Pushing the Boundaries of *Ab Initio* Nuclear Structure

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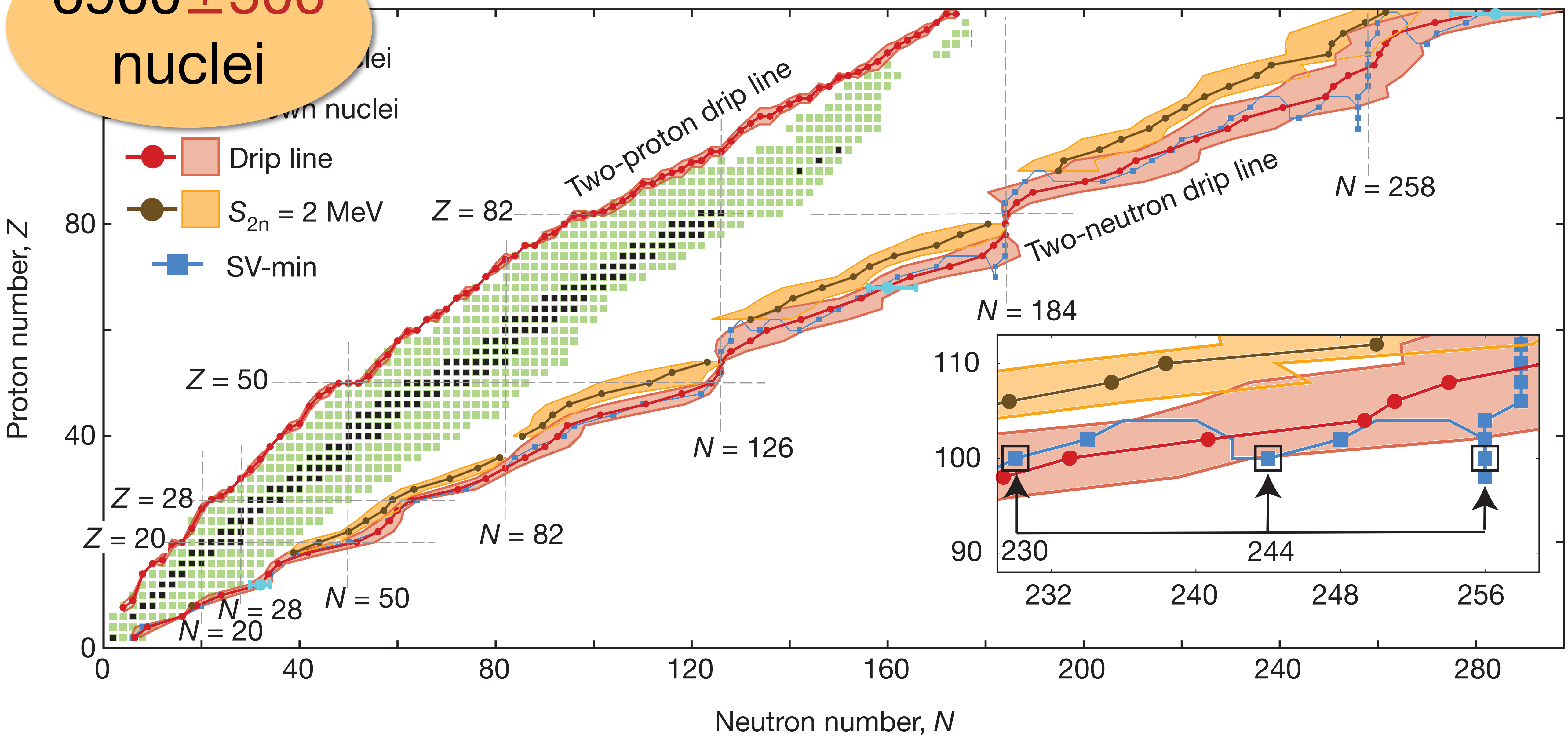
Outline

- Nuclear Interactions from Chiral Effective Field Theory
- Similarity Renormalization Group
- In-Medium SRG
- Results for Finite Nuclei
- Outlook

Why Ab Initio Nuclear Structure?

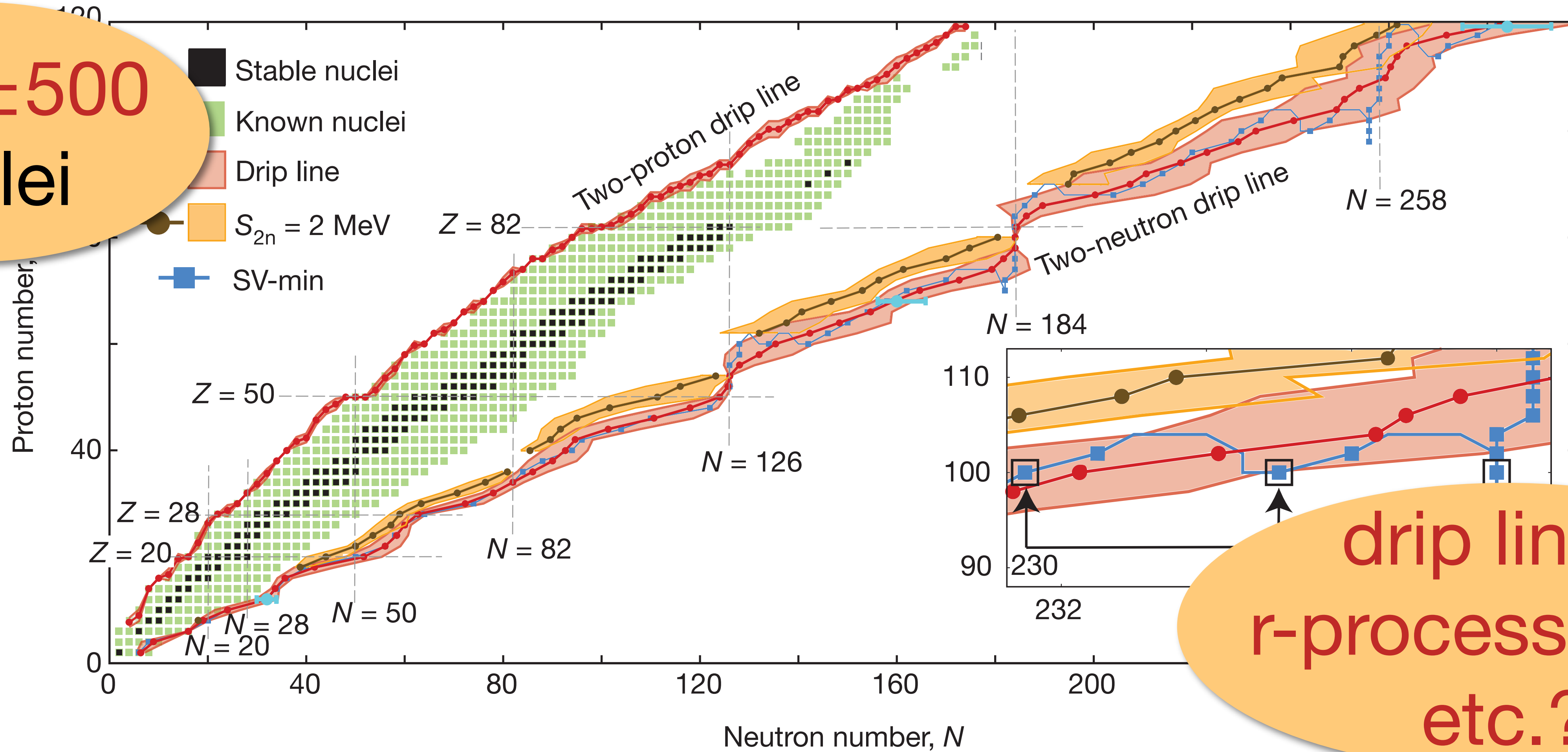
6900±500
nuclei



[from J. Erler et al., Nature 486, 509 (2012)]

Why Ab Initio Nuclear Structure?

6900±500 nuclei

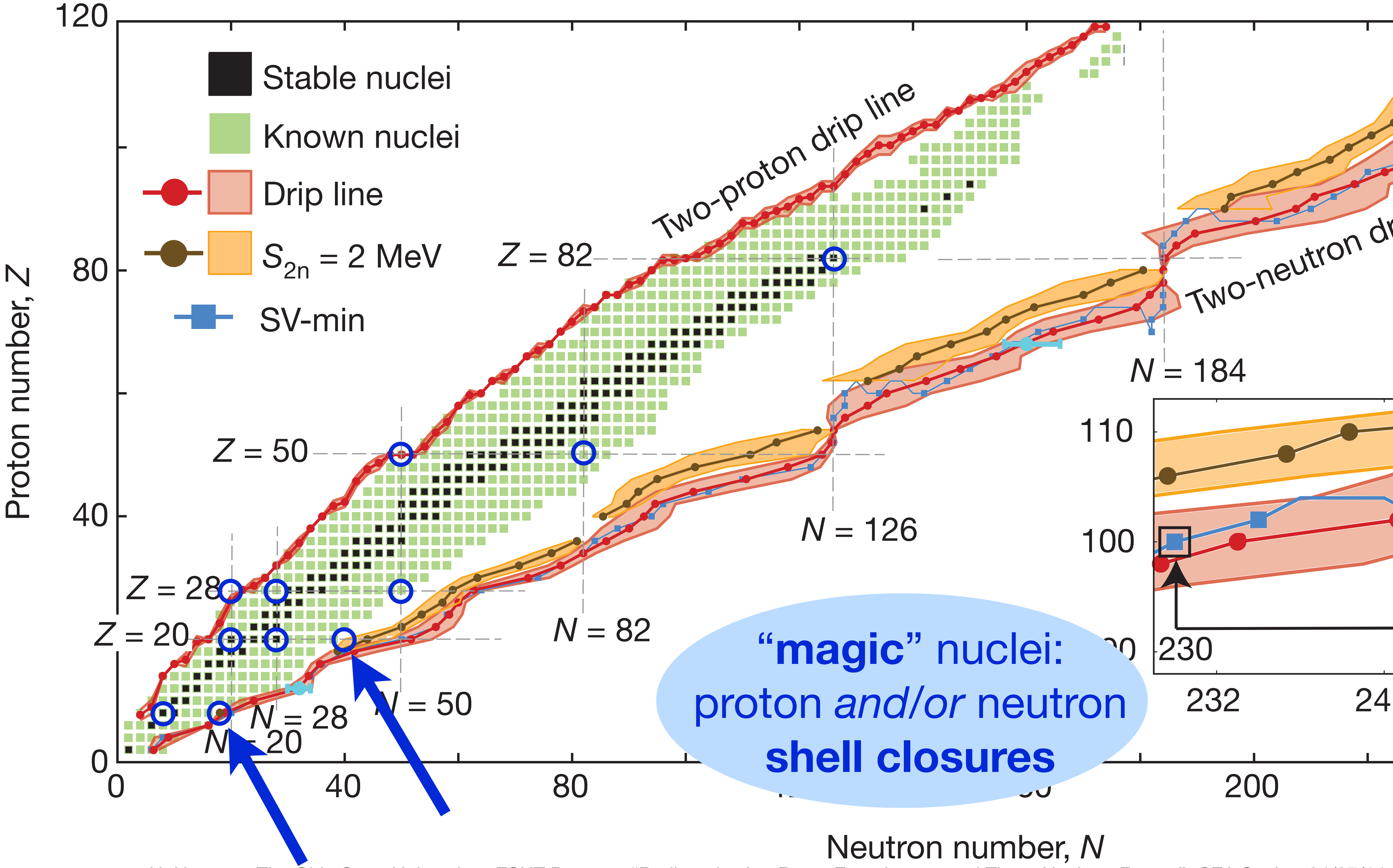


[from J. Erler et al., Nature 4

drip lines, r-process path, etc.?

- phenomenological Energy Density Functionals
  - Skyrme (~100 parameterizations), Gogny, ...
  - fit to binding energies, radii, close to valley of stability
  - uncertainty increases for exotic nuclei, spectroscopic observables

Why Ab Initio Nuclear Structure?



“magic” nuclei: proton *and/or* neutron **shell closures**

Why Ab Initio Nuclear Structure?

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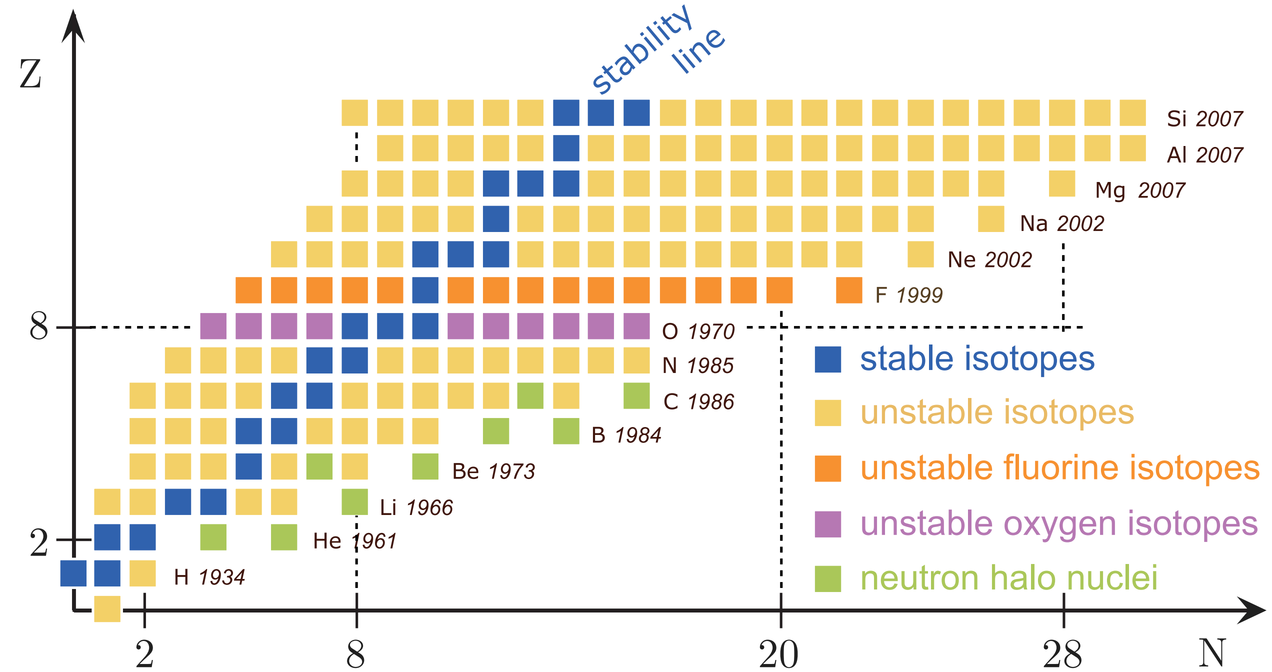
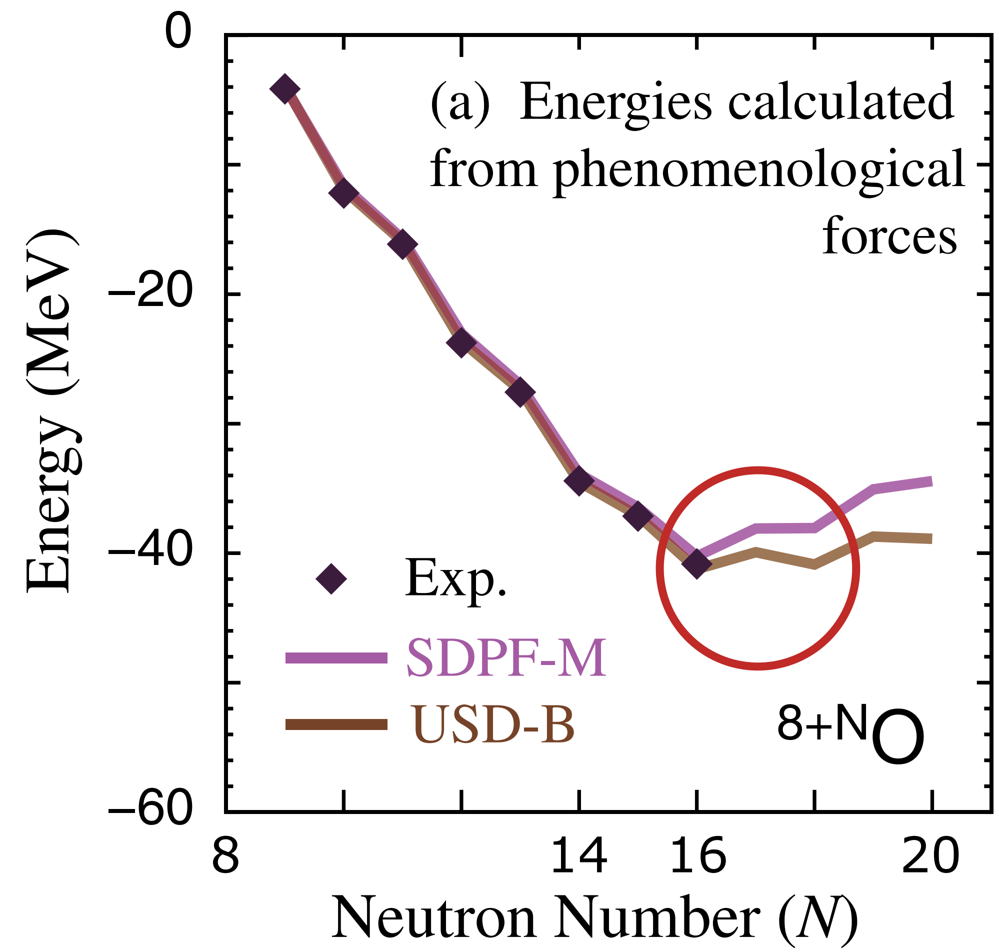
- **Interacting Shell Model**: oxygen drip line depends on interaction
- phenomen. interactions not interchangeable between many-body methods

- systematic improvements ?
- theoretical uncertainties ?
- systematic link to QCD ?





[T. Otsuka et al., Phys. Rev. Lett. 105, 032501 (2010)]

Nuclear Interactions from Chiral Effective Field Theory

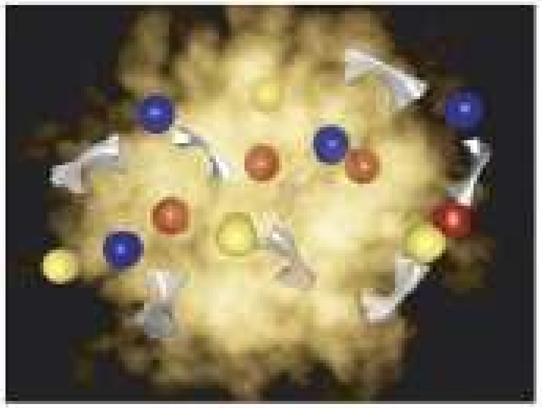
E. Epelbaum, H.-W. Hammer, and U.-G. Meissner, Rev. Mod. Phys. **81** (2009), 1773

Scales of the Strong Interaction

momentum transfer (resolution)

QCD

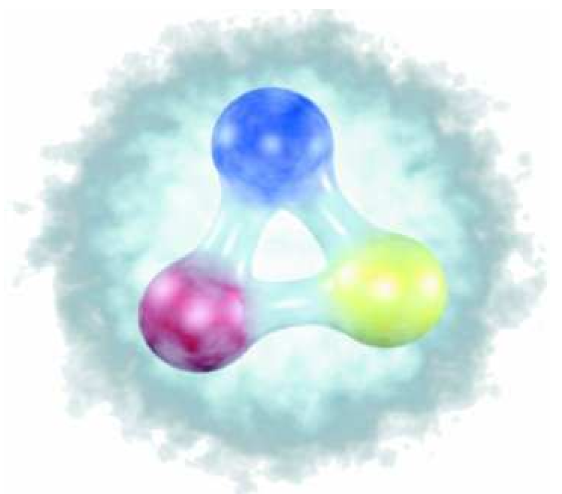
Chiral EFT

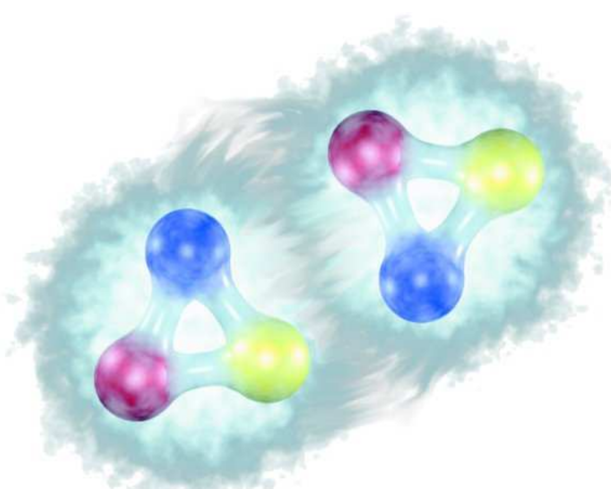


quarks, gluons

chiral phase transition

(de)confinement phase transition





Weinberg's 3rd Law of Progress in Theoretical Physics:

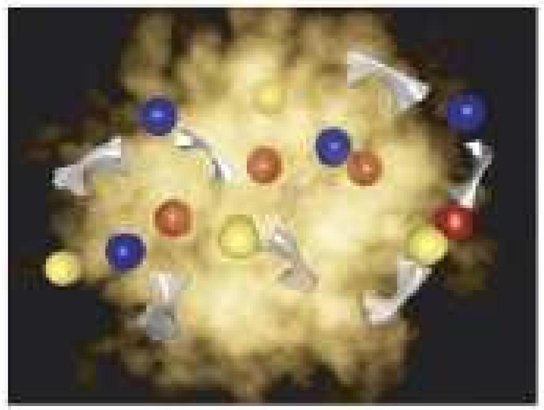
"You may use any degrees of freedom you like to describe a physical system, but if you use the wrong ones, you'll be sorry!"

Scales of the Strong Interaction

momentum transfer (resolution)

QCD

Chiral EFT



quarks, gluons

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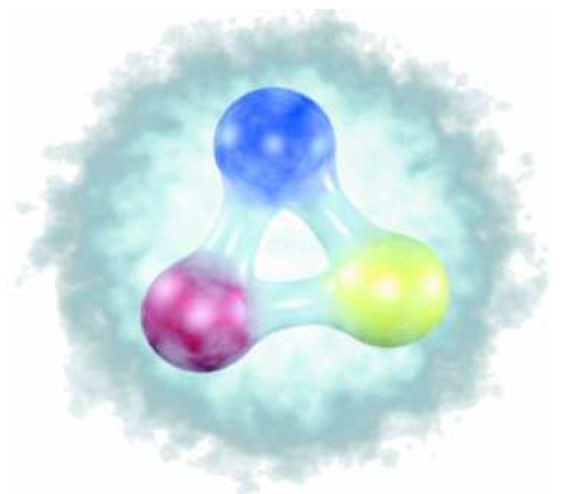
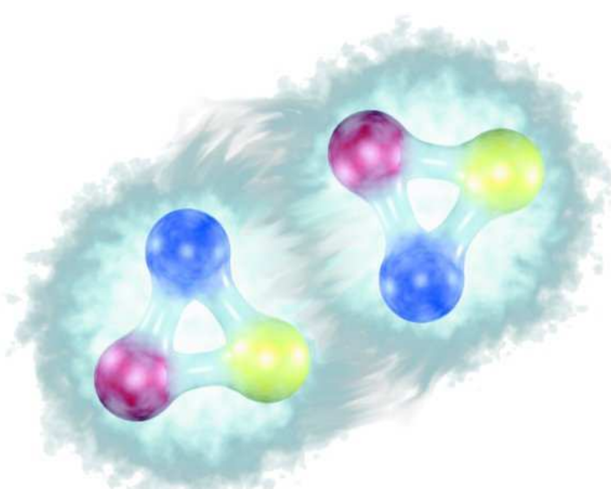


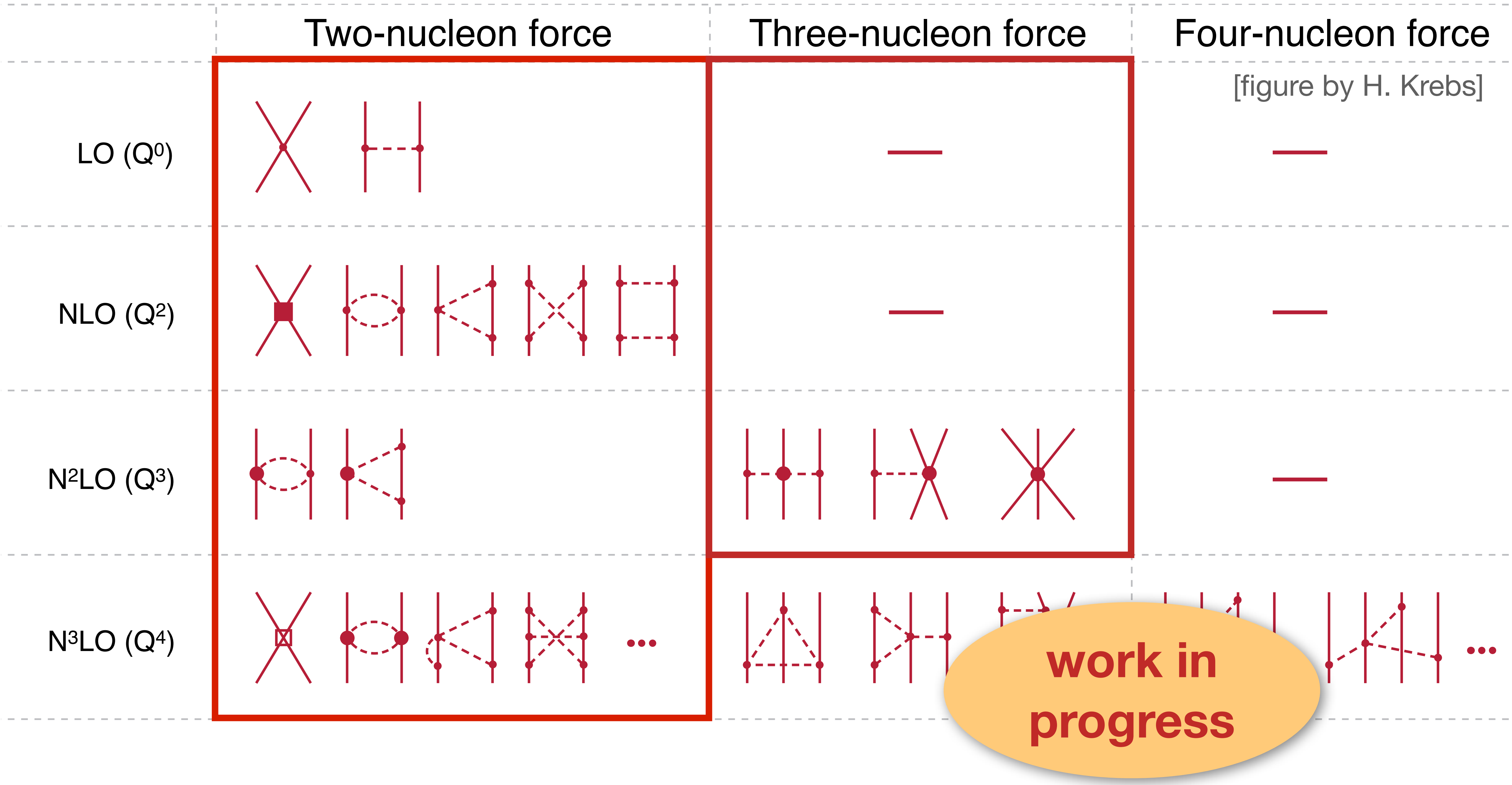
pions (π), nucleons (N), ...



chiral symmetry

spontaneously broken,
π is Goldstone boson

Interactions from Chiral EFT



- organization in powers $(Q/\Lambda_\chi)^\nu$ allows systematic improvement
- consistent NN, 3N, ... interactions & operators (electromagnetic & weak transitions, etc.)

Similarity Renormalization Group

Review:

S. Bogner, R. Furnstahl, and A. Schwenk, Prog. Part. Nucl. Phys. **65** (2010), 94

E. Anderson, S. Bogner, R. Furnstahl, and R. Perry, Phys. Rev. **C82** (2011), 054001

E. Jurgenson, P. Navratil, and R. Furnstahl, Phys. Rev. **C83** (2011), 034301

R. Roth, S. Reinhardt, and H. H., Phys. Rev. **C77** (2008), 064003

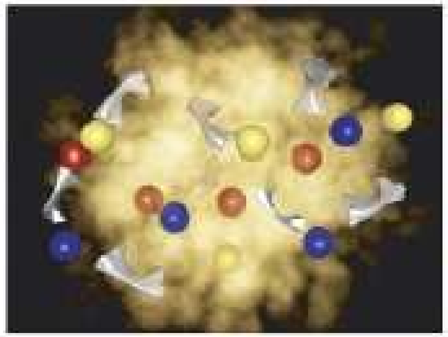
H. H. and R. Roth, Phys. Rev. **C75** (2007), 051001

Scales of the Strong Interaction

momentum transfer (resolution)

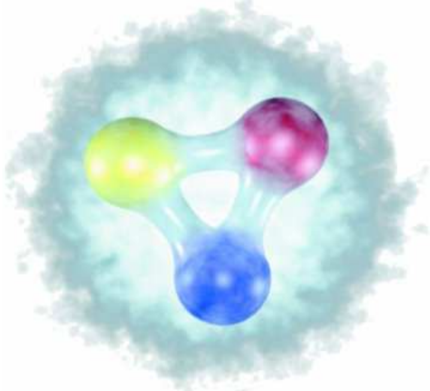
QCD

Chiral EFT

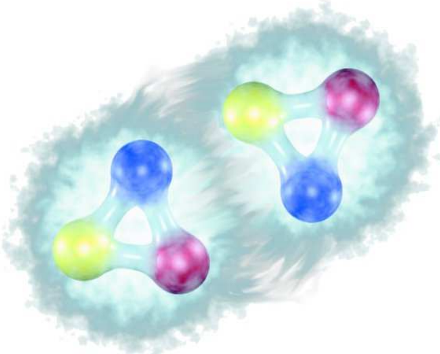


- quarks, gluons

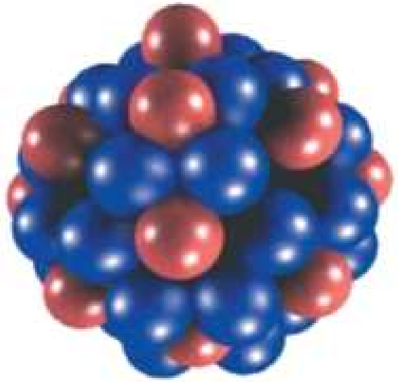
chiral symmetry



- pions, nucleons, ...
  - nuclear interactions
  - few-nucleon systems



(Which) Details necessary?



- finite nuclei
  - nuclear structure & reactions

Similarity Renormalization Group

Basic Concept

continuous unitary transformation of the Hamiltonian to band-diagonal form w.r.t. a given "uncorrelated" many-body basis

- evolved Hamiltonian

$$H(s) = U(s) H U^{\dagger}(s) \equiv T + V(s)$$

- flow equation:

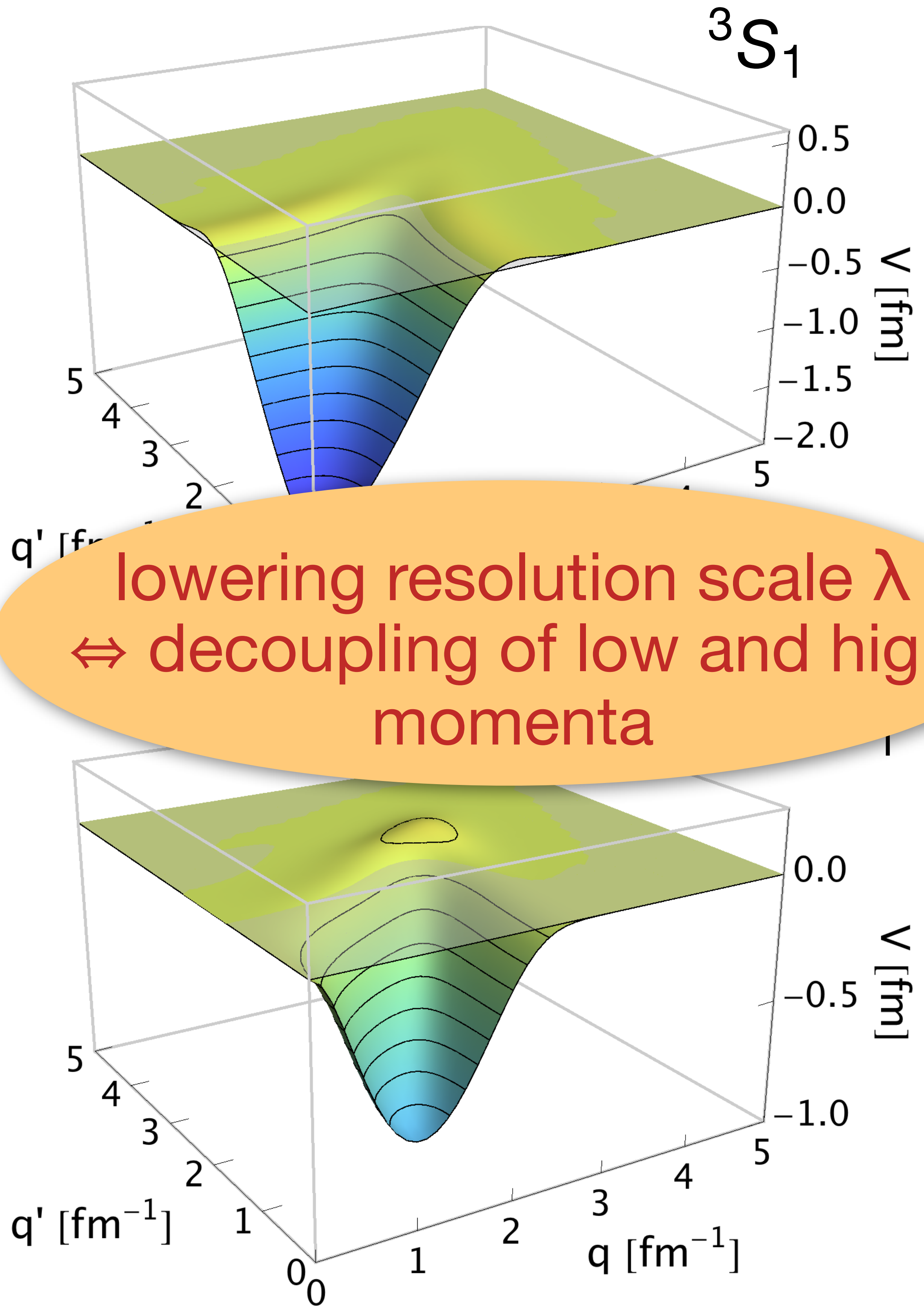
$$\frac{d}{ds} H(s) = \left[\eta(s), H(s)\right] , \quad \eta(s) = \frac{dU(s)}{ds} U^{\dagger}(s) = -\eta^{\dagger}(s)$$

- choose $\eta(s)$ to achieve desired behavior, e.g. decoupling of momentum or energy scales

- consistently evolve observables of interest

SRG in Two-Body Space

momentum space matrix elements



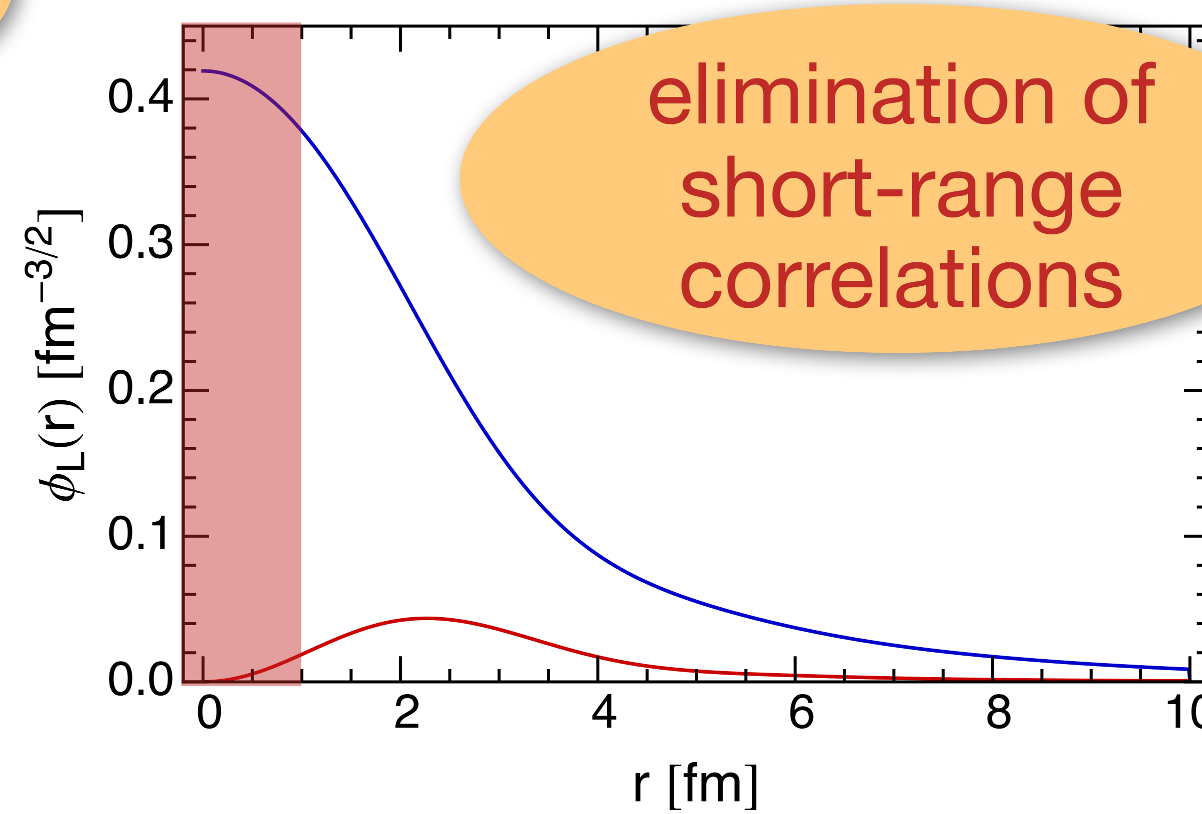
lowering resolution scale λ
⇔ decoupling of low and high momenta

$\lambda = 1.8\ \mathrm{fm}^{-1}$

$$\eta(\lambda) = 2\mu\left[T_{\mathrm{rel}}, H(\lambda)\right]$$

$$\lambda = s^{-1/4}$$

deuteron wave function



elimination of short-range correlations

Induced Interactions

- SRG is a unitary transformation in A-body space
- up to A-body interactions are induced during the flow:

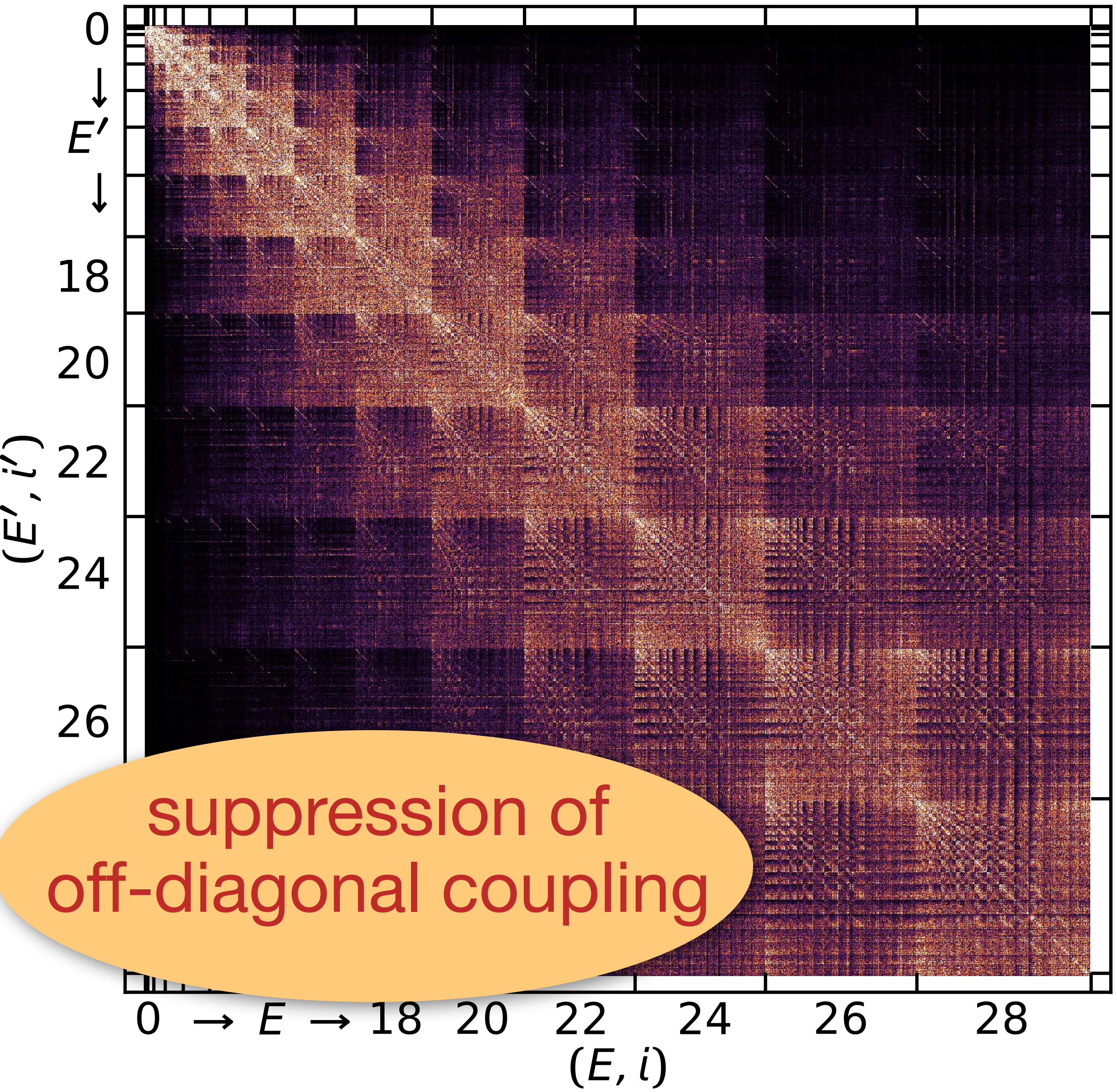
$$\frac{dH}{d\lambda} = [[\sum a^\dagger a, \sum \underbrace{a^\dagger a^\dagger aa}_{\text{2-body}}], \sum \underbrace{a^\dagger a^\dagger aa}_{\text{2-body}}] = \ldots + \sum \underbrace{a^\dagger a^\dagger a^\dagger aaa}_{\text{3-body}} + \ldots$$

- state-of-the-art: evolve in three-body space, truncate induced four- and higher many-body forces
(Jurgenson, Furnstahl, Navratil, PRL 103, 082501; Hebeler, PRC 85, 021002)
- λ-dependence of eigenvalues is a diagnostic for size of omitted induced interactions

SRG in Three-Body Space

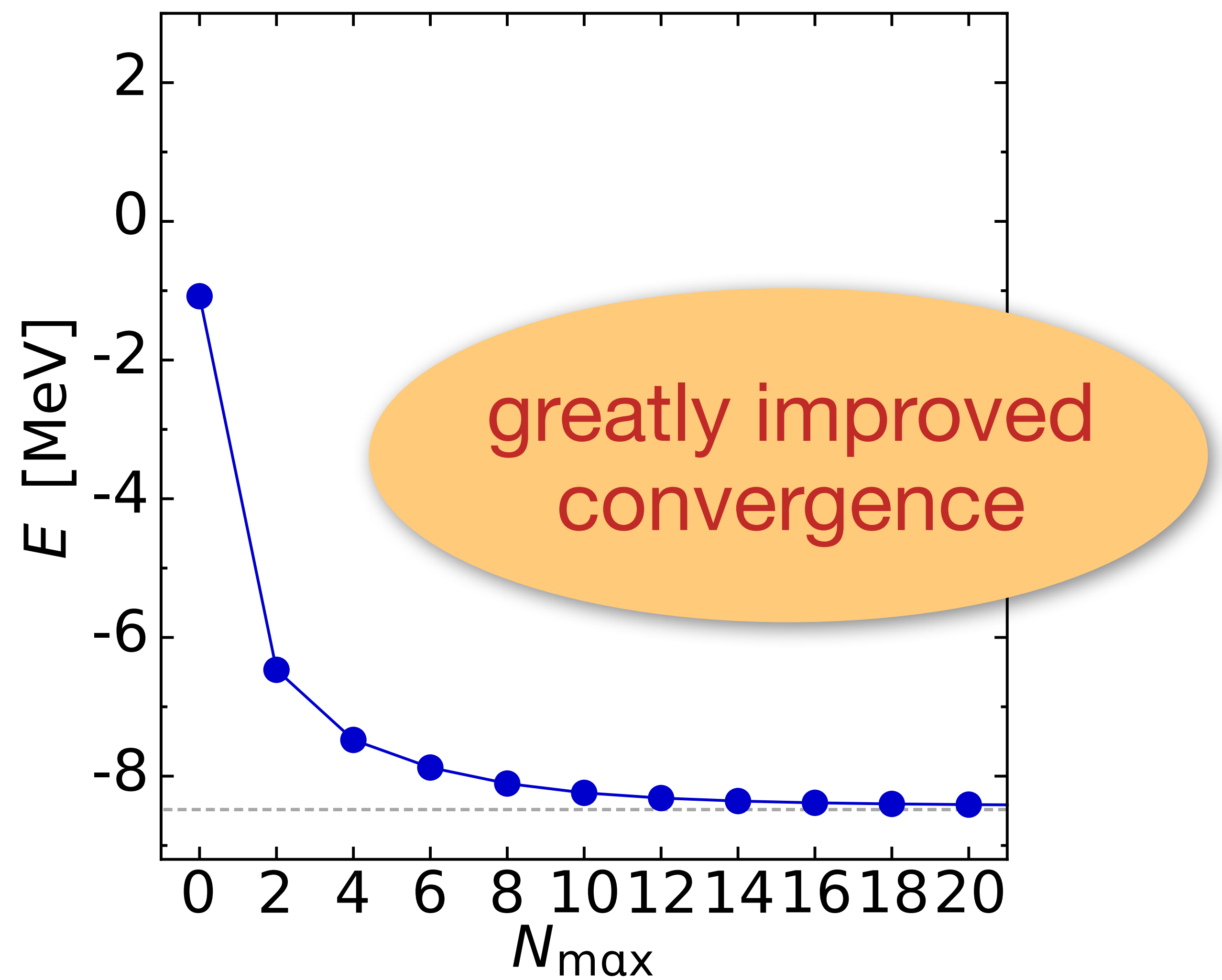
3B Jacobi-HO Matrix Elements

$J^\pi = \frac{1}{2}^+, T = \frac{1}{2}, \hbar\Omega = 28$ MeV



λ = 1.33 fm⁻¹

^{3}H ground-state (NCSM)

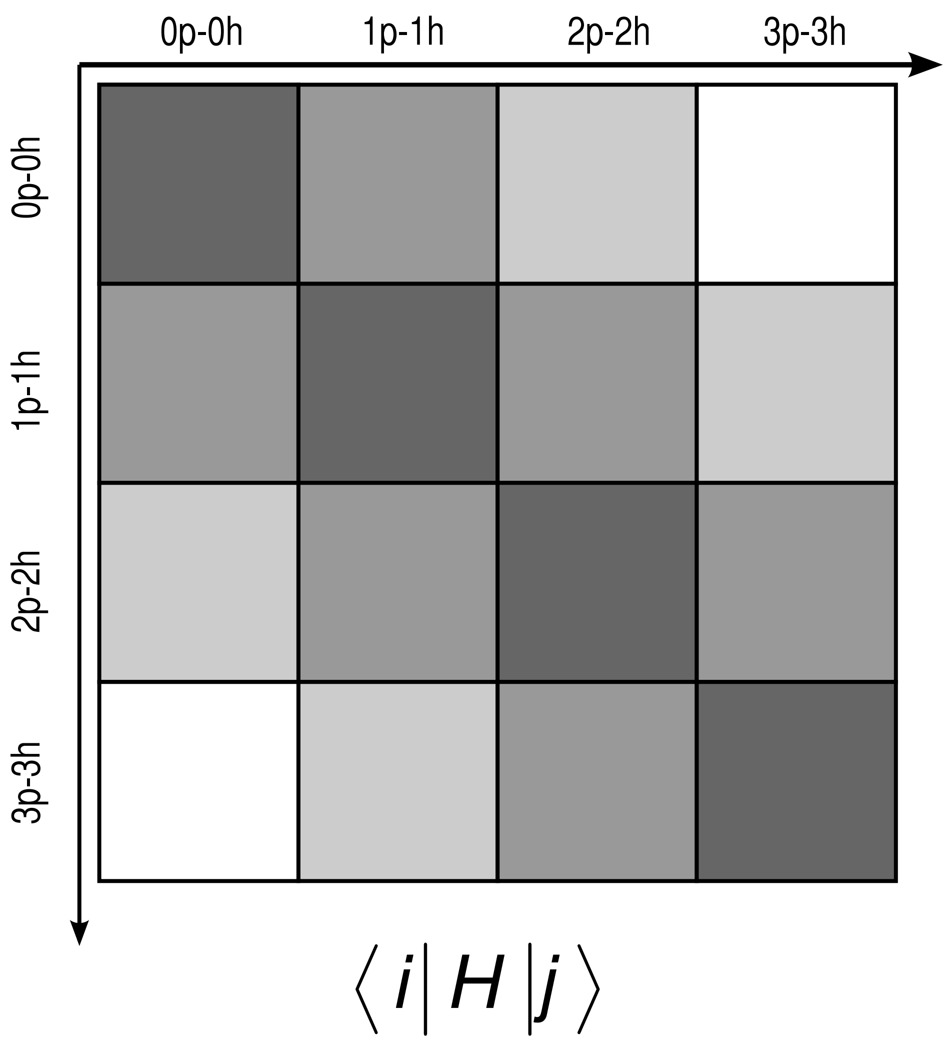


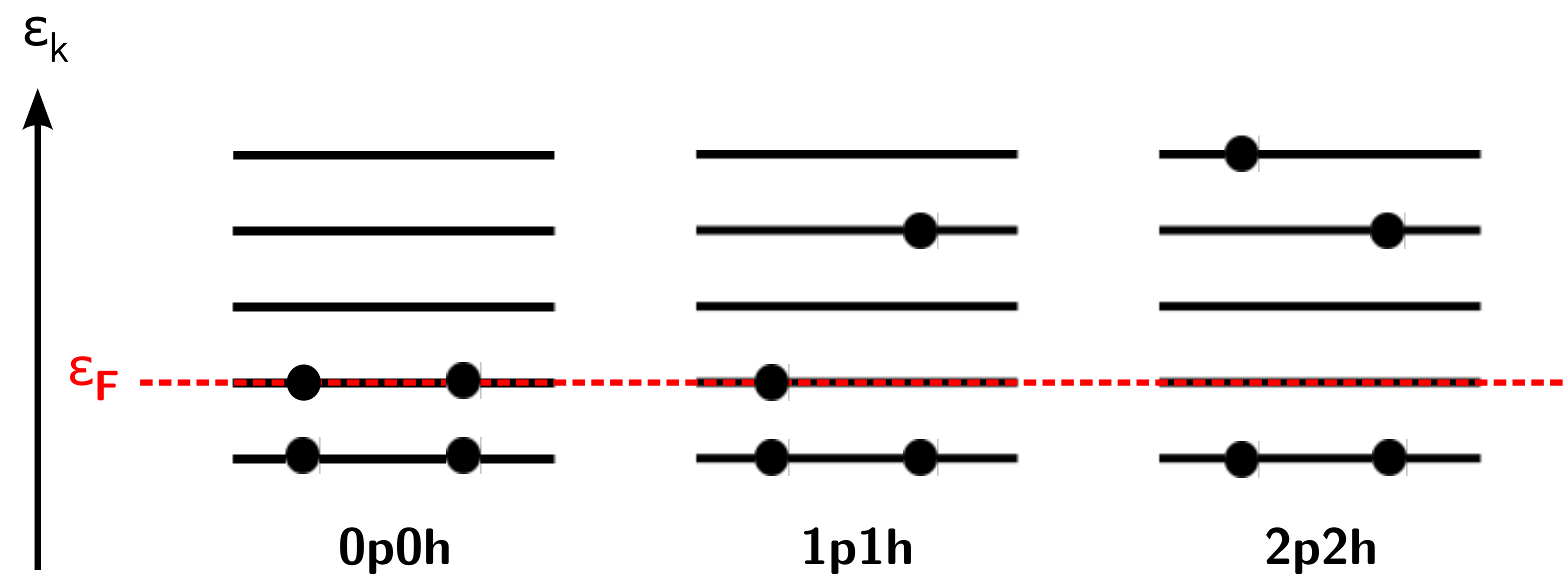
[figures by R. Roth, A. Calci, J. Langhammer]

In-Medium SRG

H. H., S. K. Bogner, S. Binder, A. Calci, J. Langhammer, R. Roth, and A. Schwenk, Phys. Rev. C **87**, 034307 (2013)
K. Tsukiyama, S. K. Bogner, and A. Schwenk, Phys. Rev. Lett. **106**, 222502 (2011)

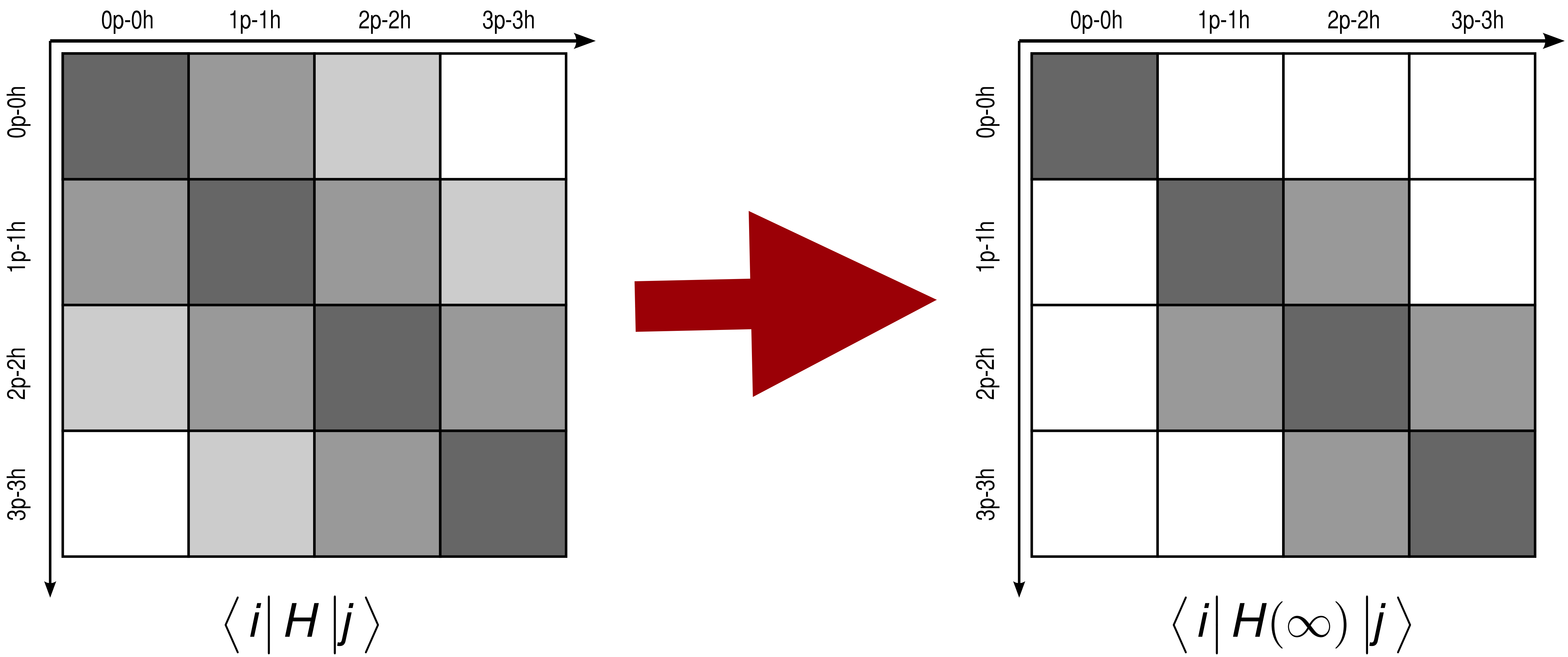
Decoupling in A-Body Space





excitations relative to reference state:
→ normal-ordering

Decoupling in A-Body Space



aim: decouple reference state $|\Phi\rangle$ (0p-0h) from excitations

Normal Ordering

- second quantization: $A^{k_1\dots k_N}_{l_1\dots l_N} = a^\dagger_{k_1}\dots a^\dagger_{k_N} a_{l_N}\dots a_{l_1}$
- particle- and hole density matrices:

$$\lambda^k_l = \left\langle \Phi \right| A^k_l \left| \Phi \right\rangle \longrightarrow n_k \delta^k_l\,, \quad n_k \in \{0,1\}$$
$$\xi^k_l = \lambda^k_l - \delta^k_l \qquad \longrightarrow -\bar{n}_k \delta^k_l \equiv -(1-n_k)\delta^k_l$$

- define normal-ordered operators recursively:

$$A^{k_1\dots k_N}_{l_1\dots l_N} = :A^{k_1\dots k_N}_{l_1\dots l_N}: + \lambda^{k_1}_{l_1} :A^{k_2\dots k_N}_{l_2\dots l_N}: + \text{singles}$$
$$+ \left(\lambda^{k_1}_{l_1}\lambda^{k_2}_{l_2} - \lambda^{k_1}_{l_2}\lambda^{k_2}_{l_1}\right) :A^{k_3\dots k_N}_{l_3\dots l_N}: + \text{doubles} + \dots$$

- algebra is simplified significantly because

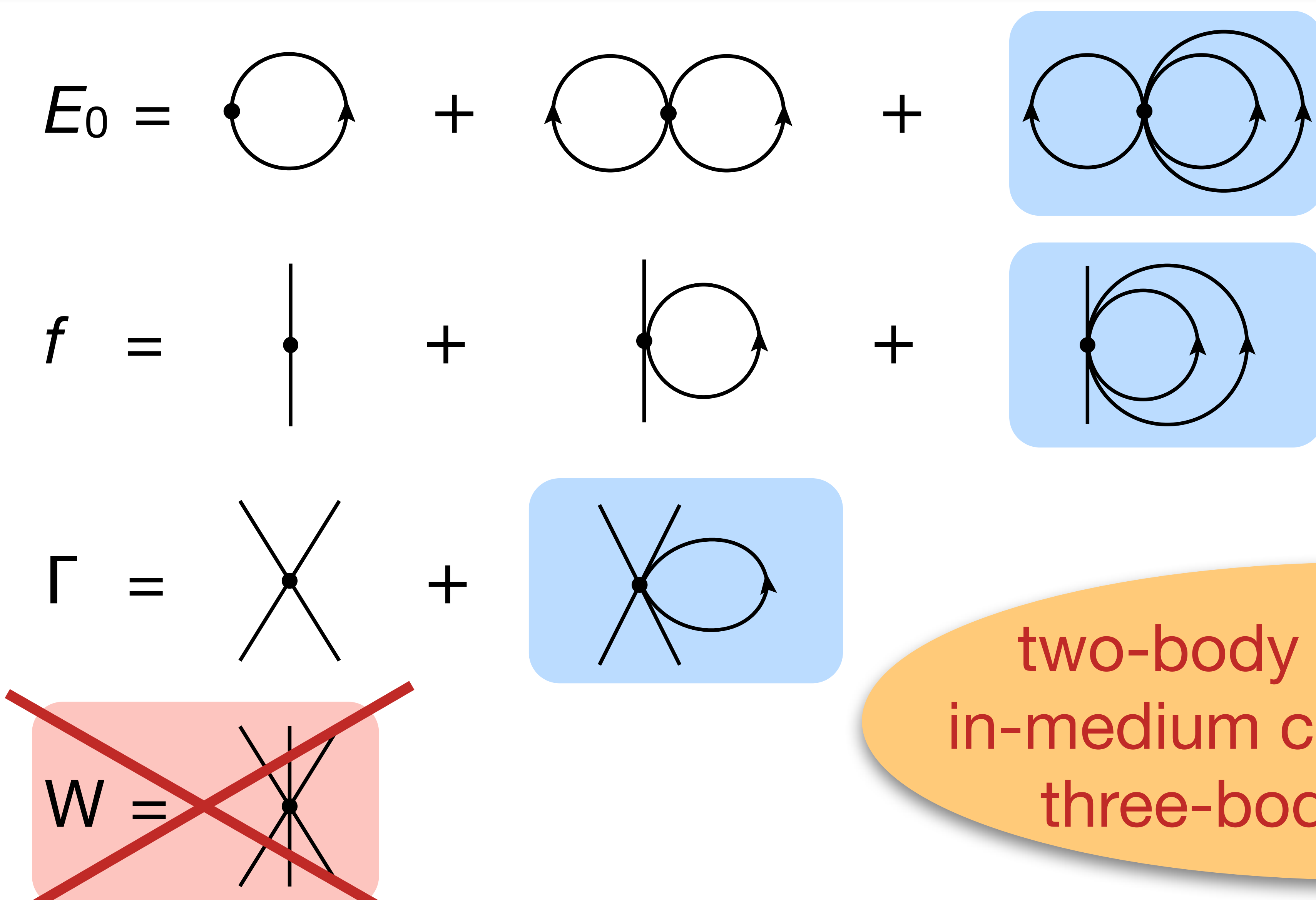
$$\left\langle \Phi \right| :A^{k_1\dots k_N}_{l_1\dots l_N}: \left| \Phi \right\rangle = 0$$

- Wick's theorem gives simplified expansions (fewer terms!) for products of normal-ordered operators

Normal-Ordered Hamiltonian

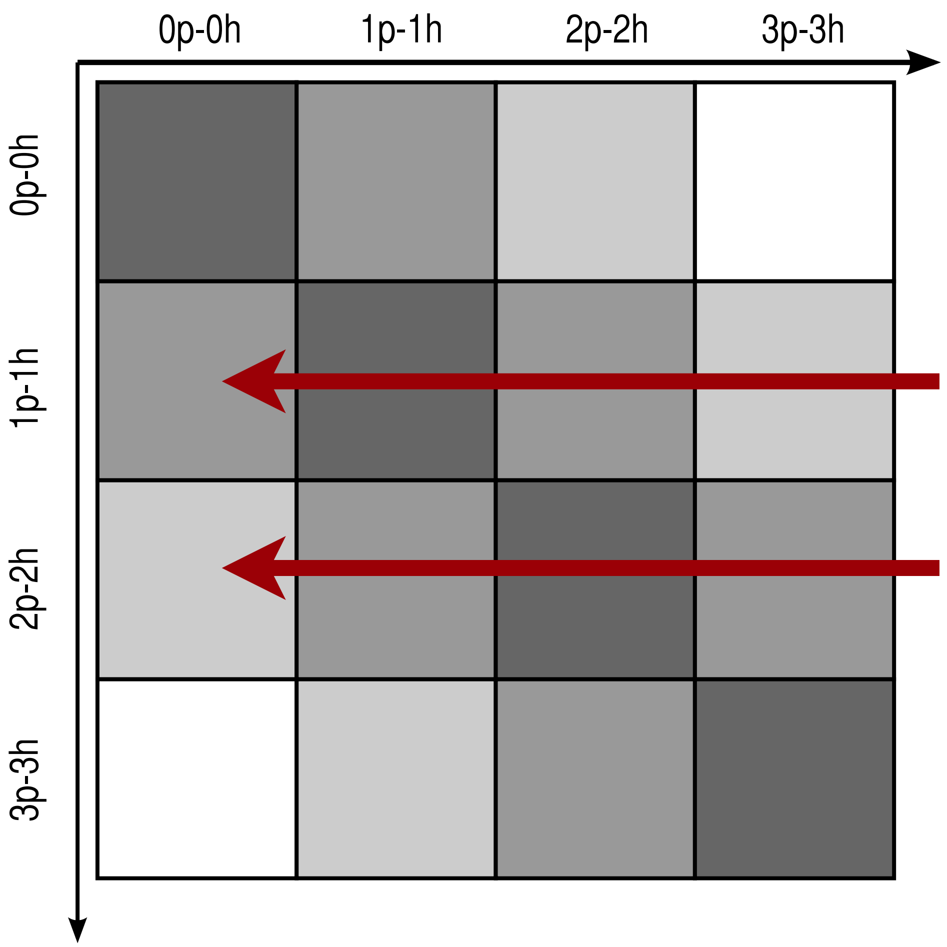
Normal-Ordered Hamiltonian

$$H = E_0 + \sum_{kl} f^k_l :A^k_l: + \frac{1}{4}\sum_{klmn} \Gamma^{kl}_{mn} :A^{kl}_{mn}: + \frac{1}{36}\sum_{ijklmn} W^{ijk}_{lmn} :A^{ijk}_{lmn}:$$



two-body formalism with in-medium contributions from three-body interactions

Choice of Generator



$$\left\langle {}^{p}_{h} \middle| H \middle| \Psi \right\rangle = \sum_{kl} f^k_l \left\langle \Psi \middle| :A^h_p :: A^k_l : \middle| \Psi \right\rangle = -n_h \bar{n}_p f^p_h$$

$$\left\langle {}^{pp'}_{hh'} \middle| H \middle| \Psi \right\rangle = \sum_{klmn} \Gamma^{kl}_{mn} \left\langle \Psi \middle| :A^{hh'}_{pp'} :: A^{kl}_{mn} : \middle| \Psi \right\rangle \sim \Gamma^{pp'}_{hh'}$$

Off-Diagonal Hamiltonian & Generator

$$H^{od} \equiv f^{od} + \Gamma^{od}\,, \quad f^{od} \equiv \sum_{ph} f^p_h :A^p_h: + \text{H.c.}\,, \quad \Gamma^{od} \equiv \sum_{pp'hh'} \Gamma^{pp'}_{hh'} :A^{pp'}_{hh'}: + \text{H.c.}$$

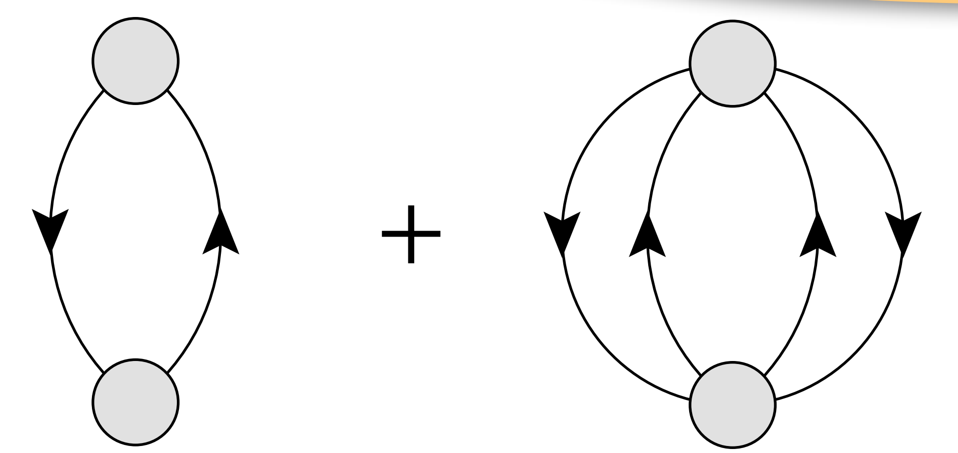
$$\rightarrow \quad \eta = \left[H^d, H^{od}\right]$$

In-Medium SRG Flow Equations

0-body Flow

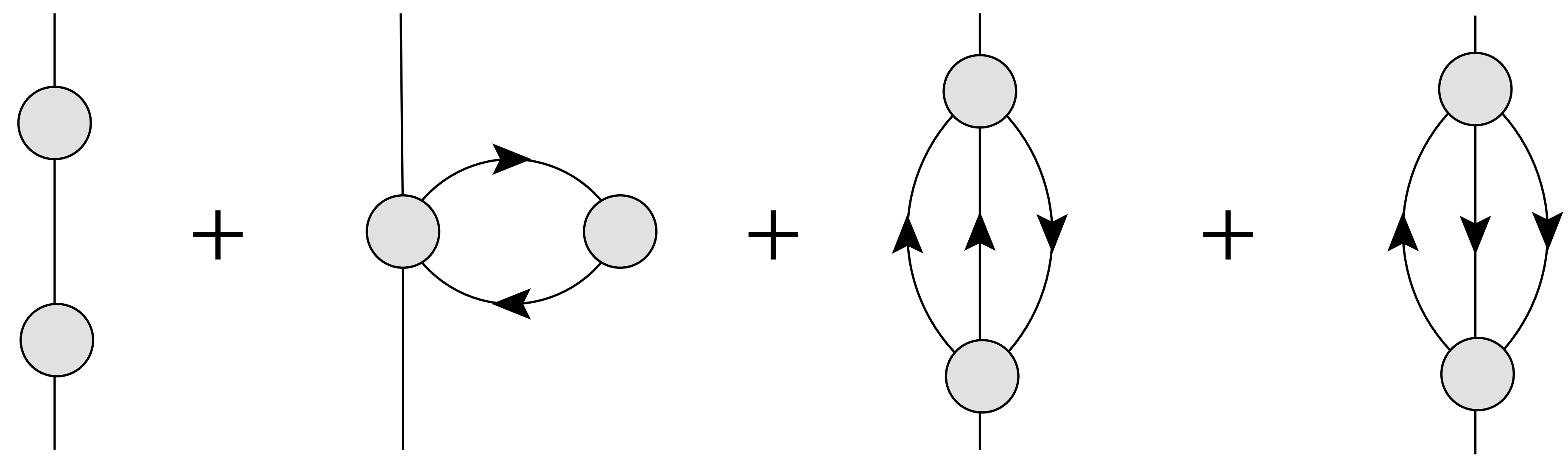
~ 2nd order MBPT for *H(s)*

$$\frac{dE}{ds} =$$



1-body Flow

$$\frac{df}{ds} =$$

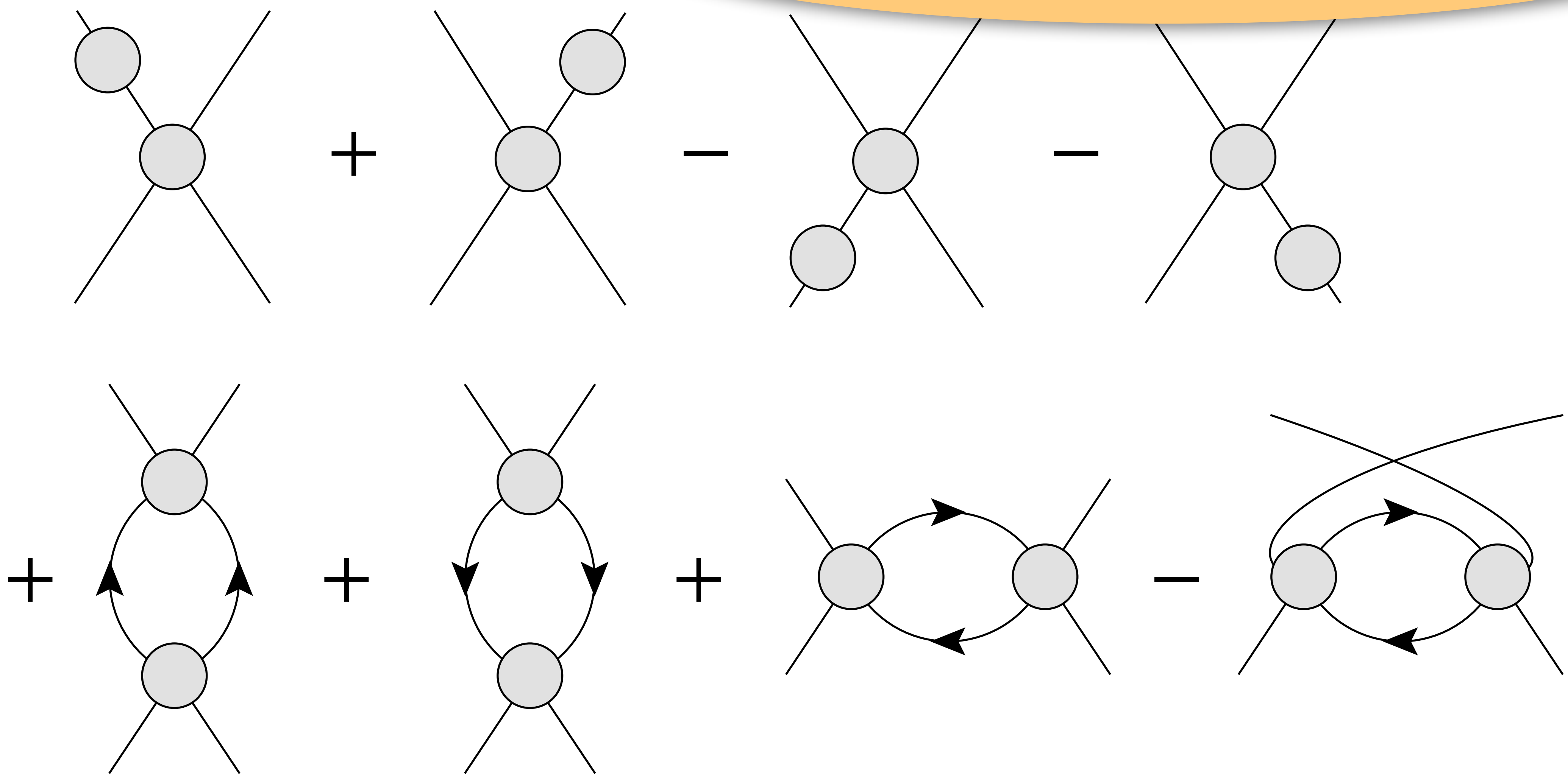


In-Medium SRG Flow Equations

2-body Flow

only linked diagrams contribute, IM-SRG size-extensive

$$\frac{d\Gamma}{ds} =$$



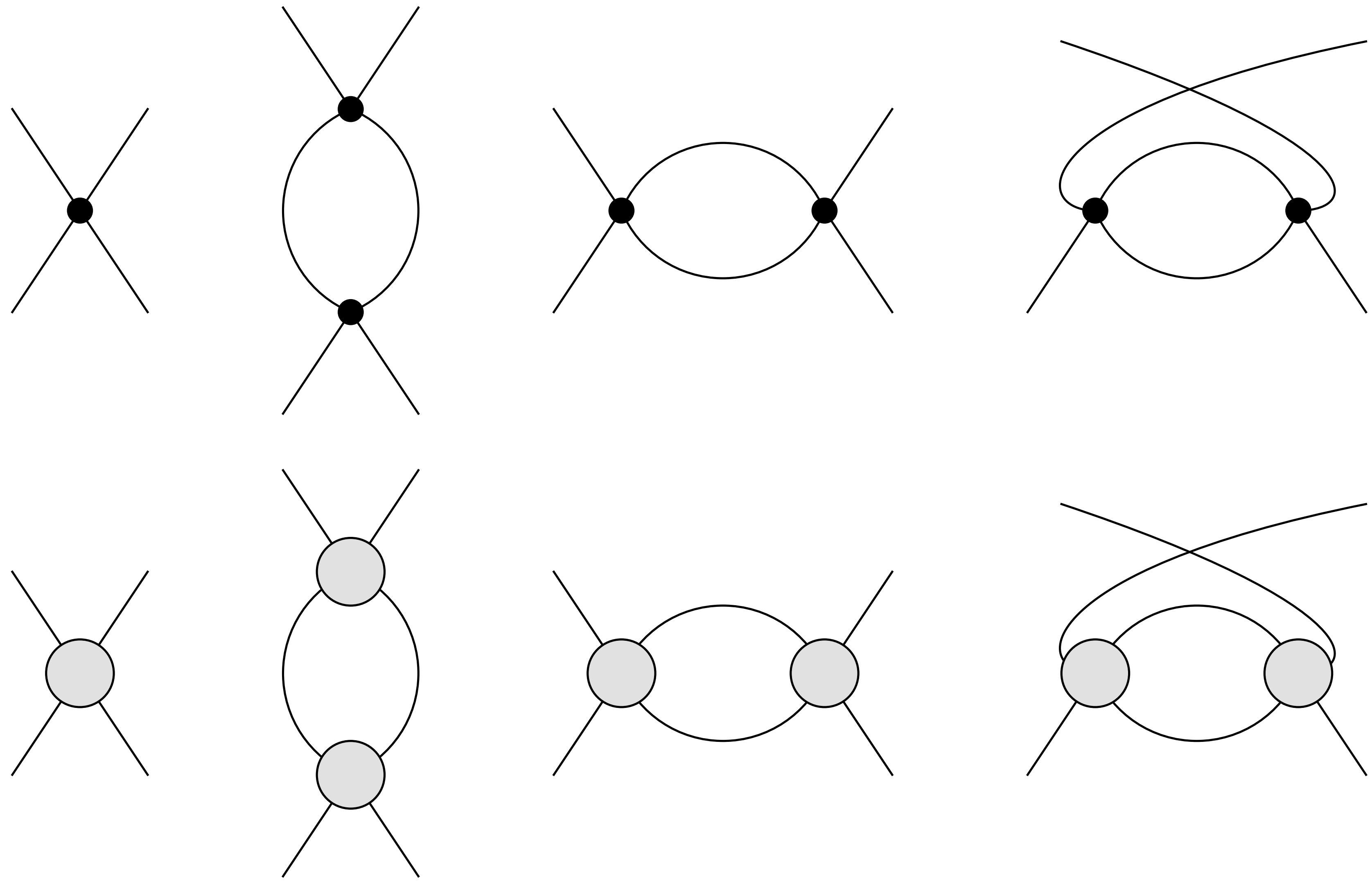
s channel — ladders

t channel, u channel — rings

In-Medium SRG Flow: Diagrams

$\Gamma(\delta s) \sim$

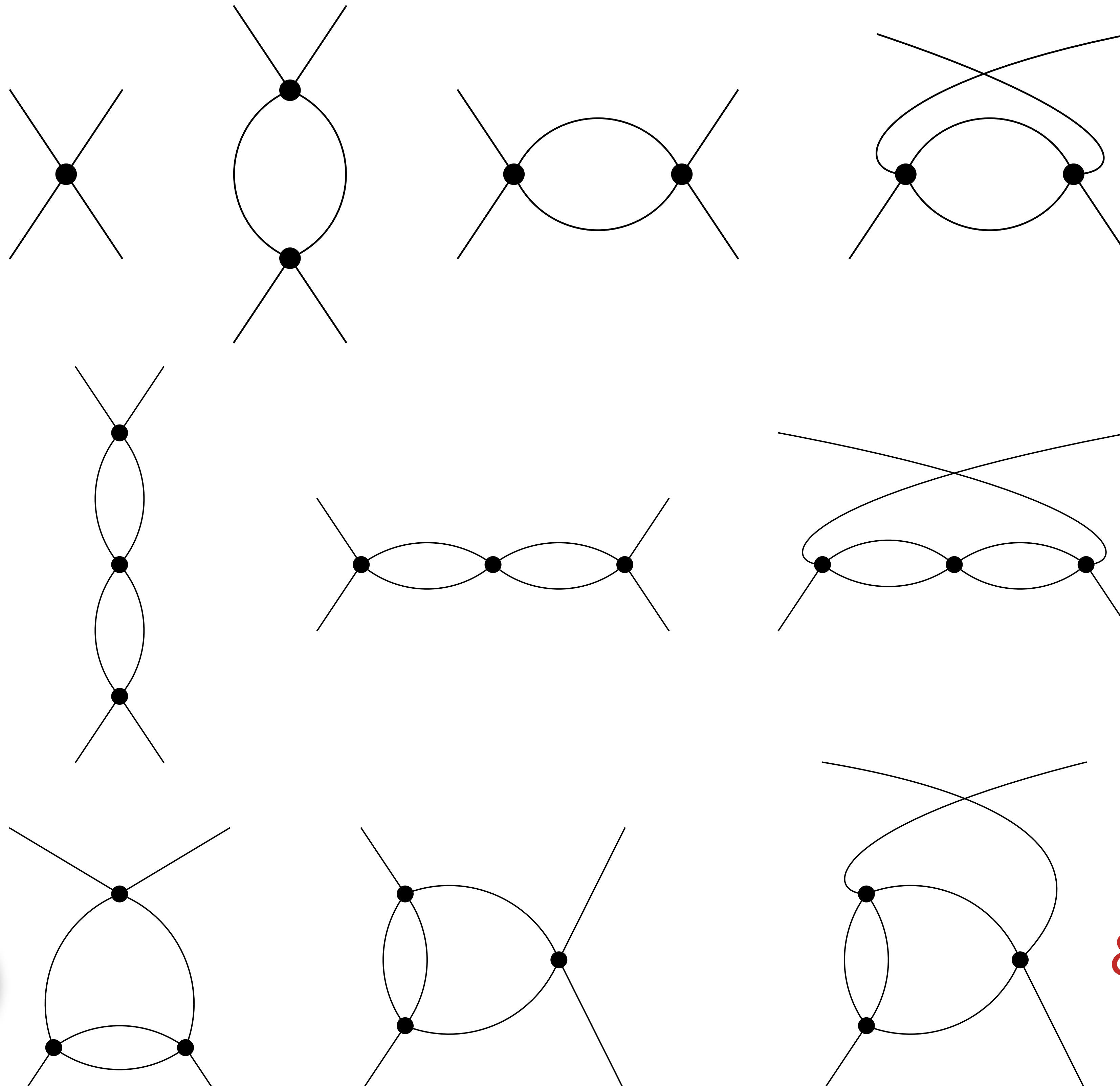
$\Gamma(2\delta s) \sim$



In-Medium SRG Flow: Diagrams

$\Gamma(\delta s) \sim$

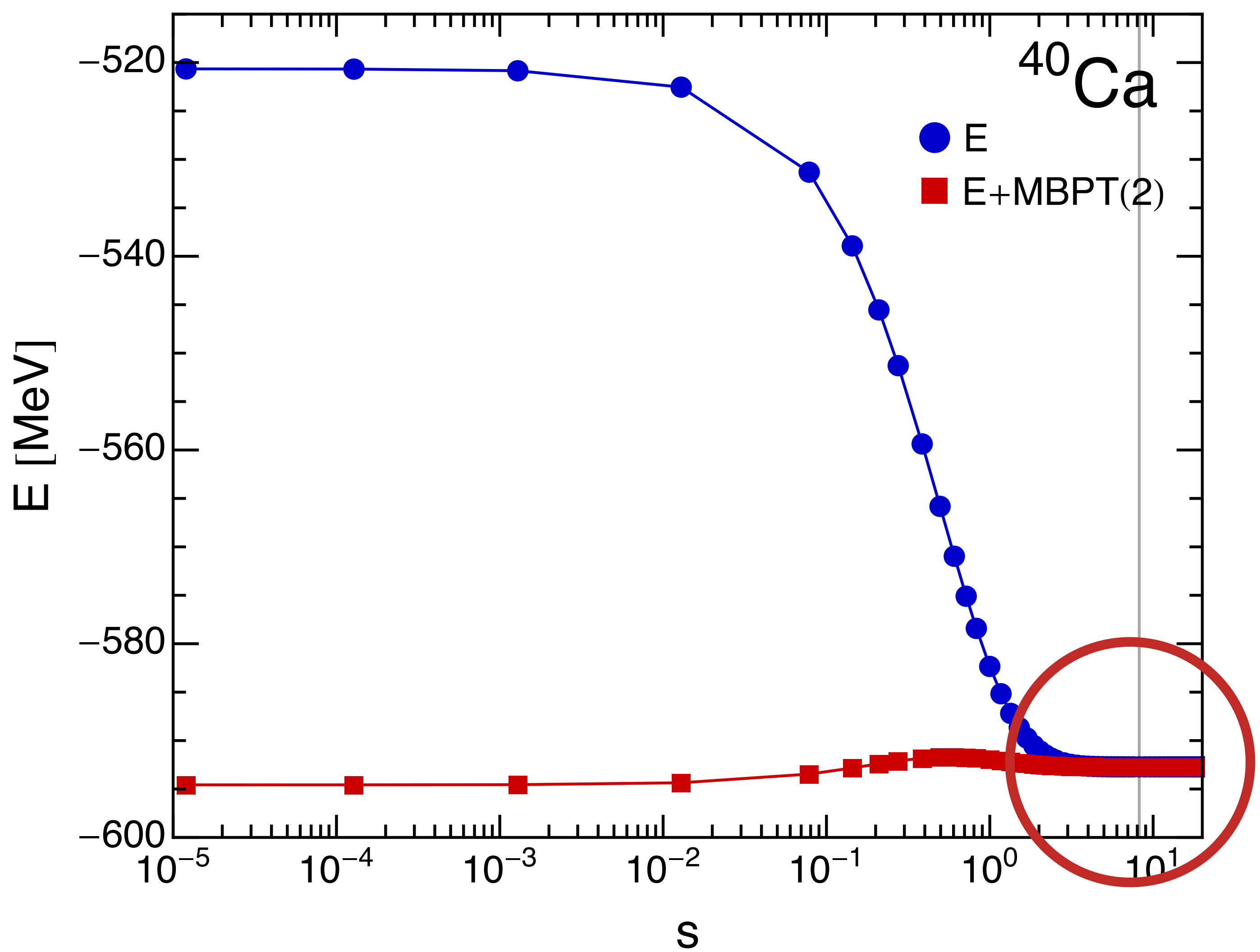
$\Gamma(2\delta s) \sim$

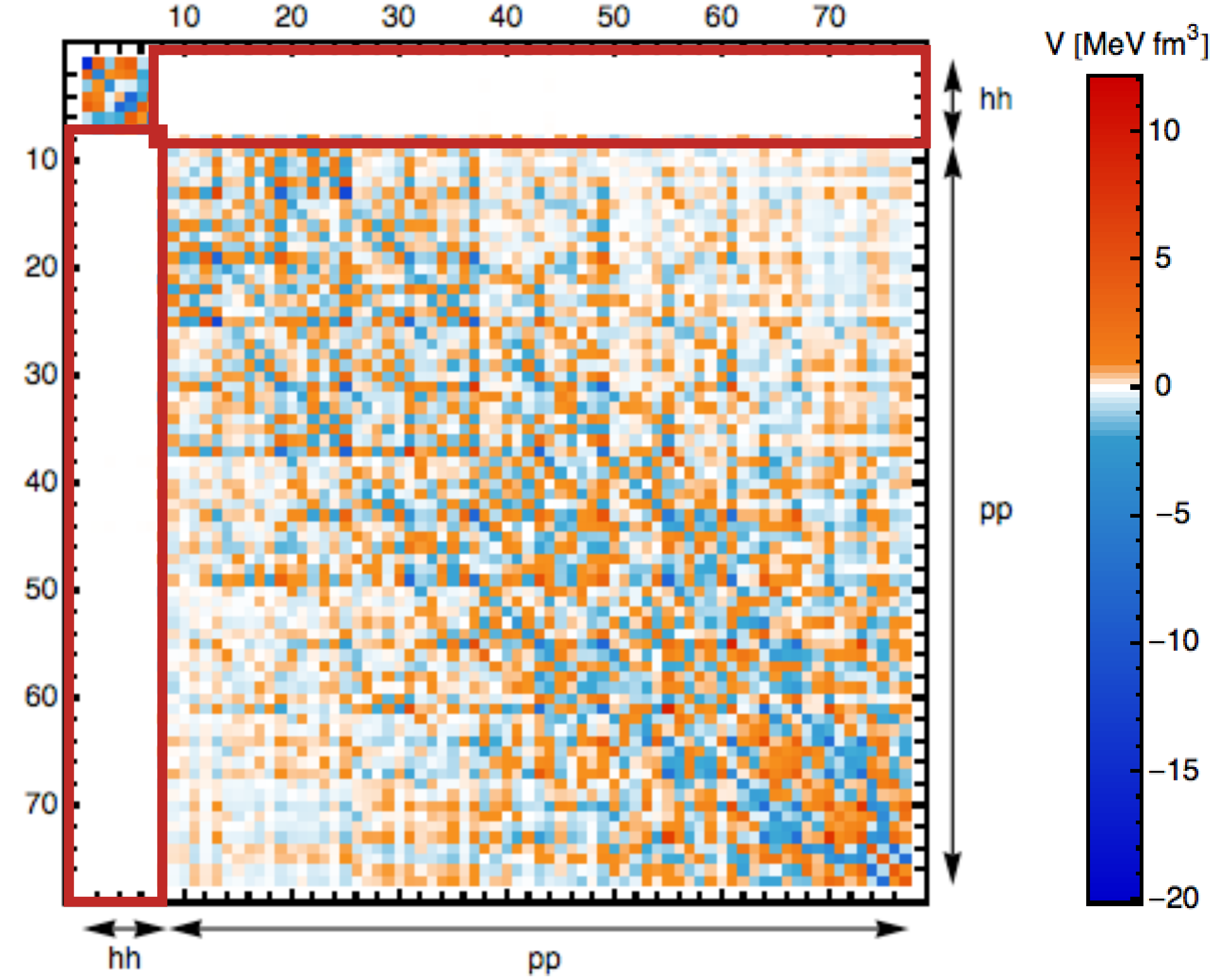


non-perturbative resummation

& many more...

Decoupling





N3LO, $\lambda = 2.0\ \text{fm}^{-1}, e_{\text{Max}} = 8$

non-perturbative resummation of MBPT series (correlations)

off-diagonal couplings are rapidly driven to zero

Results for Finite Nuclei

H. H., S. Binder, A. Calci, J. Langhammer, and R. Roth, Phys. Rev. Lett **110**, 242501 (2013)
H. H., S. K. Bogner, S. Binder, A. Calci, J. Langhammer, R. Roth, and A. Schwenk,
Phys. Rev. C **87**, 034307 (2013)

Hamiltonians

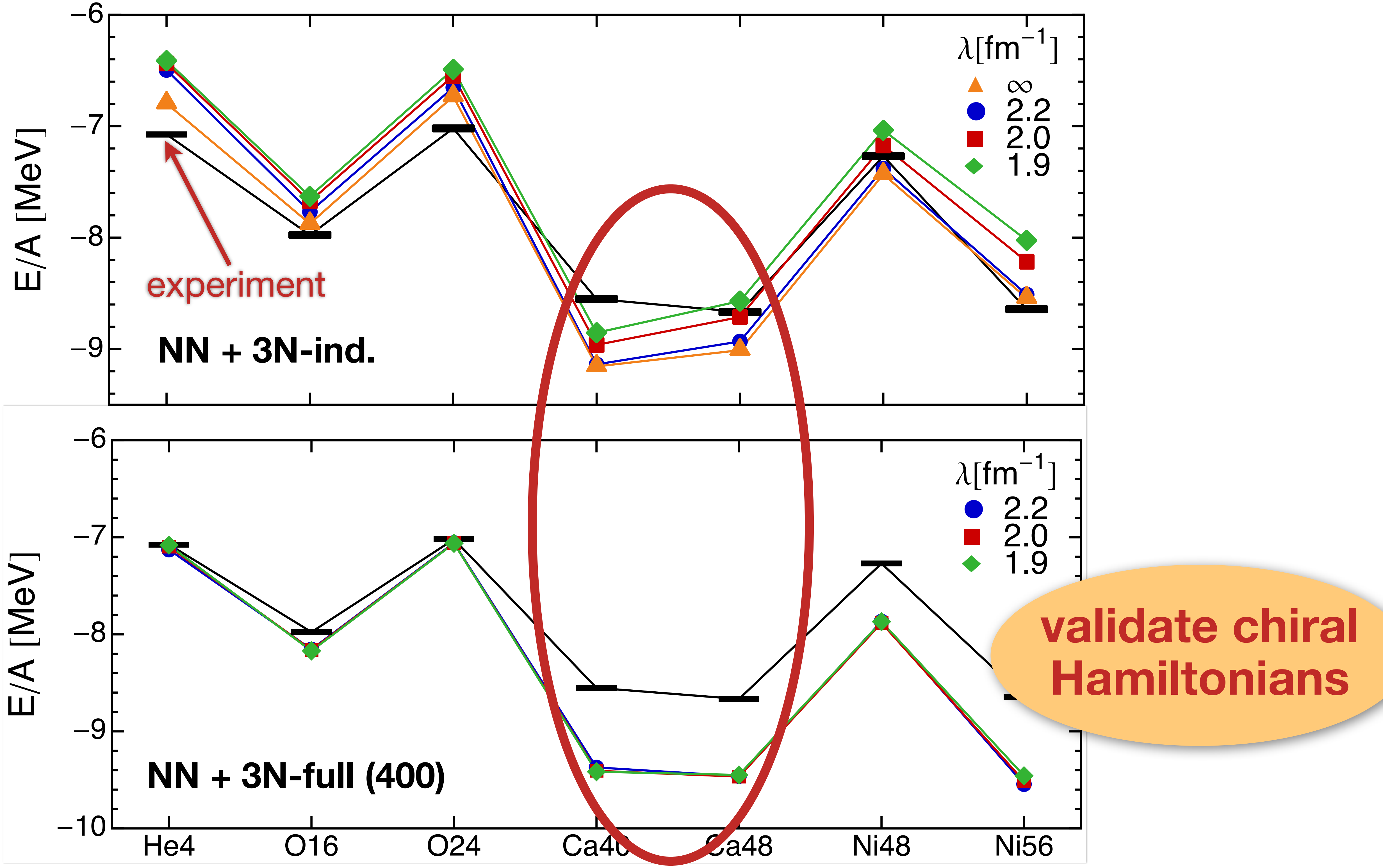
Initial Hamiltonian

- NN: chiral interaction at N^3LO (Entem & Machleidt)
- 3N: chiral interaction at N^2LO (c_D,c_E fit to ^3H energy & half-life)

SRG-Evolved Hamiltonians

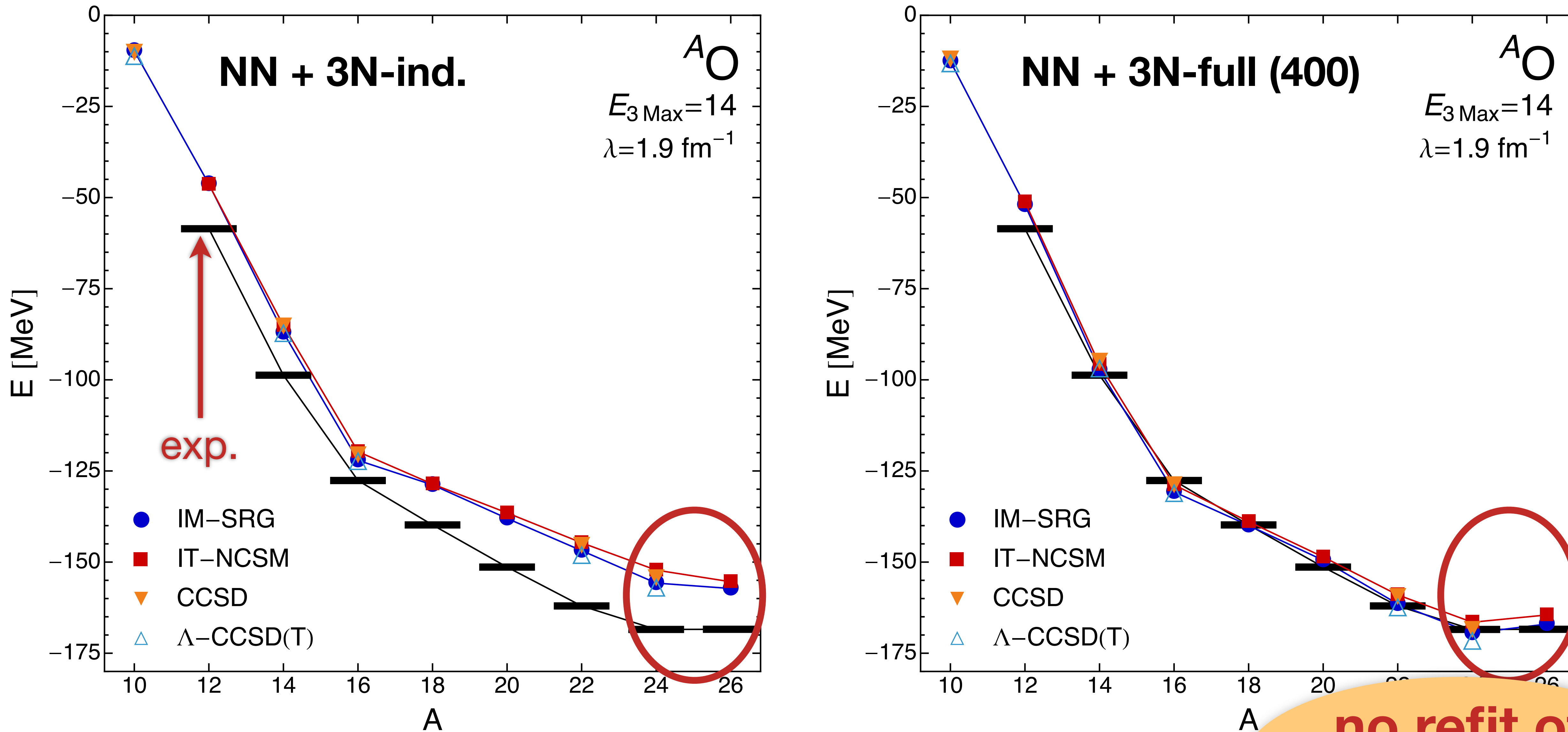
- **NN + 3N-induced:** start with initial NN Hamiltonian, keep two- and three-body terms
- **NN + 3N-full:** start with initial NN + 3N Hamiltonian, keep two- and three-body terms

Results: Closed-Shell Nuclei



Phys. Rev. C **87**, 034307 (2013), arXiv: 1212.1190 [nucl-th]

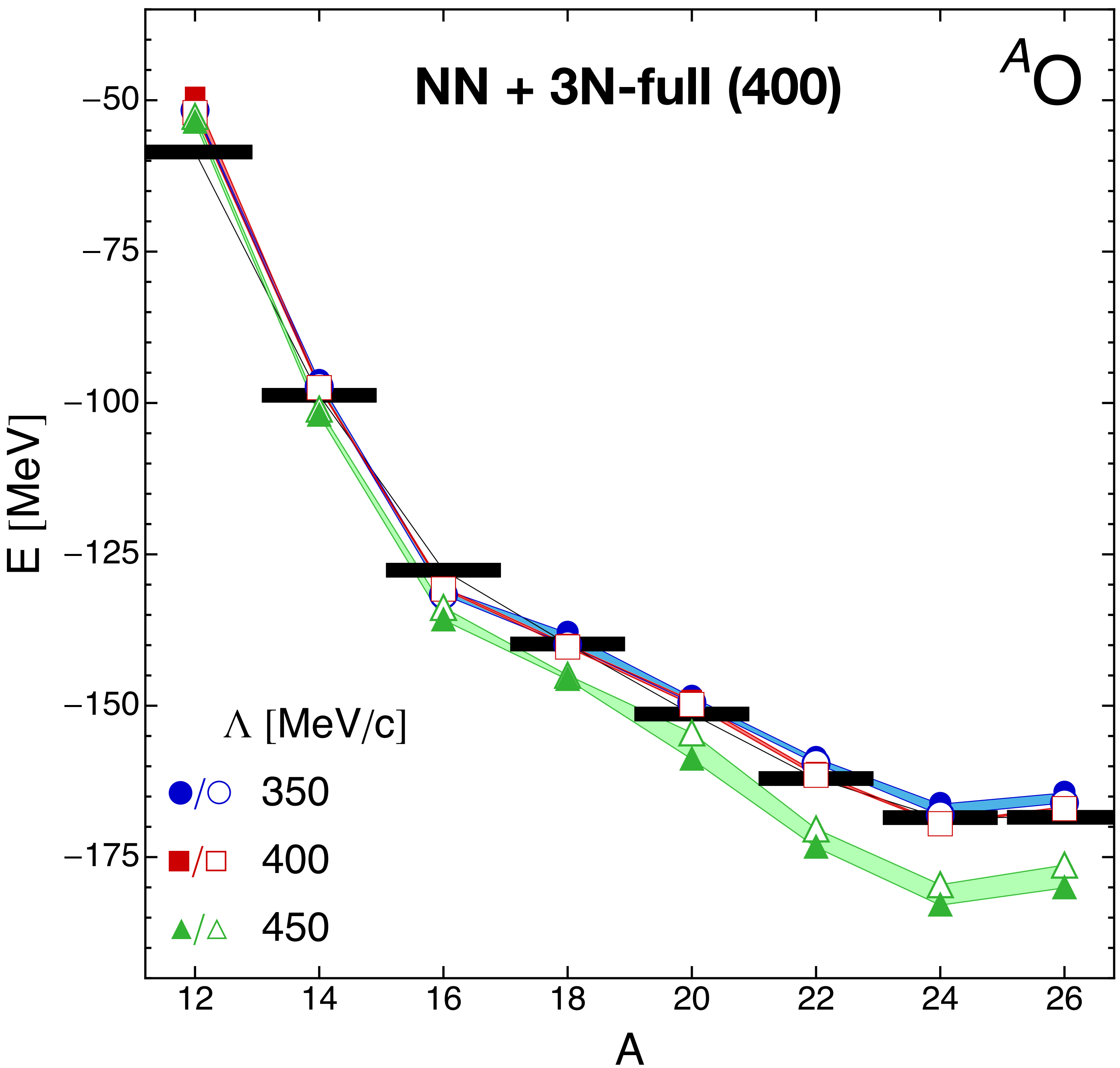
Results: Oxygen Chain



no refit of 3N interaction

- reference state: number-projected Hartree-Fock-Bogoliubov (pairing correlations)
- consistent results for different many-body methods (also SCGF)
  (HH et al., PRL **110**, 242501, (2013); Cipollone et al., PRL **111**, 062501 (2013))

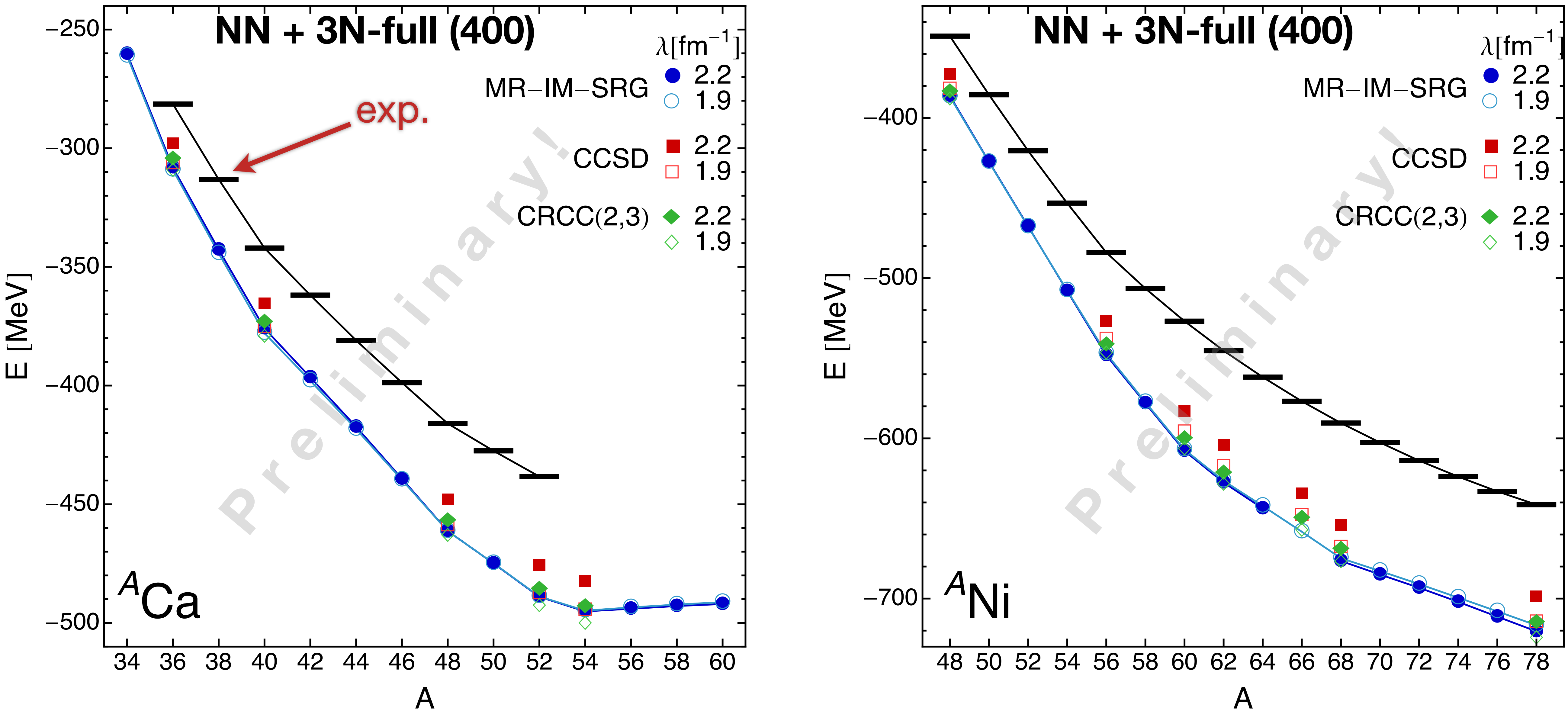
Variation of Scales



Phys. Rev. Lett. **110**, 242501 (2013)

- variation of **initial 3N cutoff only**
- diagnostics for chiral interactions
- **dripline at A=24 is robust under variations**

Calcium and Nickel Isotopes



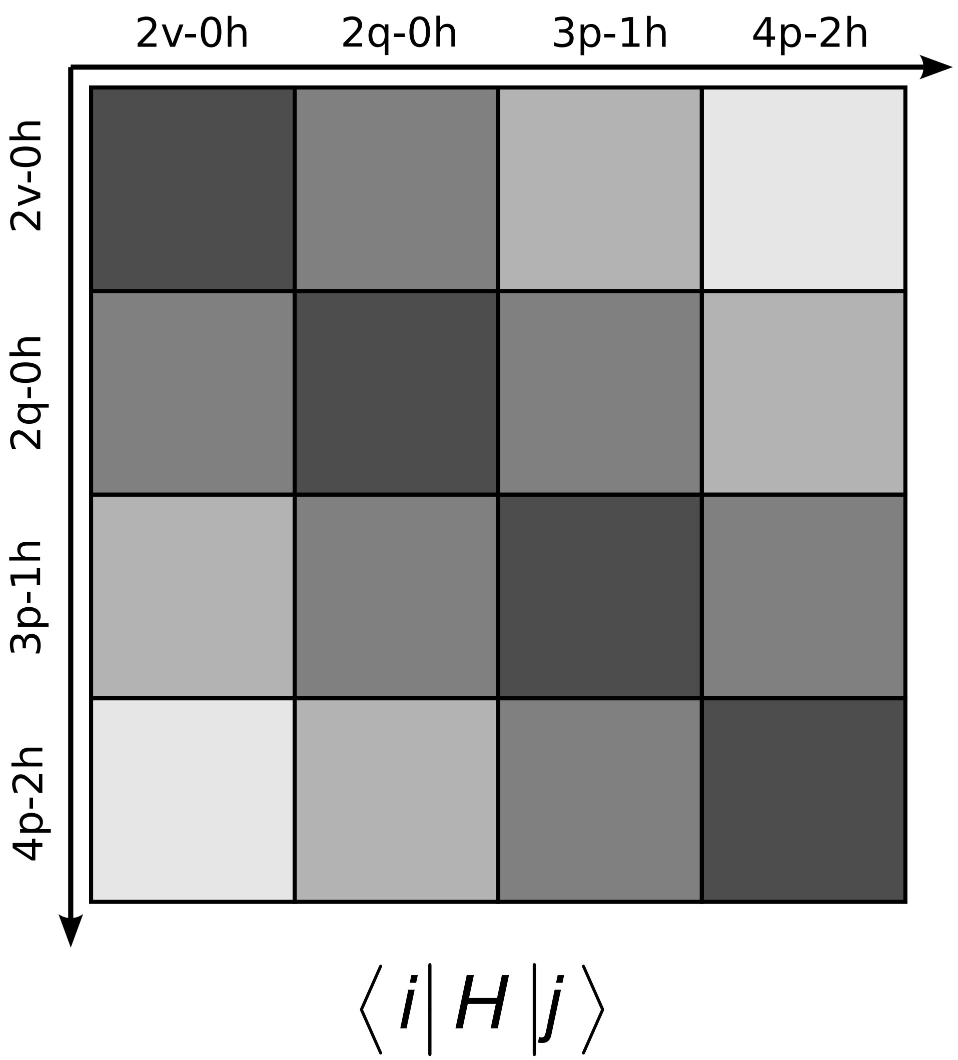
$e_{\mathrm{Max}} = 14,\ E_{3\mathrm{Max}} = 14$

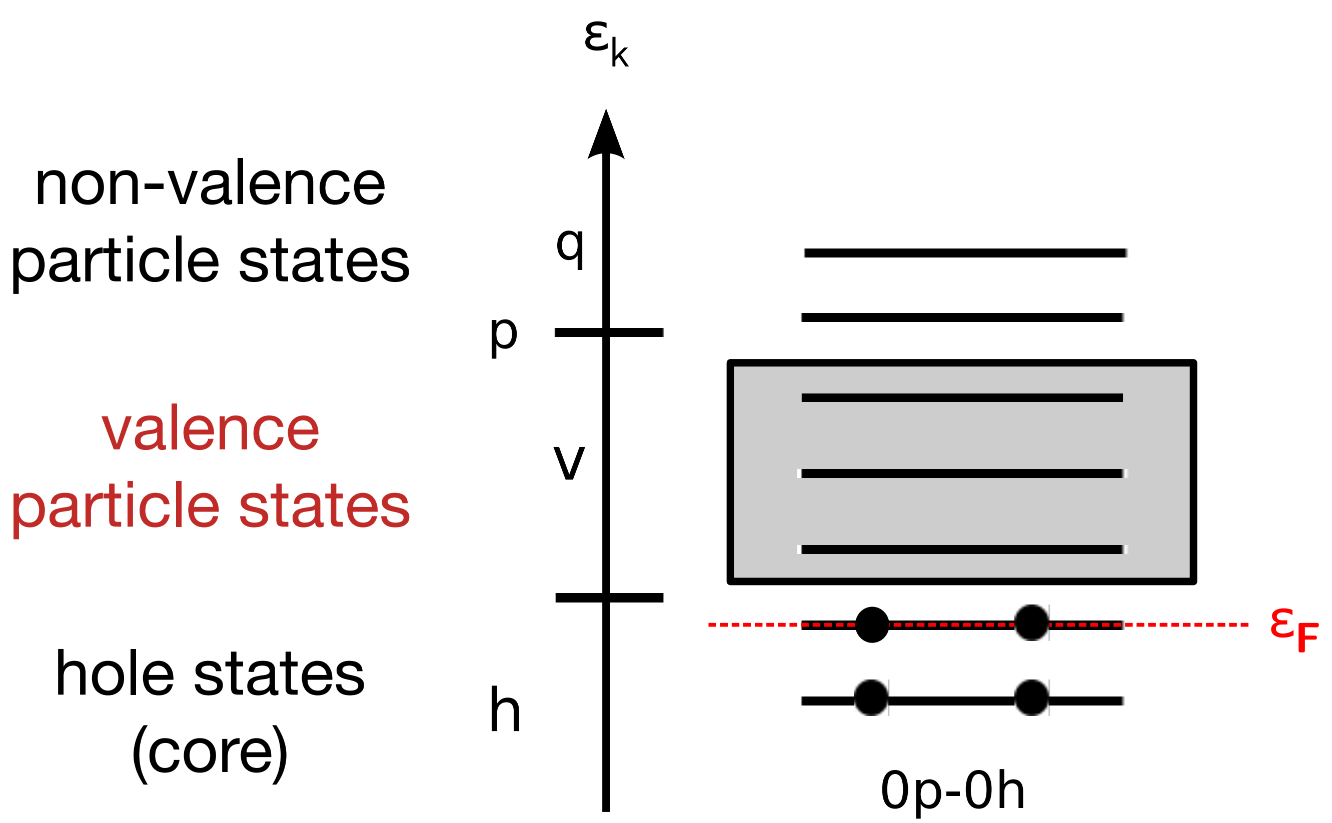
- **improved free-space 3N SRG evolution** for input Hamiltonian (S. Binder et al., arXiv:1312.5685 [nucl-th])
- calculations for pf-shell nuclei in progress, **heavier nuclei in reach**

IM-SRG + Shell Model

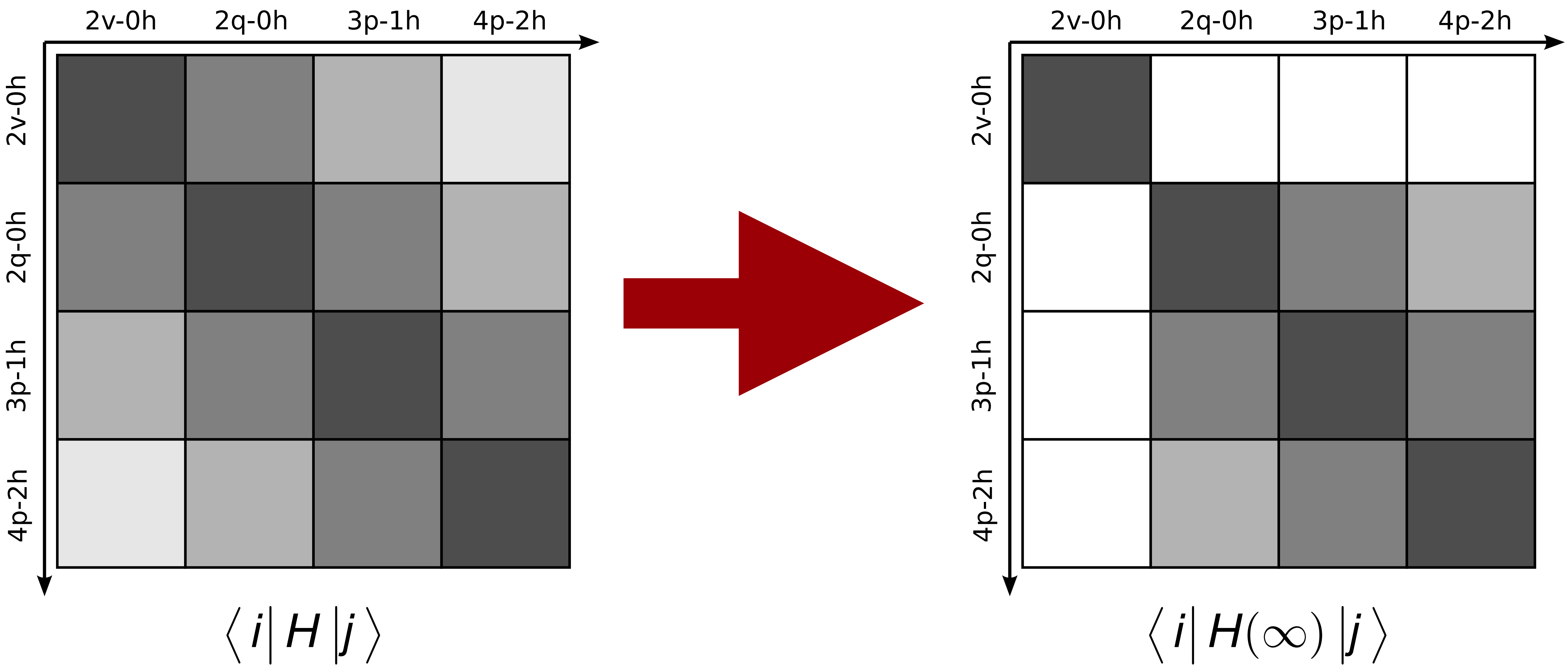
S. K. Bogner, H. H., J. D. Holt, A. Schwenk, S. Binder, A. Calci, J. Langhammer, R. Roth, arXiv:1402:1407 [nucl-th]
K. Tsukiyama, S. K. Bogner, and A. Schwenk, Phys. Rev. C **85**, 061304(R) (2012)

Valence Space Decoupling





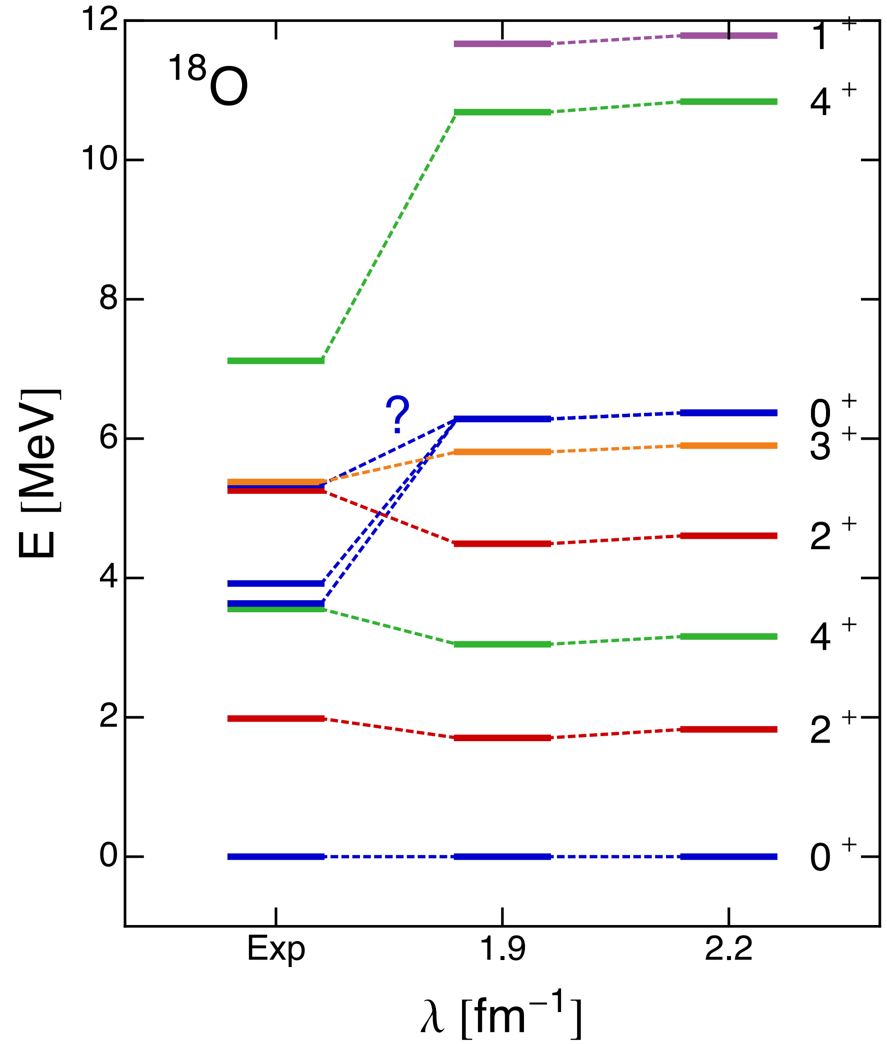
Valence Space Decoupling

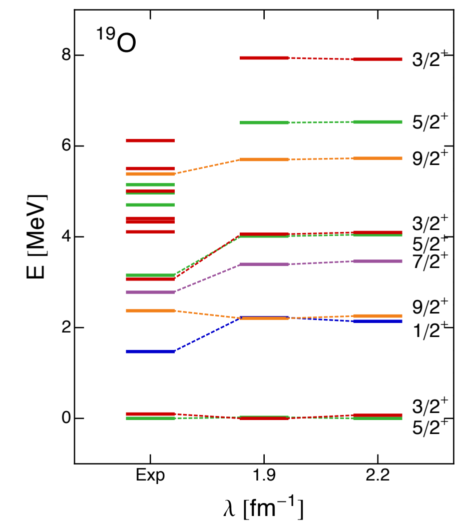


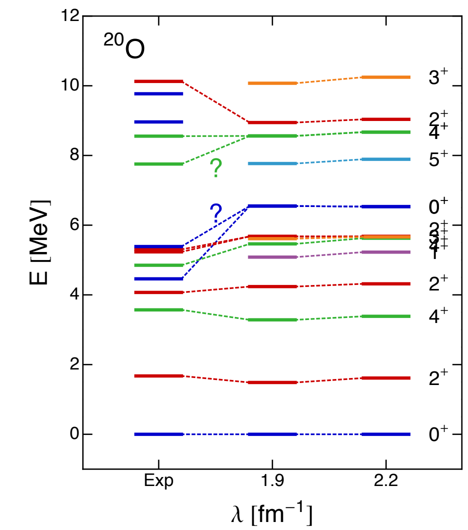
- use White-type generator with off-diagonal Hamiltonian

$$\left\{ H^{od} \right\} = \{ f^{h}_{h'}, f^{p}_{p'}, f^{p}_{h}, f^{q}_{v}, \Gamma^{pp'}_{hh'}, \Gamma^{pp'}_{hv}, \Gamma^{pq}_{vv'} \} \text{ \& H.c.}$$

Oxygen Spectra



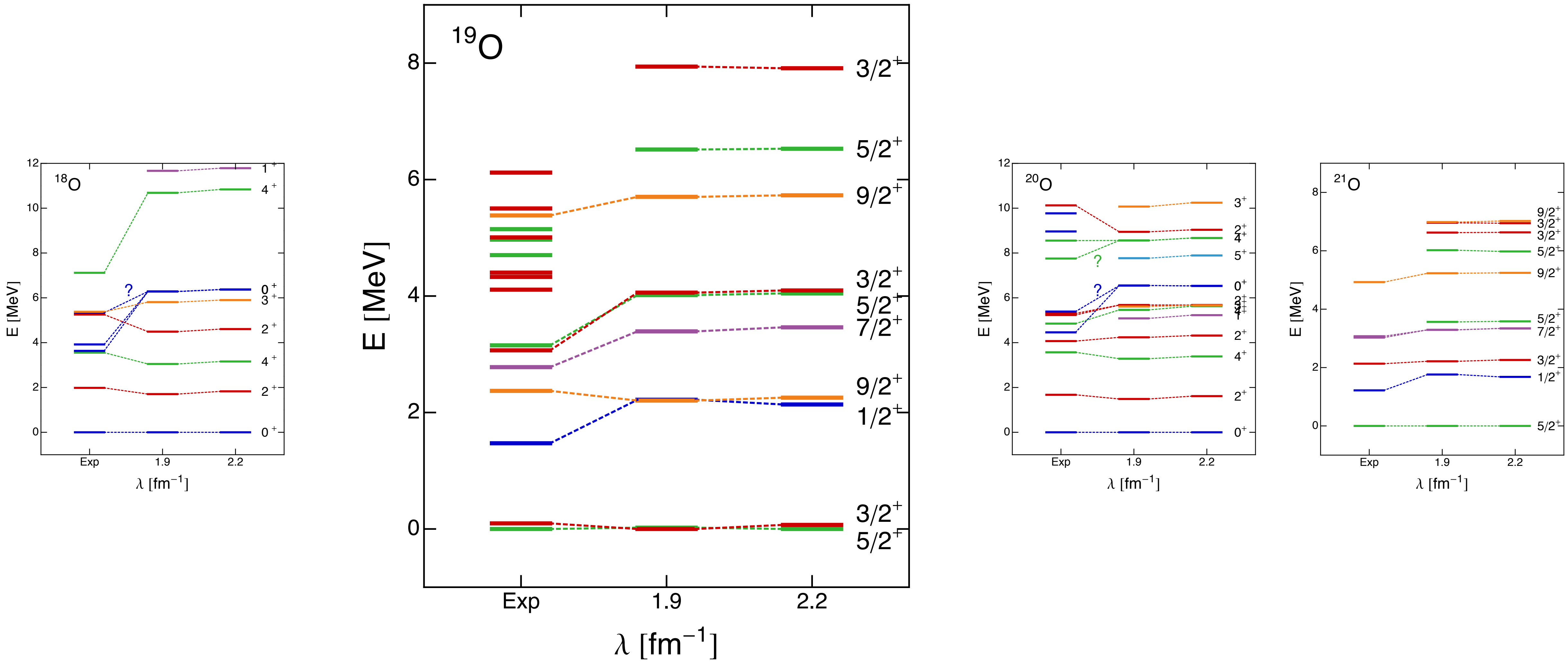




NN+3N-full (400), $e_{\mathrm{Max}} = 10$, $E_{\mathrm{3Max}} = 14$, $\hbar\Omega = 24$ MeV

- good description of low-lying states

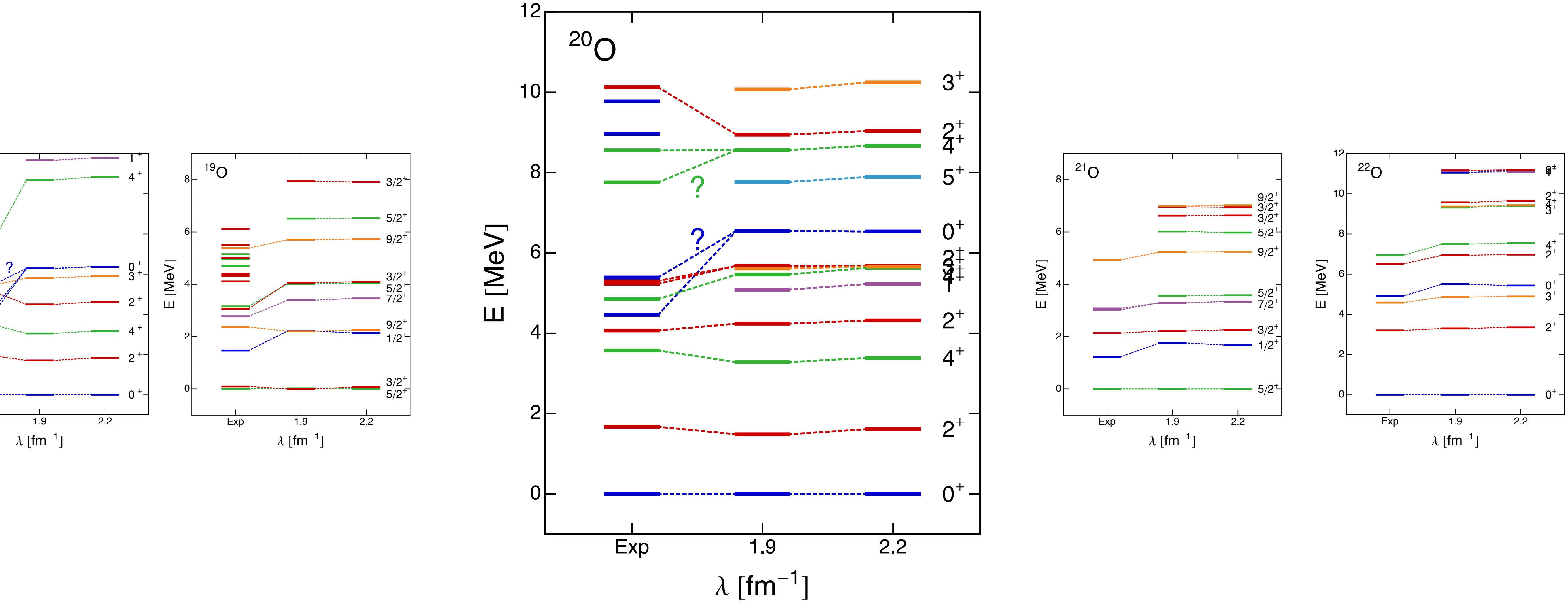
Oxygen Spectra



NN+3N-full (400), $e_{\text{Max}} = 10$, $E_{3\text{Max}} = 14$, $\hbar\Omega = 24$ MeV

- good description of low-lying states

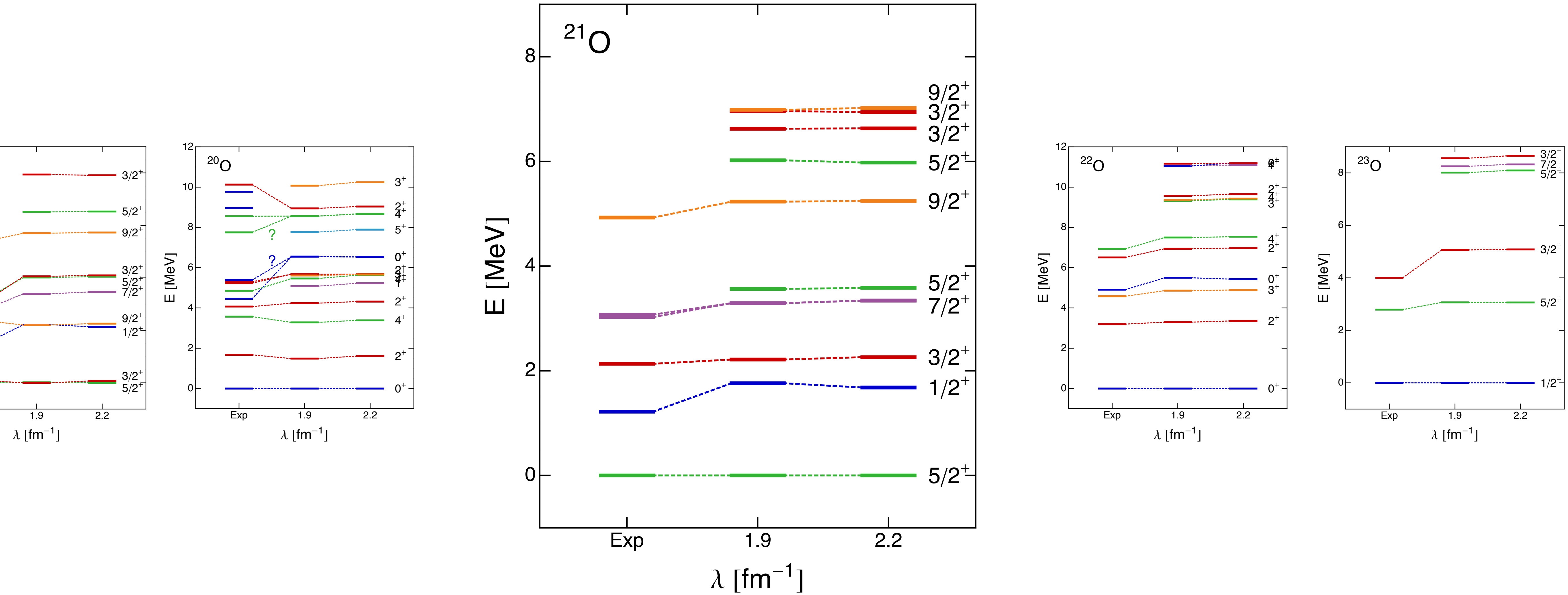
Oxygen Spectra



NN+3N-full (400), $e_{\text{Max}} = 10$, $E_{3\text{Max}} = 14$, $\hbar\Omega = 24$ MeV

- good description of low-lying states

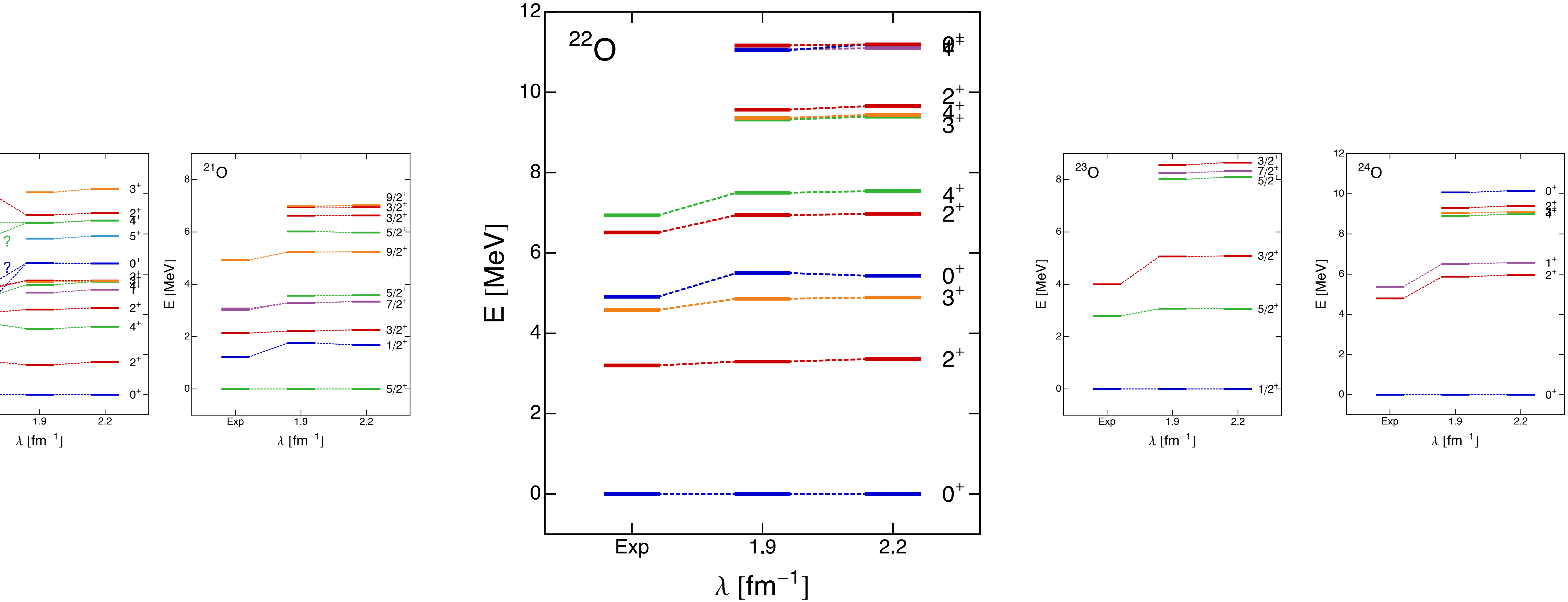
Oxygen Spectra



NN+3N-full (400), $e_{\text{Max}} = 10,\ E_{3\text{Max}} = 14,\ \hbar\Omega = 24$ MeV

- good description of low-lying states

Oxygen Spectra



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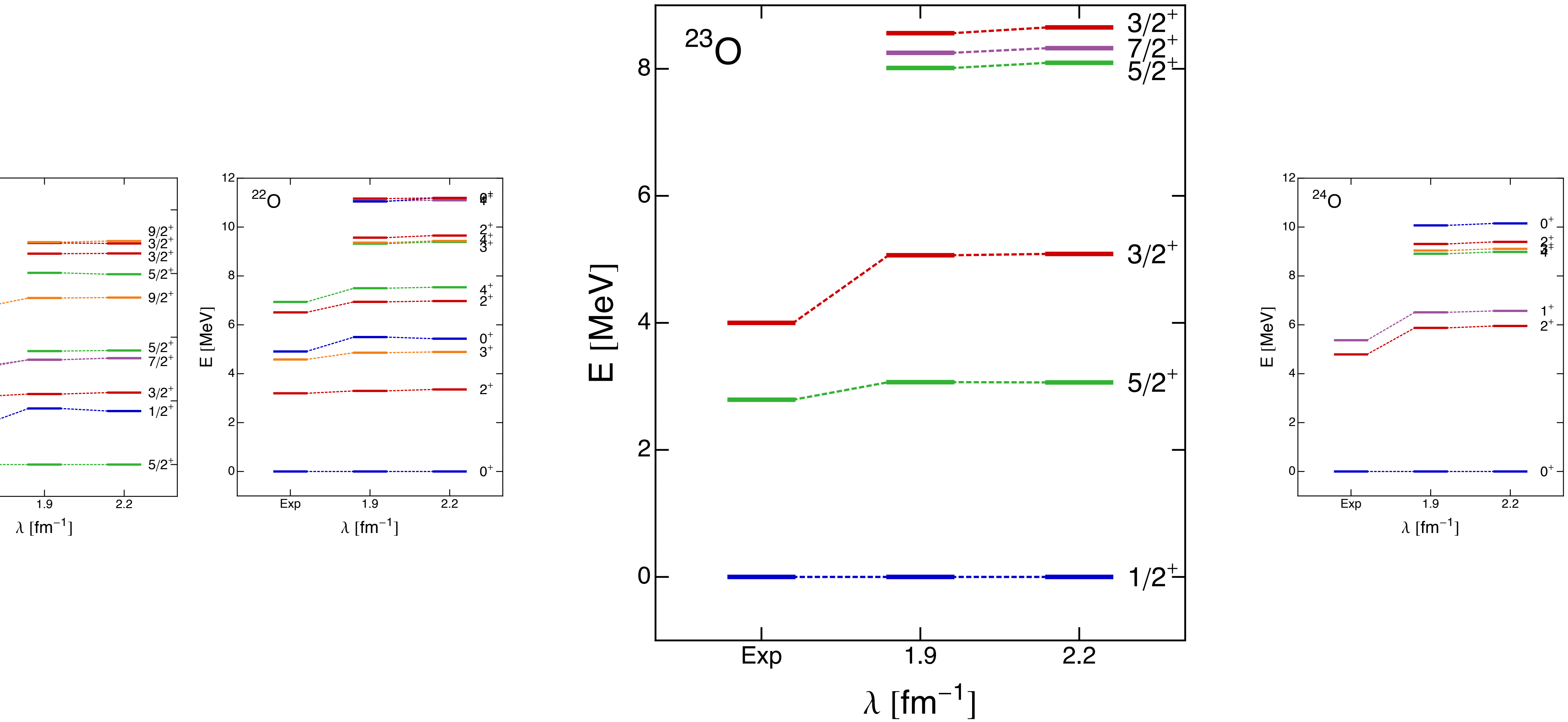
Oxygen Spectra



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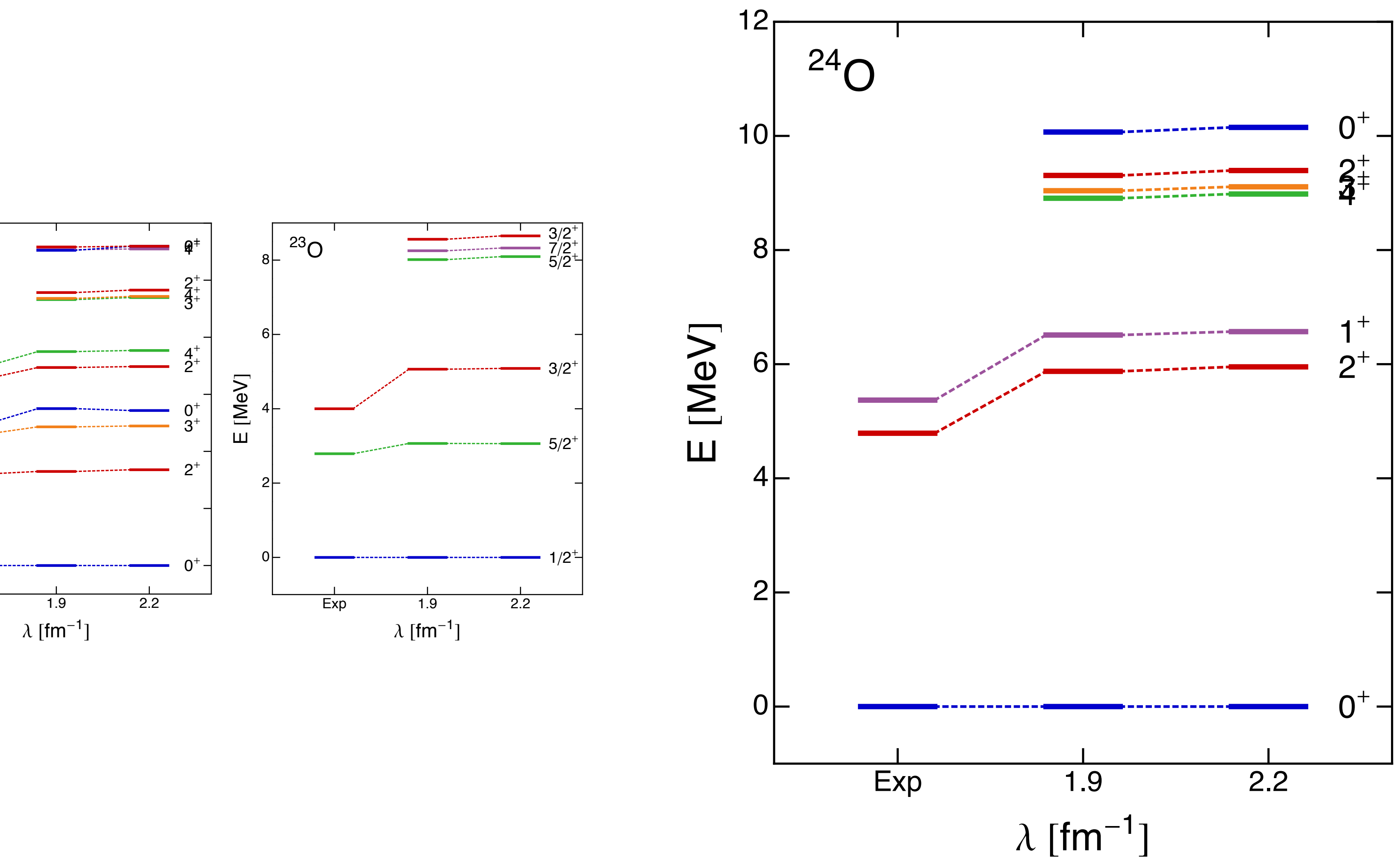
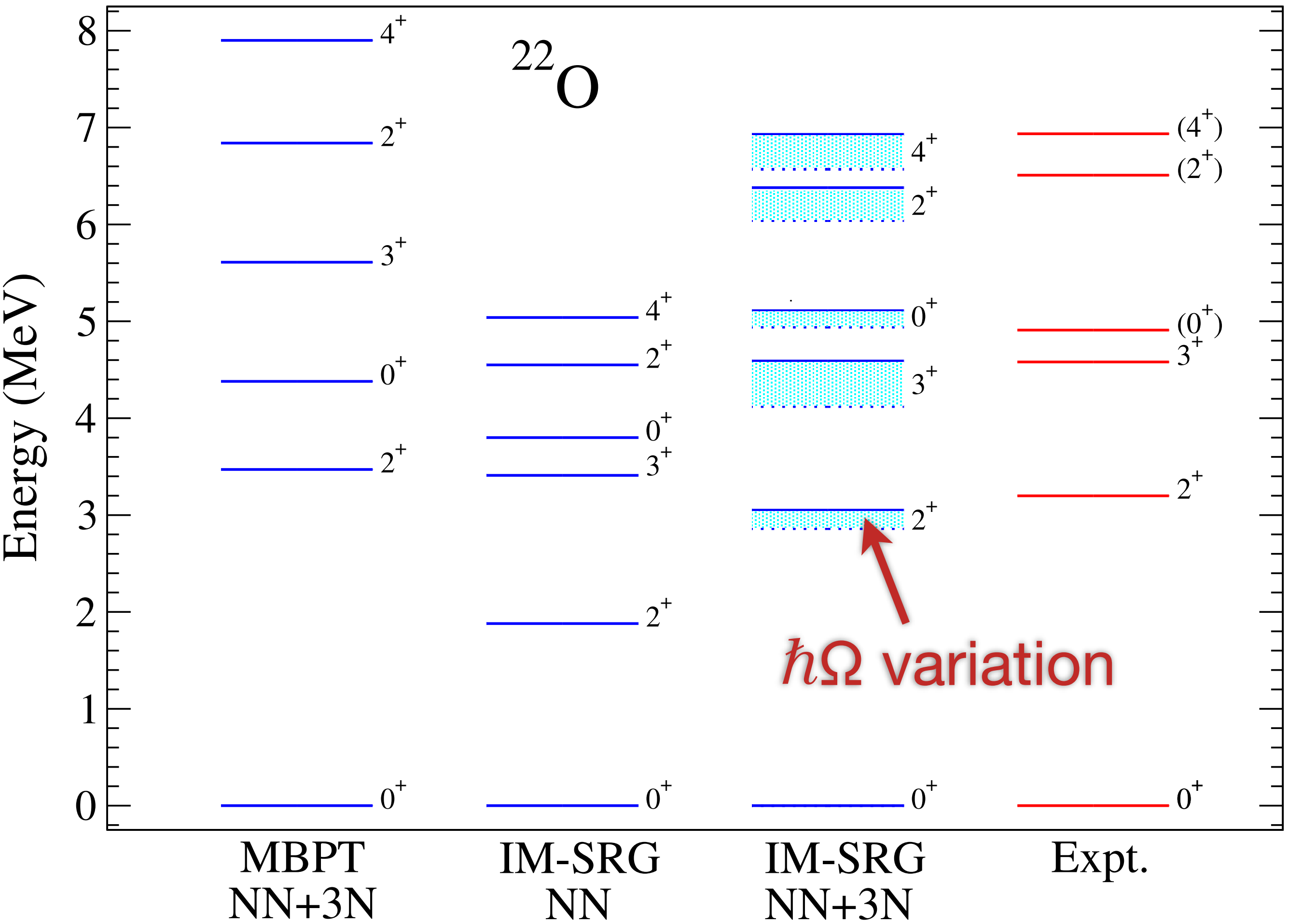


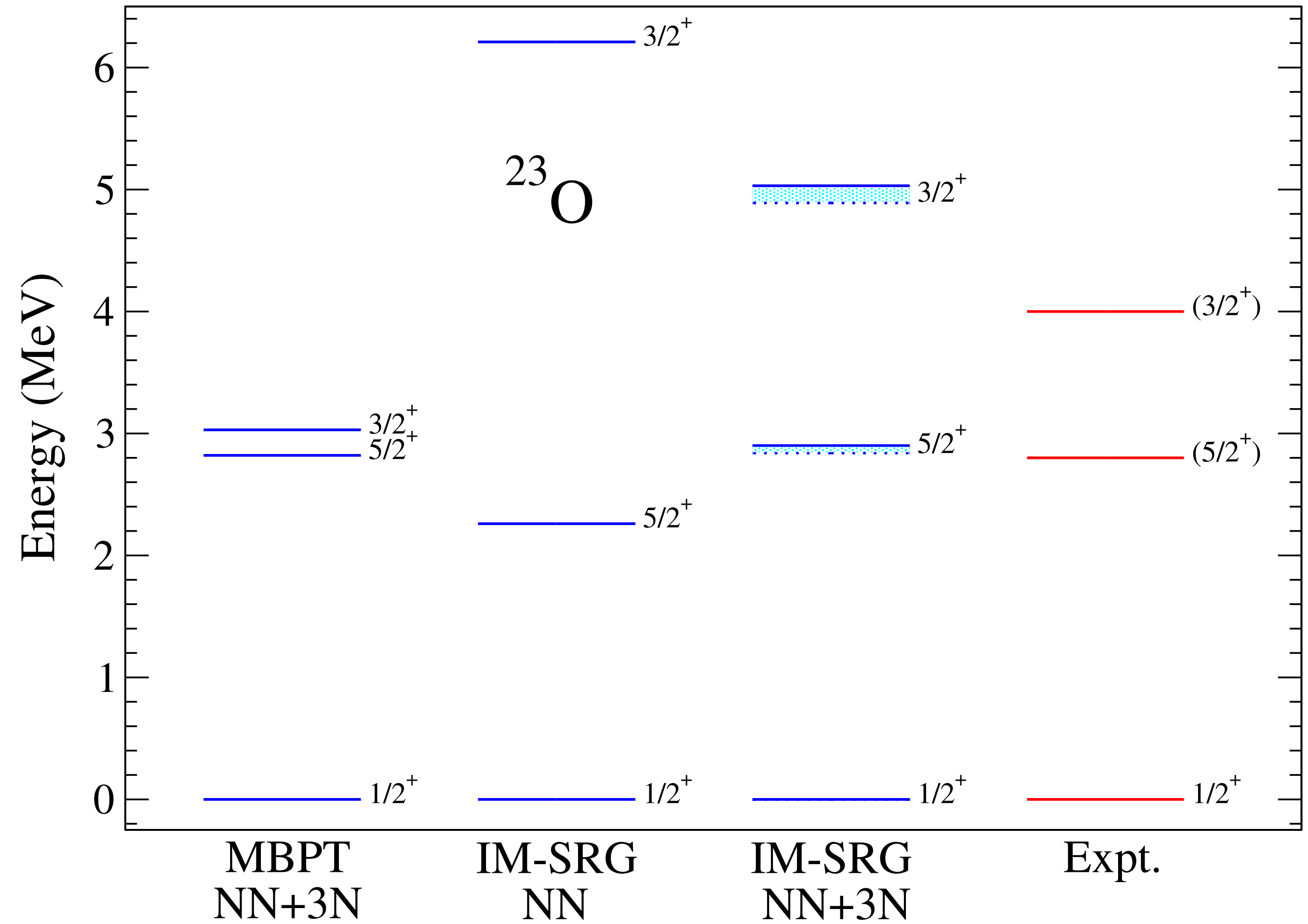
NN+3N-full (400), $e_{\text{Max}} = 10,\ E_{3\text{Max}} = 14,\ \hbar\Omega = 24$ MeV

- good description of low-lying states
- easy approach to spectra, odd nuclei, intrinsic deformation

➡ **but:** numerical effort determined by shell-model calculation

Comparison of Methods



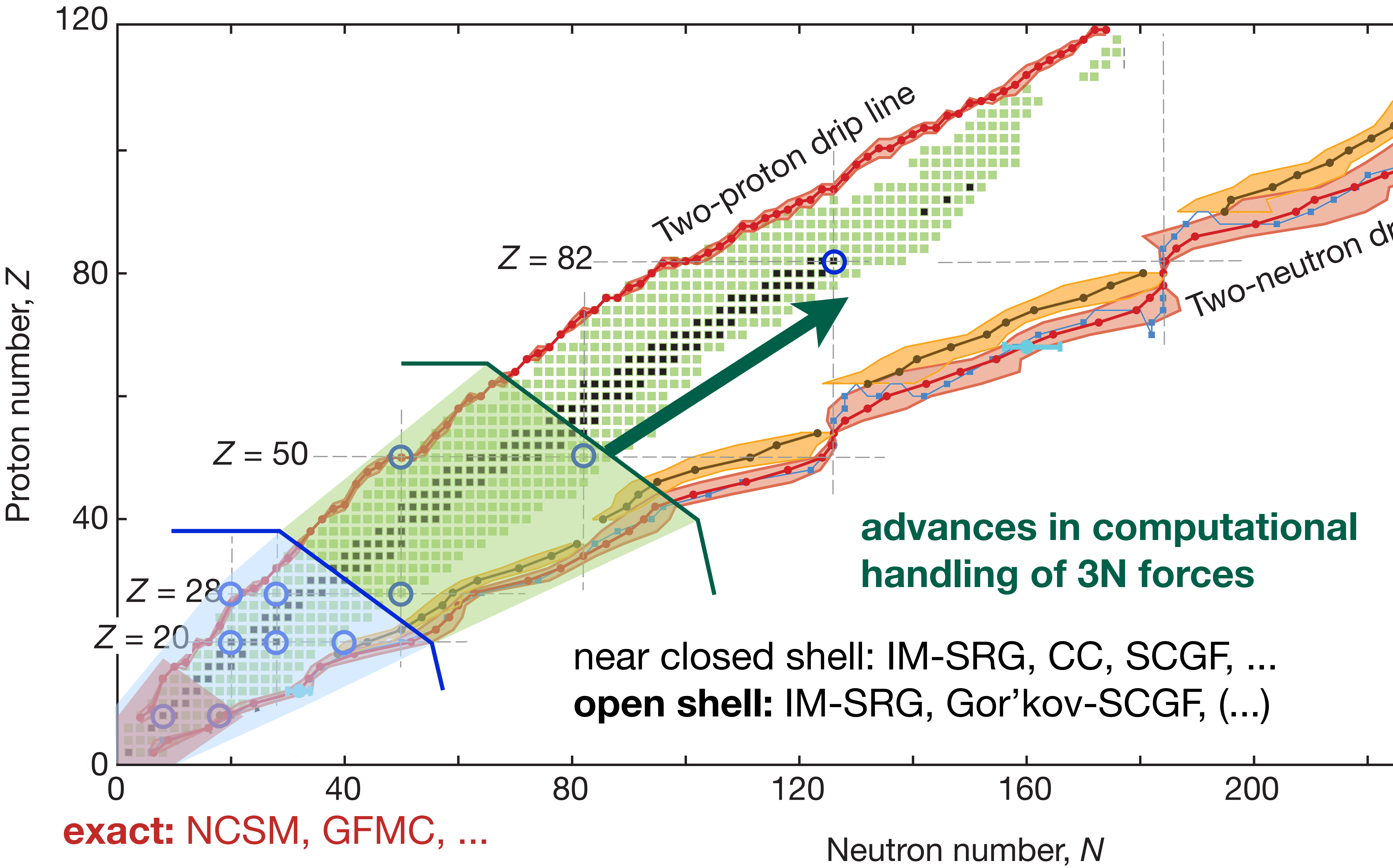


arXiv: 1402.1407 [nucl-th], [figures by J. Holt]

- **3N forces crucial**
- IM-SRG improves on finite-order effective interaction
- competitive with phenomenological calculations

Conclusions

Ab Initio Nuclear Structure



advances in computational handling of 3N forces

near closed shell: IM-SRG, CC, SCGF, ...

open shell: IM-SRG, Gor'kov-SCGF, (...)

exact: NCSM, GFMC, ...

Conclusions

- new era of ab initio nuclear structure and reaction theory, driven by SRG and EFT methods
- chiral interactions maintain stringent link to QCD
    - consistent, universal framework, but some open issues remain
- SRG to systematically change resolution scales of interactions (and observables)
    - improved convergence & control over approximations
    - enhanced reach of exact many-body methods
- In-Medium SRG as an innovative new many-body method
- many exciting applications ahead ...

Acknowledgments

THE OHIO STATE UNIVERSITY

S. Bogner, T. Morris
NSCL, Michigan State University

S. Binder, A. Calci, K. Hebeler, **J. Holt, J. Langhammer, R. Roth, A. Schwenk**
TU Darmstadt, Germany

R. J. Furnstahl, S. Koenig, S. More, R. J. Perry
The Ohio State University

K. A. Wendt
UT-Knoxville & Oak Ridge National Laboratory

P. Papakonstantinou
IBS / Rare Isotope Science Project, S. Korea

NSF
DEPARTMENT OF ENERGY · UNITED STATES OF AMERICA
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