In-Medium SRG for Closed- and Open-Shell Nuclei

Heiko Hergert
Department of Physics, The Ohio State University

Outline

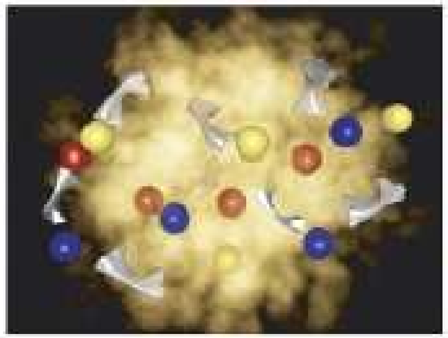
- Similarity Renormalization Group in Nuclear Physics
- In-Medium SRG for Closed Shell-Nuclei
- Multi-Reference In-Medium SRG
- Open-Shell Nuclei
- Outlook

Scales of the Strong Interaction

momentum transfer (resolution)

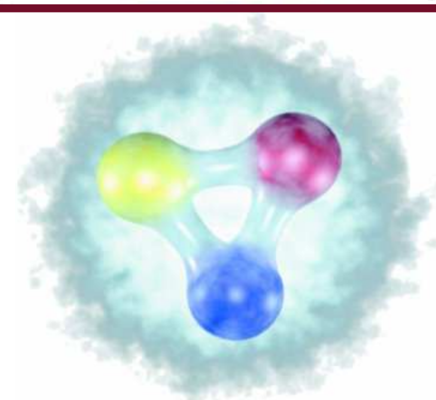
QCD

Chiral EFT

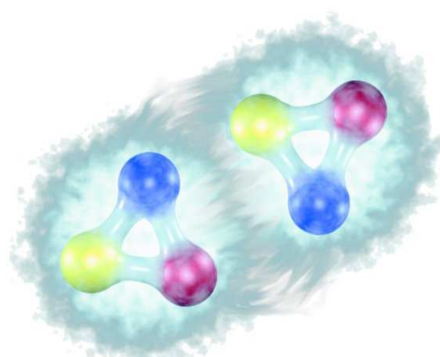


- quarks, gluons

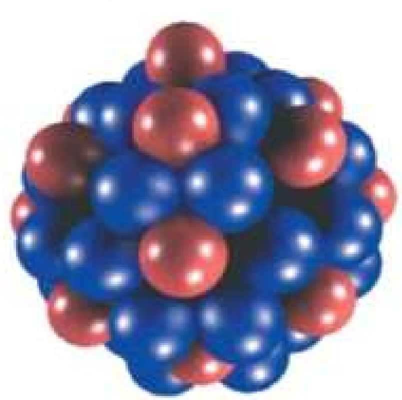
chiral symmetry



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



(Which) Details necessary?



- finite nuclei
  - nuclear structure & reactions

Similarity Renormalization Group 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

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

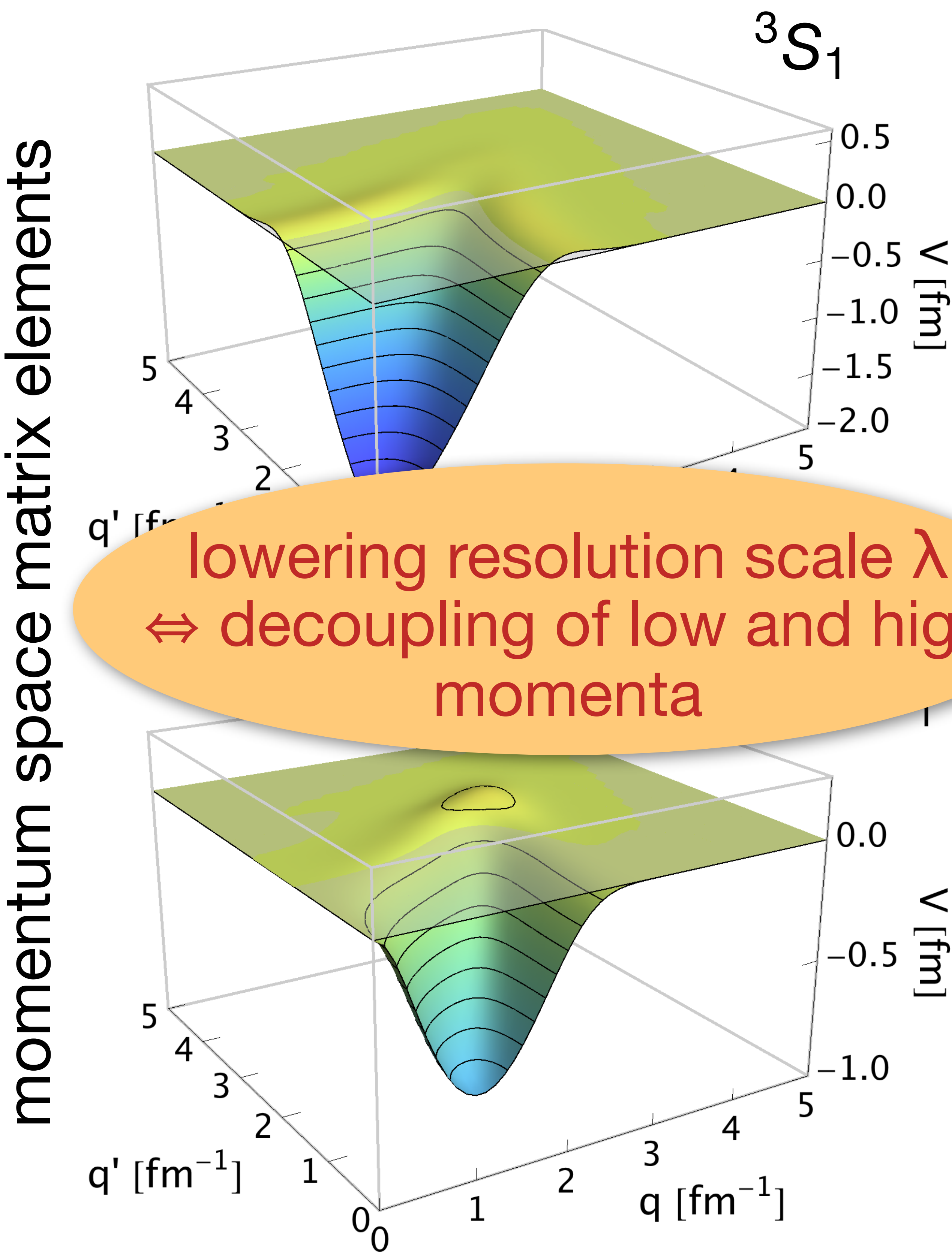
- flow equation:

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

- 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



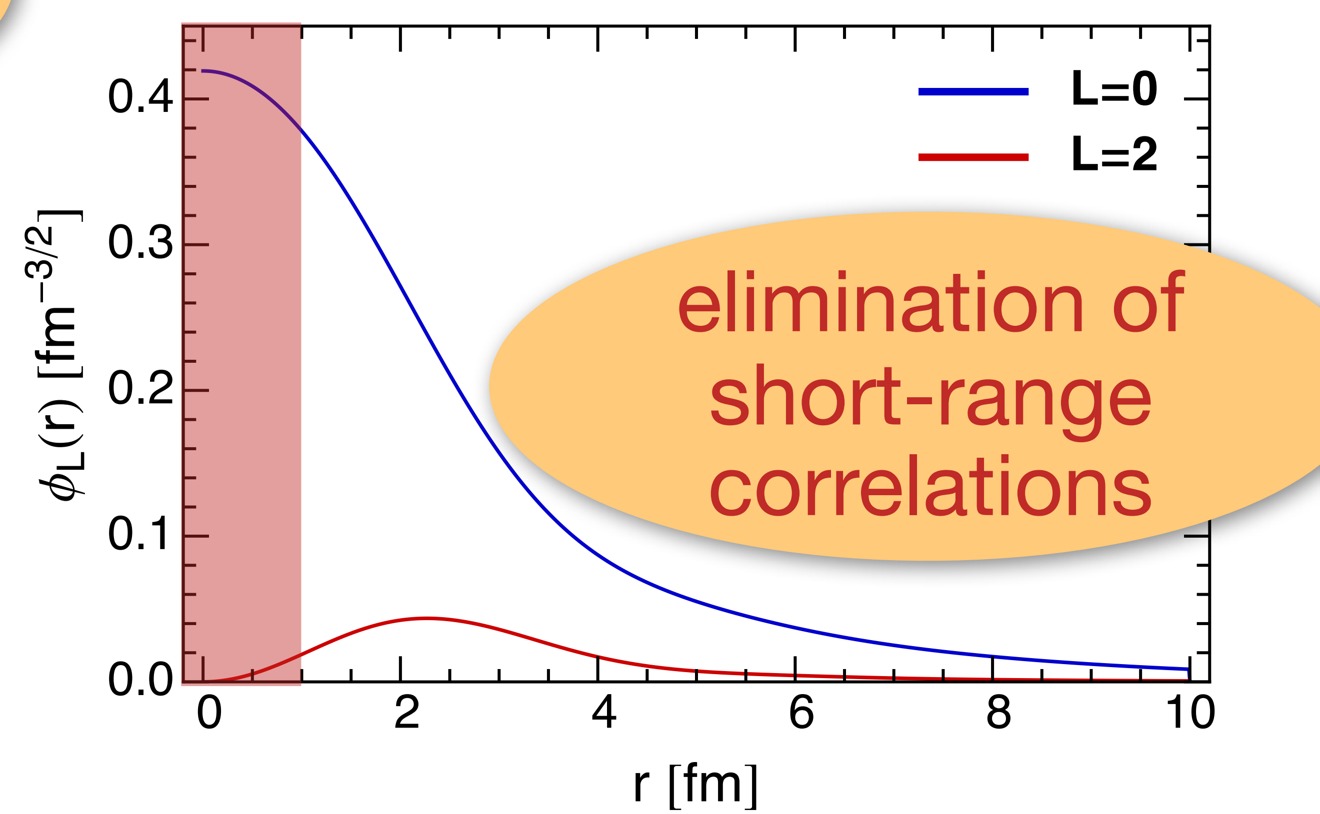
lowering resolution scale λ
⇔ decoupling of low and high momenta

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

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

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

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:

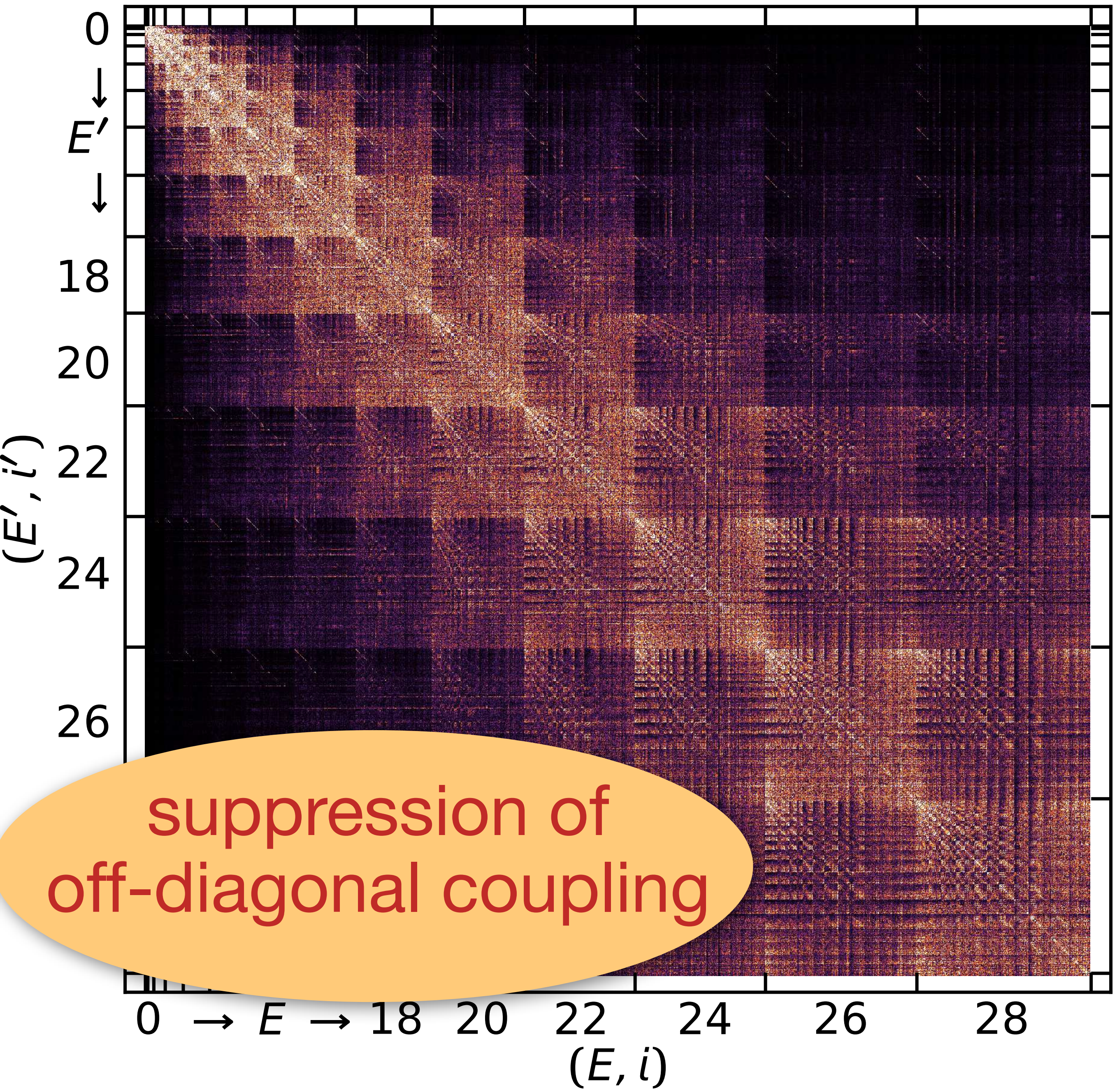
$$\frac{dH}{d\lambda} = [[\sum a^\dagger a, \sum \underbrace{a^\dagger a^\dagger aa}_{\text{2-body}}], \sum \underbrace{a^\dagger a^\dagger aa}_{\text{2-body}}] = \ldots + \sum \underbrace{a^\dagger a^\dagger a^\dagger aaa}_{\text{3-body}} + \ldots$$

- 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

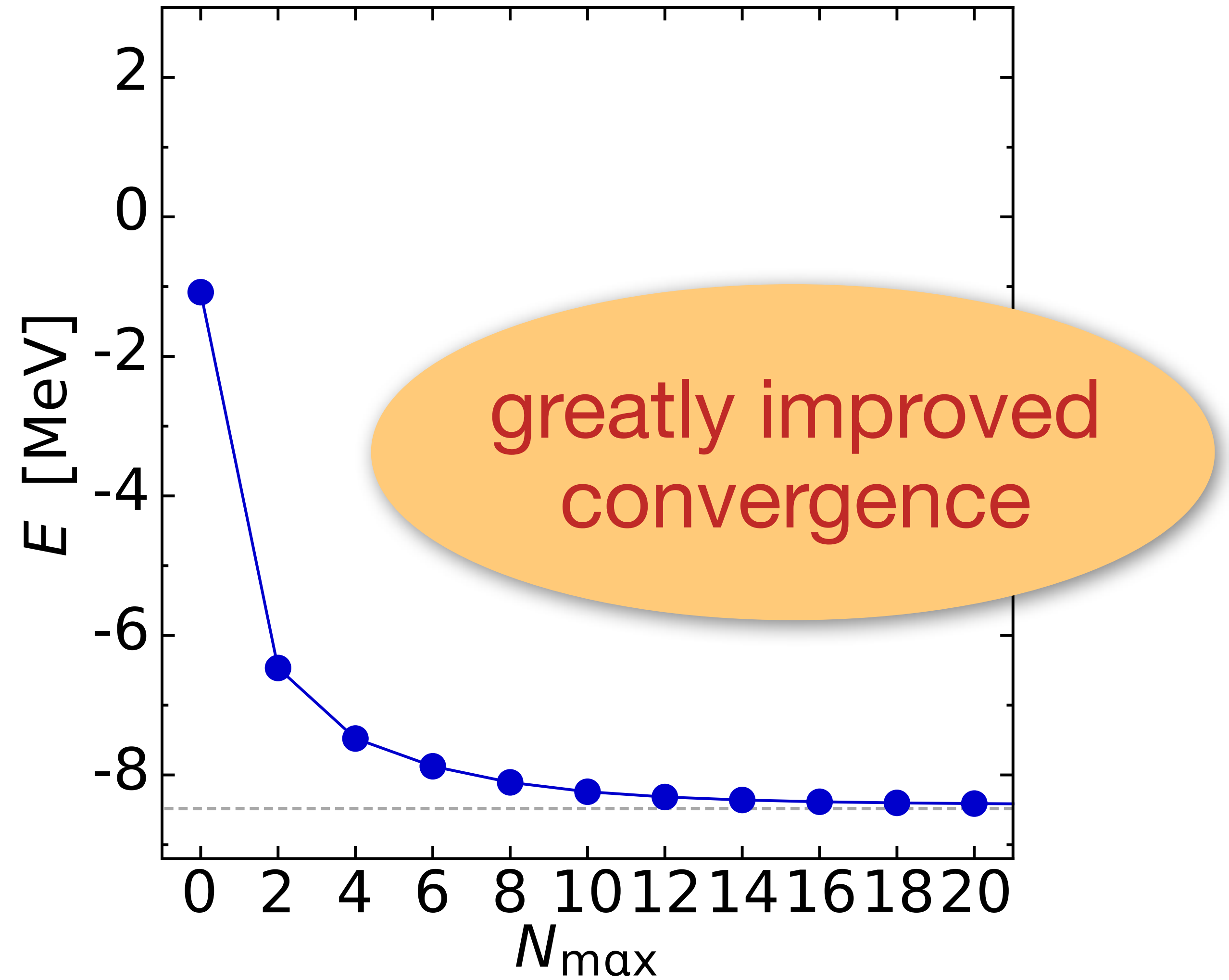
$J^{\pi} = \frac{1}{2}^{+}, T = \frac{1}{2}, \hbar\Omega = 28$ MeV



suppression of off-diagonal coupling

λ = 1.33 fm^{-1}

^{3}H ground-state (NCSM)



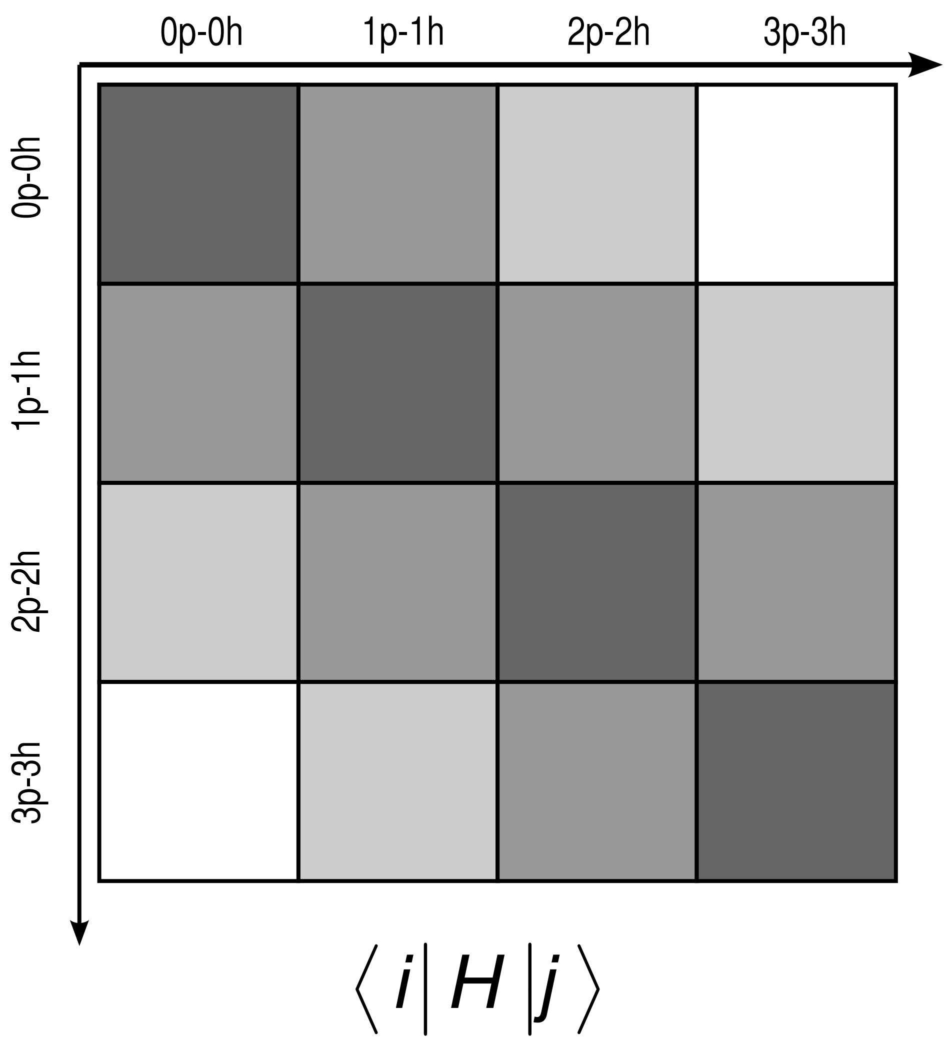
greatly improved convergence

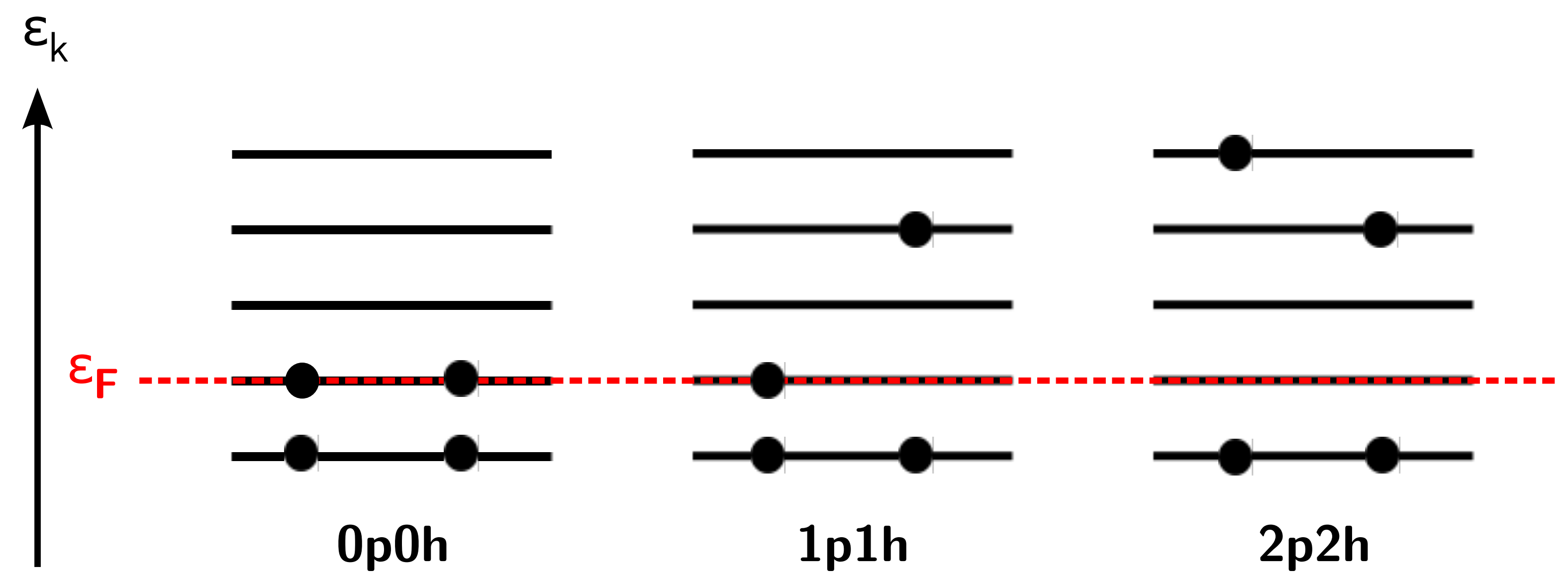
[figures by R. Roth, A. Calci, J. Langhammer]

In-Medium SRG for Closed-Shell Nuclei

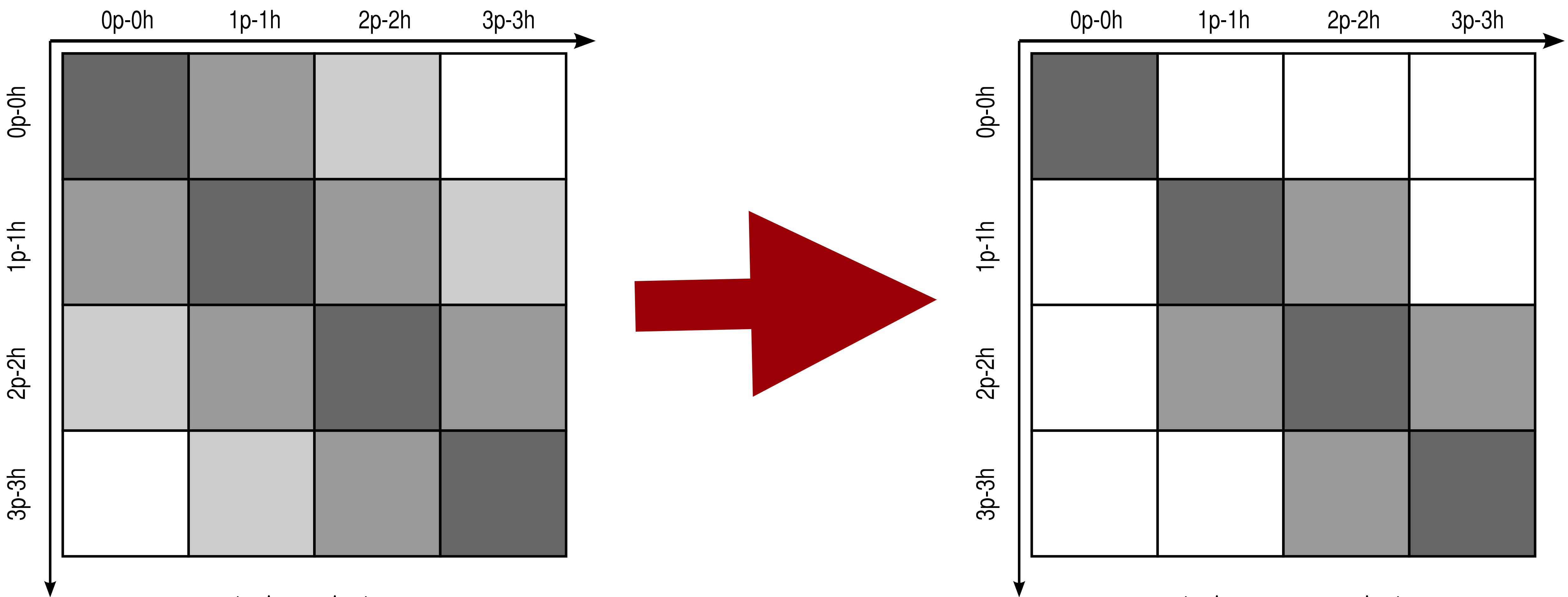
H. H., S. K. Bogner, S. Binder, A. Calci, J. Langhammer, R. Roth, and A. Schwenk, Phys. Rev. C **87**, 034307 (2013), arXiv:1212.1190 [nucl-th]
K. Tsukiyama, S. K. Bogner, and A. Schwenk, Phys. Rev. Lett. **106**, 222502 (2011)

Decoupling in A-Body Space





Decoupling in A-Body Space



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

aim: decouple reference state (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:

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

- 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

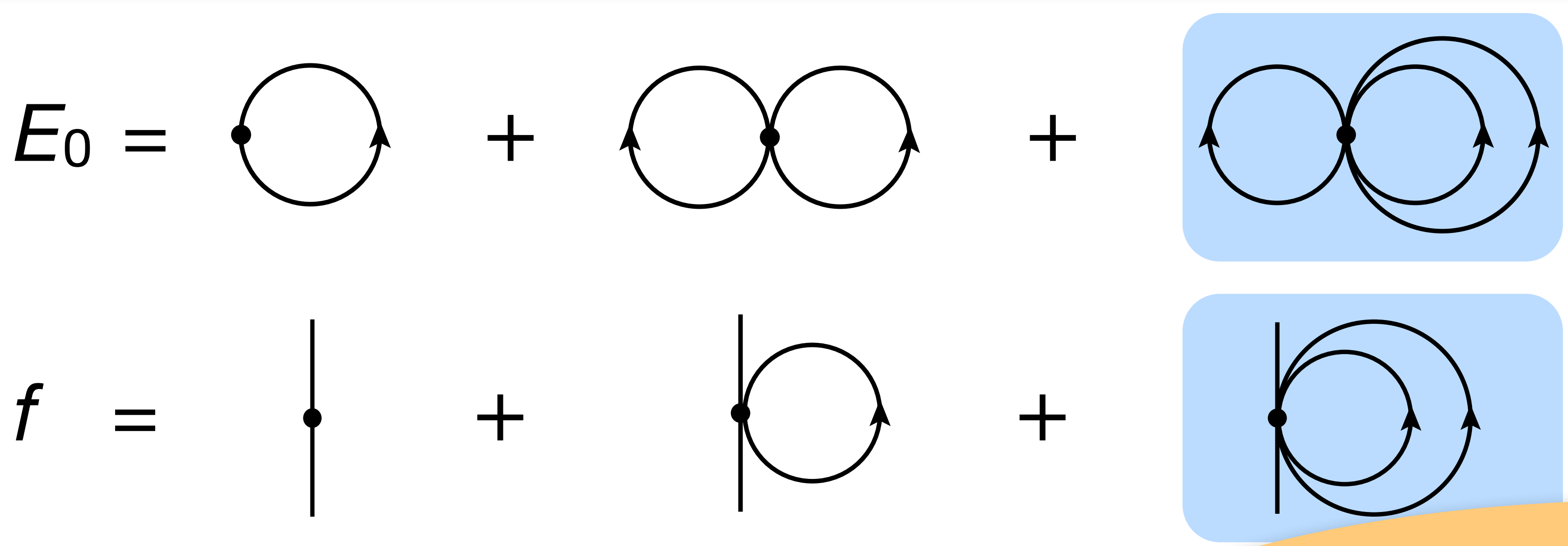
$$\langle \Phi | :A^{k_1\dots k_N}_{l_1\dots l_N}: | \Phi \rangle = 0$$

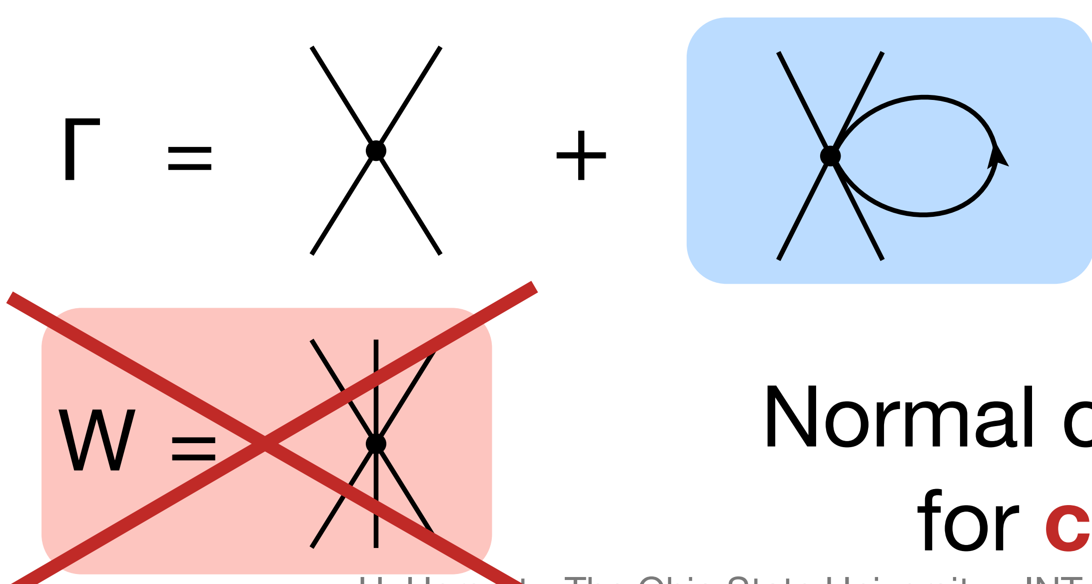
- Wick's theorem gives simplified expansions (fewer terms!) for products of normal-ordered operators

Normal-Ordered Hamiltonian

Normal-Ordered Hamiltonian

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

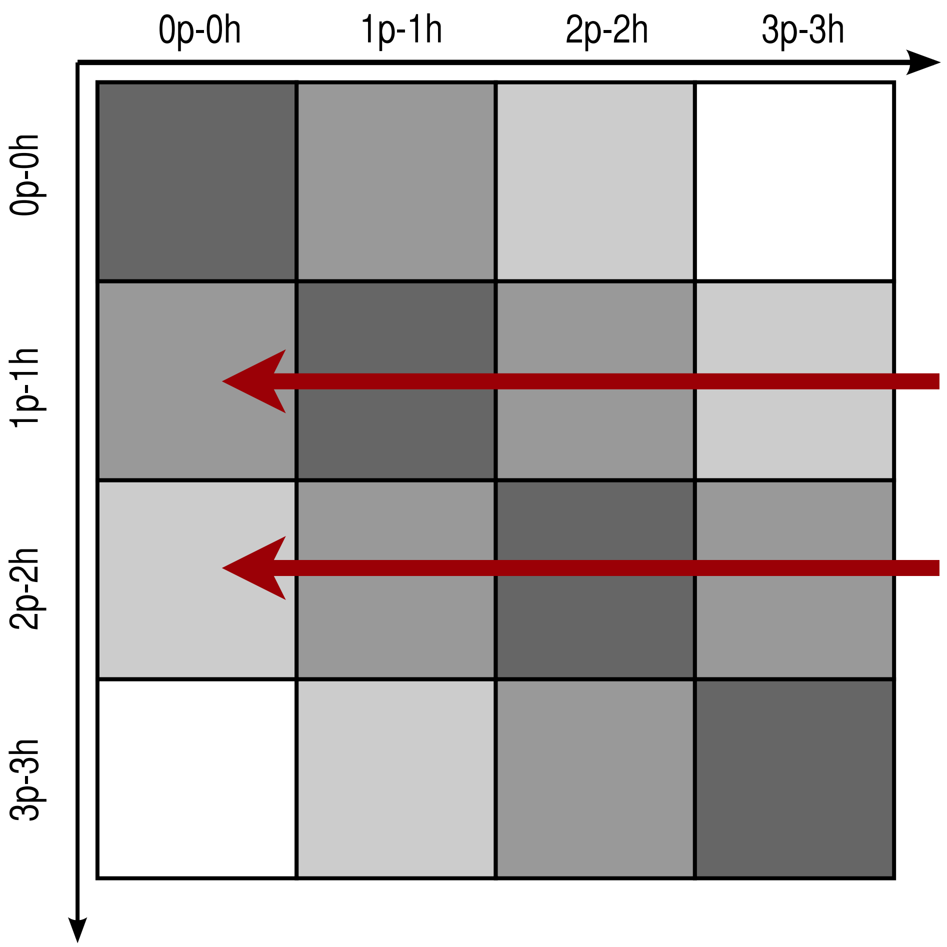




two-body formalism with in-medium contributions from three-body interactions

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

Choice of Generator



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

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

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

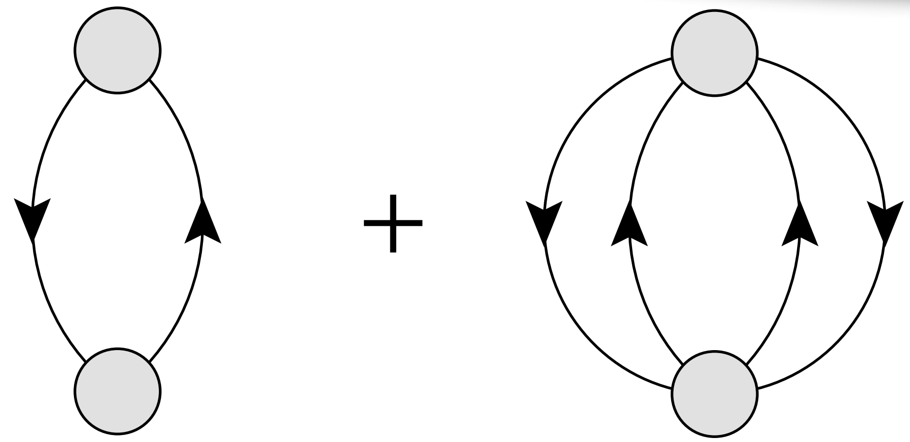
$$\frac{d}{ds}f^1_2 = \sum_a \left(\eta^1_a f^a_2 - f^1_a \eta^a_2\right) + \sum_{ab}\left(\eta^a_b \Gamma^{b1}_{a2} - f^a_b \eta^{b1}_{a2}\right)(n_a - n_b)$$
$$+ \frac{1}{2}\sum_{abcdef}\left(\eta^{1a}_{bc}\Gamma^{bc}_{2a} - \Gamma^{1a}_{bc}\eta^{bc}_{2a}\right)(n_a \bar{n}_b \bar{n}_c + \bar{n}_a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

In-Medium SRG Flow Equations

0-body Flow

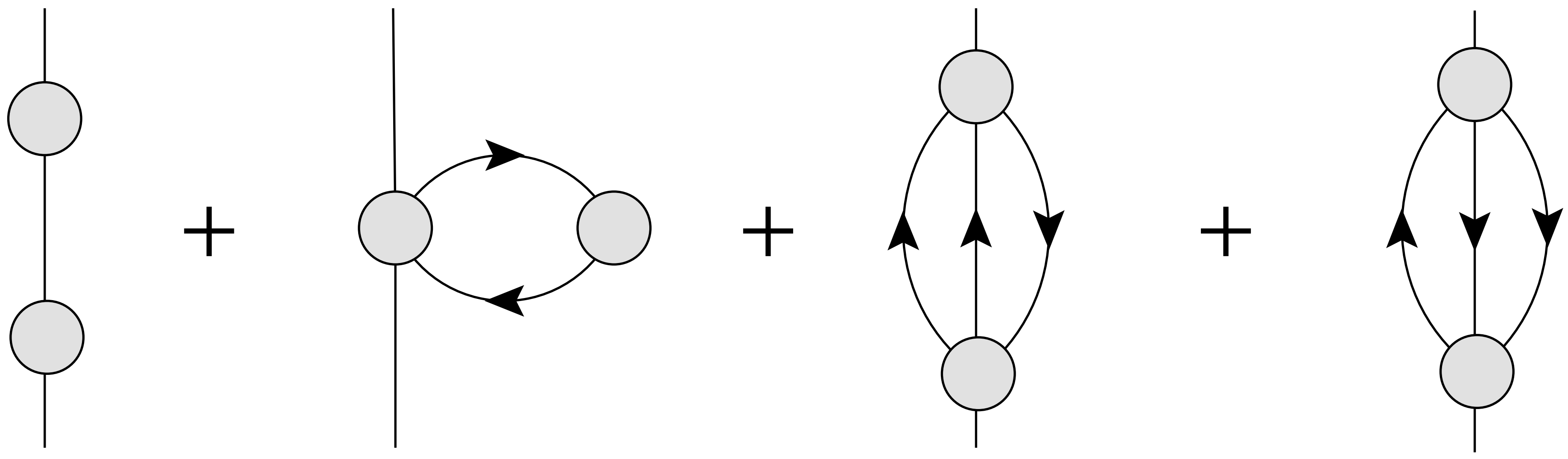
~ 2nd order MBPT for *H(s)*

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



1-body Flow

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



(White generator, Hugenholtz diagrams)

In-Medium SRG Flow Equations

2-body Flow

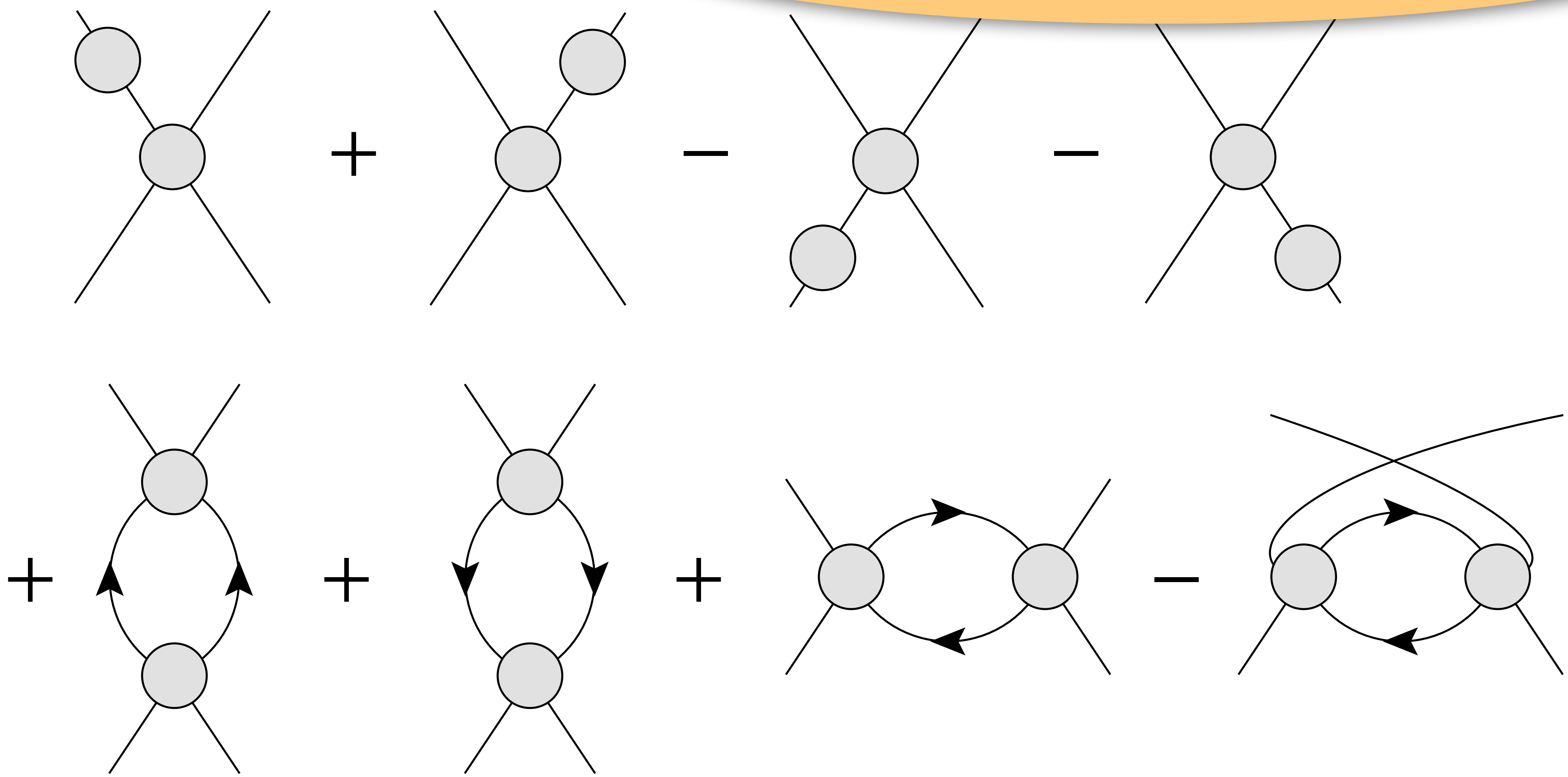
$$
\begin{aligned}
\frac{d}{ds}\Gamma^{12}_{34} = &\sum_a \left(\eta^1_a \Gamma^{a2}_{34} + \eta^2_a \Gamma^{1a}_{34} - \eta^a_3 \Gamma^{12}_{a4} - \eta^a_4 \Gamma^{12}_{3a} - f^1_a \eta^{a2}_{34} - f^2_a \eta^{1a}_{34} + f^a_3 \eta^{12}_{a4} + f^a_4 \eta^{12}_{3a}\right) \\
&+ \frac{1}{2}\sum_{ab} \left(\eta^{12}_{ab}\Gamma^{ab}_{34}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

In-Medium SRG Flow Equations

2-body Flow

only linked diagrams contribute,
IM-SRG size-extensive

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

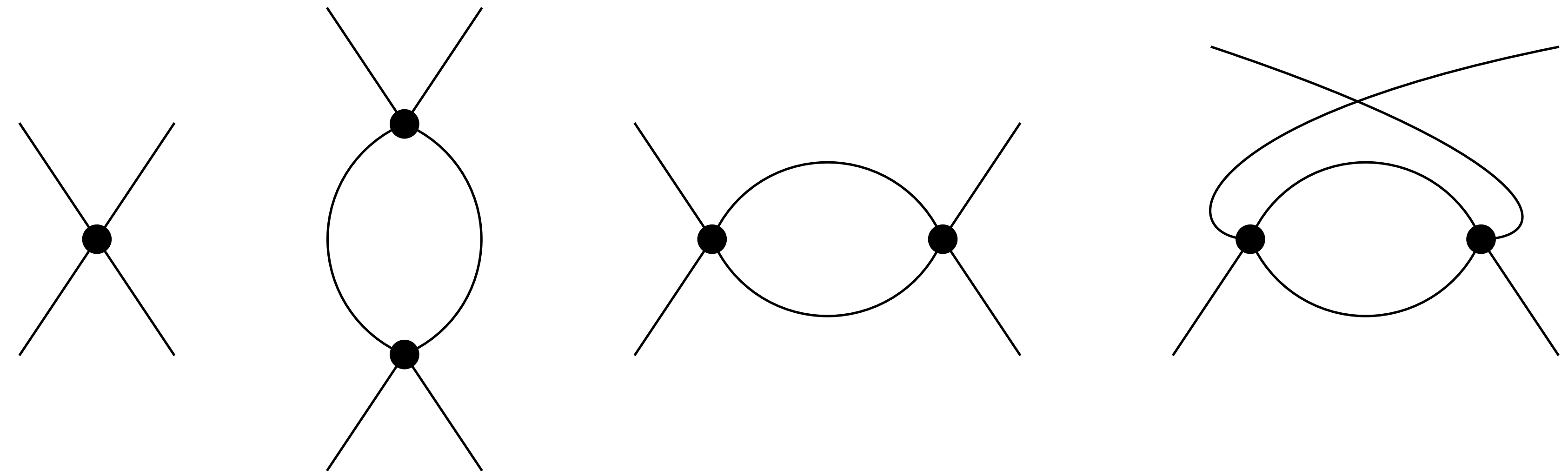


s channel — ladders

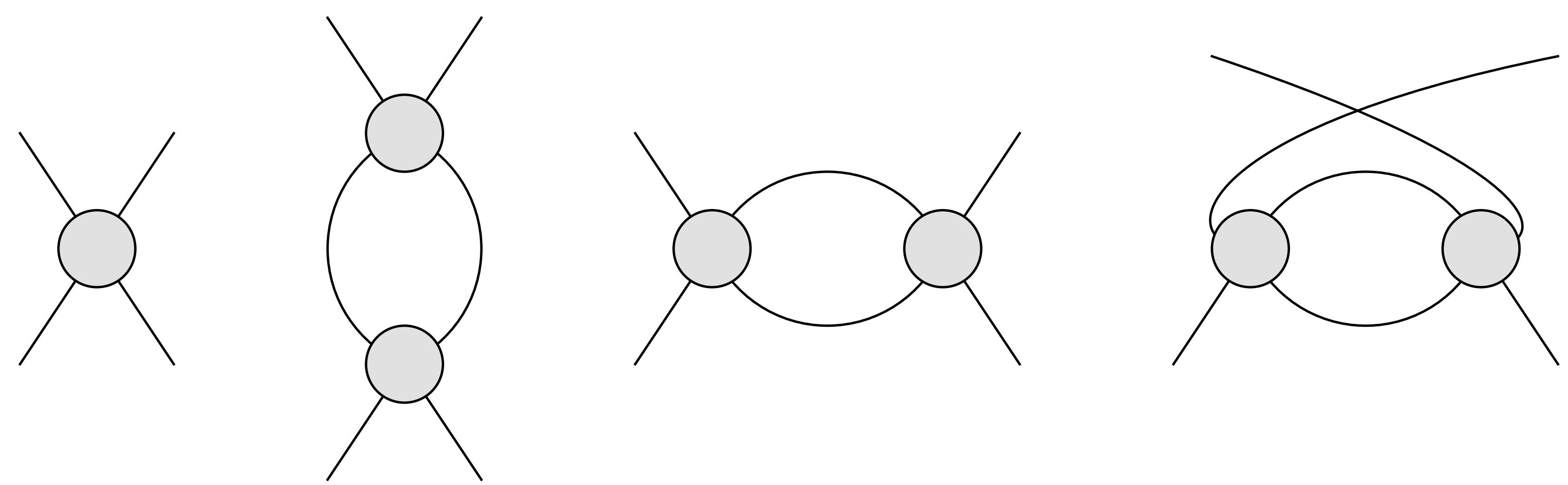
t channel, *u* channel — rings

In-Medium SRG Flow: Diagrams

$\Gamma(\delta s) \sim$



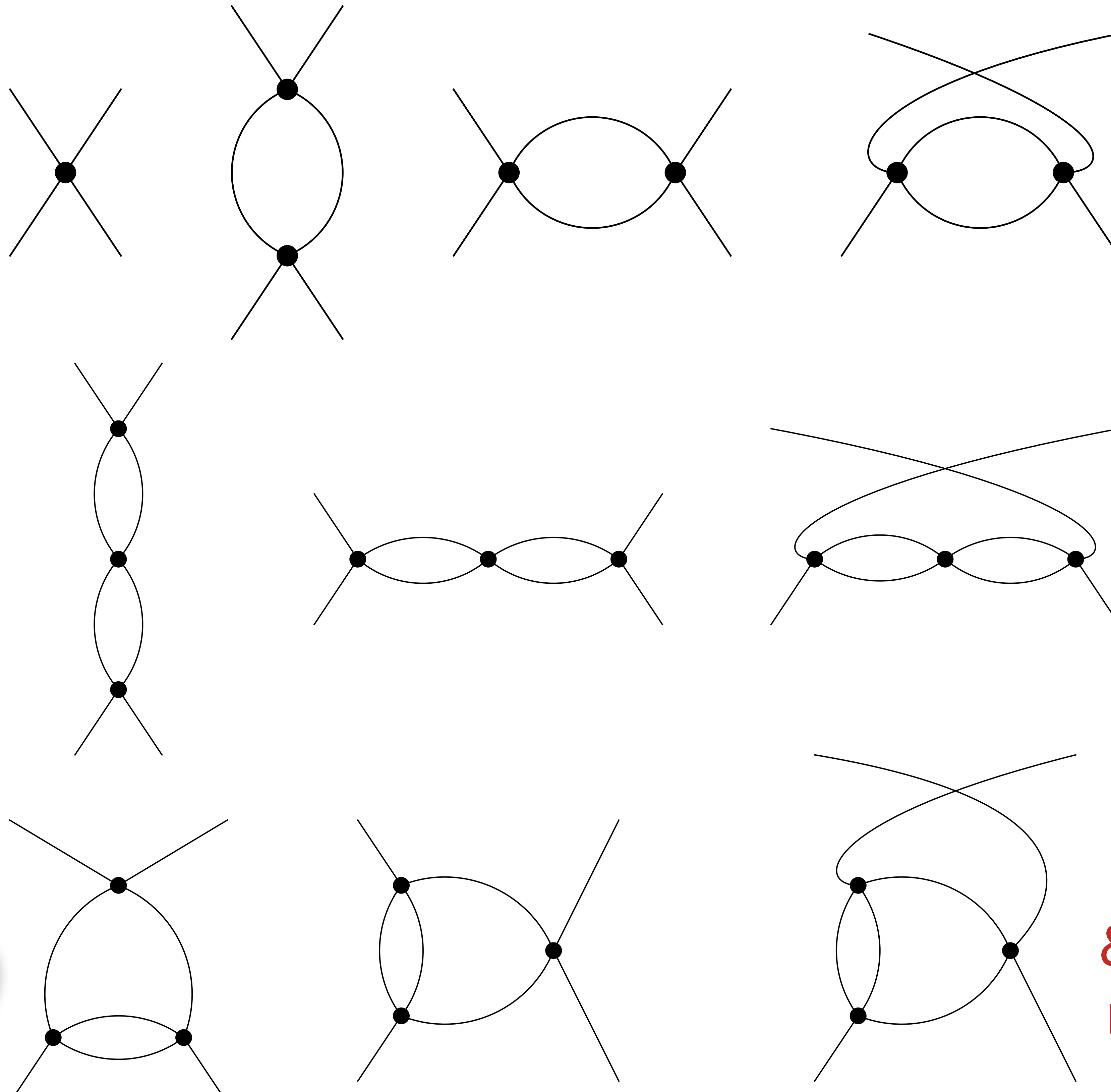
$\Gamma(2\delta s) \sim$



In-Medium SRG Flow: Diagrams

$\Gamma(\delta s) \sim$

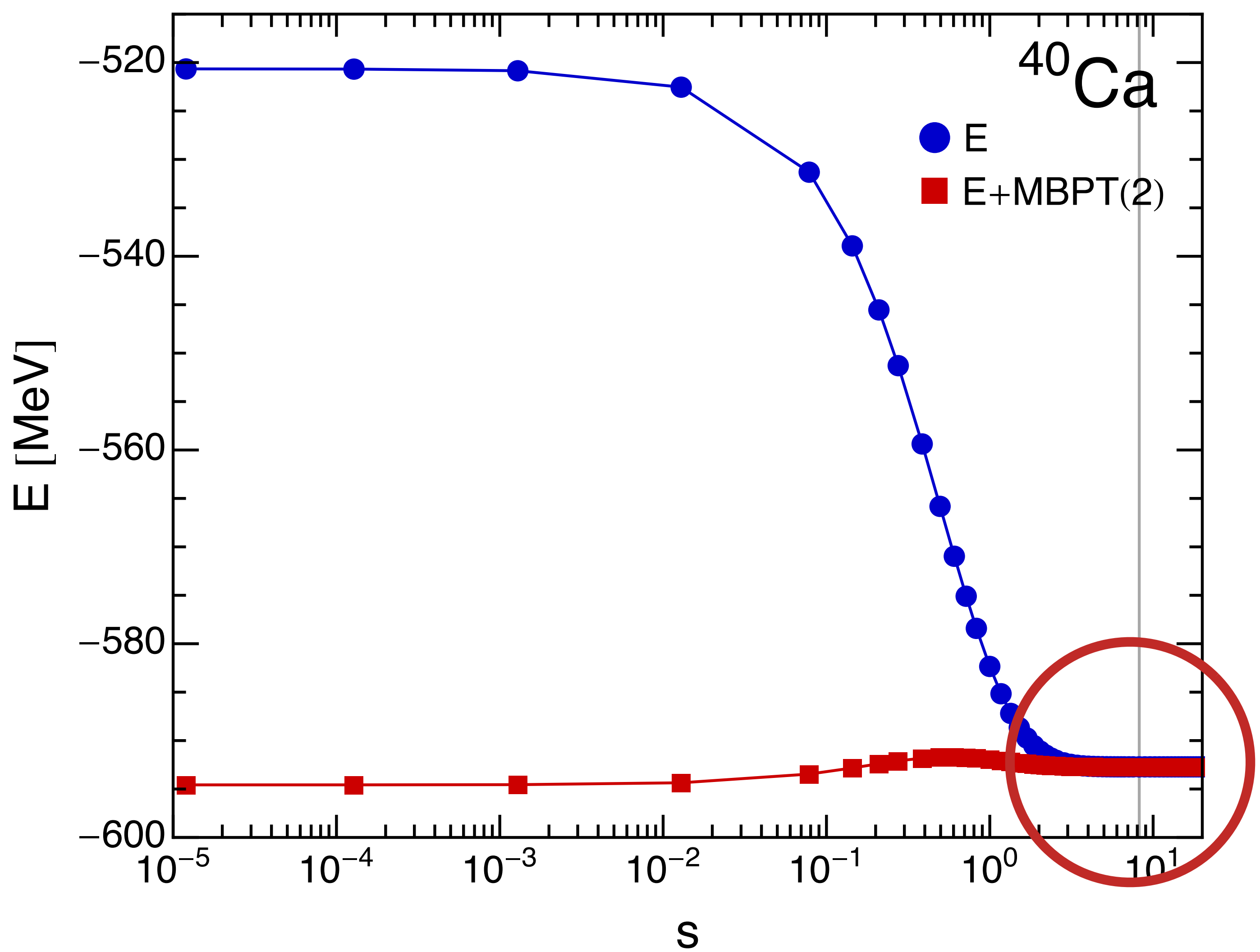
$\Gamma(2\delta s) \sim$

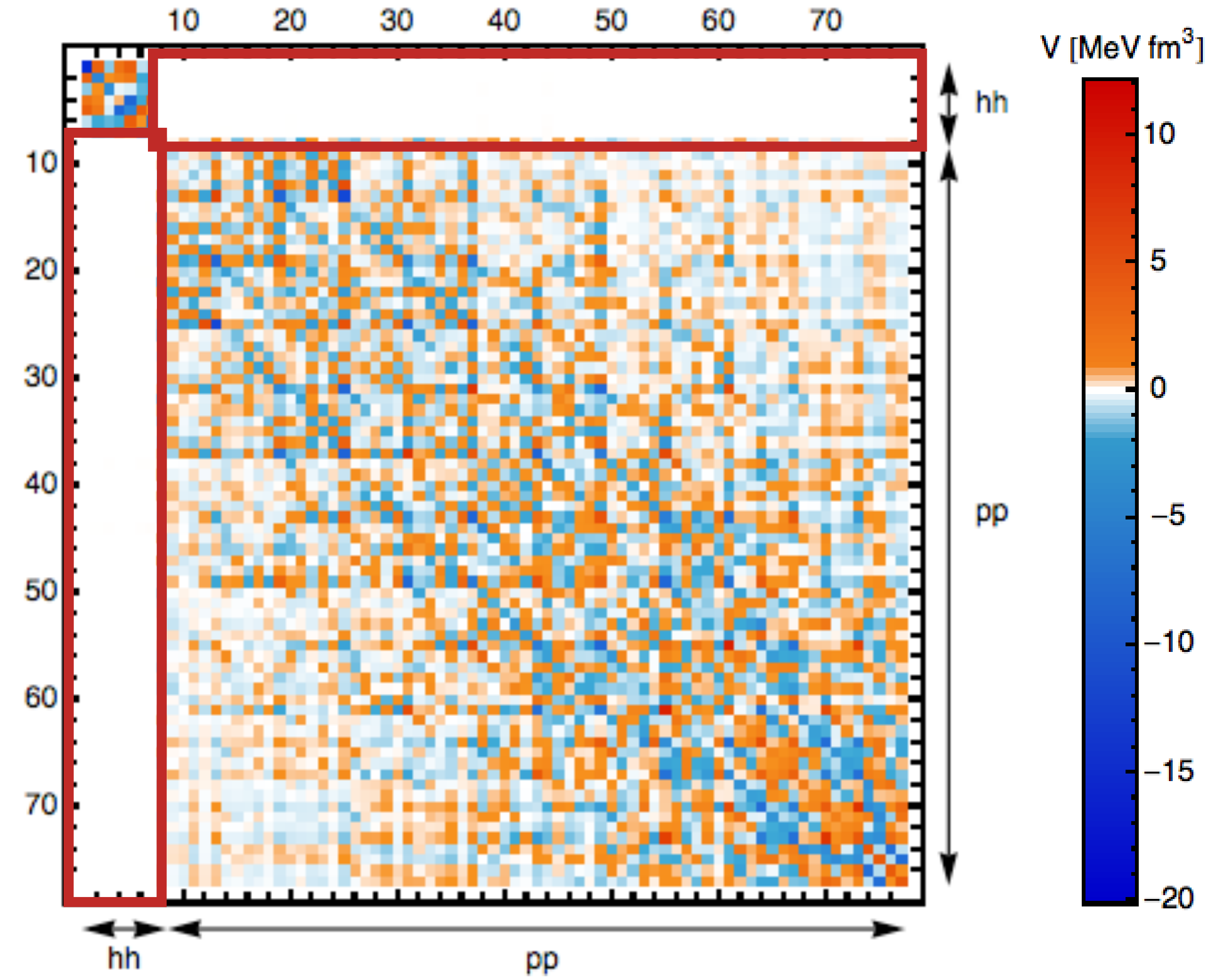


non-perturbative resummation

& many more...

Decoupling



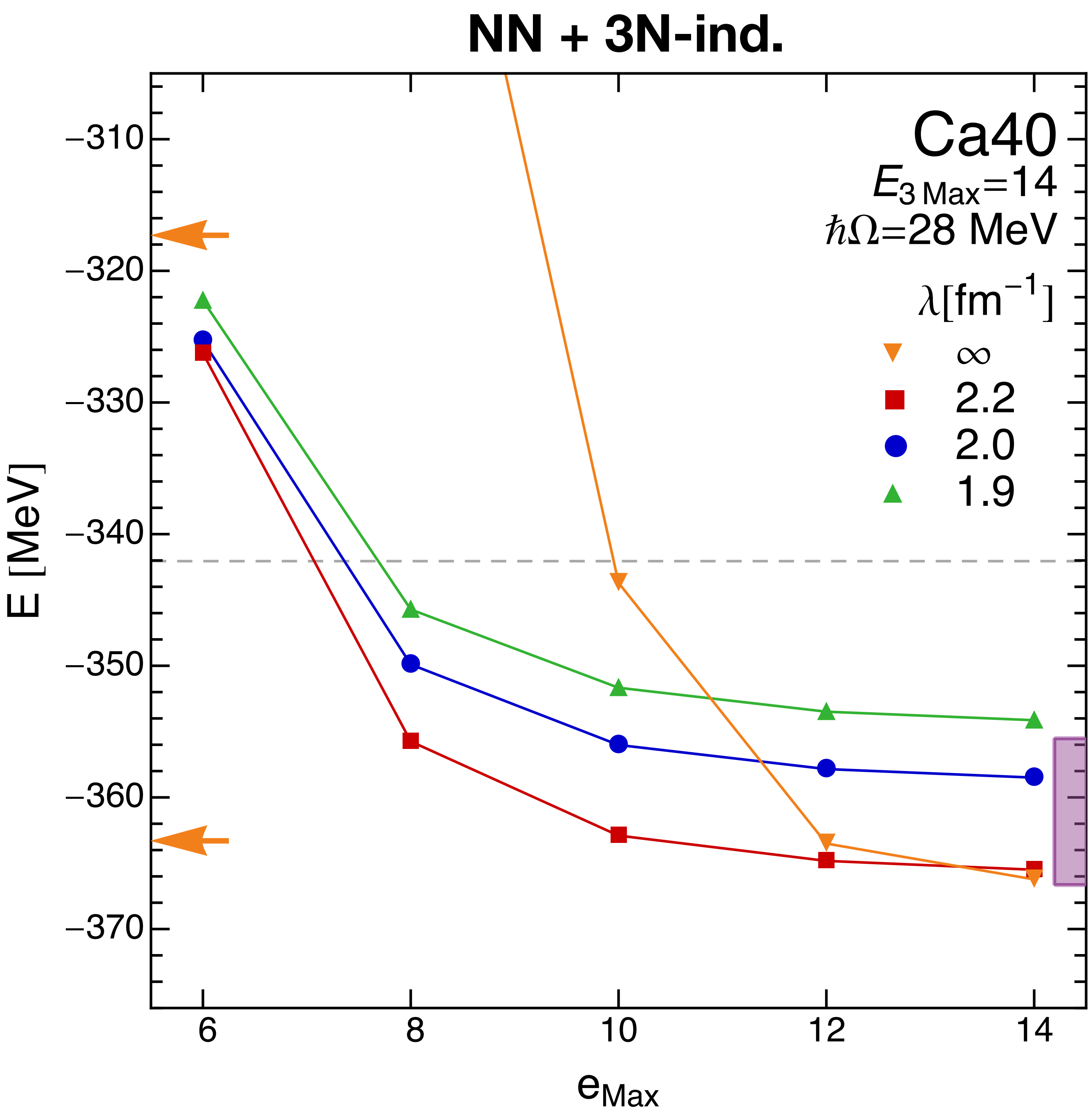


N3LO, $\lambda = 2.0\ \mathrm{fm}^{-1}, e_{\mathrm{Max}} = 8$

non-perturbative resummation of MBPT series (correlations)

off-diagonal couplings are rapidly driven to zero

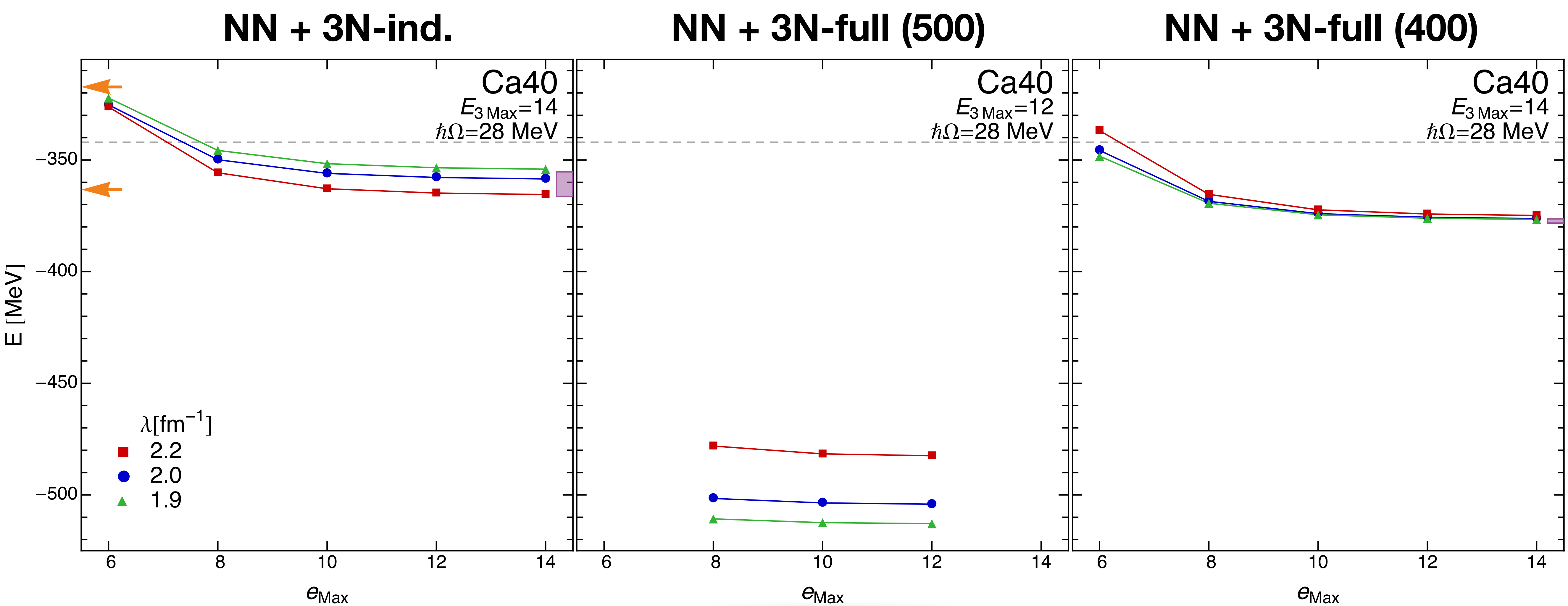
Results: Closed-Shell Nuclei



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

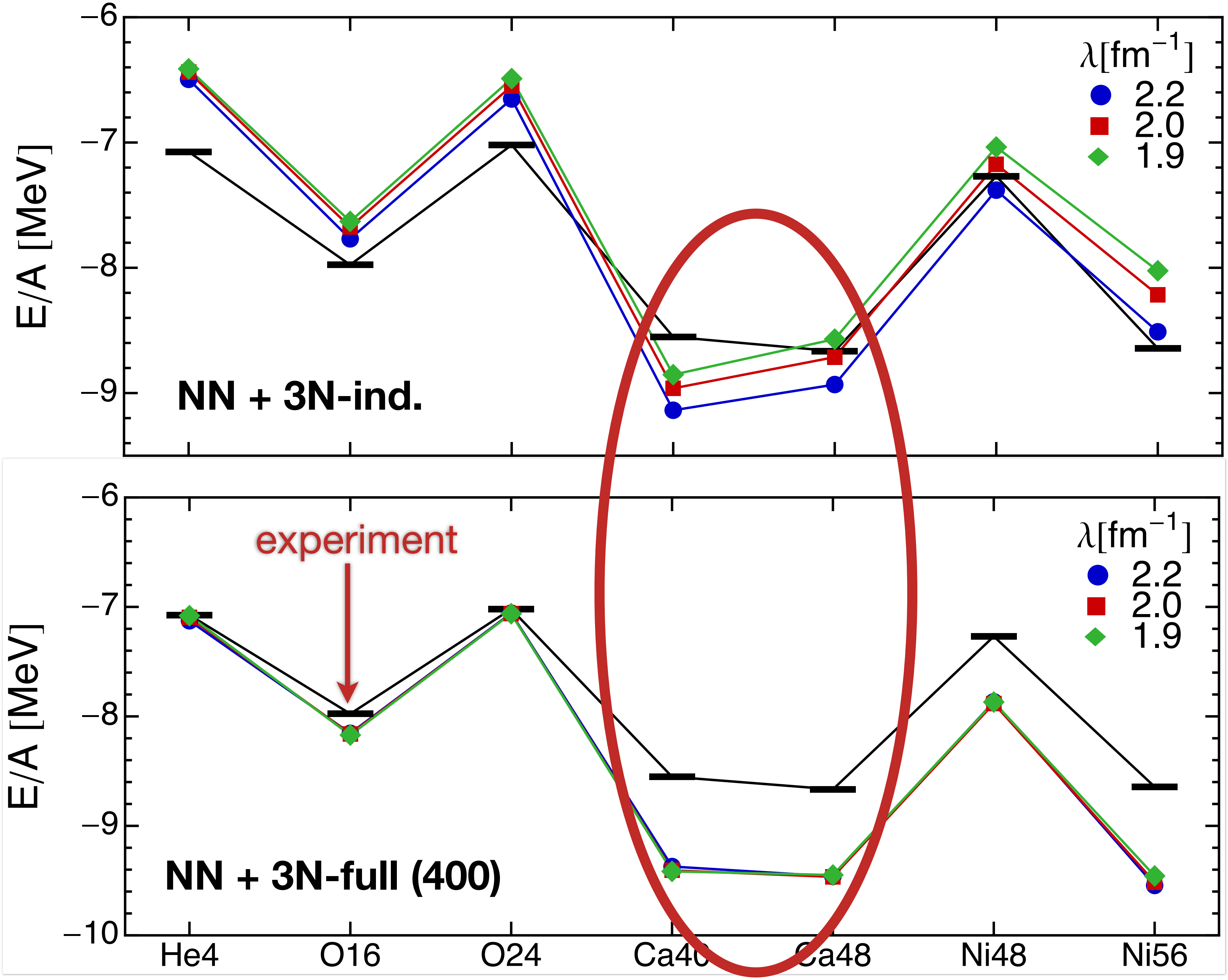


validate chiral Hamiltonians

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

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

Results: Closed-Shell Nuclei



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

Multi-Reference In-Medium SRG

Generalized Normal Ordering

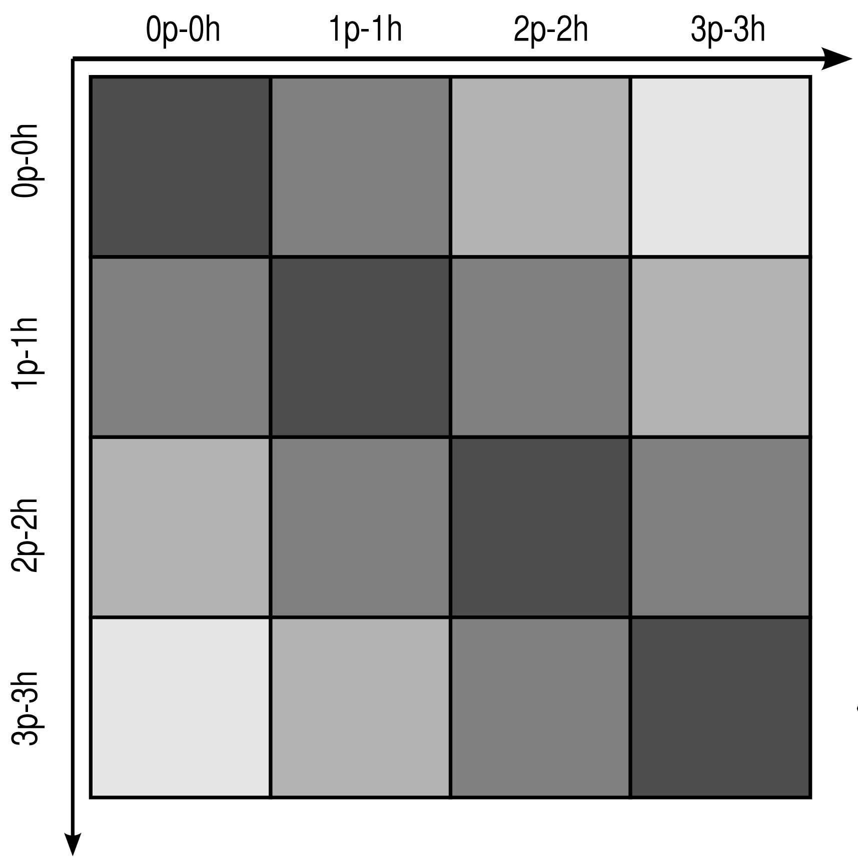
- generalized Wick theorem (Kutzelnigg & Mukherjee)
- define irreducible n-body density matrices:

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

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

$:A^{k\dots}_{m\dots}::A^{l\dots}_{n\dots}:$	λ^{k}_{n}
$:A^{k\dots}_{m\dots}::A^{l\dots}_{n\dots}:$	ξ^{l}_{m}
$:A^{ab\dots}_{cd\dots}::A^{kl\dots}_{mn\dots}:, :A^{ab\dots}_{cd\dots}::A^{kl\dots}_{mn\dots}:$, etc.	$\lambda^{ab}_{mn}, \lambda^{ab}_{cm}$, etc.
$:A^{abc\dots}_{def\dots}::A^{klm\dots}_{nop\dots}:, :A^{abc\dots}_{def\dots}::A^{klm\dots}_{nop\dots}:$, etc.	$\lambda^{abc}_{nop}, \lambda^{abk}_{nop}$, etc.
...	...

Decoupling



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

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

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

- truncation in irreducible density matrices
  - number of correlated vs. total pairs, triples, ... (caveat: 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:

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

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

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

THE OHIO STATE UNIVERSITY

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

H. H., S. Binder, A. Calci, J. Langhammer, and R. Roth, arXiv:1302.7294 [nucl-th]
K. Tsukiyama, S. K. Bogner, and A. Schwenk, Phys. Rev. C **85**, 061304(R) (2012)

Approaches to Open-Shell Nuclei

- use IM-SRG to derive effective Hamiltonians & operators for Shell Model calculations
  (K. Tsukiyama, S.K. Bogner, A. Schwenk, PRC 85, 061304 (2012))

- use IM-SRG directly with suitable open-shell reference state:

  - multi-reference state from m-scheme Hartree-Fock, (small-scale) Shell Model, DMRG, etc.

  - Hartree-Fock-Bogoliubov many-body state (allows easy implementation of spherical symmetry)

Particle-Number Projection

- HFB ground state is a superposition of states with different particle number:

$$\left|\Psi\right\rangle = \sum_{A=N,N\pm2,\dots} c_A \left|\Psi_A\right\rangle\,, \qquad \left|\Psi_N\right\rangle \equiv P_N \left|\Psi\right\rangle \equiv \frac{1}{2\pi}\int_0^{2\pi} d\phi\, e^{i\phi(\hat{N}-N)}\left|\Psi\right\rangle$$

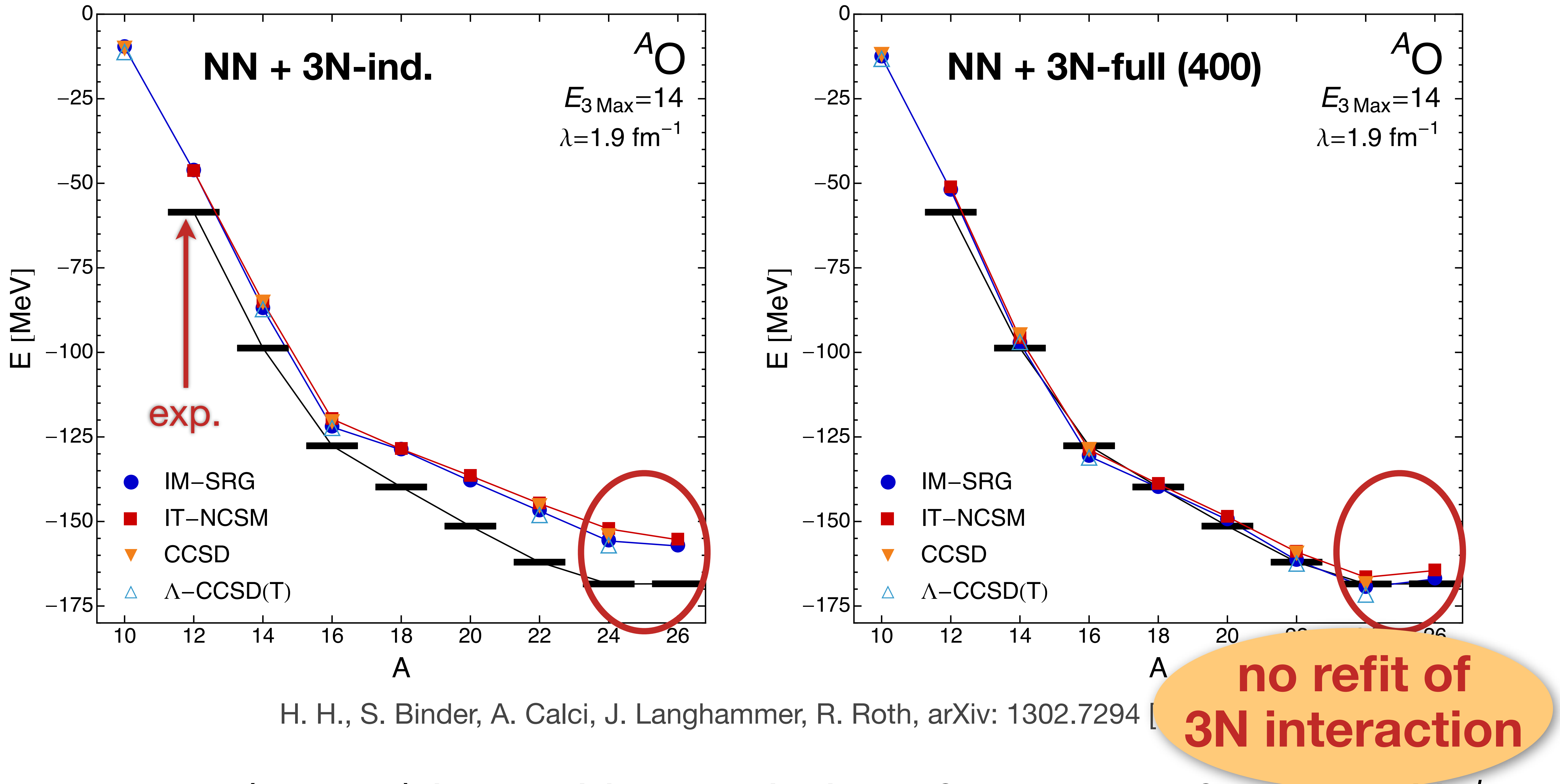
- calculate one- and two-body densities (project only once):

$$\lambda^k_l = \frac{\left\langle\Psi\right| A^k_l P_N \left|\Psi\right\rangle}{\left\langle\Psi\middle|\Psi\right\rangle}\,, \qquad \lambda^{kl}_{mn} = \frac{\left\langle\Psi\right| A^{kl}_{mn} P_N \left|\Psi\right\rangle}{\left\langle\Psi\middle|\Psi\right\rangle} - \lambda^k_m\lambda^l_m + \lambda^k_n\lambda^l_m$$

- work in natural orbitals (= HFB canonical basis):

$$\lambda^k_l = n_k\delta^k_l \left(= v^2_k\delta^k_l\right)\,, \quad 0 \leq n_k \leq 1$$

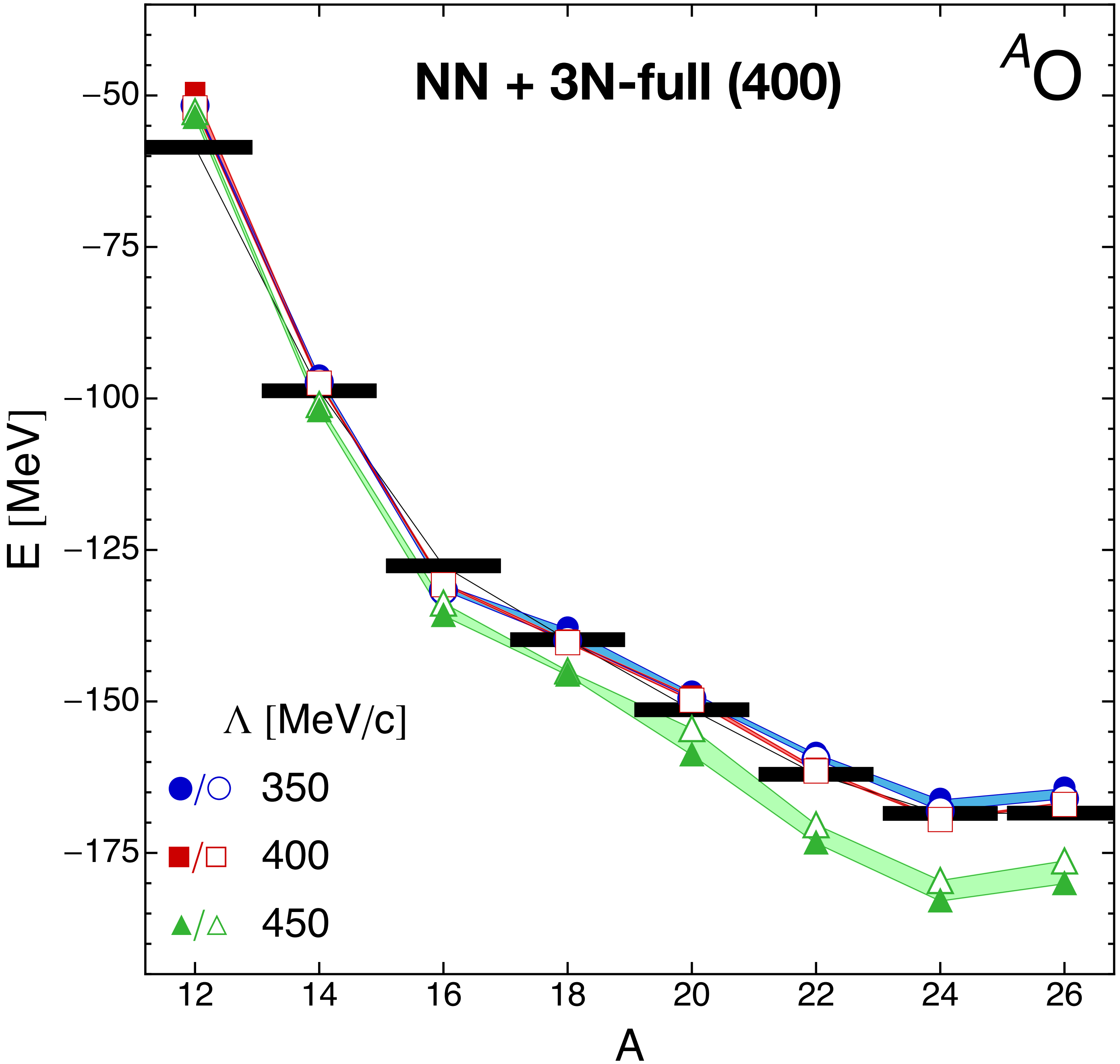
Results: Oxygen Chain



H. H., S. Binder, A. Calci, J. Langhammer, R. Roth, arXiv: 1302.7294 [

- results (mostly) insensitive to choice of generator for same H^{od}
- consistent results from different many-body methods

Variation of Scales



H. H., S. Binder, A. Calci, J. Langhammer, R. Roth, arXiv: 1302.7294 [nucl-th]

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

Conclusions

Conclusions & Outlook

- new *Ab-initio* method for medium-mass & heavy nuclei
- two-body formalism includes 3, ... , A-body forces through normal ordering
- new method for the derivation of shell-model interactions
  (K. Tsukiyama, S. K. Bogner, A. Schwenk, PRC 85, 061304 (2012))

✓ first systematic studies of closed- and open-shell nuclei based on chiral NN + 3N Hamiltonians completed
(H. H. et al. Phys. Rev. C **87**, 034307; H. H. et al., arXiv: 1302.7294 [nucl-th])

➡ analysis of Multi-Reference IM-SRG and systematic studies of other isotopic chains

➡ efficient evolution of observables ?

➡ excited states, deformation, etc. ...

Acknowledgments

S. K. Bogner
NSCL, Michigan State University

S. Binder, A. Calci, J. Langhammer, R. Roth, A. Schwenk
TU Darmstadt, Germany

R. J. Furnstahl, K. Hebeler, R. J. Perry, K. A. Wendt
The Ohio State University

P. Papakonstantinou
IPN Orsay, France

NUCLEI
Nuclear Computational Low-Energy Initiative

Ohio Supercomputer Center