In-Medium SRG with Chiral NN+3N Interactions

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Outline

- Similarity Renormalization Group in Nuclear Physics
- In-Medium SRG for Closed Shell-Nuclei
- Multi-Reference In-Medium SRG
- Open-Shell Nuclei
- IM-SRG + Shell Model
- Outlook

Similarity Renormalization Group in Nuclear Physics

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 HH, Phys. Rev. **C77** (2008), 064003

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

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

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

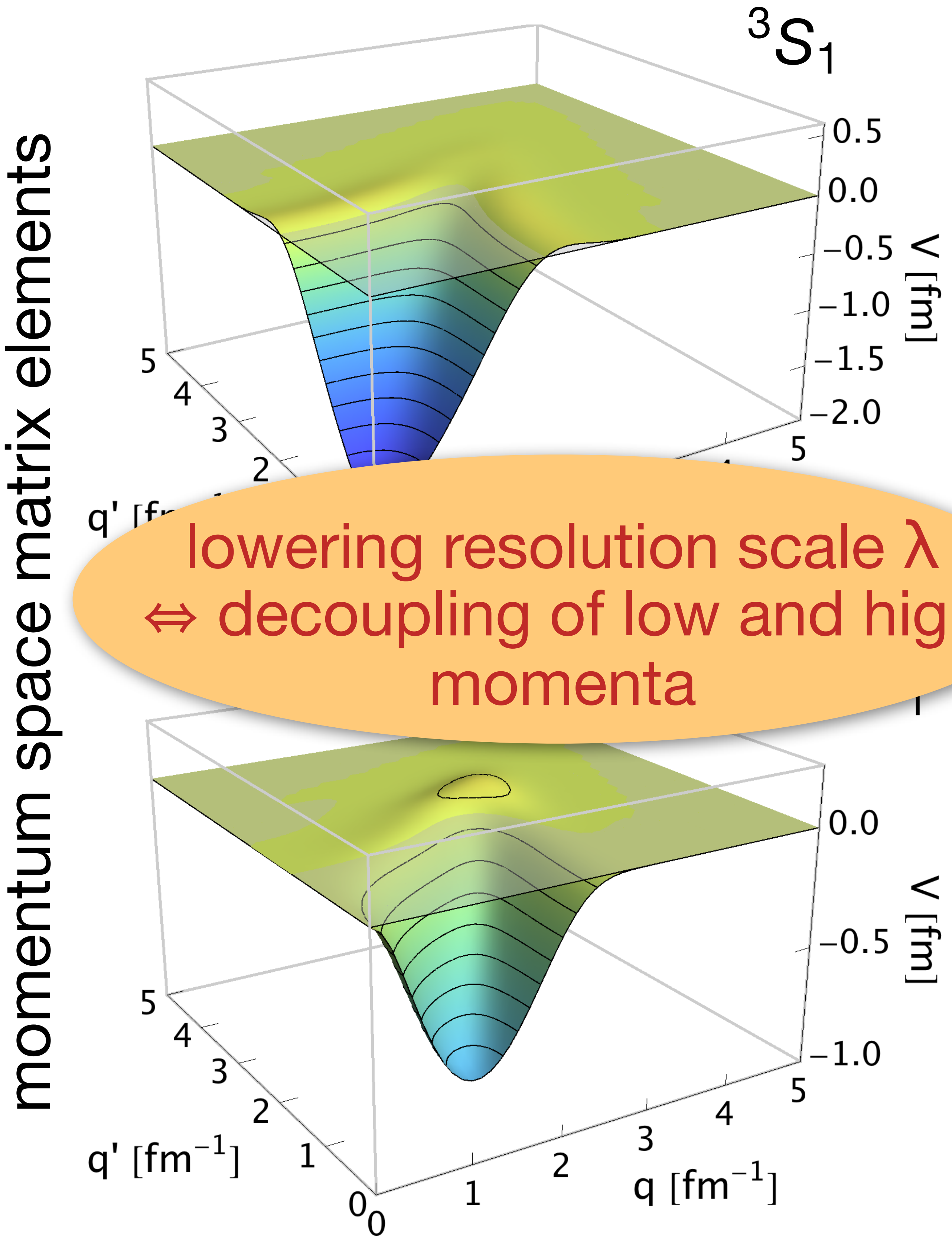
- flow equation:

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

- 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



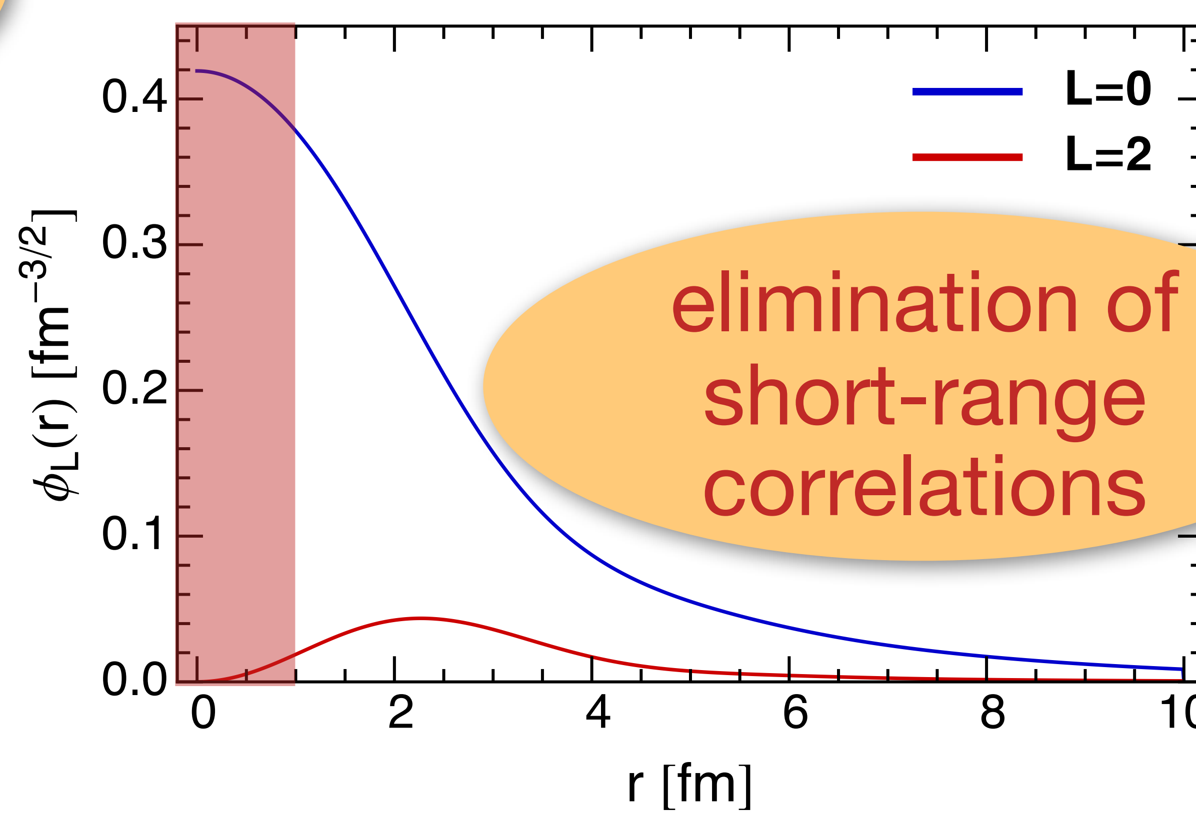
lowering resolution scale λ
⇔ decoupling of low and high momenta

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

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

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

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:

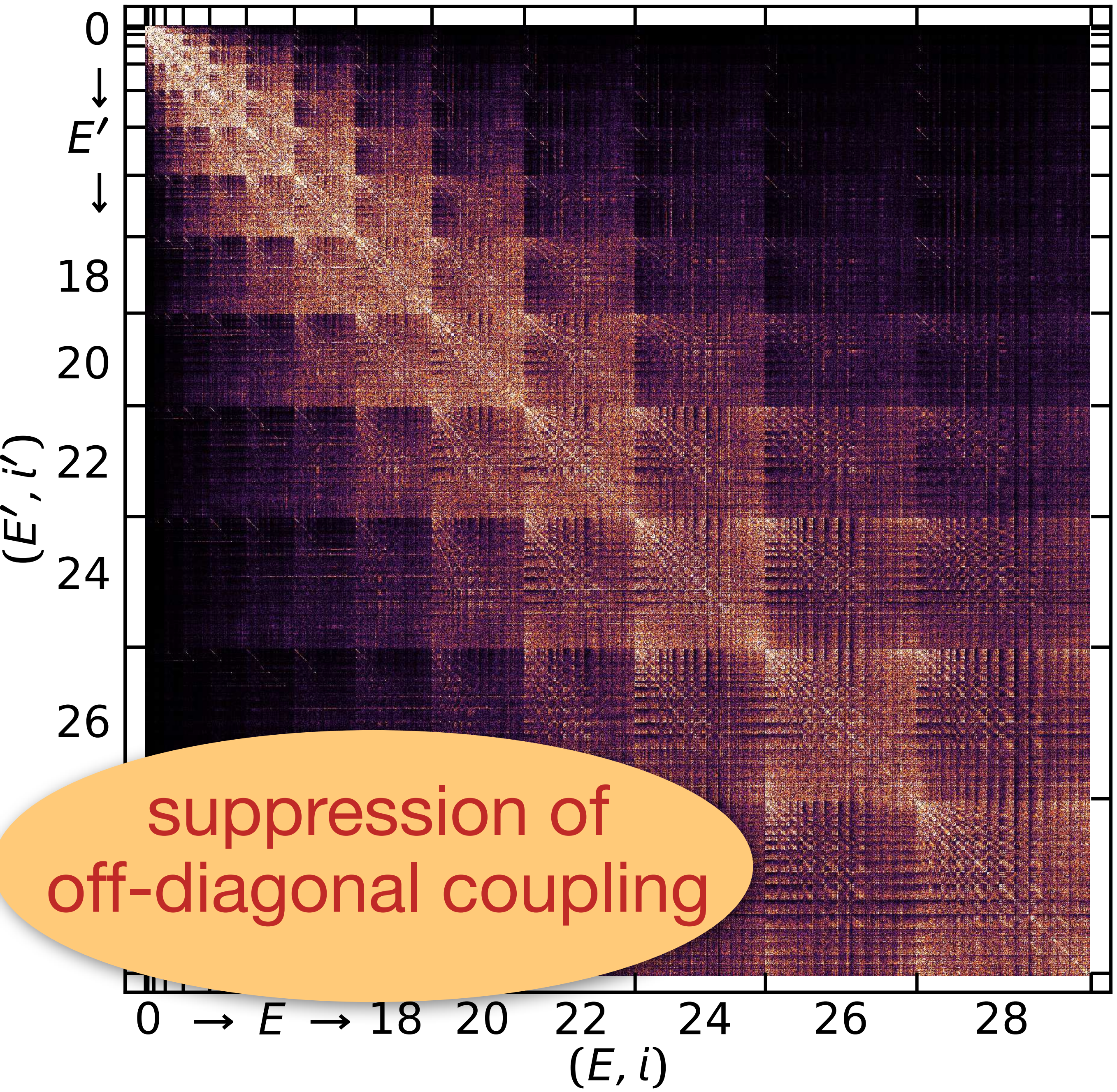
$$\frac{dH}{d\lambda} = [[\sum a^\dagger a, \sum \underbrace{a^\dagger a^\dagger a a}_{2-body}], \sum \underbrace{a^\dagger a^\dagger a a}_{2-body}] + \ldots = \sum \underbrace{a^\dagger a^\dagger a^\dagger a a a}_{3-body} + \ldots$$

- 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; Wendt, arXiv:1304.1431 [nucl-th])
- use λ-dependence of eigenvalues as a diagnostic for size of omitted induced interactions

SRG in Three-Body Space

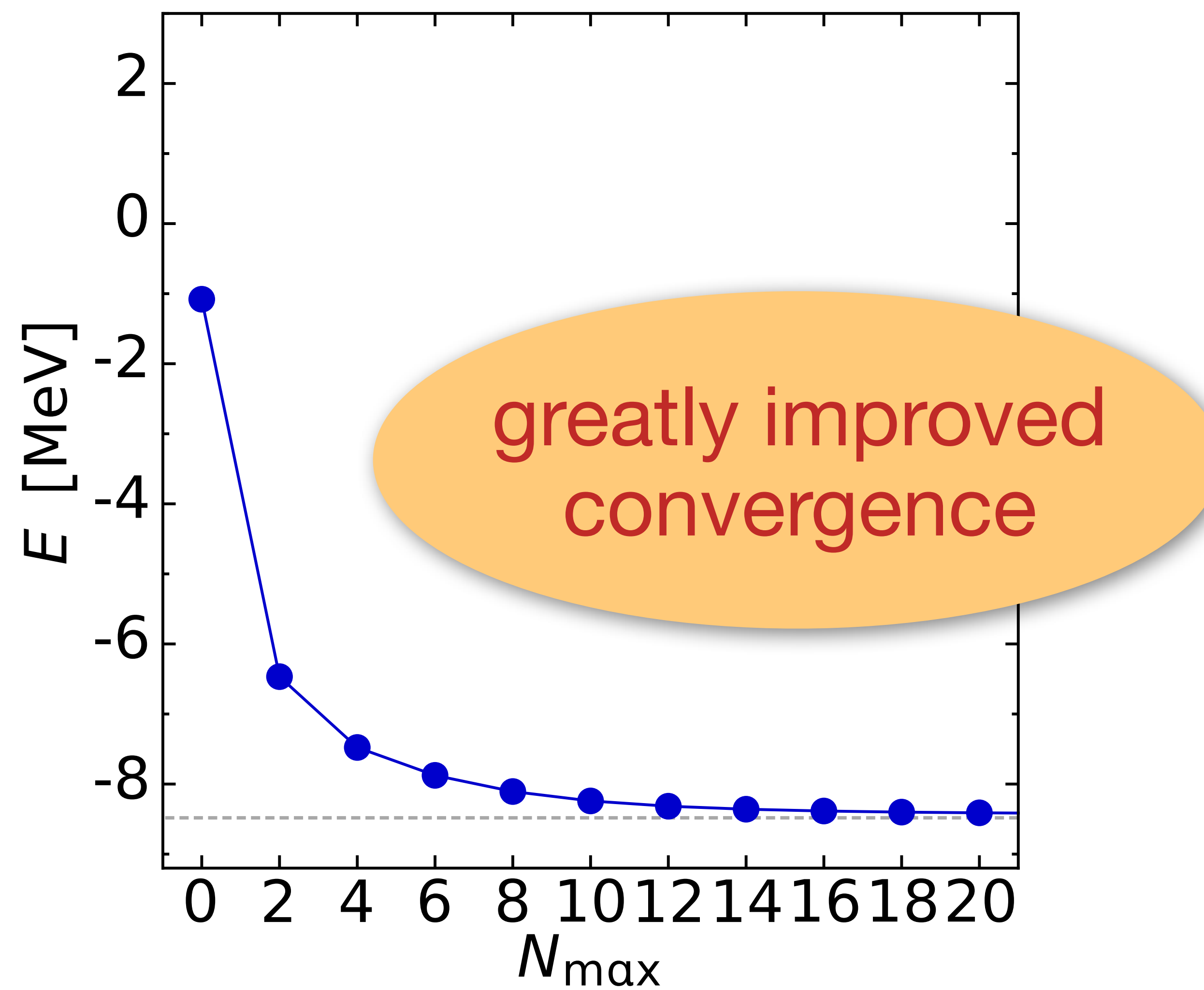
3B Jacobi-HO Matrix Elements

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



λ = 1.33 fm^{-1}

^{3}H ground-state (NCSM)

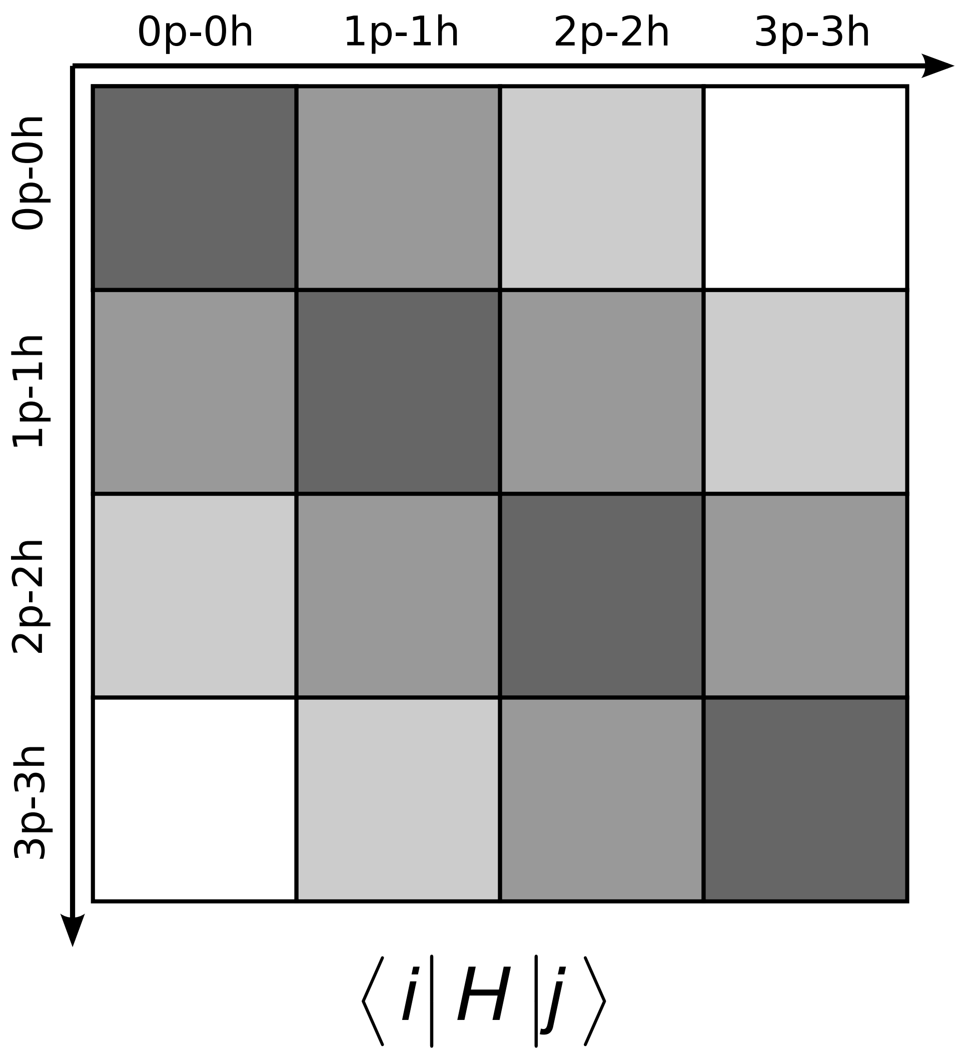


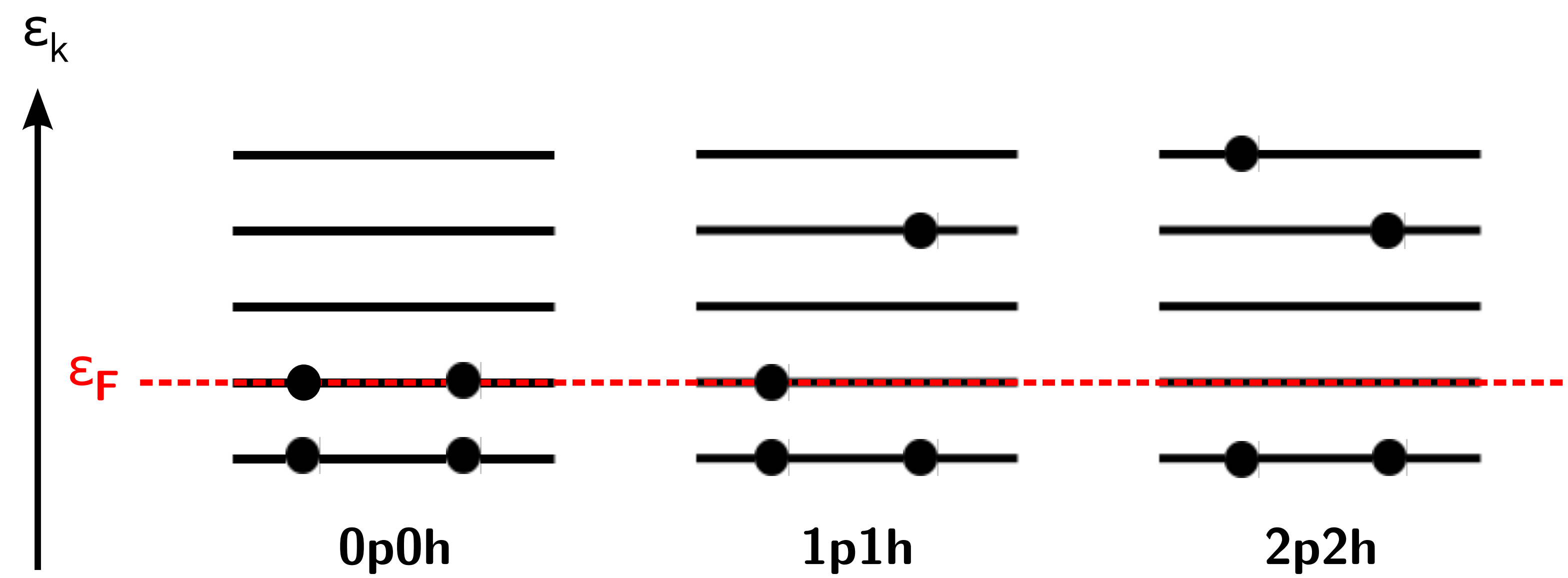
[figures by R. Roth, A. Calci, J. Langhammer]

In-Medium SRG for Closed-Shell Nuclei

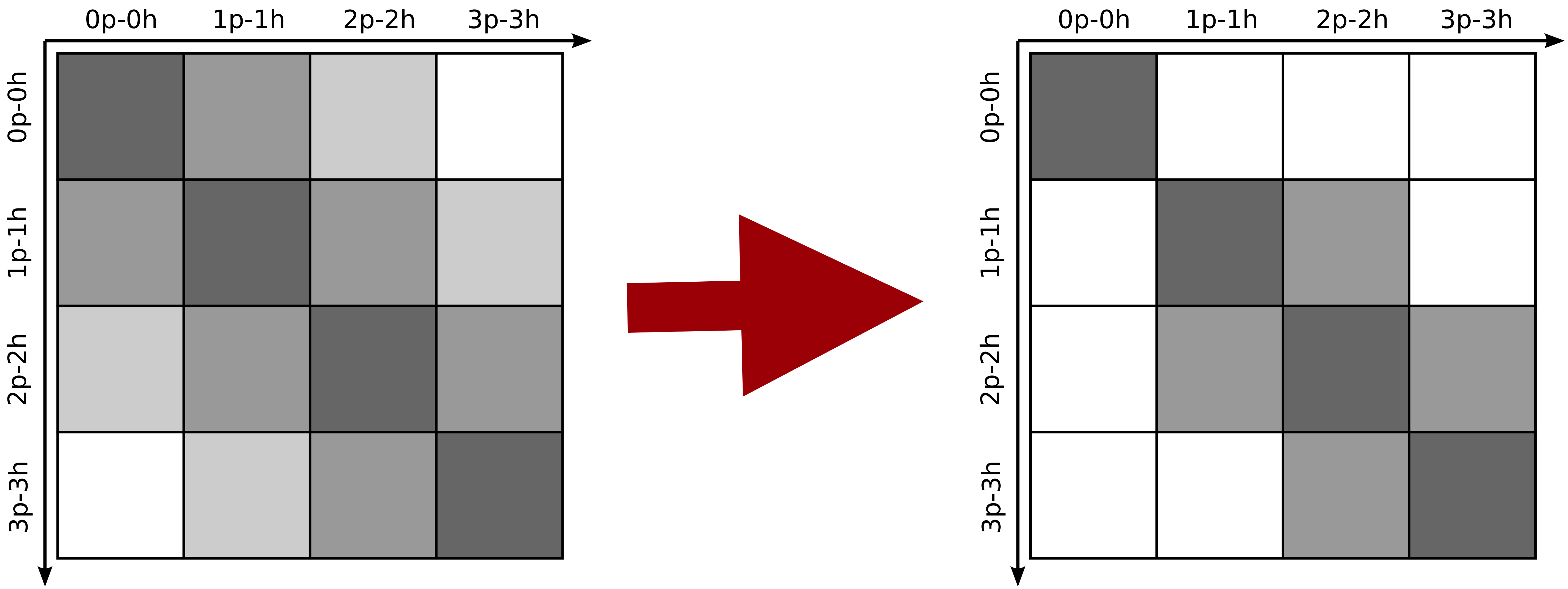
HH, S. K. Bogner, S. Binder, A. Calci, J. Langhammer, R. Roth, and A. Schwenk,
Phys. Rev. C **87**, 034307 (2013)
K. Tsukiyama, S. K. Bogner, and A. Schwenk, Phys. Rev. Lett. **106**, 222502 (2011)

Decoupling in A-Body Space





Decoupling in A-Body Space



$\langle i | H | j \rangle$ $\qquad$ $\langle i | H(\infty) | j \rangle$

aim: decouple reference state (0p-0h) from excitations

Normal Ordering

- second quantization: $A^{k_1 \ldots k_N}_{l_1 \ldots l_N} = a^\dagger_{k_1} \ldots a^\dagger_{k_N} a_{l_N} \ldots a_{l_1}$
- 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:

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

- algebra is simplified significantly because

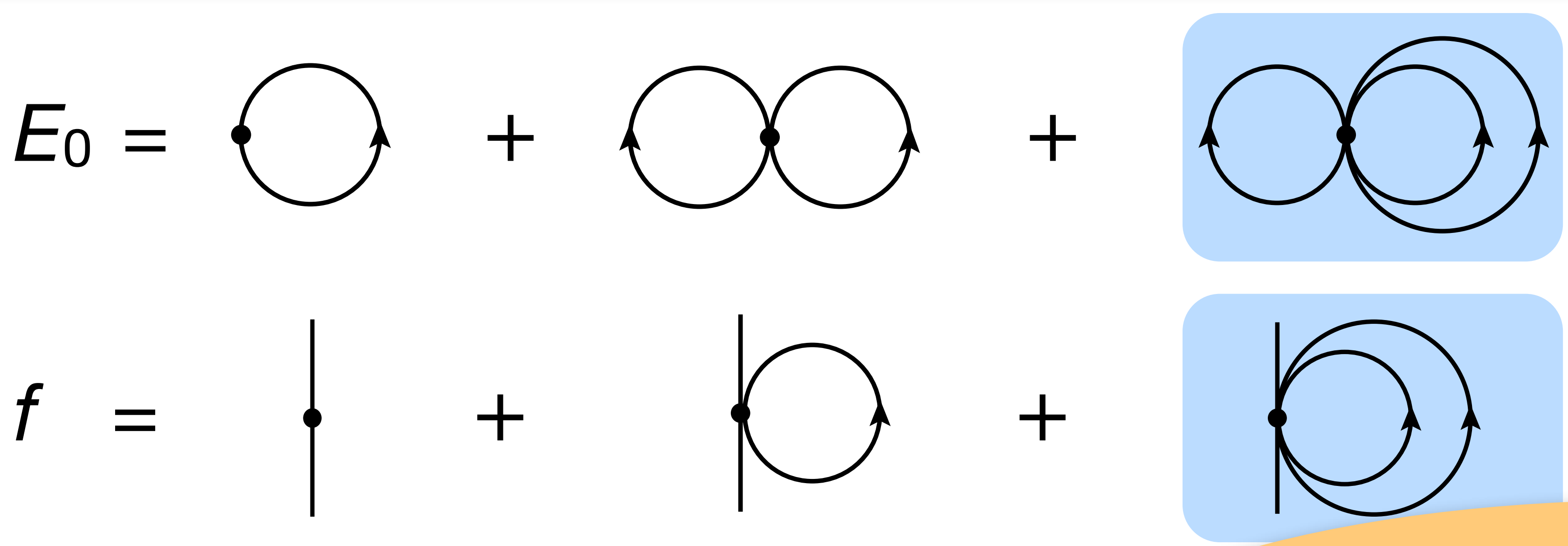
$$\left\langle \Phi \right| :A^{k_1 \ldots k_N}_{l_1 \ldots l_N}: \left| \Phi \right\rangle = 0$$

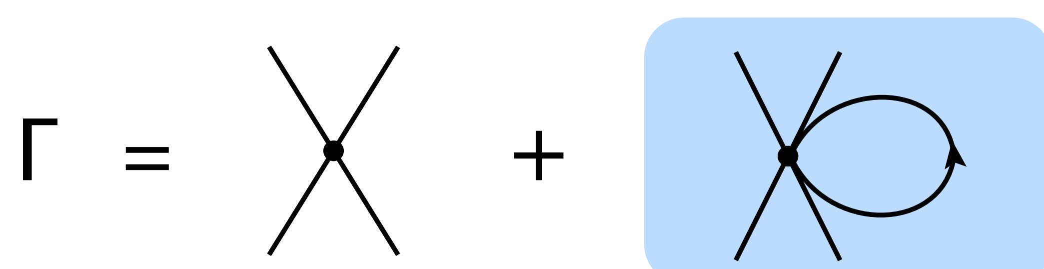
- Wick's theorem gives simplified expansions (fewer terms!) for products of normal-ordered operators

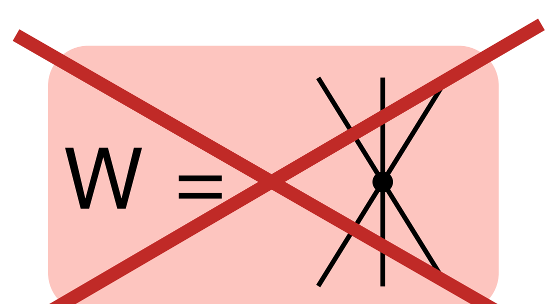
Normal-Ordered Hamiltonian

Normal-Ordered Hamiltonian

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



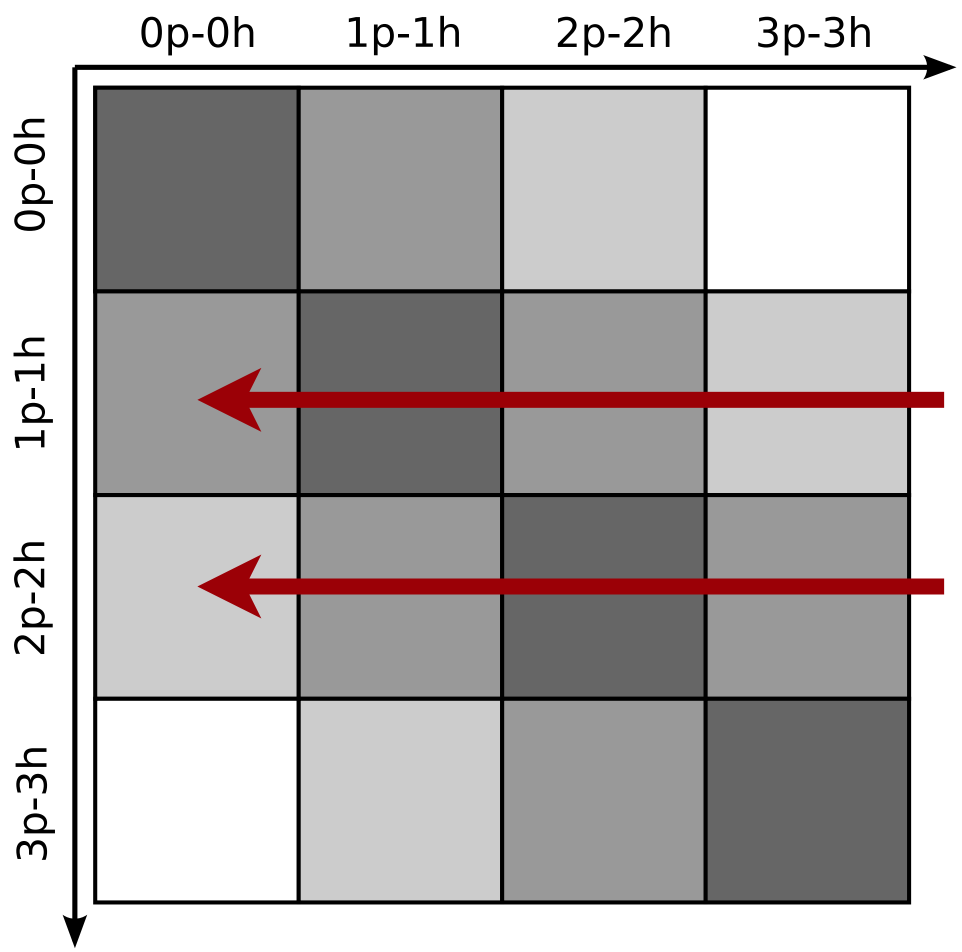




two-body formalism with in-medium contributions from three-body interactions

Normal ordering w.r.t. Hartree-Fock solution for **complete** NN(+3N) Hamiltonian!

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

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

Choice of Generator

- Wegner

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

- White (J. Chem. Phys. 117, 7472)

$$\eta^{II} = \sum_{ph} \frac{f^{p}_{h}}{E_p - E_h} :A^{p}_{h}: + \sum_{pp'hh'} \frac{\Gamma^{pp'}_{hh'}}{E_{pp'} - E_{hh'}} :A^{pp'}_{hh'}: + \text{H.c.}$$

$E_p - E_h, E_{pp'} - E_{hh'}$: approx. 1p1h, 2p2h excitation energies

- off-diagonal matrix elements are suppressed like $e^{-\Delta E^2 s}$ (Wegner) or e^{-s} (White)
- g.s. energies ($s \to \infty$) for both generators agree within a few keV

In-Medium SRG Flow Equations

0-body Flow

$$\frac{dE}{ds} = \sum_{ab}(n_a - n_b)\left(\eta^a_b f^b_a - f^a_b \eta^b_a\right) + \frac{1}{4}\sum_{abcd}\left(\eta^{ab}_{cd}\Gamma^{cd}_{ab} - \Gamma^{ab}_{cd}\eta^{cd}_{ab}\right) n_a n_b \bar{n}_c \bar{n}_d$$

1-body Flow

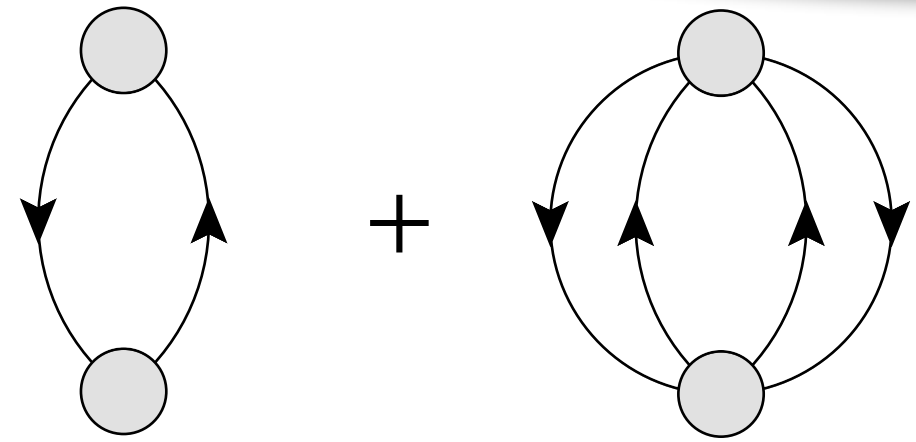
$$\frac{d}{ds}f^1_2 = \sum_a \left(\eta^1_a f^a_2 - f^1_a \eta^a_2\right) + \sum_{ab}\left(\eta^a_b \Gamma^{b1}_{a2} - f^a_b \eta^{b1}_{a2}\right)(n_a - n_b)$$
$$+ \frac{1}{2}\sum_{abcdef}\left(\eta^{1a}_{bc}\Gamma^{bc}_{2a} - \Gamma^{1a}_{bc}\eta^{bc}_{2a}\right)(n_a \bar{n}_b \bar{n}_c + \bar{n}_a n_b n_c)$$

In-Medium SRG Flow Equations

0-body Flow

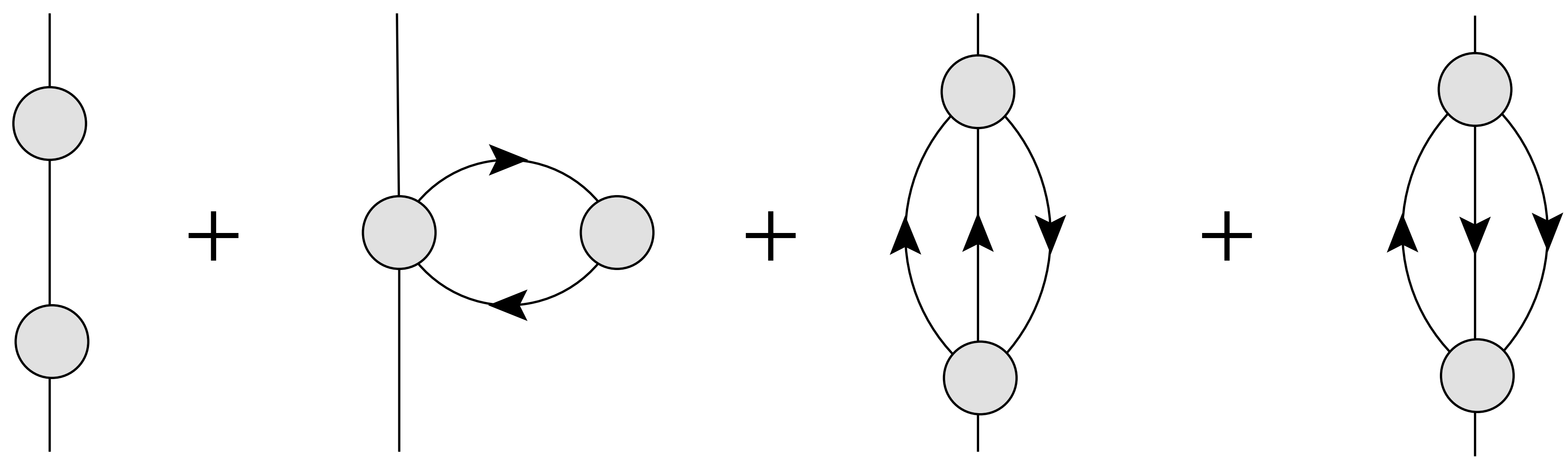
~ 2nd order MBPT for *H(s)*

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



1-body Flow

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



(White generator, Hugenholtz diagrams)

In-Medium SRG Flow Equations

2-body Flow

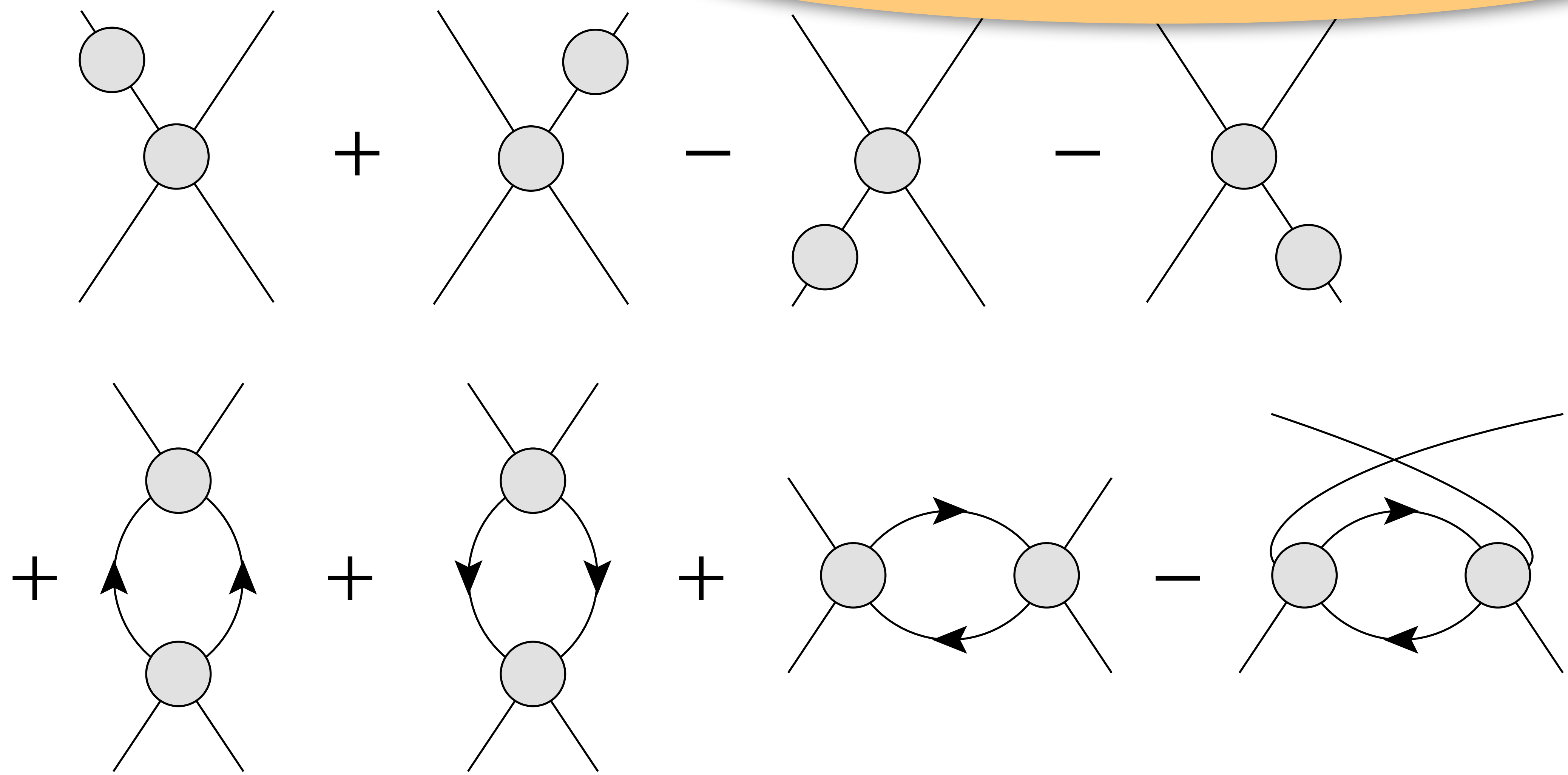
$$
\begin{aligned}
\frac{d}{ds}\Gamma^{12}_{34} = \sum_a \Big(&\eta^1_a \Gamma^{a2}_{34} + \eta^2_a \Gamma^{1a}_{34} - \eta^a_3 \Gamma^{12}_{a4} - \eta^a_4 \Gamma^{12}_{3a} - f^1_a \eta^{a2}_{34} - f^2_a \eta^{1a}_{34} + f^a_3 \eta^{12}_{a4} + f^a_4 \eta^{12}_{3a}\Big) \\
&+ \frac{1}{2}\sum_{ab}\left(\eta^{12}_{ab}\Gamma^{ab}_{34} - \Gamma^{12}_{ab}\eta^{ab}_{34}\right)(1 - n_a - n_b) \\
&+ \sum_{ab}(n_a - n_b)\left(\left(\eta^{1a}_{3b}\Gamma^{2b}_{4a} - \Gamma^{1a}_{3b}\eta^{2b}_{4a}\right) - \left(\eta^{2a}_{3b}\Gamma^{1b}_{4a} - \Gamma^{2a}_{3b}\eta^{1b}_{4a}\right)\right)
\end{aligned}
$$

In-Medium SRG Flow Equations

2-body Flow

only linked diagrams contribute, IM-SRG size-extensive

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



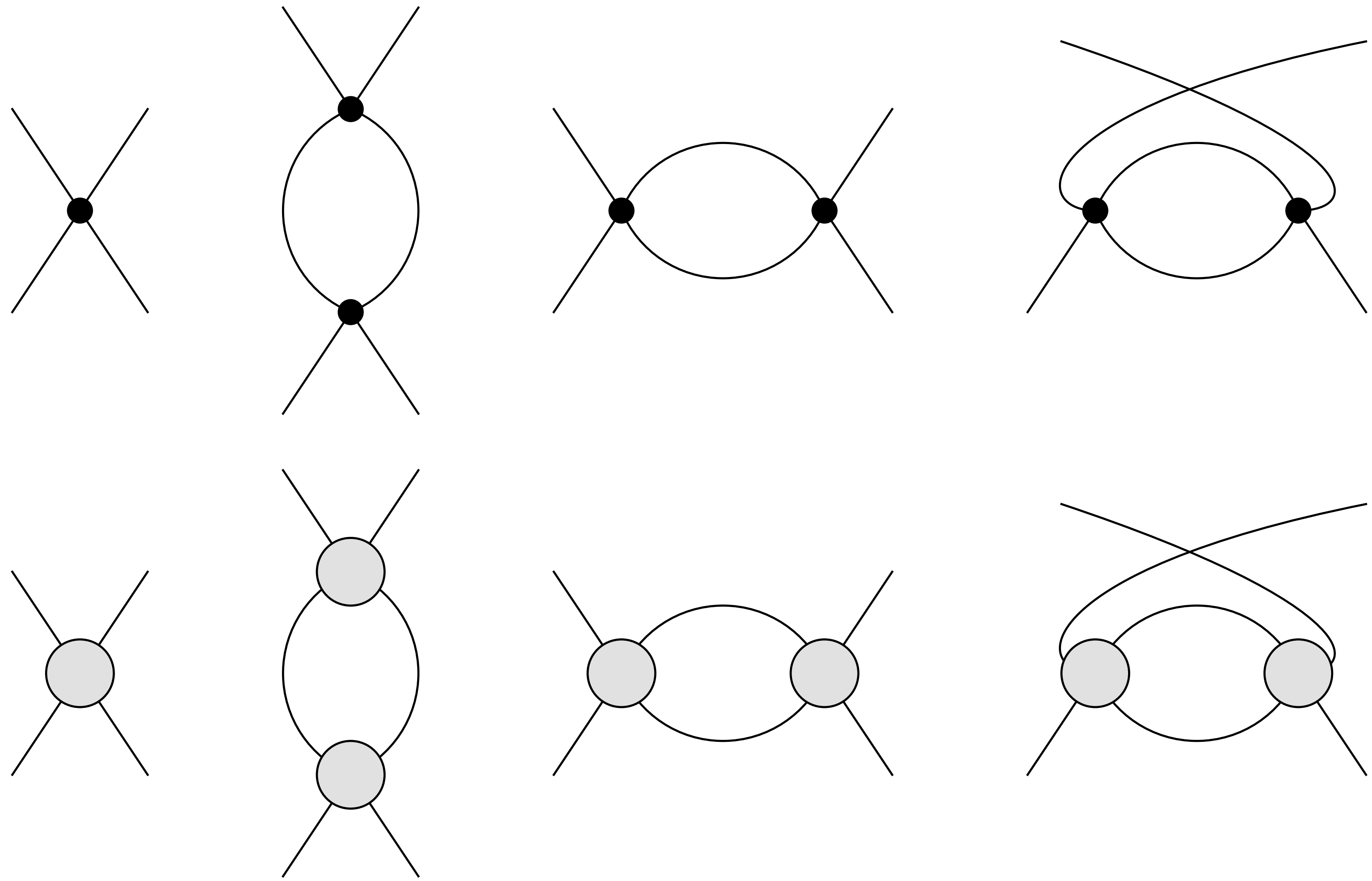
s channel — ladders

t channel, *u* channel — rings

In-Medium SRG Flow: Diagrams

$\Gamma(\delta s) \sim$

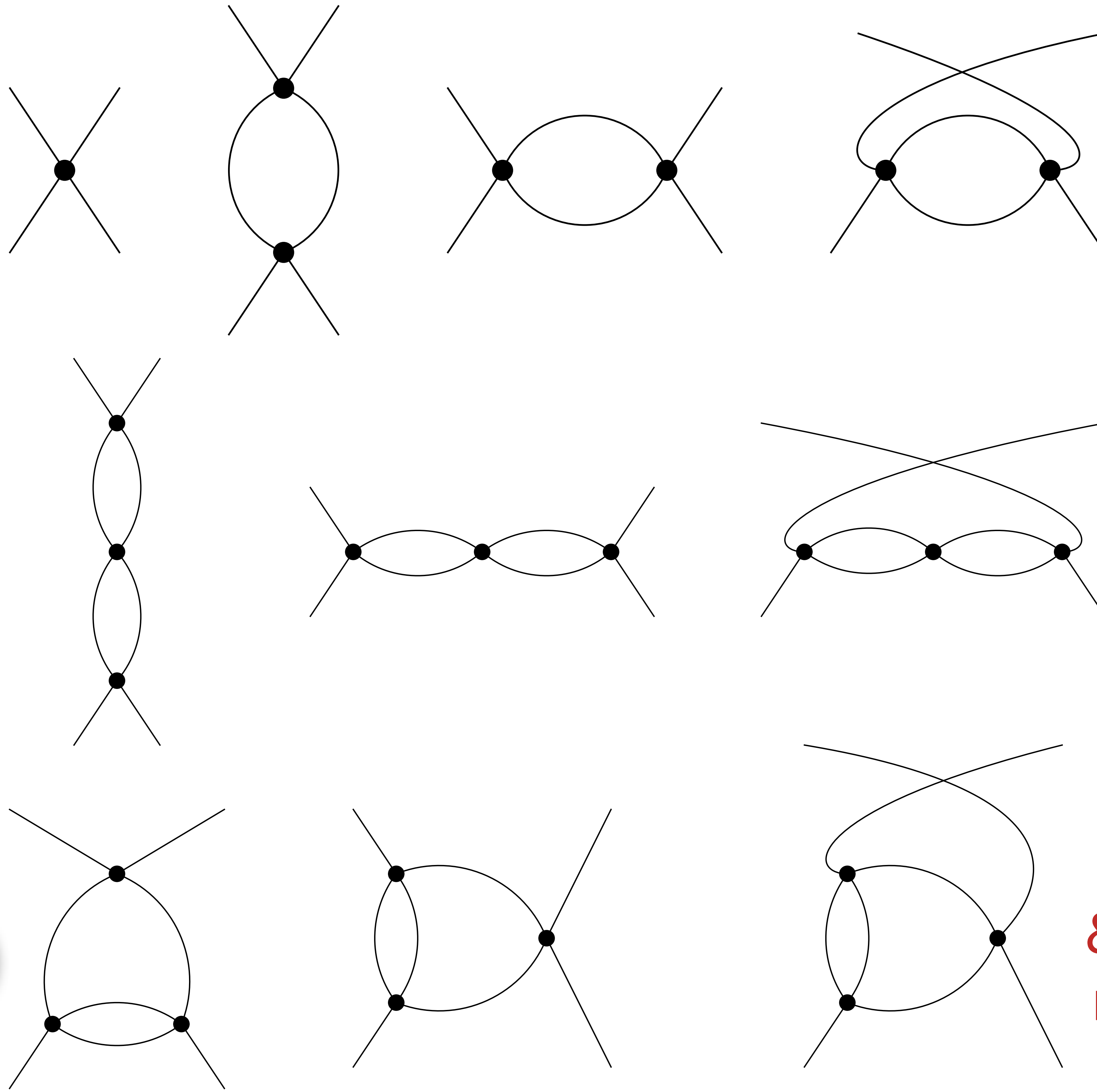
$\Gamma(2\delta s) \sim$



In-Medium SRG Flow: Diagrams

$\Gamma(\delta s) \sim$

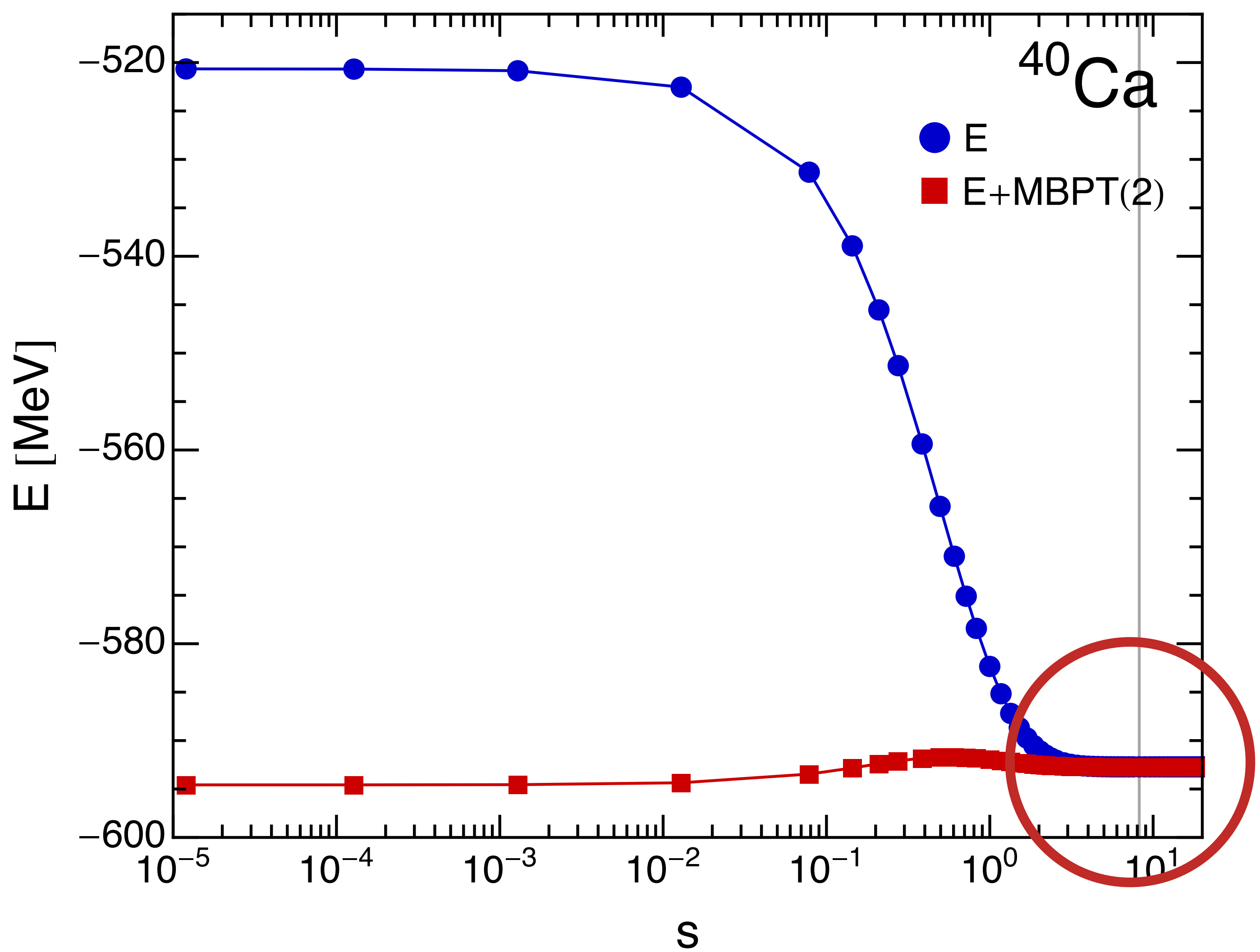
$\Gamma(2\delta s) \sim$

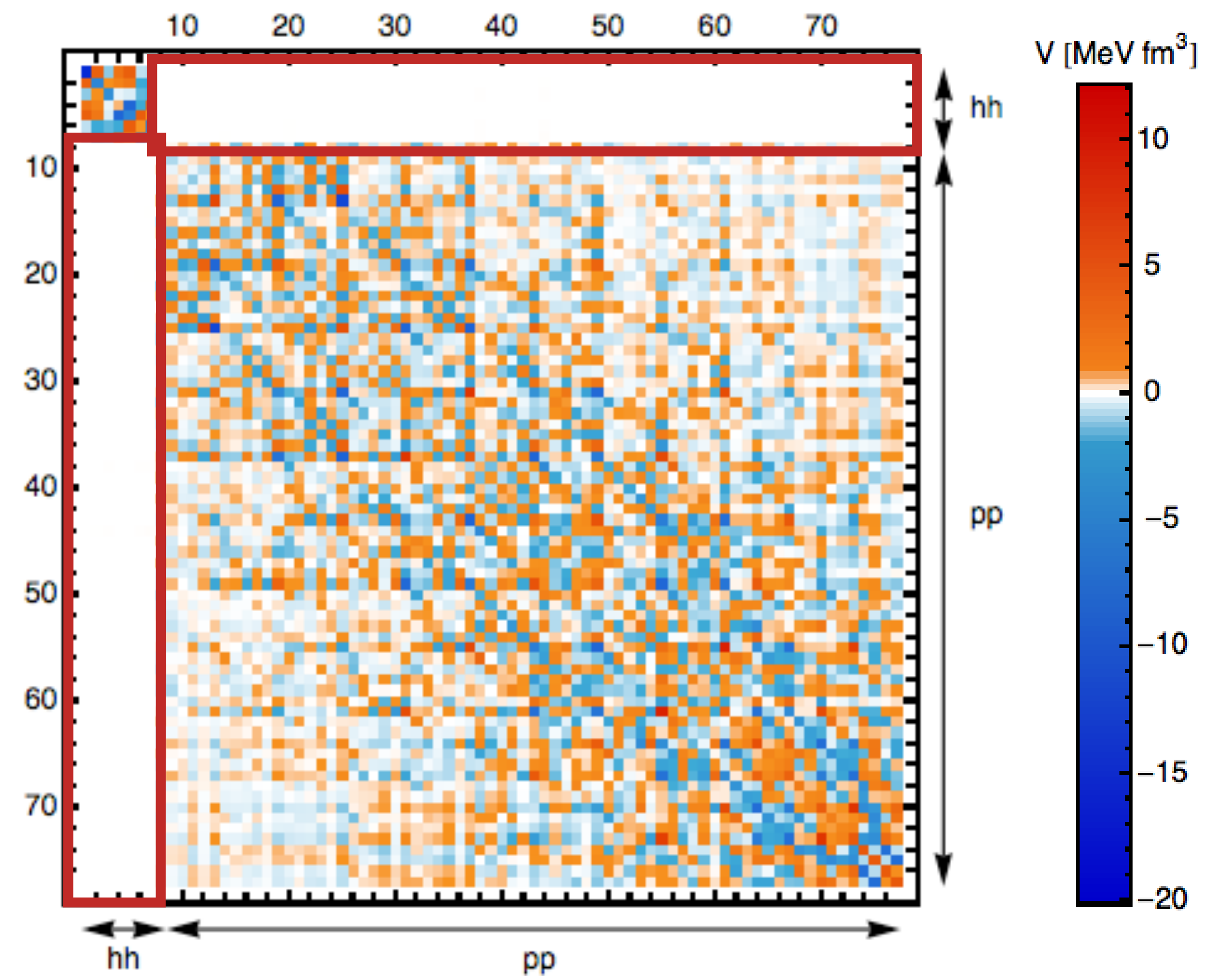


non-perturbative resummation

& many more...

Decoupling



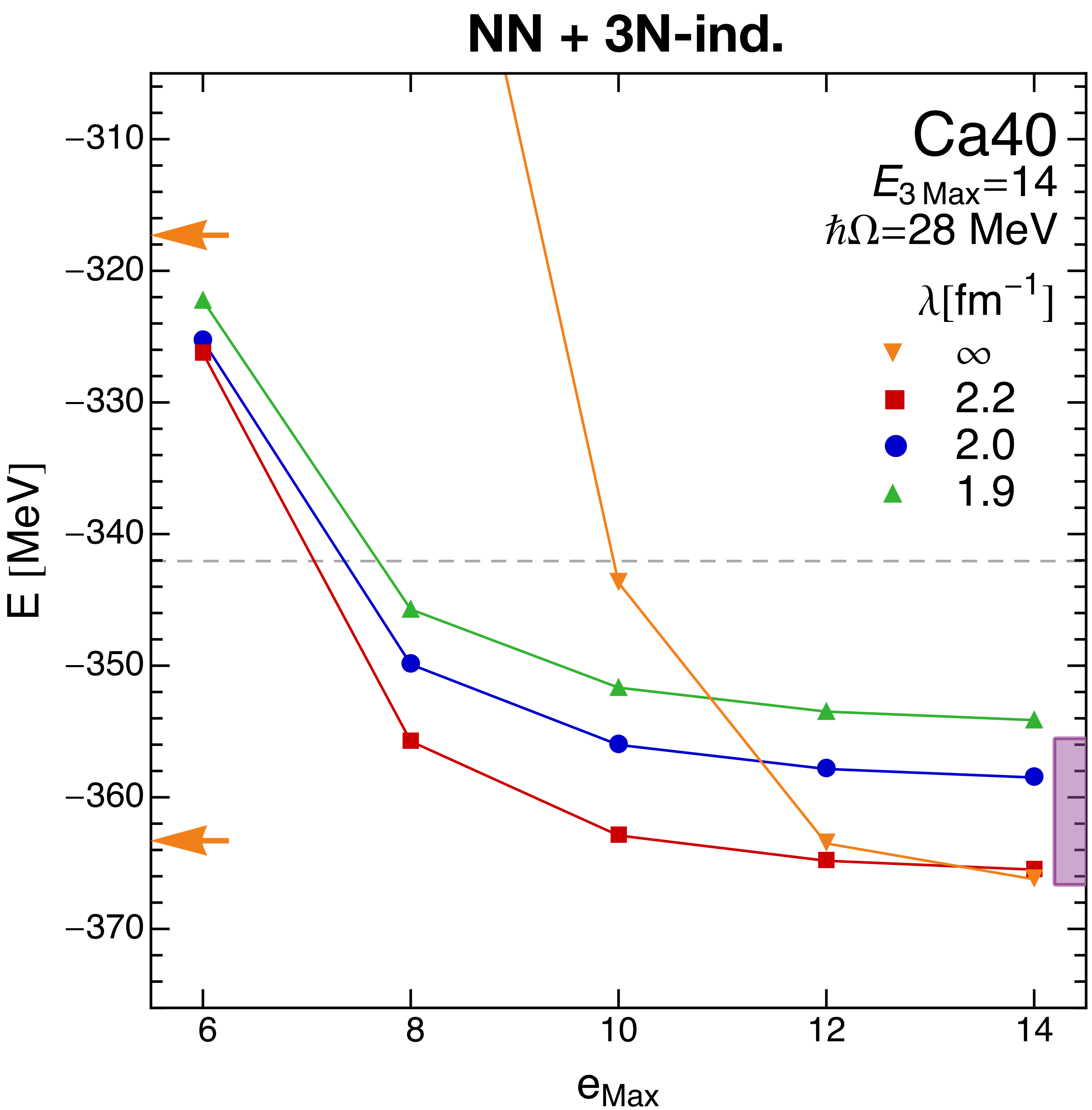


N3LO, $\lambda = 2.0\ \mathrm{fm}^{-1}, e_{\mathrm{Max}} = 8$

non-perturbative resummation of MBPT series (correlations)

off-diagonal couplings are rapidly driven to zero

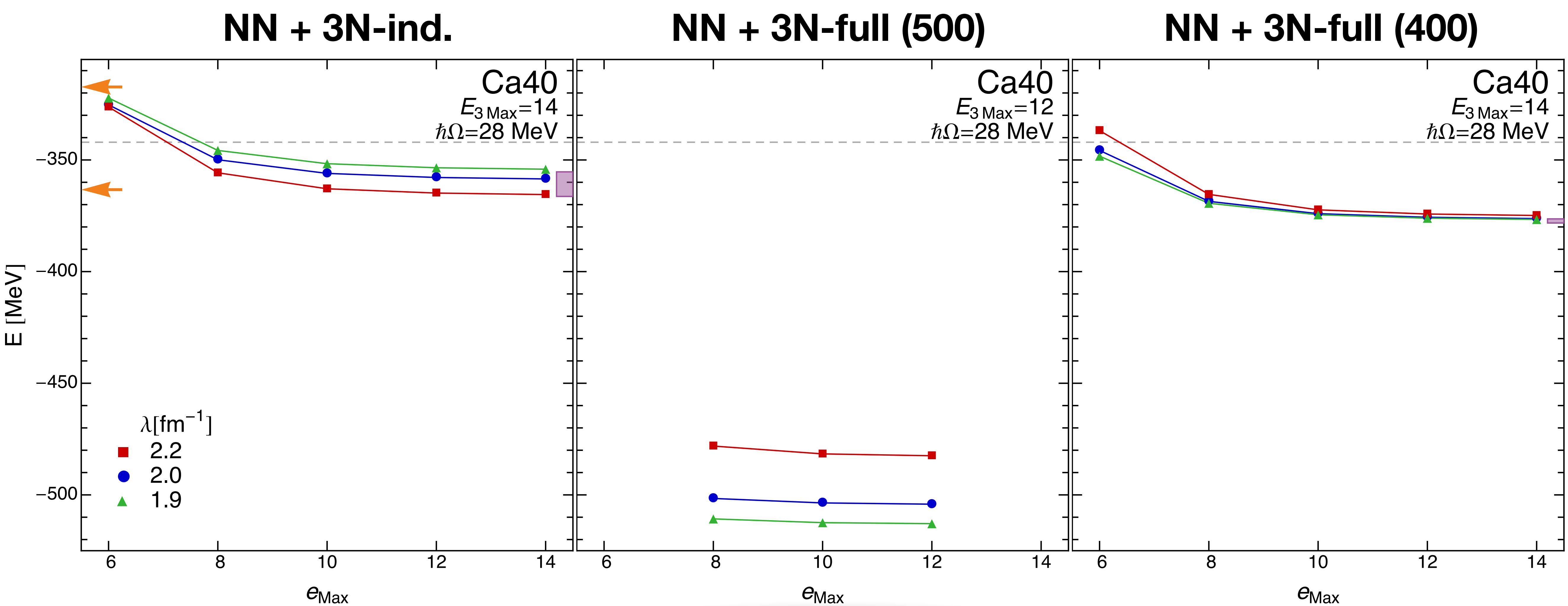
Results: Closed-Shell Nuclei



CCSD/Λ-CCSD(T), $\lambda = \infty$, G. Hagen et al., PRL 109, 032502 (2012)

Λ-CCSD(T), $\lambda = 1.9 - 2.2\ \mathrm{fm}^{-1}$, S.Binder et al., arXiv:1211.4748 [nucl-th] & PRL 109, 052501 (2012)

Results: Closed-Shell Nuclei

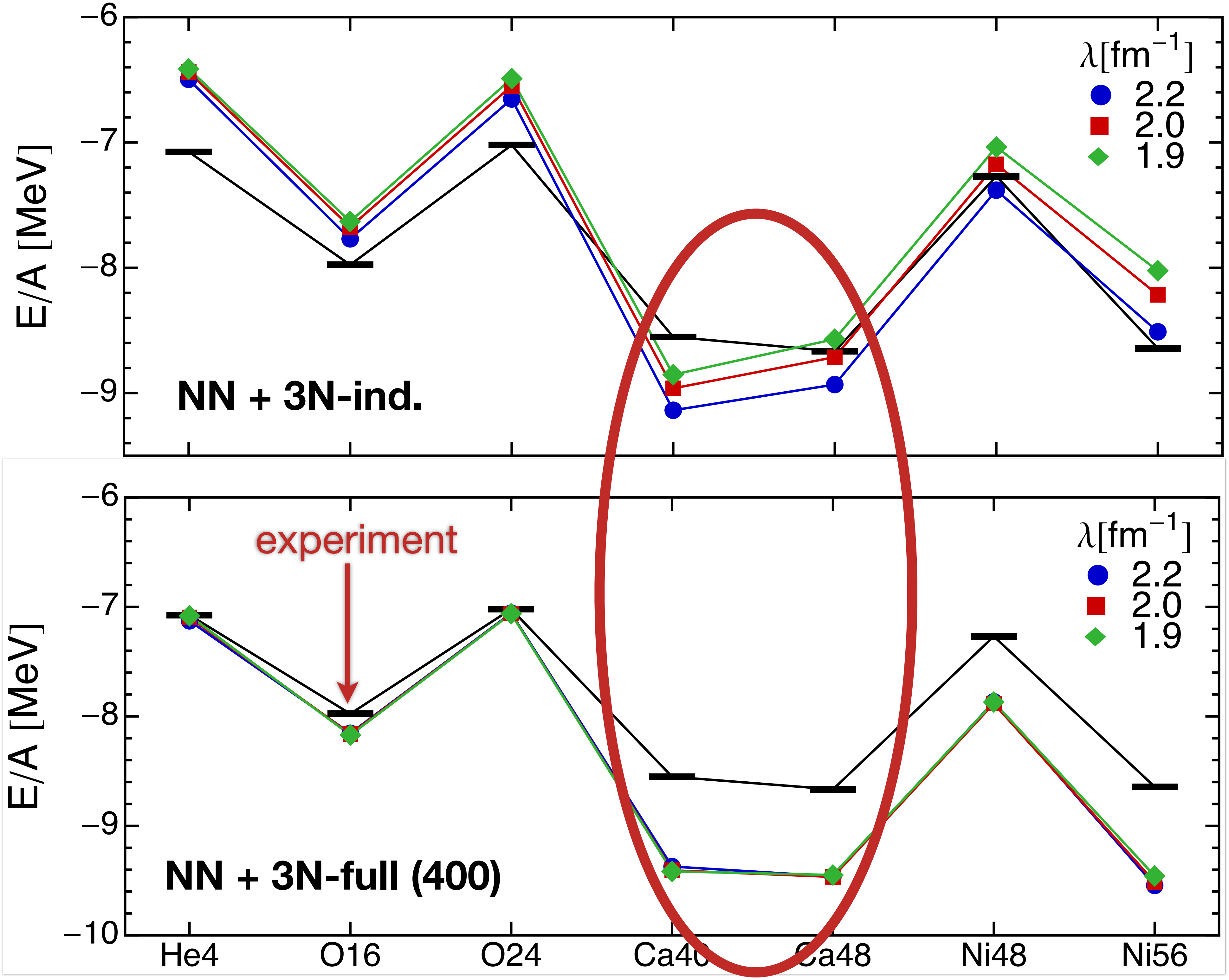


validate chiral Hamiltonians

CCSD/Λ-CCSD(T), $\lambda = \infty$, G. Hagen et al., PRL 109, 032502 (2012)

Λ-CCSD(T), $\lambda = 1.9 - 2.2\ \mathrm{fm}^{-1}$, S.Binder et al., PRL 109, 052501 (2012) & PRC 87, 021303 (2013)

Results: Closed-Shell Nuclei



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

Multi-Reference In-Medium SRG

HH, S. Binder, A. Calci, J. Langhammer, and R. Roth, Phys. Rev. Lett **110**, 242501 (2013)

Generalized Normal Ordering

- generalized normal ordering & Wick theorem for arbitrary reference state (Kutzelnigg & Mukherjee)
- ref. state correlations are encoded in irreducible n-body density matrices:

$$\rho^{kl}_{mn} = \lambda^{kl}_{mn} + \lambda^{k}_{m}\lambda^{l}_{n} - \lambda^{k}_{n}\lambda^{l}_{m}$$

$$\rho^{ijk}_{lmn} = \lambda^{ijk}_{lmn} + \lambda^{i}_{l}\lambda^{jk}_{mn} + \lambda^{i}_{l}\lambda^{j}_{m}\lambda^{k}_{n} + \text{permutations}$$

- additional terms in normal-ordered operators:

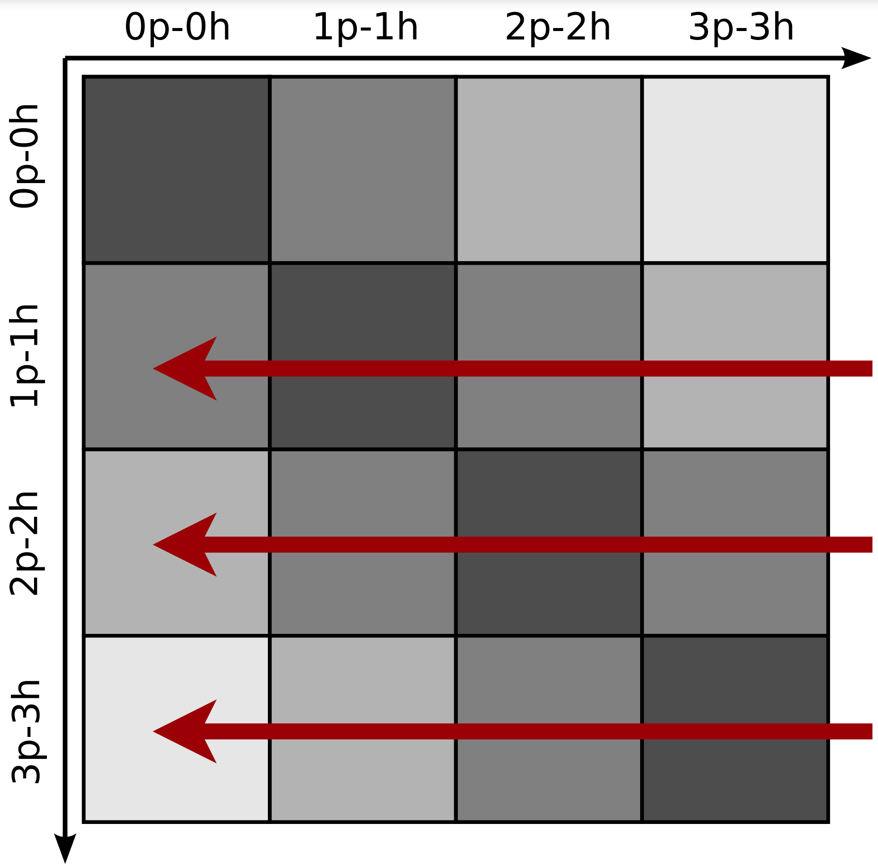
$$A^{k_1\dots k_N}_{l_1\dots l_N} = :A^{k_1\dots k_N}_{l_1\dots l_N}: + \lambda^{k_1}_{l_1} :A^{k_2\dots k_N}_{l_2\dots l_N}: + \text{singles}$$
$$+ \left(\lambda^{k_1}_{l_1}\lambda^{k_2}_{l_2} - \lambda^{k_1}_{l_2}\lambda^{k_2}_{l_1} + \lambda^{k_1 k_2}_{l_1 l_2}\right) :A^{k_3\dots k_N}_{l_3\dots l_N}: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

- additional contractions, e.g.,

$$:A^{ab}_{cd}::A^{kl}_{mn}: = \lambda^{ab}_{mn} :A^{kl}_{cd}:$$

$$:A^{abc}_{def}::A^{klm}_{nop}: = -\lambda^{abm}_{dop} :A^{ckl}_{efn}:$$

Decoupling Revisited



$$\left\langle {}^{p}_{h} \middle| H \middle| \Psi \right\rangle \sim f^{p}_{h}, \sum_{kl} f^{k}_{l} \lambda^{hk}_{pl}, \sum_{klmn} \Gamma^{kl}_{mn} \lambda^{hkl}_{pmn}, \dots$$

$$\left\langle {}^{pp'}_{hh'} \middle| H \middle| \Psi \right\rangle \sim \Gamma^{pp'}_{hh'}, \sum_{km} \Gamma^{pk}_{hm} \lambda^{h'k}_{p'm}, \sum_{kl} f^{k}_{l} \lambda^{hh'k}_{pp'l}, \sum_{klmn} \Gamma^{kl}_{mn} \lambda^{hh'kl}_{pp'mn}, \dots$$

$$\left\langle {}^{pp'p''}_{hh'hh'} \middle| H \middle| \Psi \right\rangle \sim \dots$$

- truncation in irreducible density matrices
  - number of correlated vs. total pairs, triples, ... (caveat for highly collective reference states)
  - perturbative analysis (e.g. for shell-model like states)
- verify for chosen multi-reference state when possible

Multi-Reference Flow Equations

0-body flow:

$$
\frac{dE}{ds} = \sum_{ab} (n_a - n_b) \left(\eta^a_b f^b_a - f^a_b \eta^b_a \right) + \frac{1}{4} \sum_{abcd} \left(\eta^{ab}_{cd} \Gamma^{cd}_{ab} - \Gamma^{ab}_{cd} \eta^{cd}_{ab} \right) n_a n_b \bar{n}_c \bar{n}_d
$$

$$
+ \frac{1}{4} \sum_{abcd} \left(\frac{d}{ds} \Gamma^{ab}_{cd} \right) \lambda^{ab}_{cd} + \cancel{\frac{1}{4} \sum_{abcdklm} \left(\eta^{ab}_{cd} \Gamma^{kl}_{am} - \Gamma^{ab}_{cd} \eta^{kl}_{am} \right) \lambda^{bkl}_{cdm}}
$$

1-body flow:

$$
\frac{d}{ds} f^1_2 = \sum_{a} \left(\eta^1_a f^a_2 - f^1_a \eta^a_2 \right) + \sum_{ab} \left(\eta^a_b \Gamma^{b1}_{a2} - f^a_b \eta^{b1}_{a2} \right) (n_a - n_b)
$$

$$
+ \frac{1}{2} \sum_{abcdef} \left(\eta^{1a}_{bc} \Gamma^{bc}_{2a} - \Gamma^{1a}_{bc} \eta^{bc}_{2a} \right) (n_a \bar{n}_b \bar{n}_c + \bar{n}_a n_b n_c)
$$

$$
+ \frac{1}{4} \sum_{abcde} \left(\eta^{1a}_{bc} \Gamma^{de}_{2a} - \Gamma^{1a}_{bc} \eta^{de}_{2a} \right) \lambda^{de}_{bc} + \sum_{abcde} \left(\eta^{1a}_{bc} \Gamma^{be}_{2d} - \Gamma^{1a}_{bc} \eta^{be}_{2d} \right) \lambda^{ae}_{cd}
$$

$$
- \frac{1}{2} \sum_{abcde} \left(\eta^{1a}_{2b} \Gamma^{cd}_{ae} - \Gamma^{1a}_{2b} \eta^{cd}_{ae} \right) \lambda^{cd}_{be} + \frac{1}{2} \sum_{abcde} \left(\eta^{1a}_{2b} \Gamma^{bc}_{de} - \Gamma^{1a}_{2b} \eta^{bc}_{de} \right) \lambda^{ac}_{de}
$$

Multi-Reference Flow Equations

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2-body flow:

$$\frac{d}{ds}\Gamma^{12}_{34} = \sum_a \left(\eta^1_a \Gamma^{a2}_{34} + \eta^2_a \Gamma^{1a}_{34} - \eta^a_3 \Gamma^{12}_{a4} - \eta^a_4 \Gamma^{12}_{3a} - f^1_a \eta^{a2}_{34} - f^2_a \eta^{1a}_{34} + f^a_3 \eta^{12}_{a4} + f^a_4 \eta^{12}_{3a}\right)$$

$$+ \frac{1}{2}\sum_{ab}\left(\eta^{12}_{ab}\Gamma^{ab}_{34} - \Gamma^{12}_{ab}\eta^{ab}_{34}\right)(1 - n_a - n_b)$$

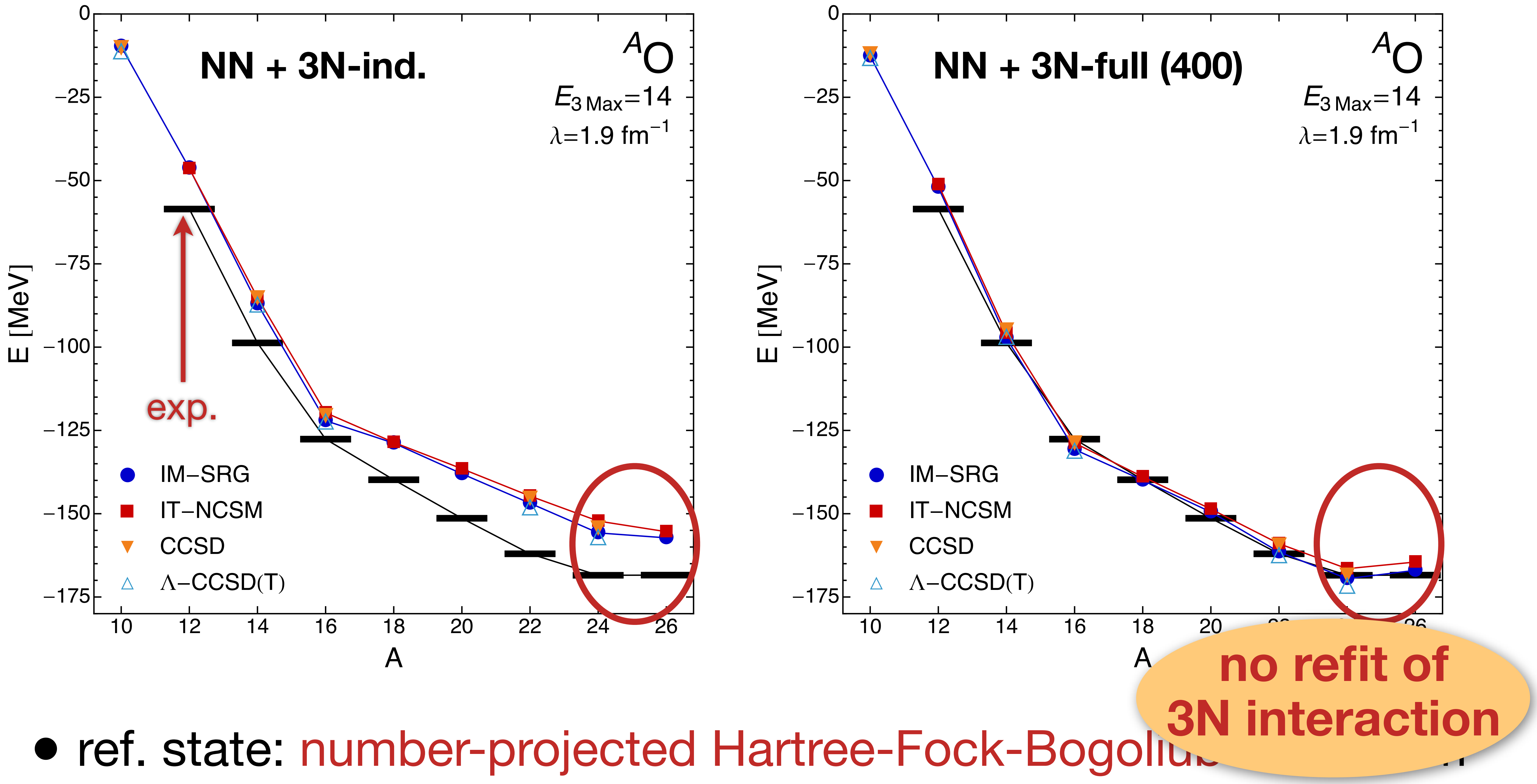
$$+ \sum_{ab}(n_a - n_b)\left(\left(\eta^{1a}_{3b}\Gamma^{2b}_{4a} - \Gamma^{1a}_{3b}\eta^{2b}_{4a}\right) - \left(\eta^{2a}_{3b}\Gamma^{1b}_{4a} - \Gamma^{2a}_{3b}\eta^{1b}_{4a}\right)\right)$$

2-body flow unchanged

Open-Shell Nuclei

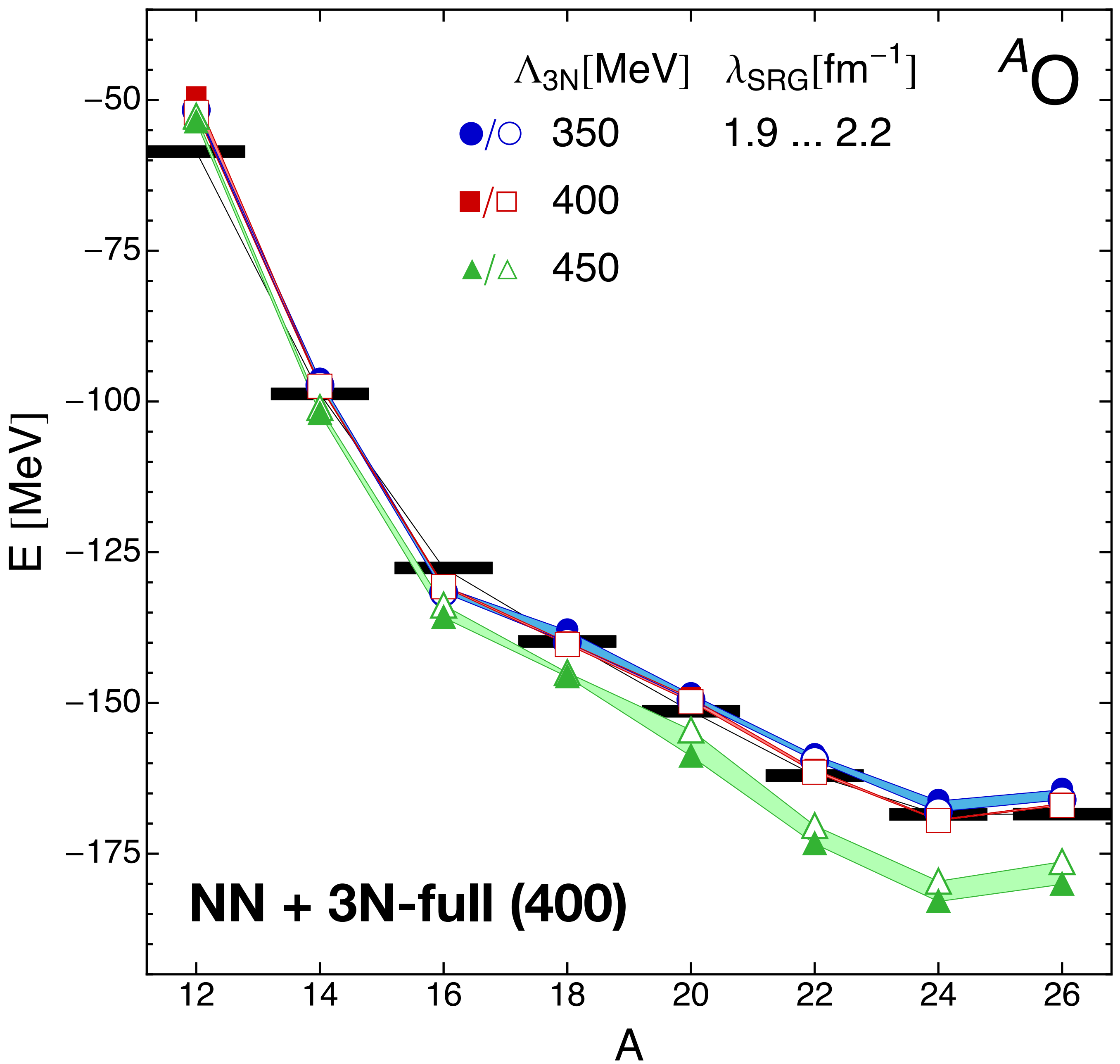
HH, S. Binder, A. Calci, J. Langhammer, and R. Roth, Phys. Rev. Lett **110**, 242501 (2013)

Results: Oxygen Chain



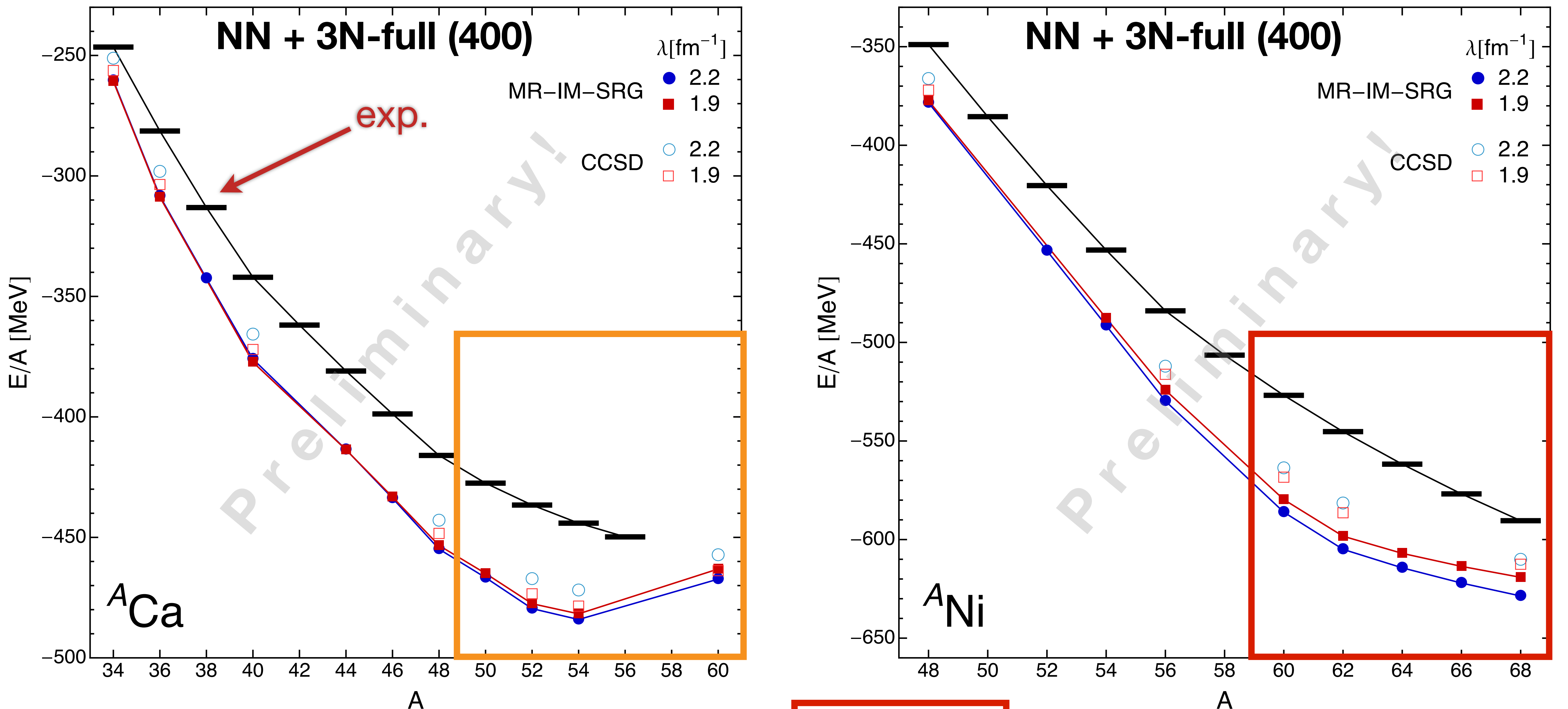
- ref. state: number-projected Hartree-Fock-Bogoliubov
- results (mostly) insensitive to choice of generator for same H^{od}
- **consistency between different many-body methods**

Variation of Scales



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

Calcium and Nickel Isotopes



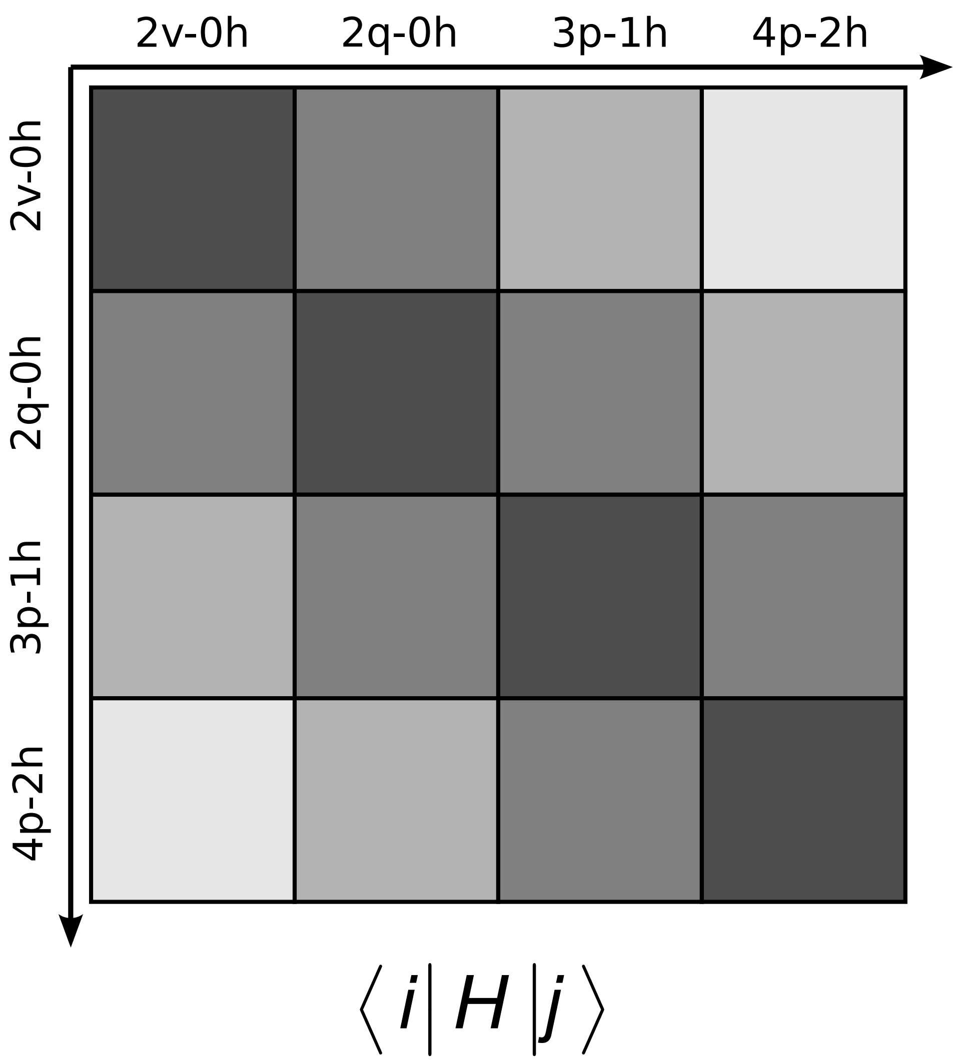
$e_{\text{Max}} = 14$, $E_{\text{3Max}} = 14$

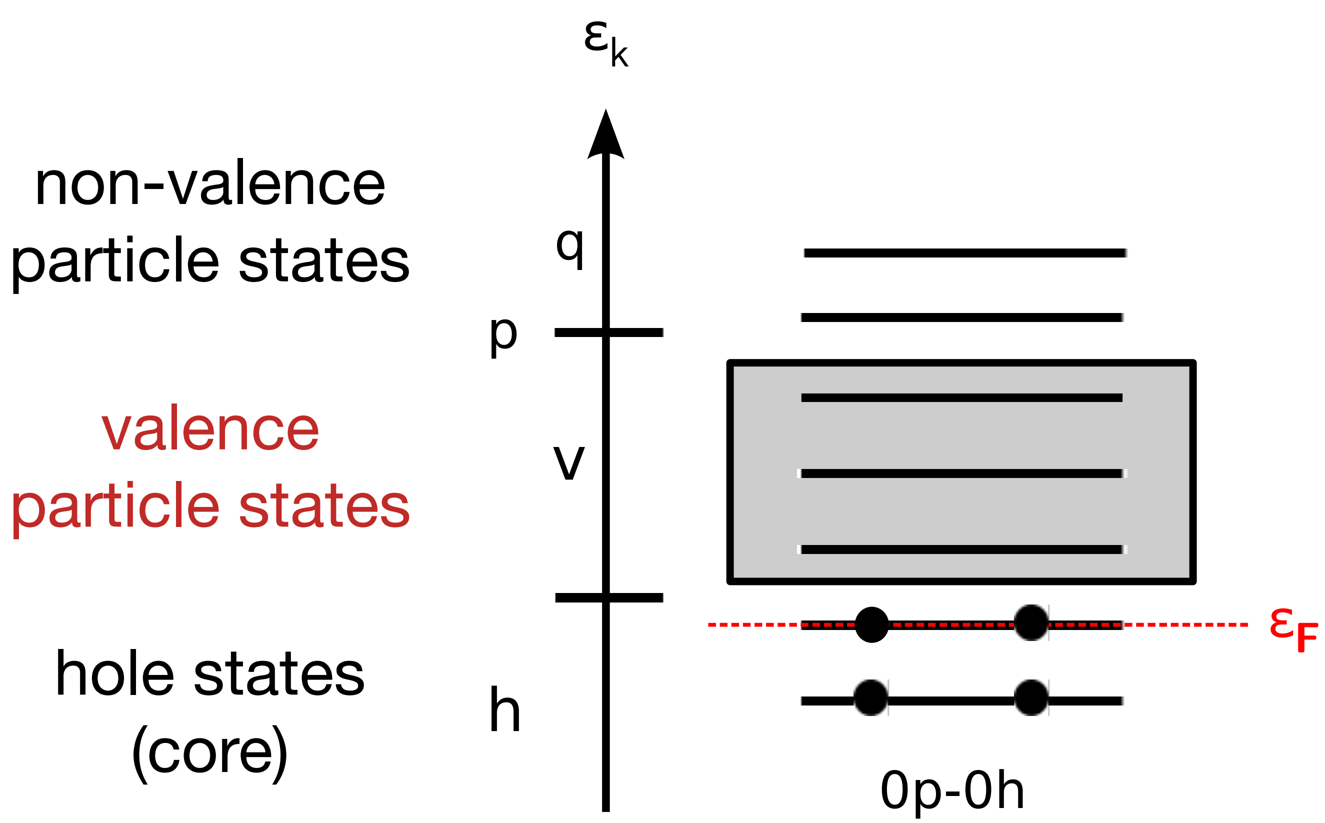
$E_{\text{3Max}} = 14$ insufficient for neutron-rich pf-shell nuclei, extension to ~20 coming soon !

IM-SRG + Shell Model

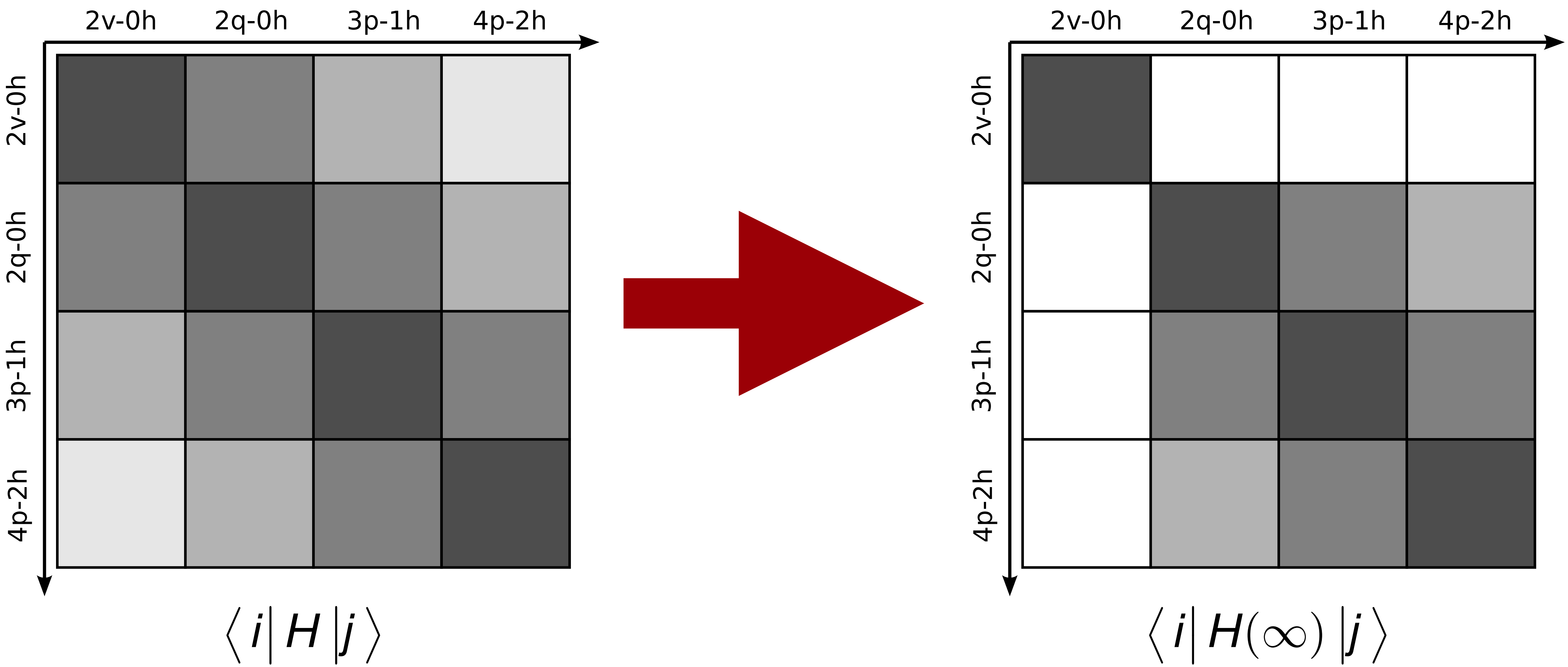
S. K. Bogner, HH, J. D. Holt, A. Schwenk, in preparation
K. Tsukiyama, S. K. Bogner, and A. Schwenk, Phys. Rev. C **85**, 061304(R) (2012)

Valence Space Decoupling





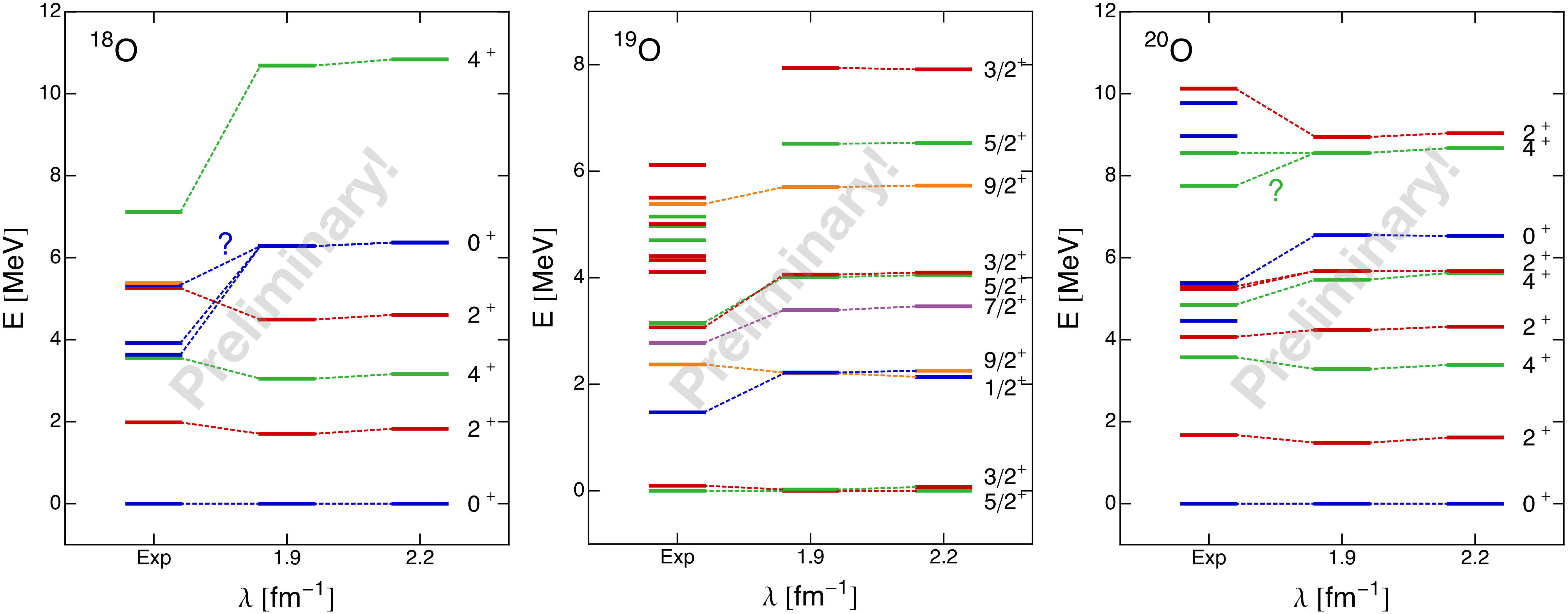
Valence Space Decoupling



- 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), $e_{\text{Max}} = 10$, $E_{3\text{Max}} = 14$, $\hbar\Omega = 24$ MeV

- ✓ good description of low-lying states
- ✓ easy approach to spectra, odd nuclei, intrinsic deformation
- ➡ **but:** numerical effort determined by shell-model calculation

Conclusions

Conclusions & Outlook

- powerful and flexible new *Ab-initio* method:
  - ground-state properties of closed- and open-shell nuclei
  - derivation of microscopic shell-model interactions

✓ first systematic studies of closed- and open-shell nuclei based on chiral NN + 3N Hamiltonians completed
(H. H. et al. PRC **87**, 034307, and PRL **110**, 242501)

➡ efficient evolution of observables / effective shell-model operators ?

➡ EoM formalism for excited states, odd nuclei

➡ deformation, continuum effects, etc. ...

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