In-Medium SRG with Chiral NN+3N Interactions

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Outline

- In-Medium SRG for Closed Shell-Nuclei
- Multi-Reference In-Medium SRG
- Open-Shell Nuclei
- 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

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:

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

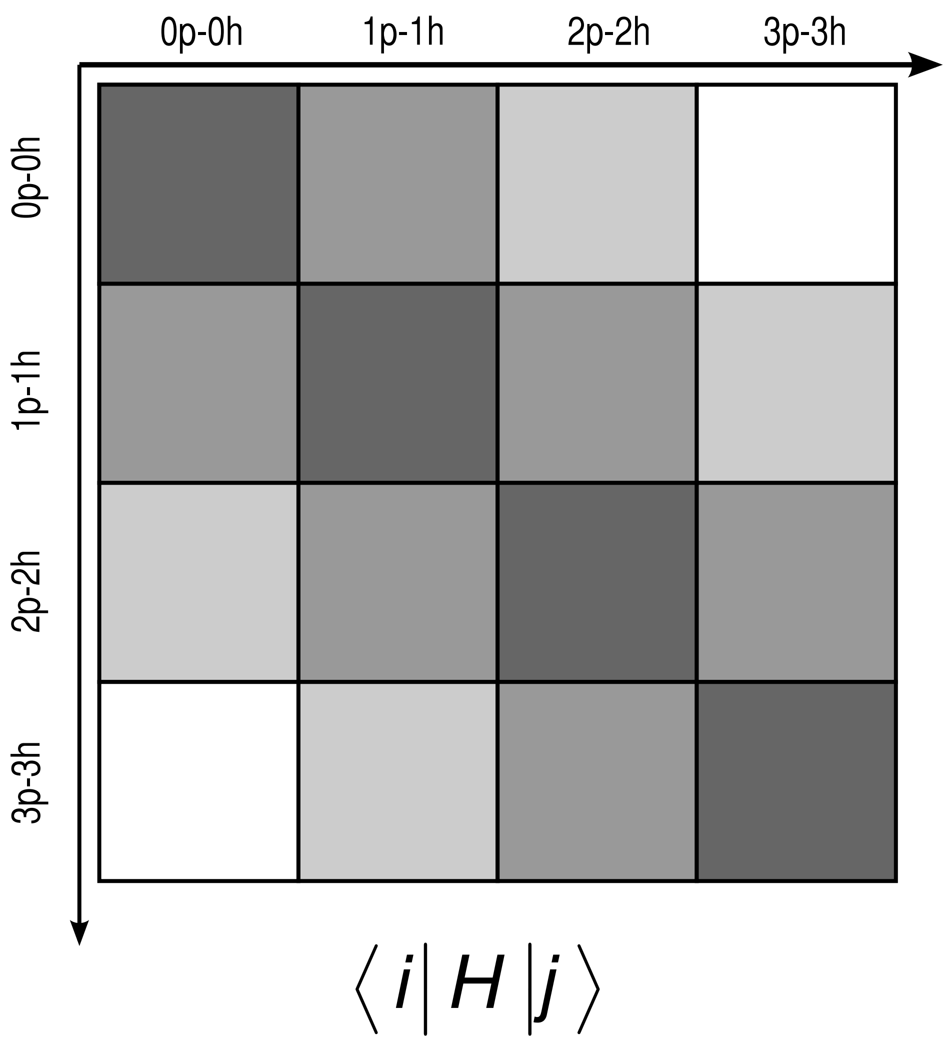
- choose $\eta(s)$ to achieve desired behavior, e.g. decoupling of momentum or energy scales

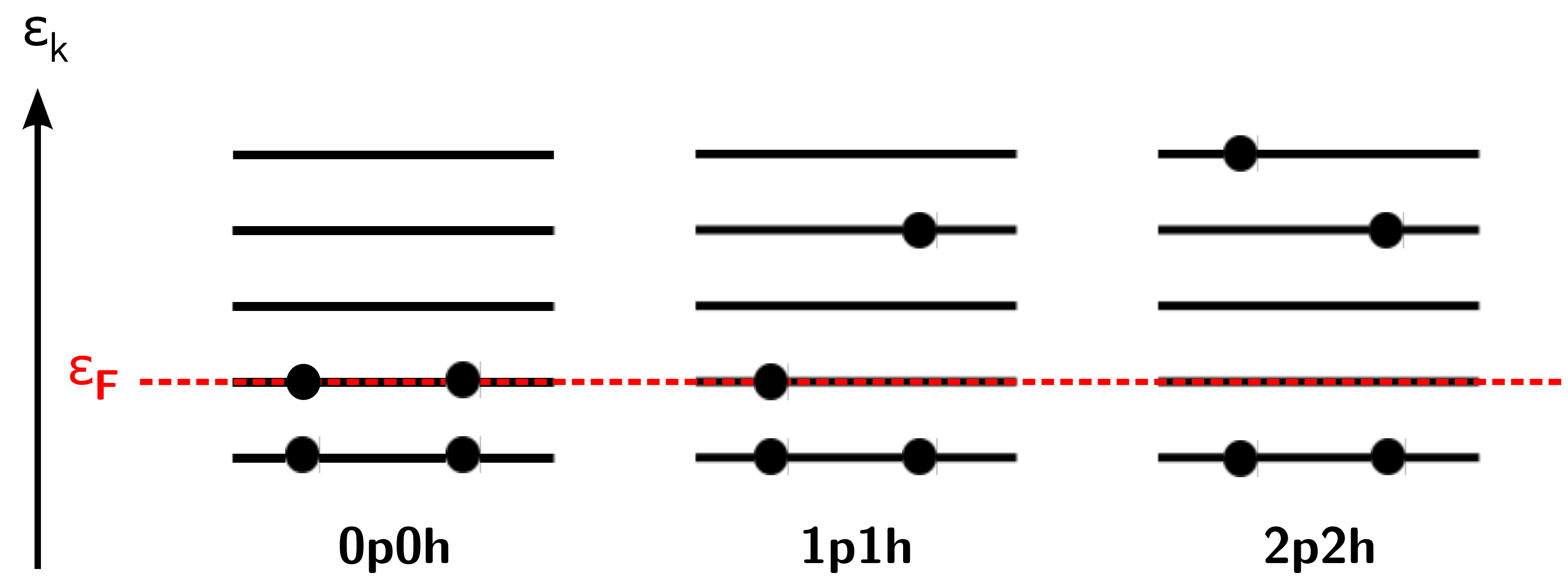
- consistently evolve observables of interest

In-Medium SRG for Closed-Shell Nuclei

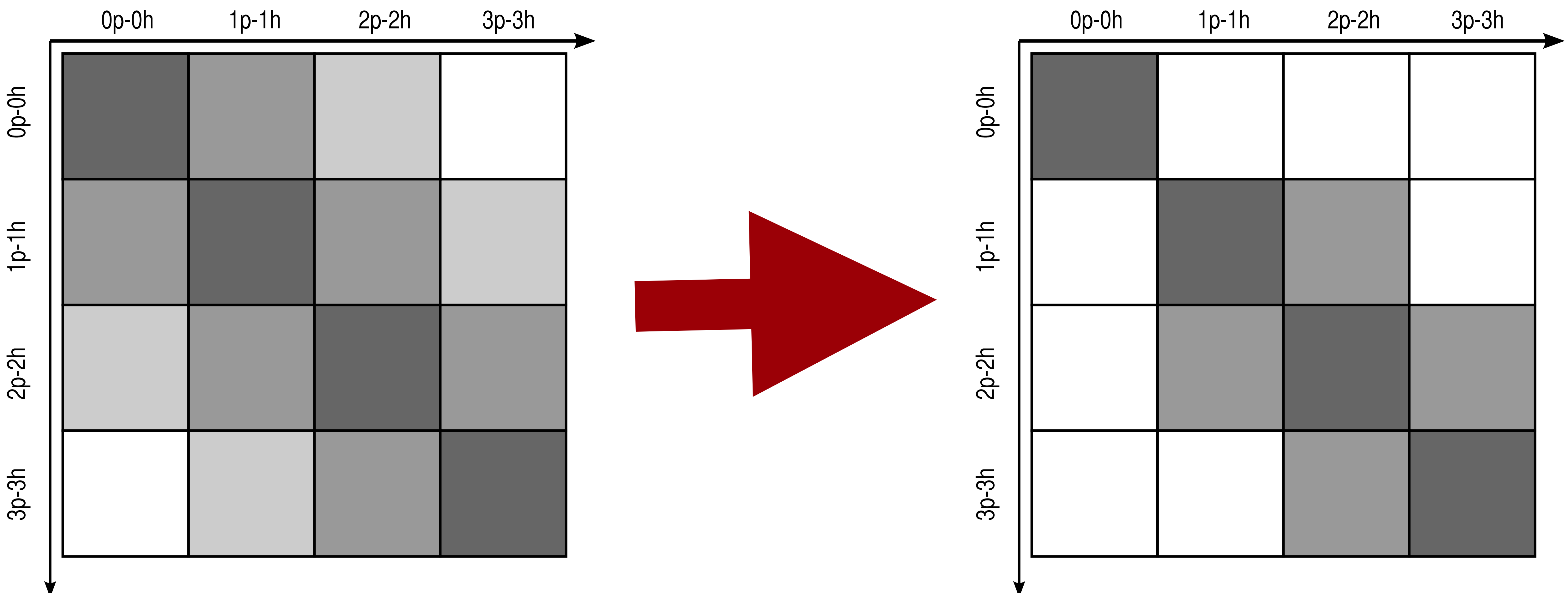
H. H., S. K. Bogner, S. Binder, A. Calci, J. Langhammer, R. Roth, and A. Schwenk,
to appear in Phys. Rev. C, arXiv:1212.1190 [nucl-th]
K. Tsukiyama, S. K. Bogner, and A. Schwenk, Phys. Rev. Lett. **106** (2011), 222502

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-Ordered Hamiltonian

Normal-Ordered Hamiltonian

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

$$E_0 = \left(1 - \frac{1}{A}\right)\sum_h t_{hh} n_h + \frac{1}{2}\sum_{hh'} \langle hh' | V_2 + T_2 | hh' \rangle n_h n_{h'} + \frac{1}{6}\sum_{hh'h''} \langle hh'h'' | V_3 | hh'h'' \rangle n_h n_{h'} n_{h''}$$

$$f^k_l = \left(1 - \frac{1}{A}\right) t_{kl} + \sum_h \langle kh | V_2 + T_2 | lh \rangle n_h + \frac{1}{2}\sum_{hh'} \langle khh' | V_3 | lhh' \rangle n_h n_{h'}$$

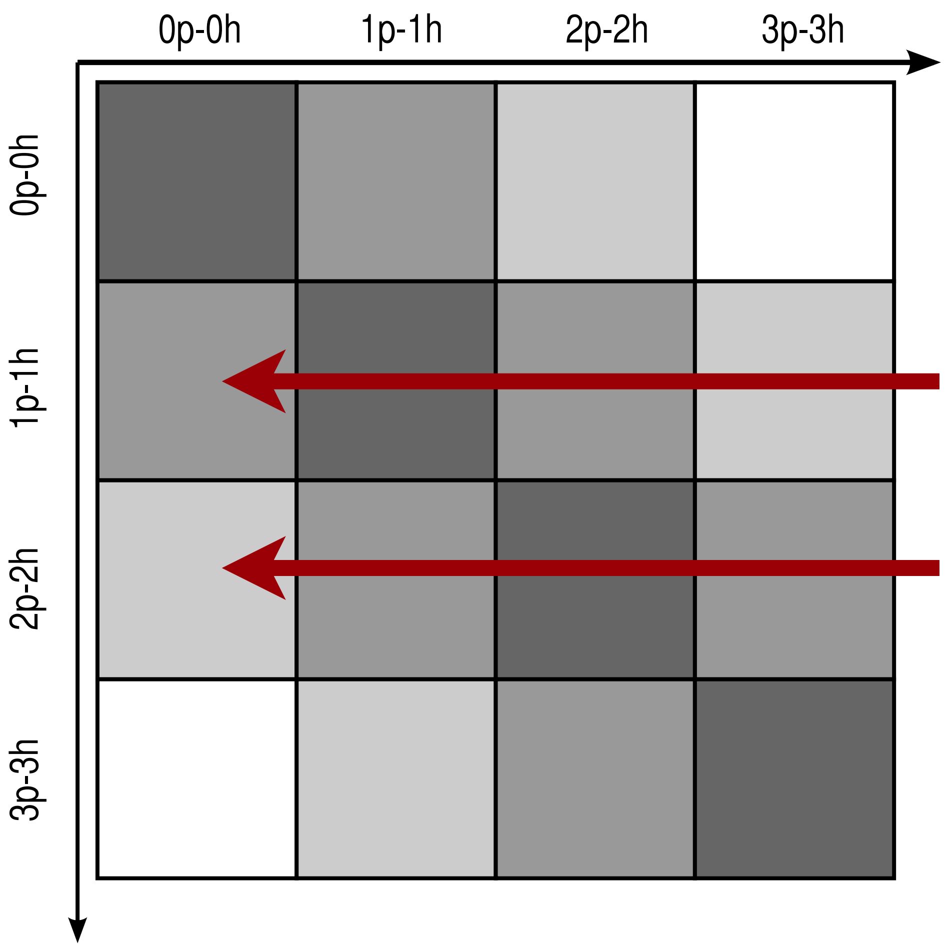
$$\Gamma^{kl}_{mn} = \langle kl | V_2 + T_2 | mn \rangle + \sum_h \langle klh | V_3 | mnh \rangle n_h$$

$$W^{ijk}_{lmn} = \langle ijk | V_3 | lmn \rangle$$

two-body formalism includes in-medium contribution from three-body interactions

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

Choice of Generator



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

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

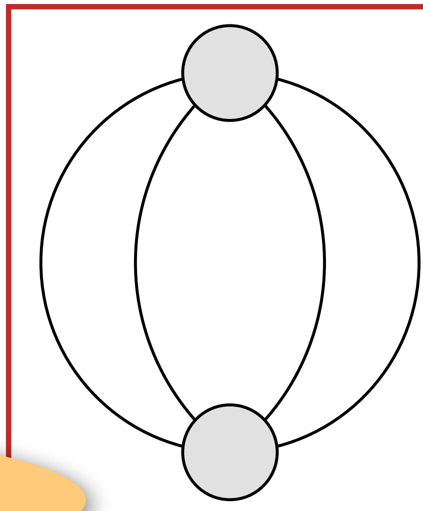
Off-Diagonal Hamiltonian

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

In-Medium SRG Flow Equations

0-body Flow

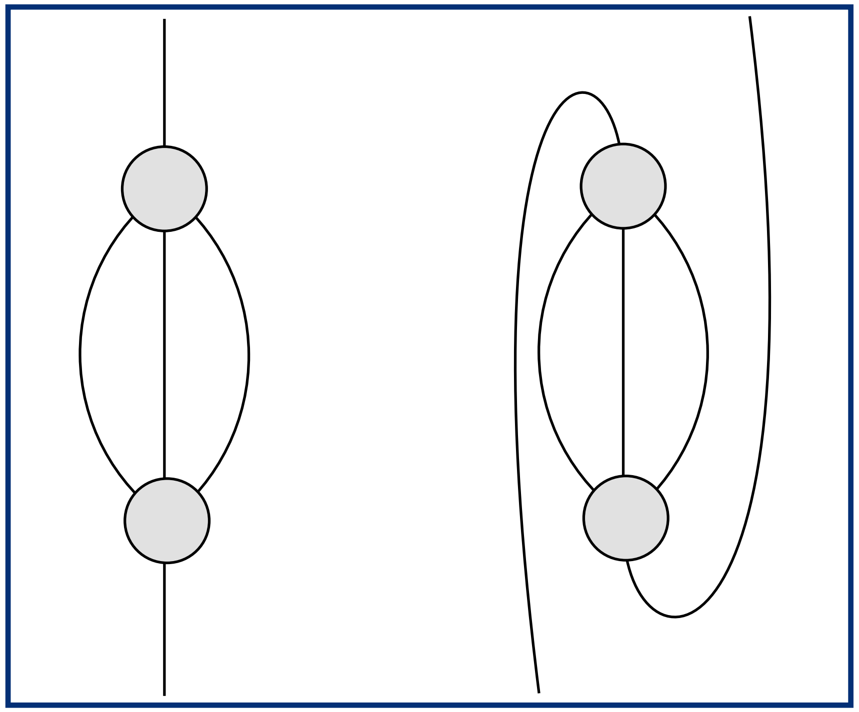
$$\frac{dE}{ds} = \sum_{ab}(n_a - n_b)\left(\eta^a_b f^b_a - f^a_b \eta^b_a\right) + \frac{1}{4}\sum_{abcd}\left(\eta^{ab}_{cd}\Gamma^{cd}_{ab} - \Gamma^{ab}_{cd}\eta^{cd}_{ab}\right) n_a n_b \bar{n}_c \bar{n}_d$$



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

1-body Flow

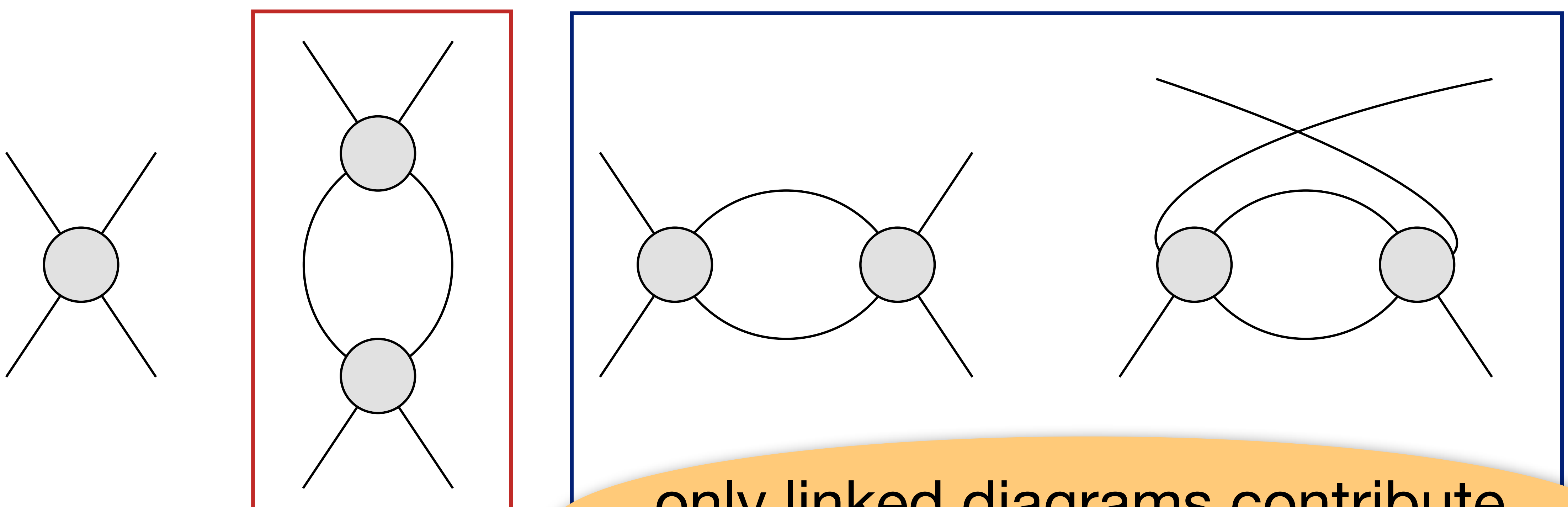
$$\frac{d}{ds}f^1_2 = \sum_a\left(\eta^1_a f^a_2 - f^1_a \eta^a_2\right) + \sum_{ab}\left(\eta^a_b \Gamma^{b1}_{a2} - f^a_b \eta^{b1}_{a2}\right)(n_a - n_b)$$
$$+ \frac{1}{2}\sum_{abcdef}\left(\eta^{1a}_{bc}\Gamma^{bc}_{2a} - \Gamma^{1a}_{bc}\eta^{bc}_{2a}\right)\left(n_a \bar{n}_b \bar{n}_c + \bar{n}_a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



In-Medium SRG Flow Equations

2-body Flow

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

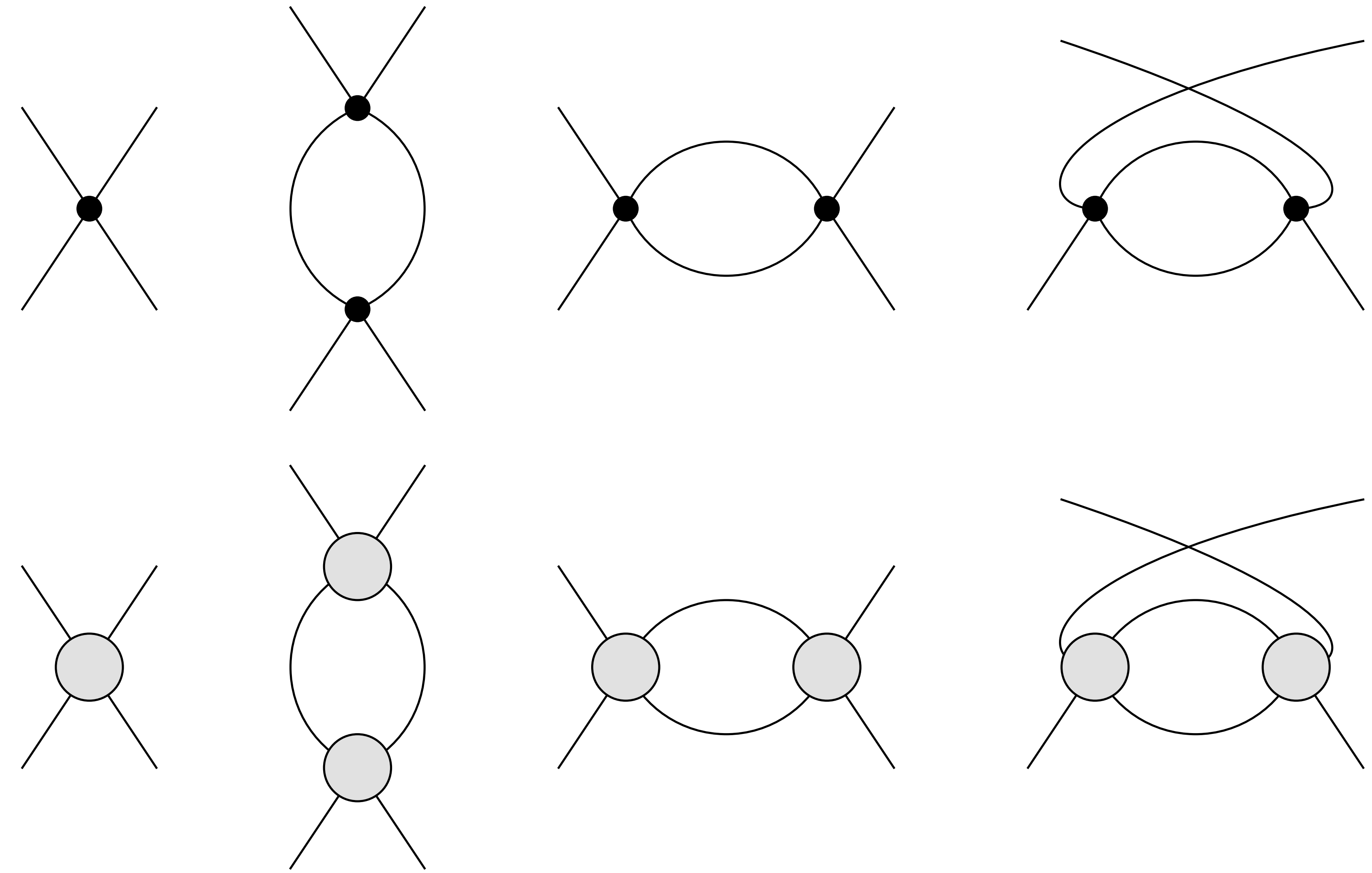


only linked diagrams contribute,
IM-SRG size-extensive

In-Medium SRG Flow: Diagrams

$\Gamma(\delta s) \sim$

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



In-Medium SRG Flow: Diagrams

$\Gamma(\delta s) \sim$

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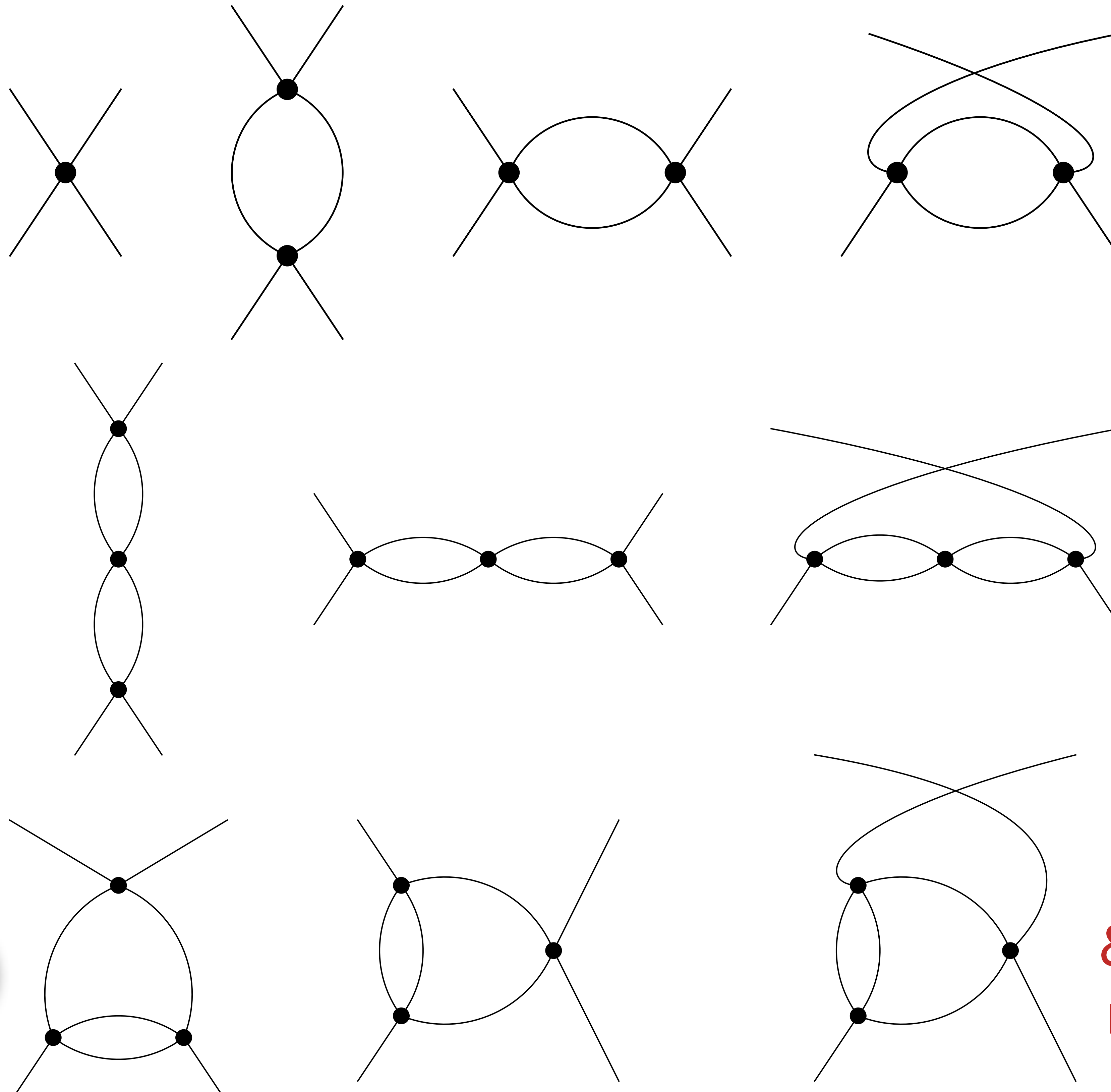
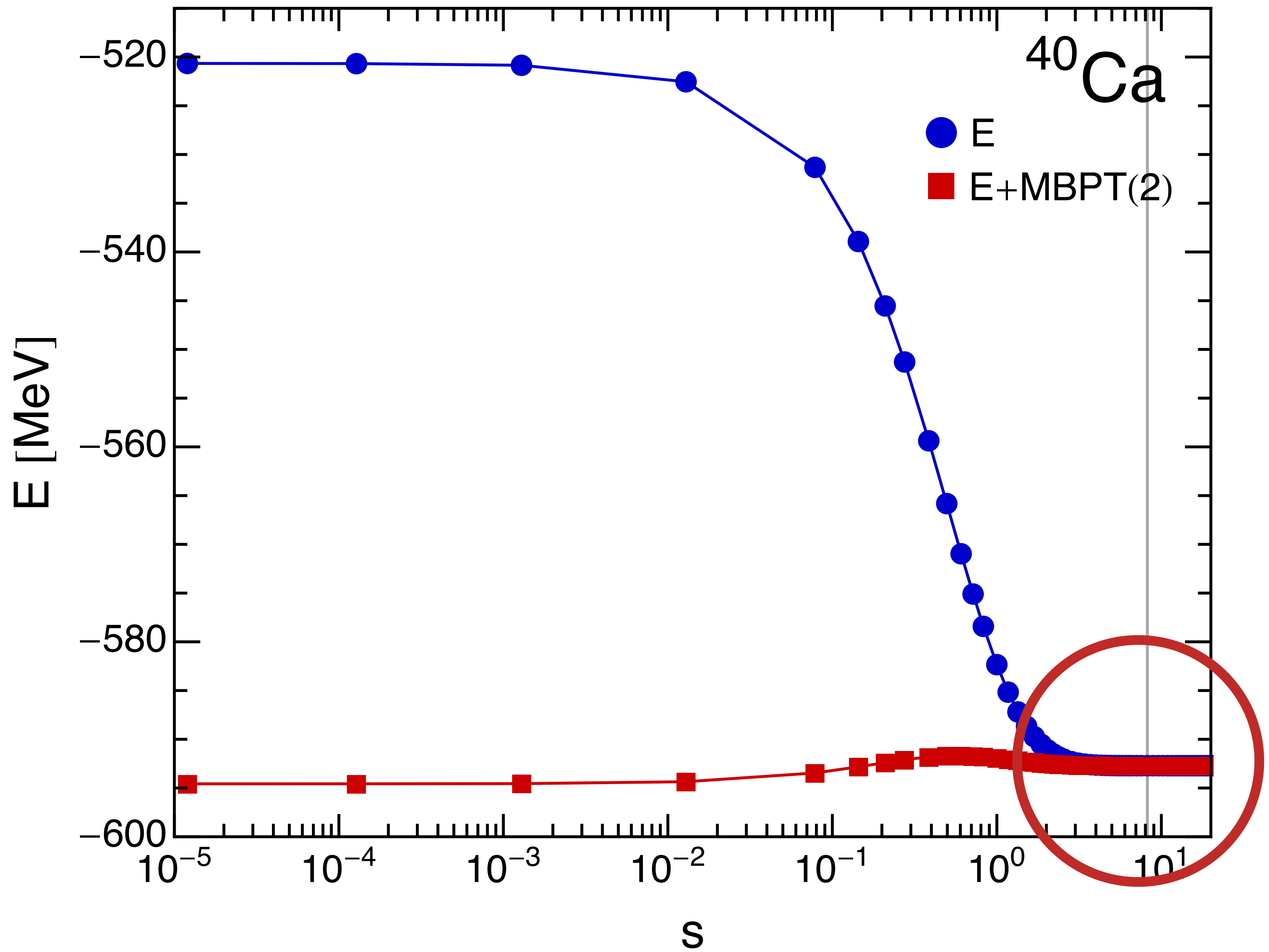
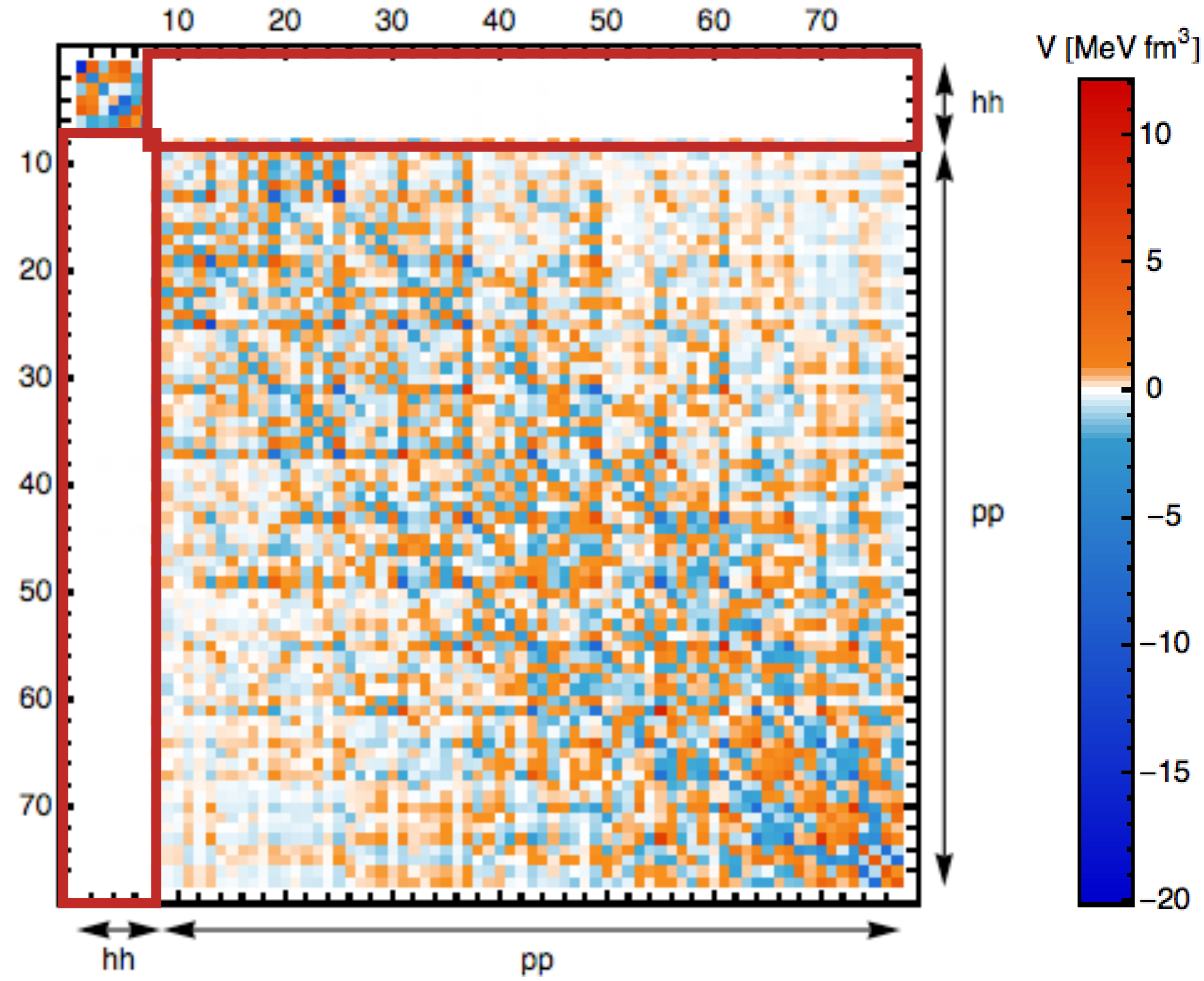


non-perturbative resummation

& many more...

Decoupling



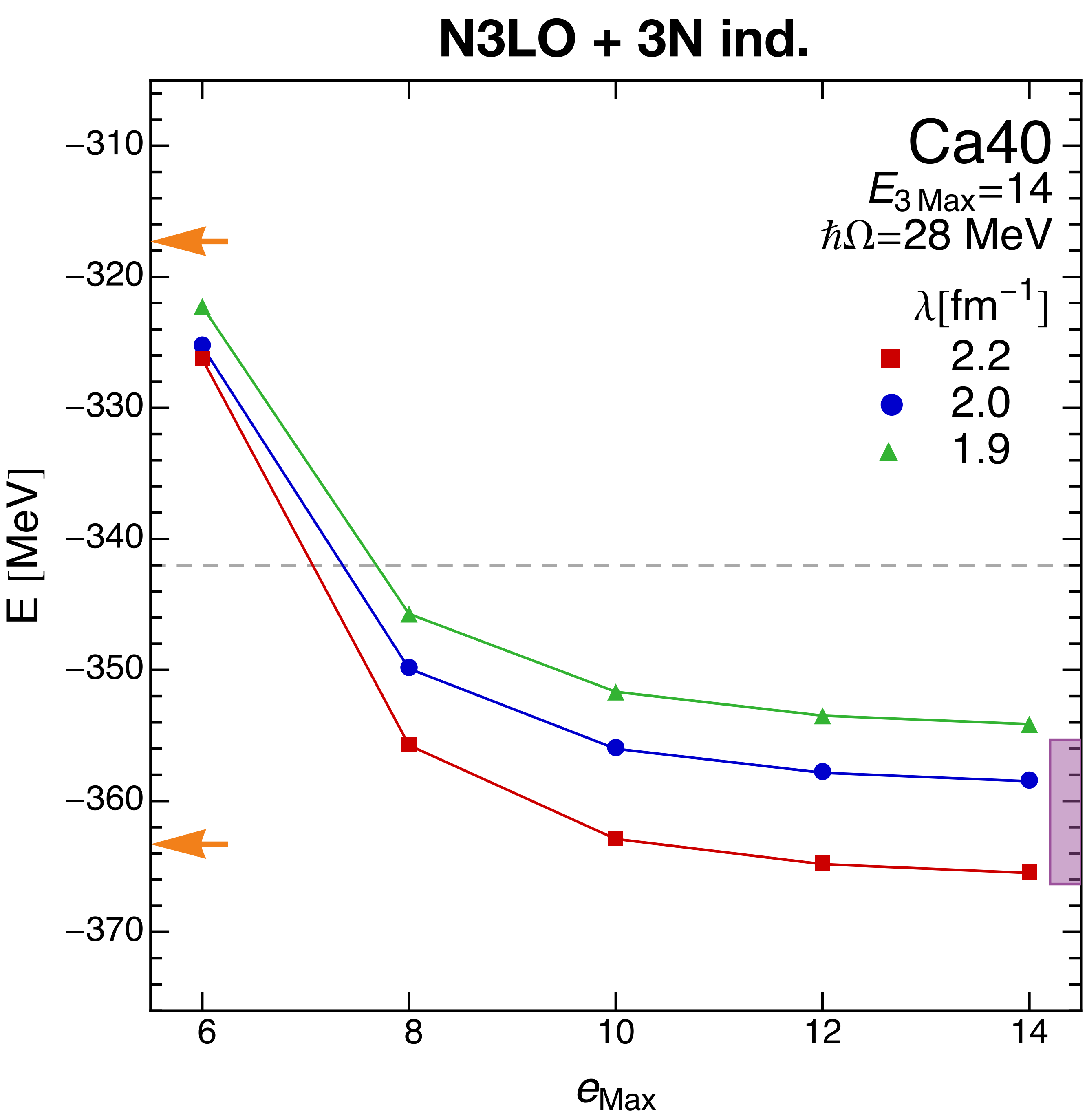


N3LO, $\lambda = 2.0\ \mathrm{fm}^{-1}, e_{\mathrm{Max}} = 8$

non-perturbative resummation of MBPT series (correlations)

off-diagonal couplings are rapidly driven to zero

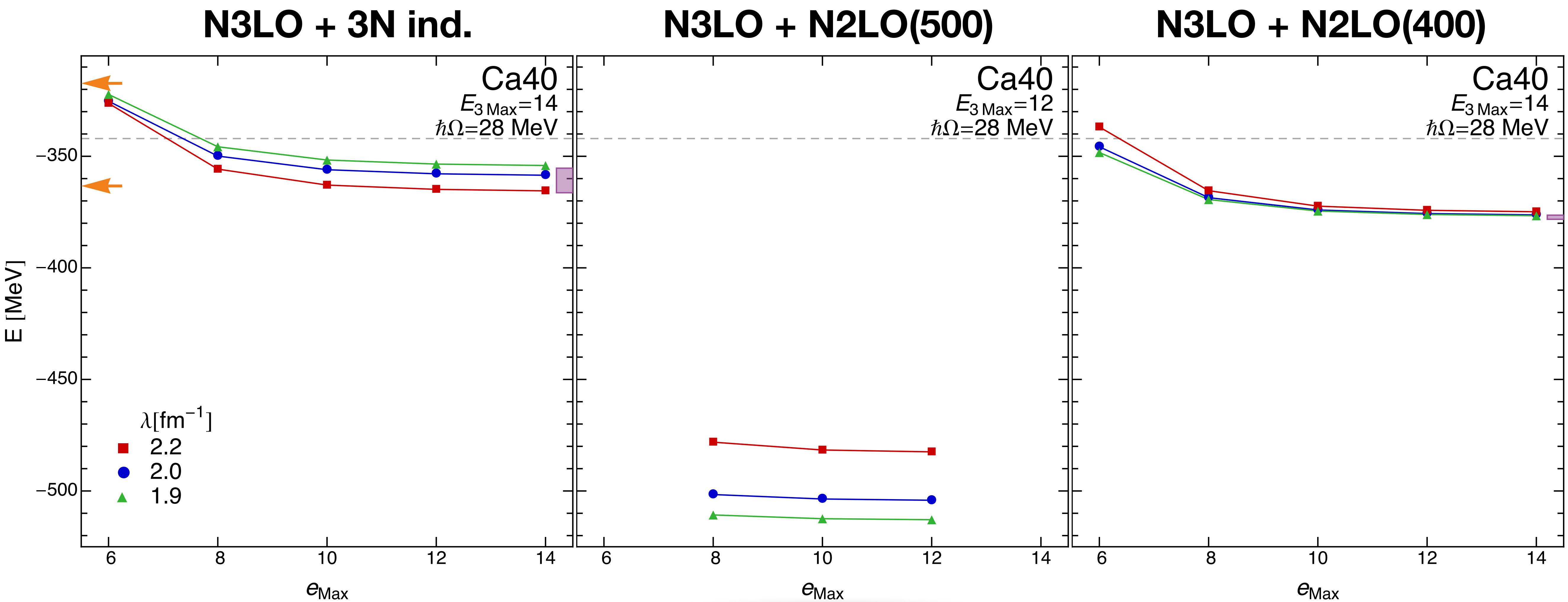
Results: Closed-Shell Nuclei



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

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

Results: Closed-Shell Nuclei

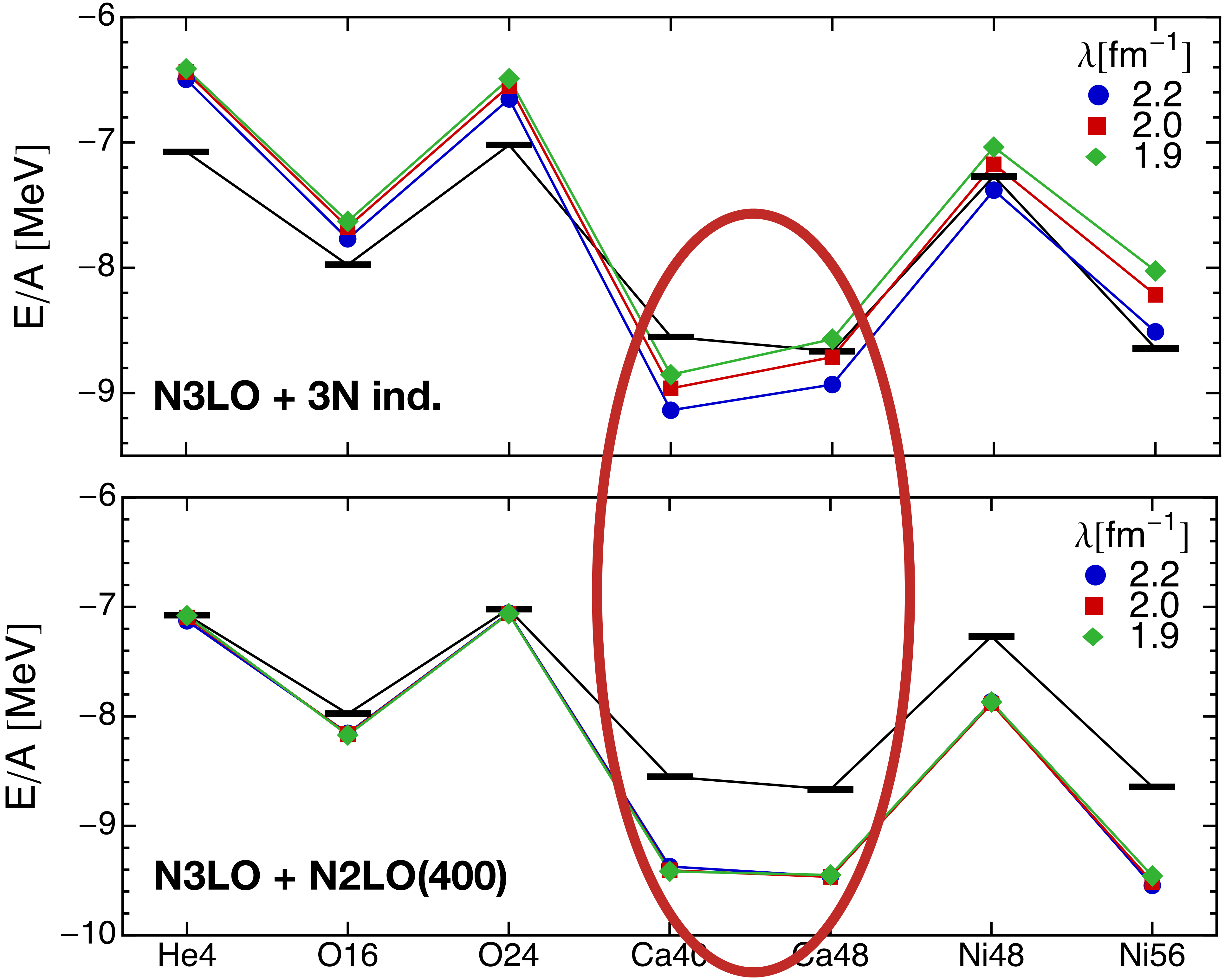


constraints & diagnostics for chiral Hamiltonians

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., arXiv:1211.4748 [nucl-th] & PRL 109, 052501 (2012)

Results: Closed-Shell Nuclei



H. Hergert et al., to appear in Phys. Rev. C, arXiv: 1212.1190 [nucl-th]

Multi-Reference
In-Medium SRG

Generalized Normal Ordering

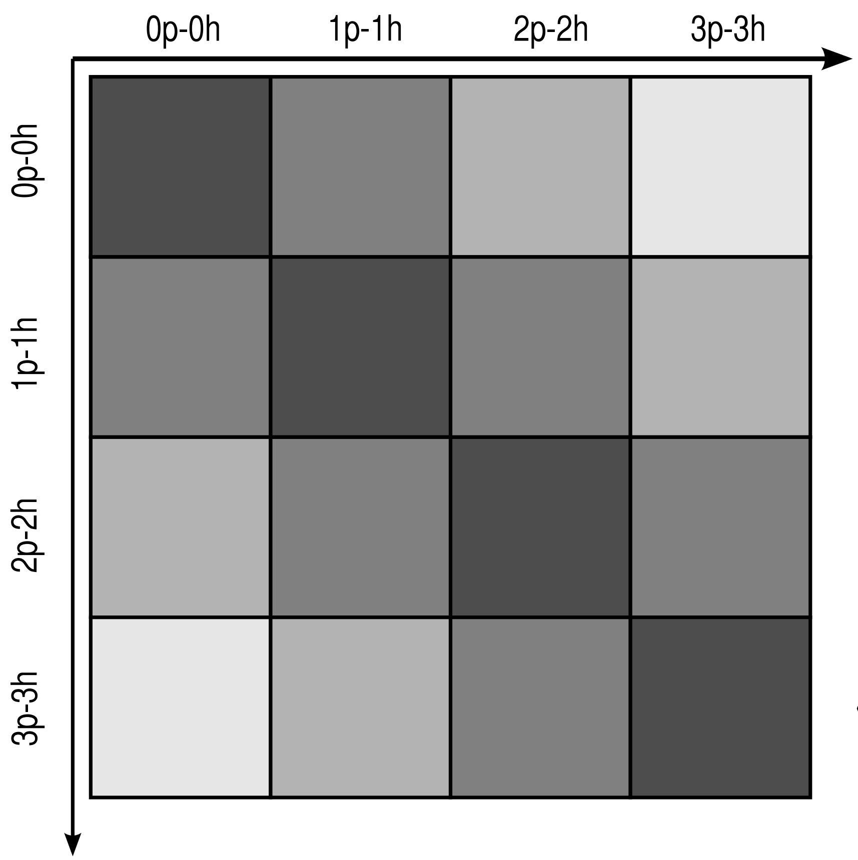
- generalized Wick theorem (Kutzelnigg & Mukherjee)
- define irreducible n-body density matrices:

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

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

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

Decoupling



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

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

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

- 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

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

Particle-Number Projection

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

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

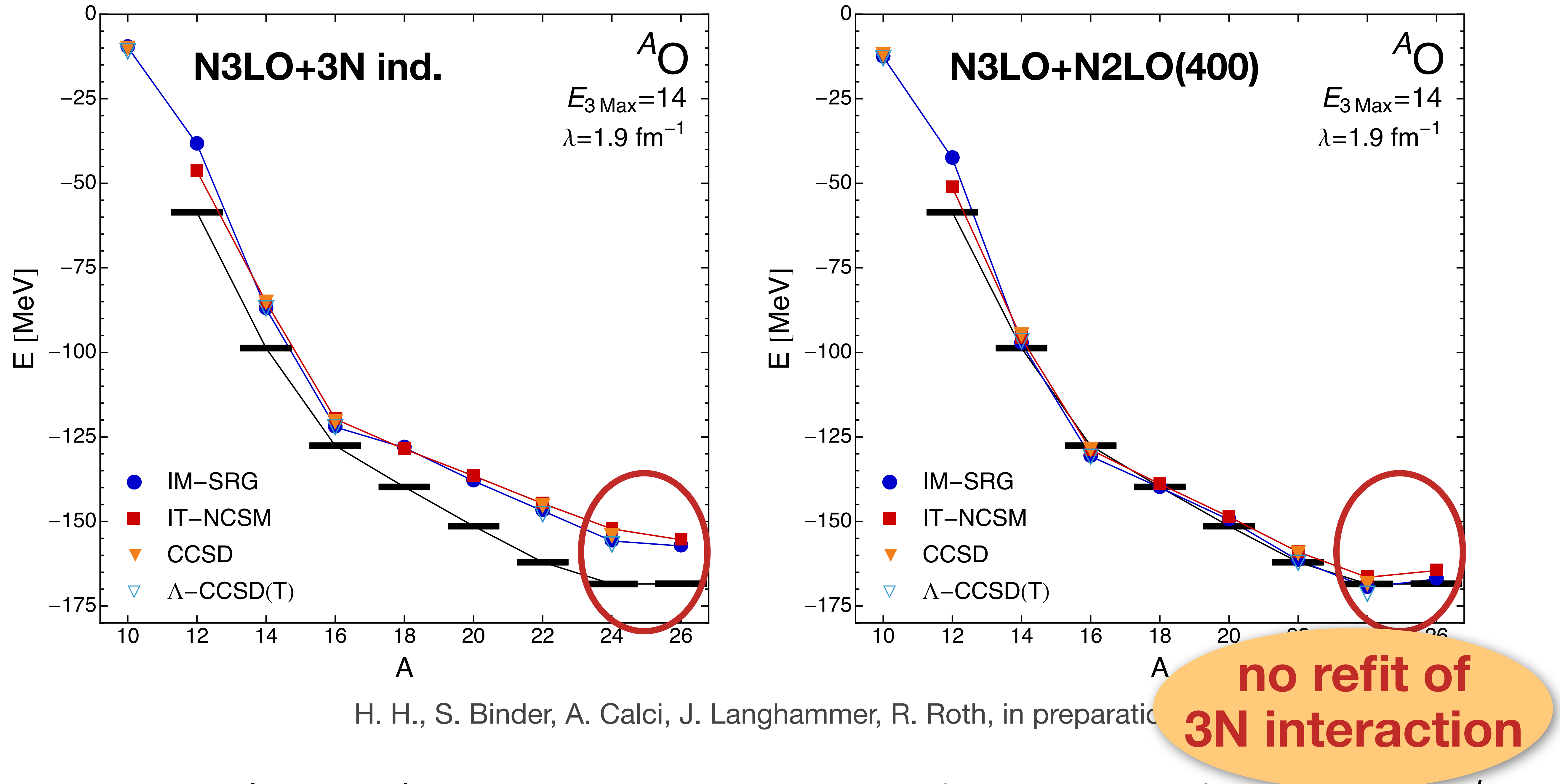
- calculate one- and two-body densities (project only once):

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

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

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

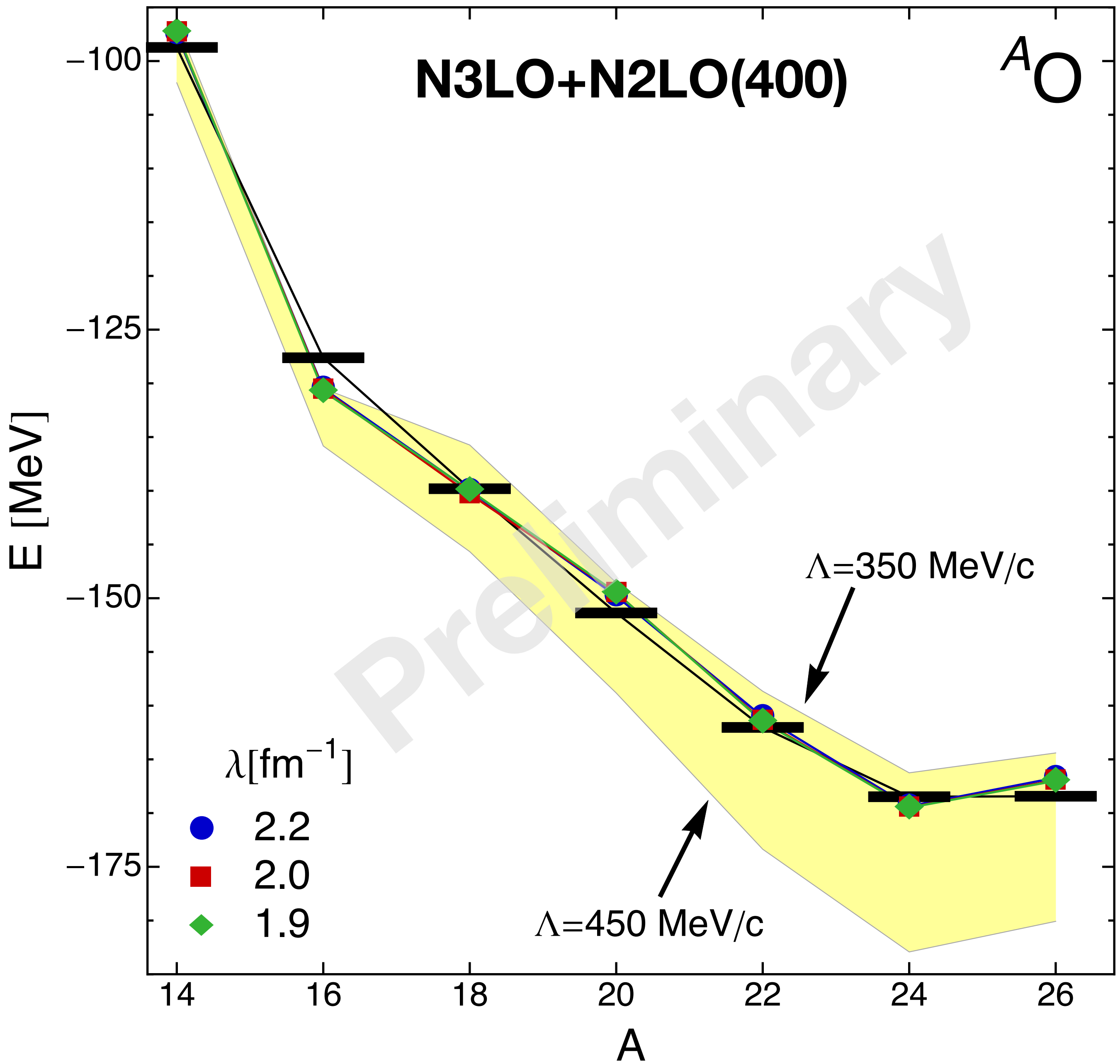
Results: Oxygen Chain



H. H., S. Binder, A. Calci, J. Langhammer, R. Roth, in preparation

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

Variation of Scales



- 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, suitable 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 study of closed-shell nuclei based on chiral NN + 3N Hamiltonians completed
(H. H. et al., arXiv: 1212.1190 [nucl-th])

➡ analysis of multi-reference IM-SRG & systematic study of open-shell nuclei

➡ efficient evolution of observables ?

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

Supplements

Normal-Ordering & Wick's Theorem

- define elementary contractions of a one-body operator w.r.t. a given reference state as

$$A^k_l \equiv a^\dagger_k a_l\,, \quad \lambda^k_l \equiv \left\langle \Psi \right| A^k_l \left| \Psi \right\rangle, \quad \xi^k_l \equiv \lambda^k_l - \delta^k_l$$

- define normal-ordered operators recursively through all possible internal contractions:

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

- Wick's Theorem: products of normal-ordered operators can be expanded in terms of external contractions alone

$$:A^{k_1\dots k_N}_{m_1\dots m_N}::A^{l_1\dots l_N}_{n_1\dots n_N}: = (-1)^{N-1}\lambda^{k_1}_{n_1} :A^{k_2\dots k_N l_1\dots l_N}_{m_1\dots m_N n_2\dots n_N}:$$
$$+ (-1)^{N-1}\xi^{l_1}_{m_1} :A^{k_1\dots k_N l_2\dots l_N}_{m_2\dots m_N n_1\dots n_N}: + \dots$$

Choice of Generator

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- Wegner

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

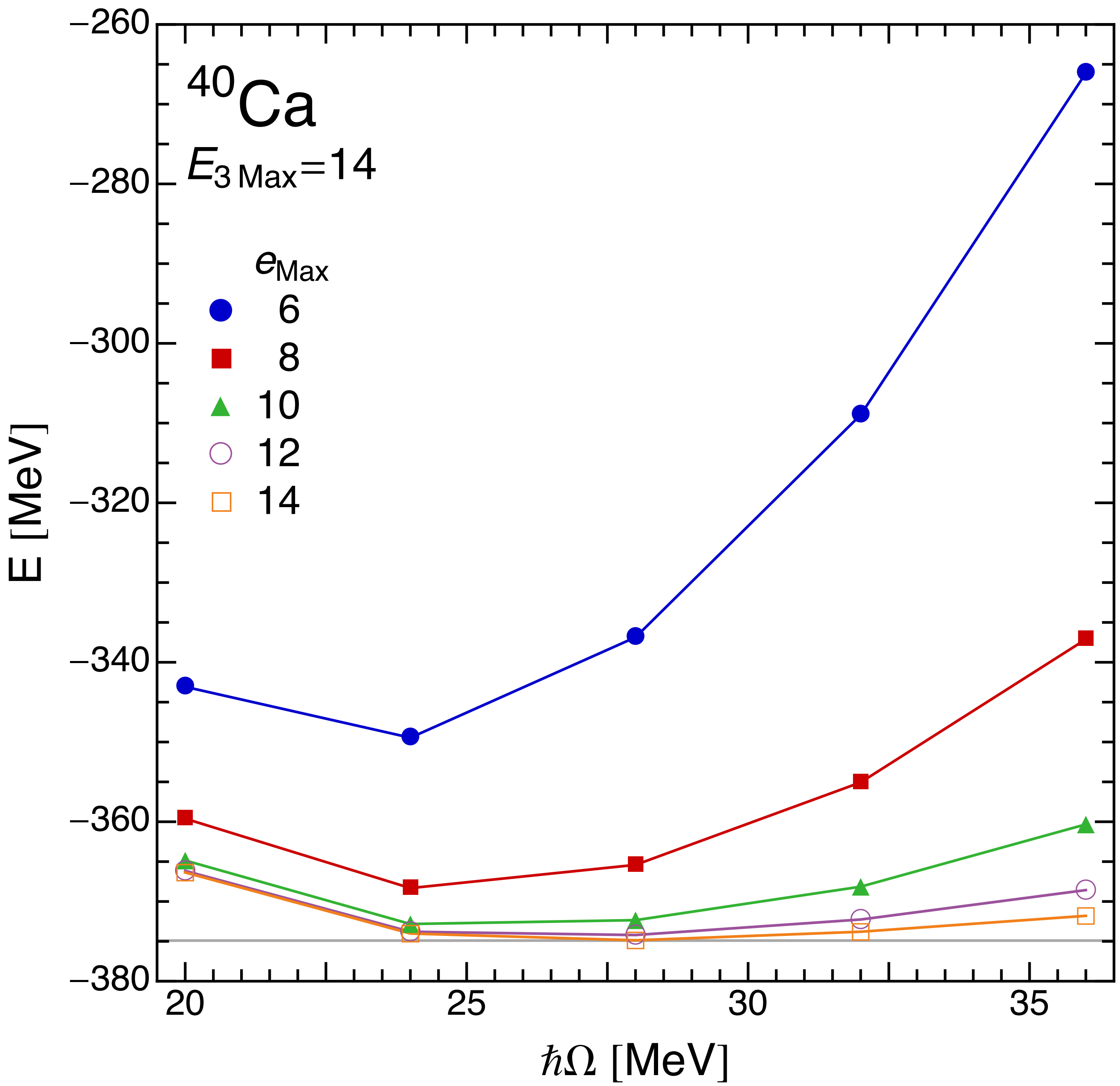
- White (J. Chem. Phys. 117, 7472)

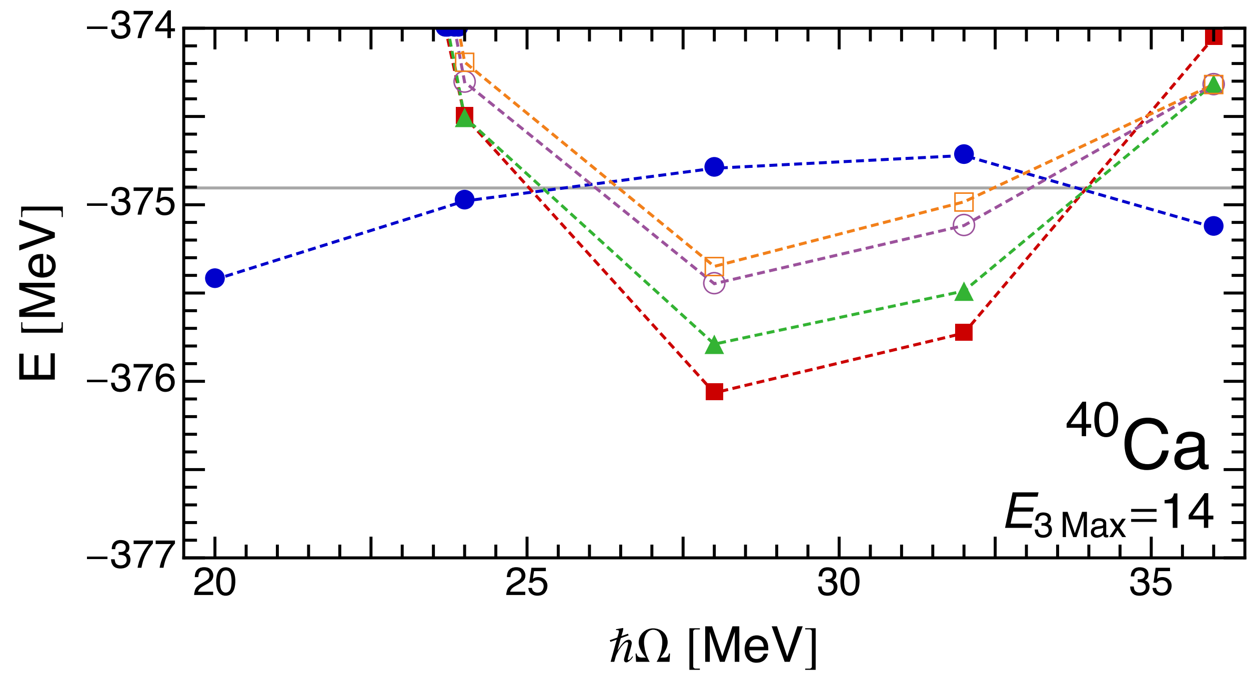
$$\eta^{II} = \sum_{ph} \frac{f^{p}_{h}}{E_p - E_h} :A^{p}_{h}: + \sum_{pp'hh'} \frac{\Gamma^{pp'}_{hh'}}{E_{pp'} - E_{hh'}} :A^{pp'}_{hh'}: + \text{H.c.}$$

$E_p - E_h, E_{pp'} - E_{hh'}$: 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

Extraplation





max./UV momentum:

$$\Lambda_{\mathrm{UV}} = \sqrt{2m(e_{\mathrm{Max}} + 3/2)\hbar\Omega}$$

radial extent:

$$L = \sqrt{2(e_{\mathrm{Max}} + 3/2)\hbar/m\Omega}$$

simultaneous ultraviolet & infrared extrapolation:

$$E(\Lambda_{\mathrm{UV}}, L) = E_\infty + A_0 \exp\left(-2\Lambda_{\mathrm{UV}}^2/A_1^2\right) + A_2 \exp\left(-2k_\infty L\right)$$

(R. Furnstahl, G. Hagen & T. Papenbrock, PRC 86,031301 (2012))