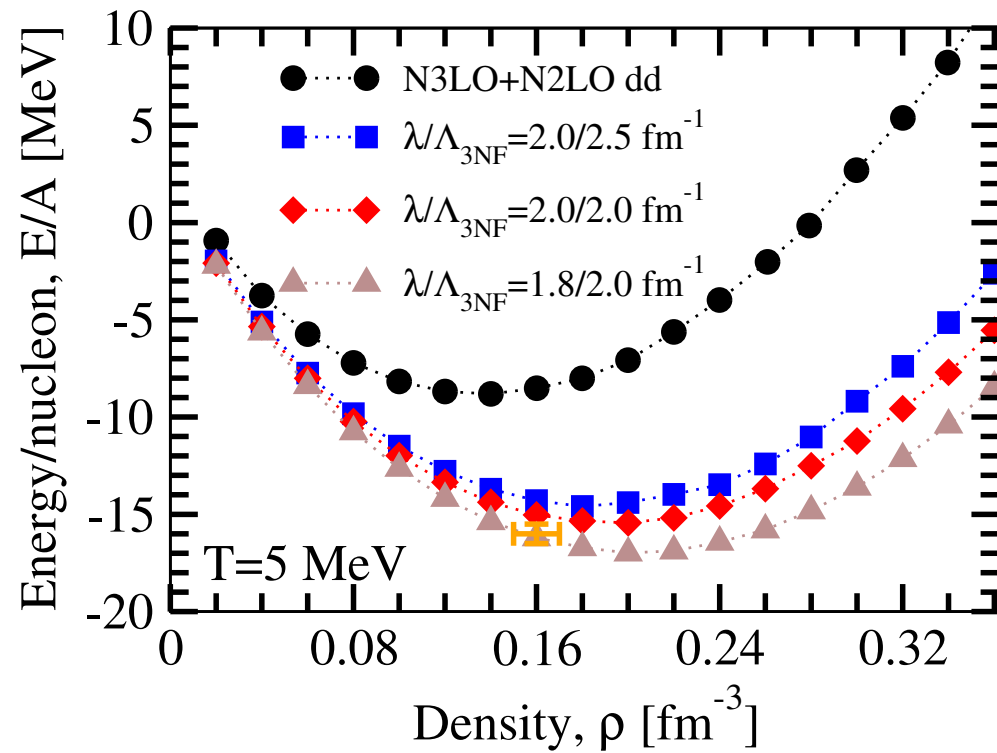
- ⇒ Results confirmed within different many-body approaches
- ⇒ NN + full 3N **correct the trend** of binding energies
- ⇒ Systematic **overbinding** through all chains around $Z=20$

Two-neutron separation energies around Ca

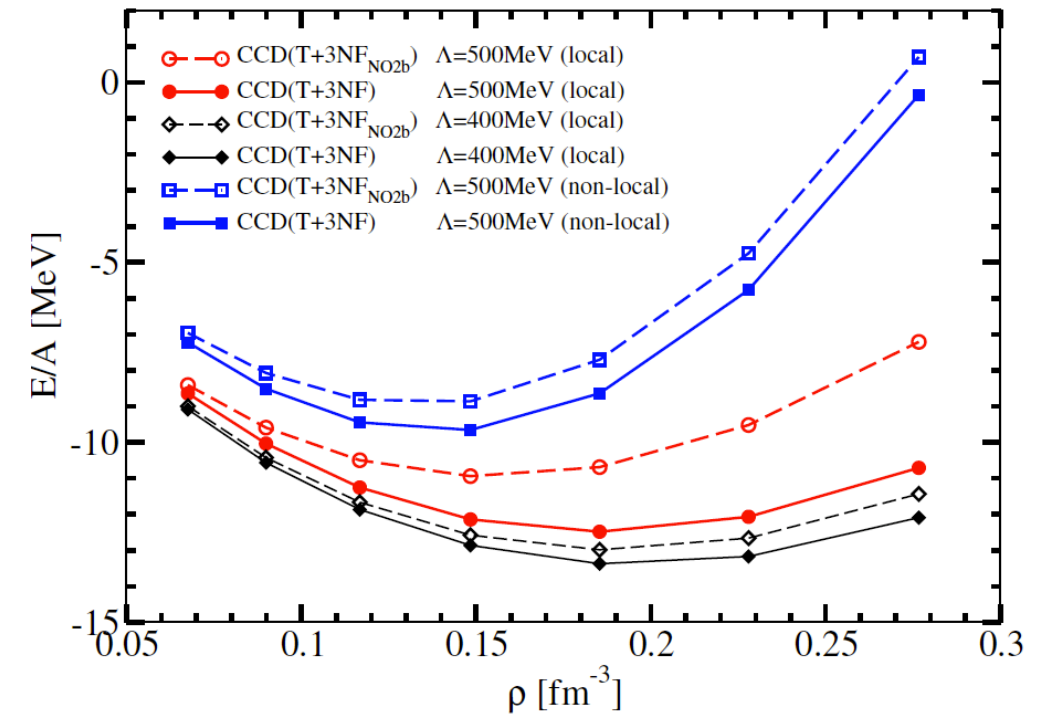


- ⇒ S_{2n} **well reproduced** with chiral NN + 3N interactions
- ⇒ Microscopic calculations extended to the whole Ca chain
- ⇒ Neighbouring **Z=18-22 chains** computed within the **same GGF framework**
- ⇒ Overestimation of N=20 gap traced back to spectrum too spread out

The nuclear matter mess



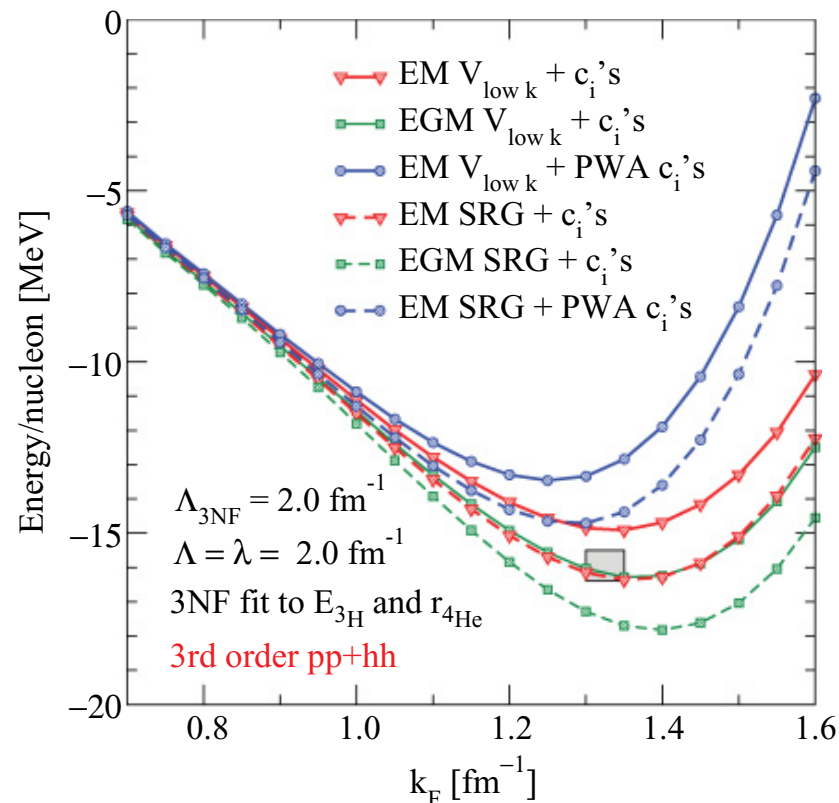
[Carbone *et al.* 2013]



[Hagen *et al.* 2014]

CC, non-perturbative, $\text{N}^2\text{LO}_{\text{opt}}$

SCGF, non-perturbative, EM + dd (500 MeV)



[Hebel *et al.* 2011]

Perturbation theory

The “EFT” approach: status

- EFT

- ▶ power counting

- ▶ inclusion of deltas? [Krebs *et al.*]

- ▶ consistency (N2LO, N3LO...) [Hebeler *et al.*]

- benchmarks of nuclear systems based on **the same** Hamiltonians in different many-body frameworks

- ▶ light nuclei, halo nuclei, medium-mass nuclei and heavy nuclei

- ▶ matter (saturation, symmetry energy, ...)

- fitting procedures of NN+3N forces,

- ▶ few-body systems and/or medium mass nuclei [Ekström *et al.*]

- ▶ ‘overfitting’?

- ▶ choices of regulator functions and cutoff ranges

- experimental signatures for 3NF effects in nuclei

- ▶ observability

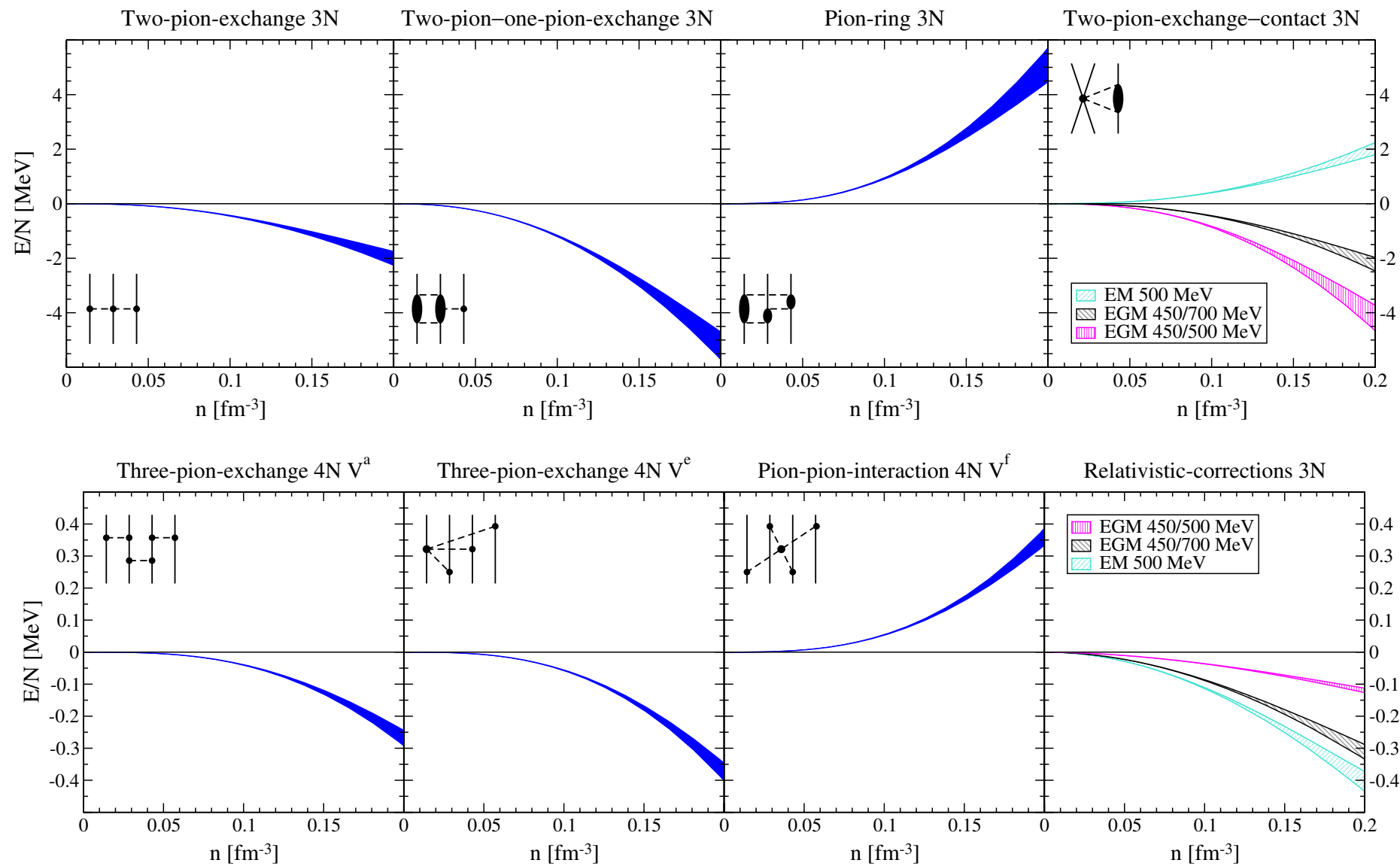
- ▶ scheme/scale dependence

- ▶ role of the Renormalization Group

[From ECT* workshop *Three-body forces from matter to nuclei*, 5-9 May 2014]

Order-by-order convergence

★ Estimated N³LO (HF level) in (infinite) neutron matter



⇒ N³LO 3N contributions **significant**

⇒ N³LO 4N contributions **small**

[Tews *et al.* 2013]

Error estimates in ab initio calculations

★ Long-term goal: **predictive** calculations with quantified **theoretical errors**

★ Possible sources of error:

1) Numerical algorithms

⇒ Usually the smallest source of error

⇒ Comparison within **one method**

2) Model space truncation

⇒ Enters at different stages of the calculation

⇒ Comparison within **one method** + results from other methods

3) Many-body expansion

⇒ Roughly under control, but difficult to assess precisely

⇒ Comparison within **one method & different methods**

4) Hamiltonian

⇒ Currently the hardest to assess in a thorough way

⇒ Comparison within **one method, different methods & data**

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 $A\pm 1$ 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, arXiv:1312.2068 (2013)

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

$$i G_{ab}^{11}(t, t') \equiv \langle \Psi_0 | T \{ a_a(t) a_b^\dagger(t') \} | \Psi_0 \rangle \equiv$$



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



$$i G_{ab}^{12}(t, t') \equiv \langle \Psi_0 | T \{ a_a(t) \bar{a}_b(t') \} | \Psi_0 \rangle \equiv$$



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



Inside the Green's function

★ Separation energy spectrum

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

Lehmann representation

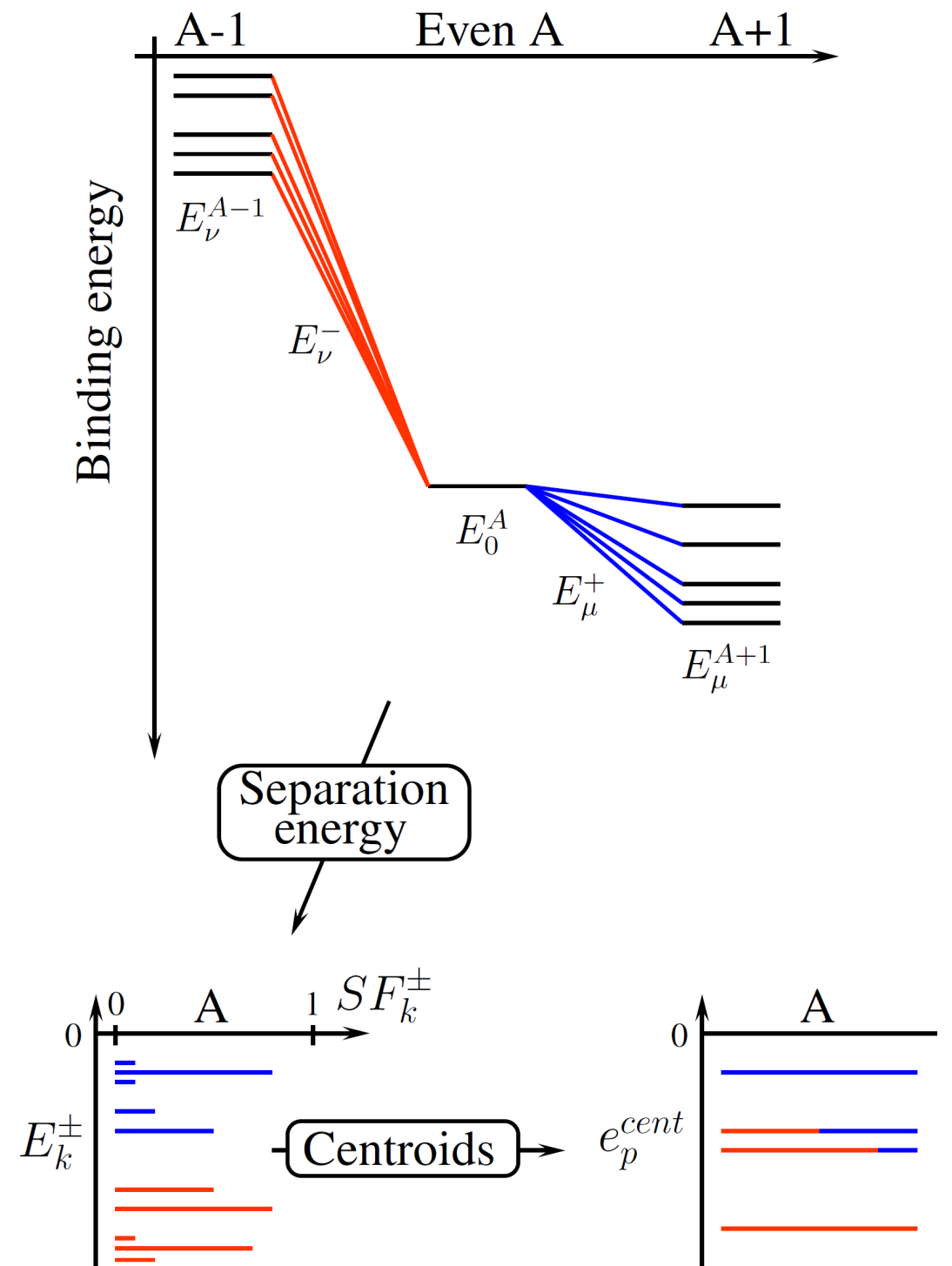
where
$$\begin{cases} \mathcal{U}_a^{k*} \equiv \langle \Psi_k | a_a^\dagger | \Psi_0 \rangle \\ \mathcal{V}_a^{k*} \equiv \langle \Psi_k | \bar{a}_a | \Psi_0 \rangle \end{cases}$$

and
$$\begin{cases} E_k^{+(A)} \equiv E_k^{A+1} - E_0^A \equiv \mu + \omega_k \\ E_k^{-(A)} \equiv E_0^A - E_k^{A-1} \equiv \mu - \omega_k \end{cases}$$

★ Spectroscopic factors

$$SF_k^+ \equiv \sum_{a \in \mathcal{H}_1} |\langle \psi_k | a_a^\dagger | \psi_0 \rangle|^2 = \sum_{a \in \mathcal{H}_1} |\mathcal{U}_a^k|^2$$

$$SF_k^- \equiv \sum_{a \in \mathcal{H}_1} |\langle \psi_k | a_a | \psi_0 \rangle|^2 = \sum_{a \in \mathcal{H}_1} |\mathcal{V}_a^k|^2$$



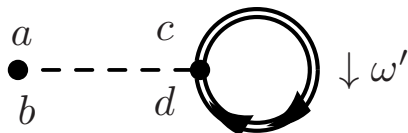
[figure from J. Sadoudi]

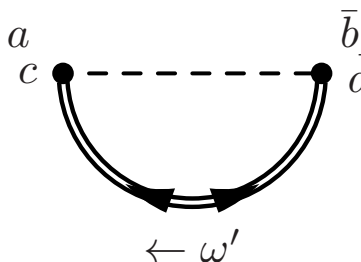
Gorkov equation & self-energy

★ Many-body Schrödinger equation \longrightarrow Dyson/Gorkov equation

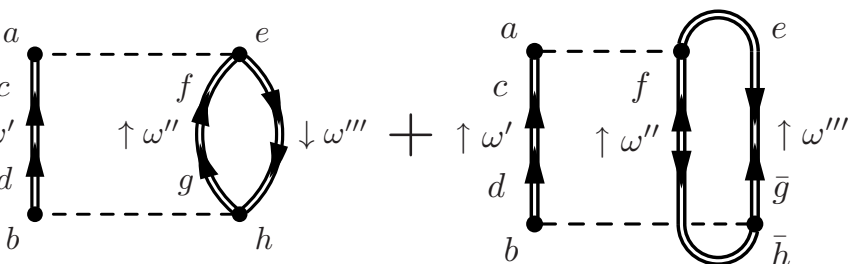
$$\mathbf{G}_{ab}(\omega) = \mathbf{G}_{ab}^{(0)}(\omega) + \sum_{cd} \mathbf{G}_{ac}^{(0)}(\omega) \Sigma_{cd}^*(\omega) \mathbf{G}_{db}(\omega)$$

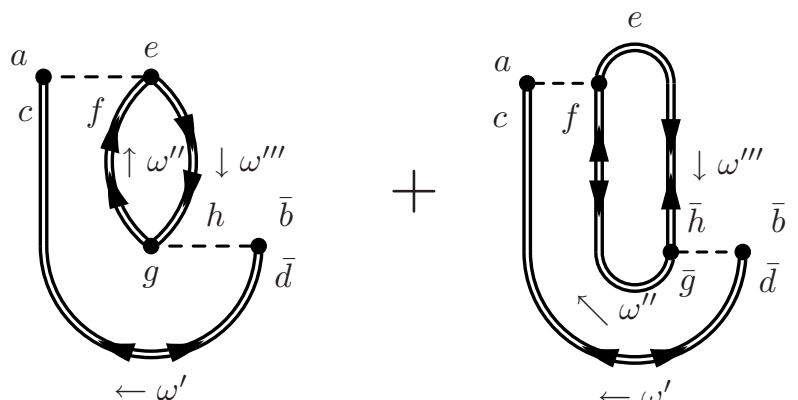
★ 1st order \Rightarrow energy-independent self-energy

$$\Sigma_{ab}^{11(1)} =$$


$$\Sigma_{ab}^{12(1)} =$$


★ 2nd order \Rightarrow energy-dependent self-energy

$$\Sigma_{ab}^{11(2)}(\omega) =$$


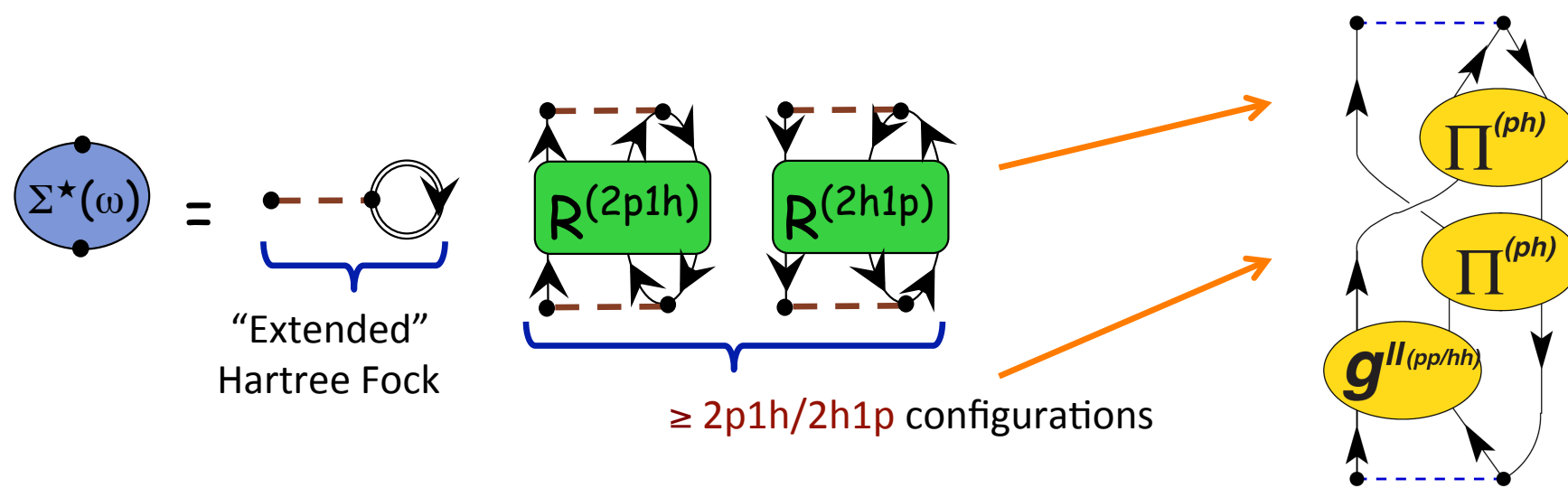
$$\Sigma_{ab}^{12(2)}(\omega) =$$


Gorkov equation & self-energy

★ Many-body Schrödinger equation \longrightarrow Dyson/Gorkov equation

$$\text{Dyson equation diagram: } \text{double line} = \text{single line} + \text{self-energy loop } \Sigma^I$$

★ More advanced formulation for closed-shell nuclei (Dyson GF)



[Barbieri *et al.*]

Green's functions calculations with (consistent) EFT interactions

★ Self-energy expansion has to be revisited

- ⇒ Part of the interaction resummed, part treated perturbatively
- ⇒ Alternative sets of diagrams?

★ RG invariance to be checked for large variations of the cutoff

- ⇒ Thorough assessment of errors from many-body truncation mandatory
- ⇒ Disentangle sources of cutoff dependence

★ Possible first steps and applications

- ⇒ Tests of pionless EFT in systems with $A > 6$
- ⇒ Application of chiral EFT potentials to light and medium-mass nuclei