In-Medium SRG for Finite Nuclei

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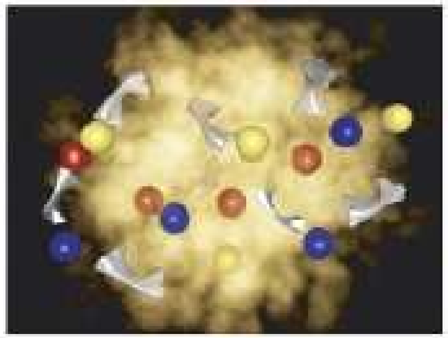
Outline

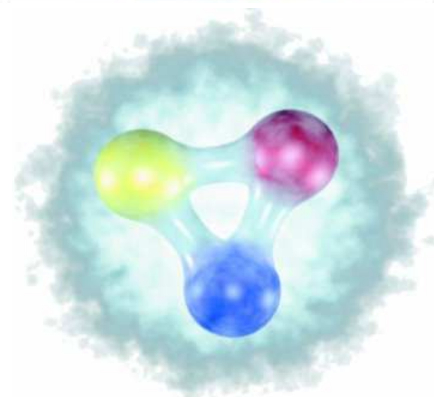
THE OHIO STATE UNIVERSITY

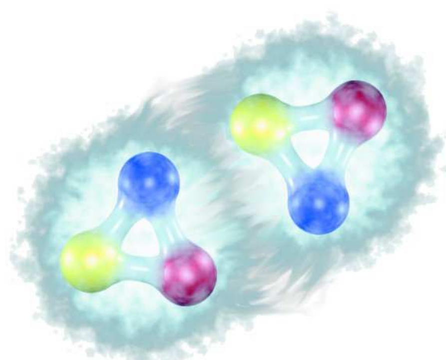
- Similarity Renormalization Group in Nuclear Physics
- In-Medium SRG for Closed Shell-Nuclei
- Multi-Reference In-Medium SRG
- Open-Shell Nuclei
- Outlook

Scales of the Strong Interaction

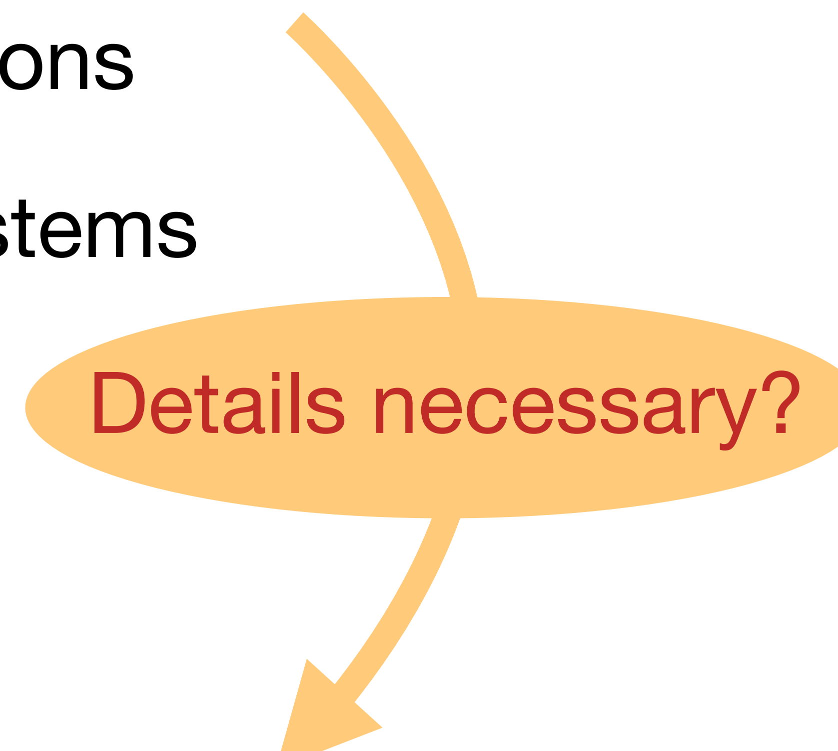


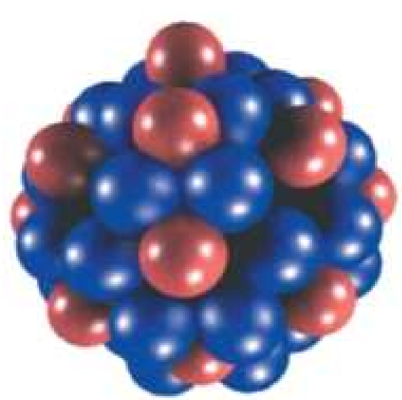
- quarks, gluons





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

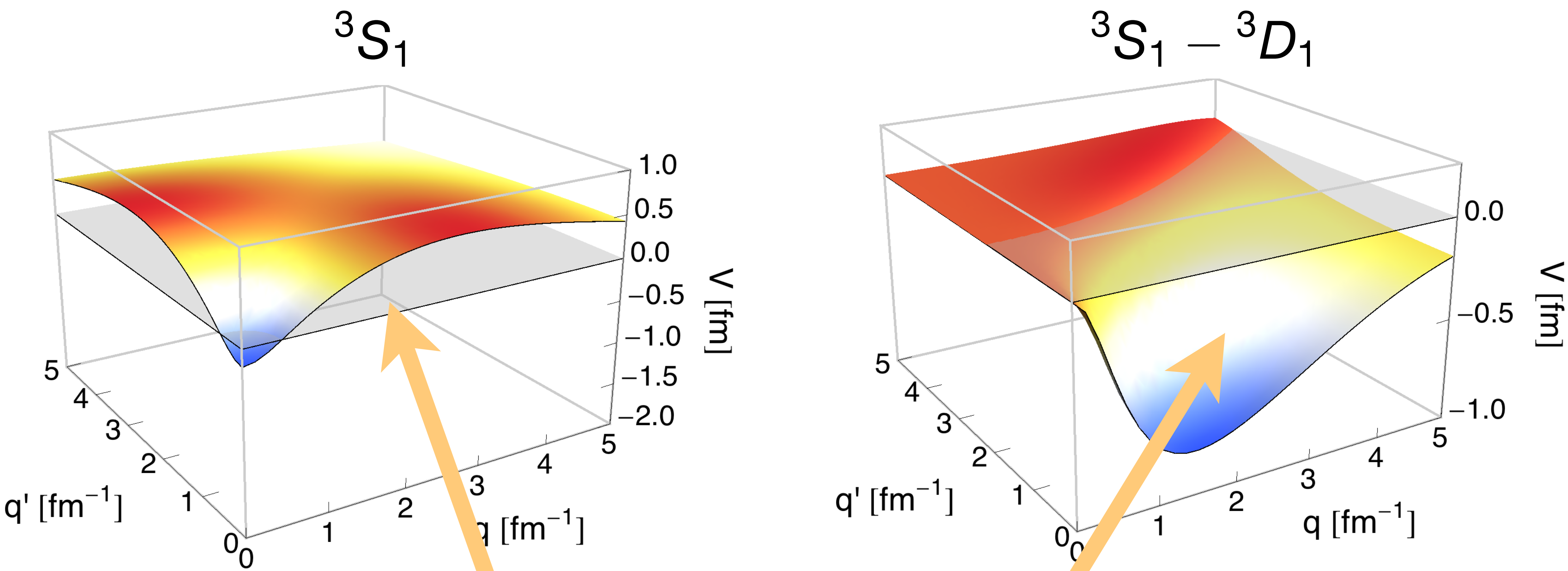




- finite nuclei
  - nuclear structure & reactions

Correlations in the NN System

Argonne V18



strong short-range correlations
$\Longleftrightarrow$ strong coupling of low and high momenta

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:

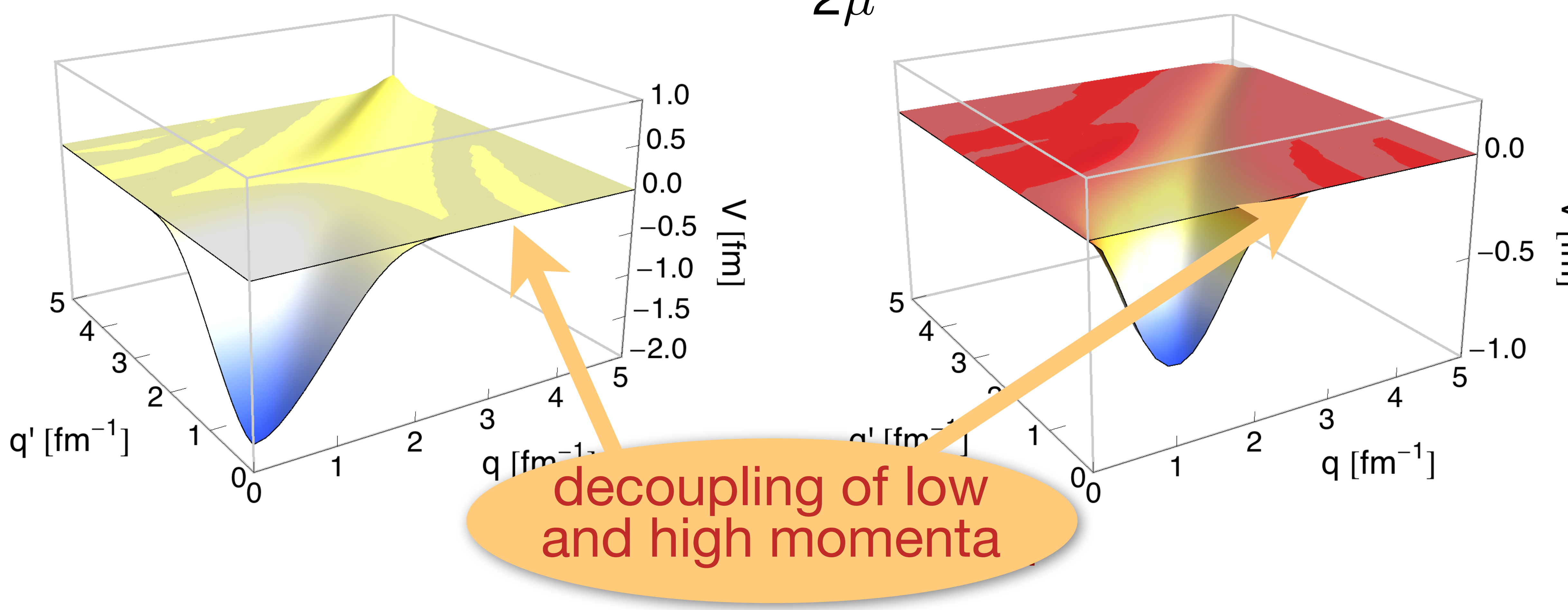
$$\frac{d}{ds} H(s) = \left[\eta(s), H(s)\right] , \quad \eta(s) = \frac{dU(s)}{ds} U^\dagger(s) = -\eta^\dagger(s)$$

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

- consistently evolve observables of interest

SRG Evolution of NN Interactions

$$\eta(s) \stackrel{2B}{=} \left[\frac{q^2}{2\mu}, V(s)\right]$$

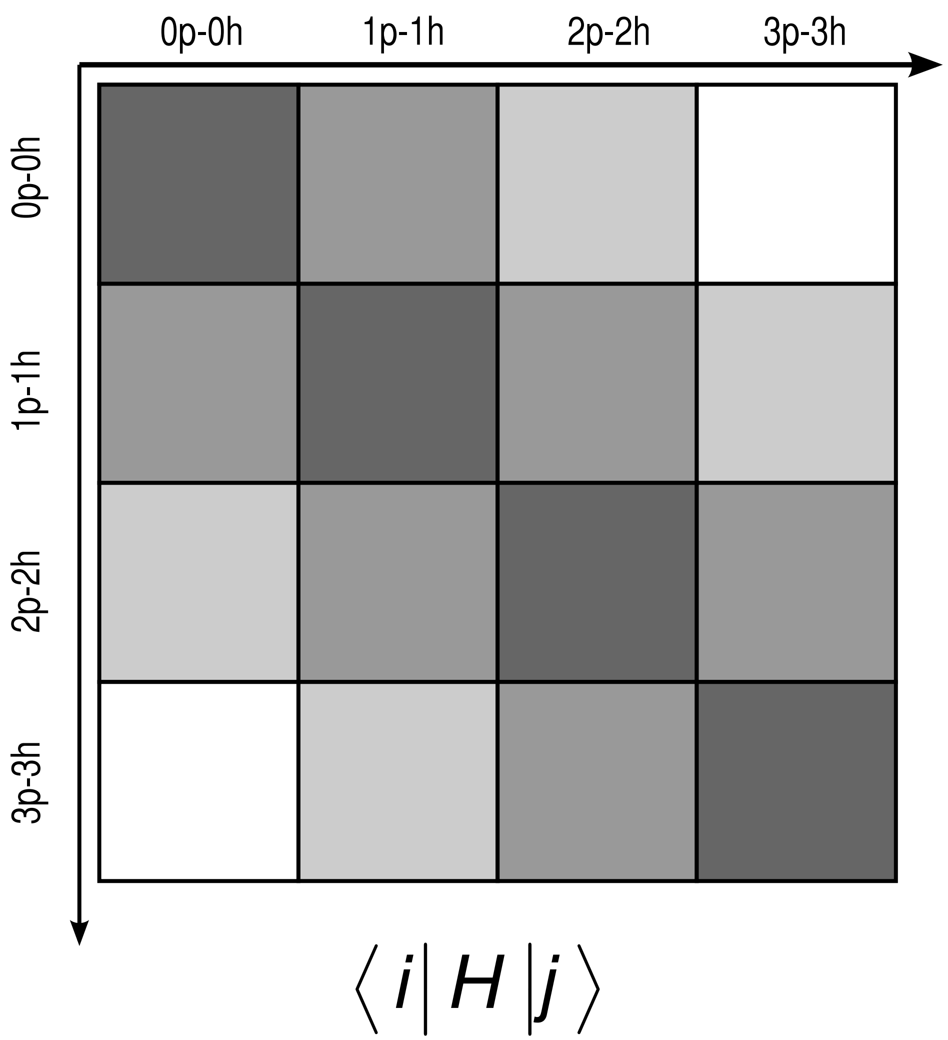


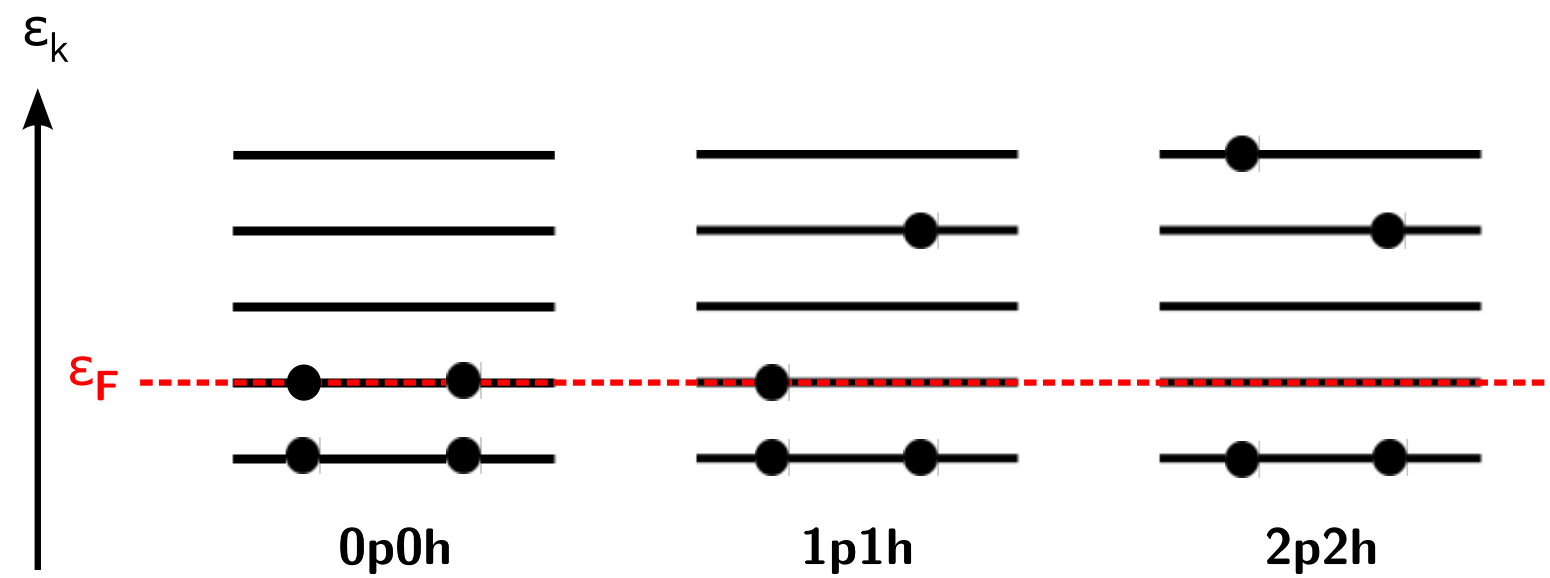
- decoupling drastically improves convergence
- SRG evolution induces many-body forces: inclusion of three-body sector has been achieved
(Jurgenson, Furnstahl, Navratil, PRL 103, 082501; Hebeler, PRC 85, 021002)

In-Medium SRG for Closed-Shell Nuclei

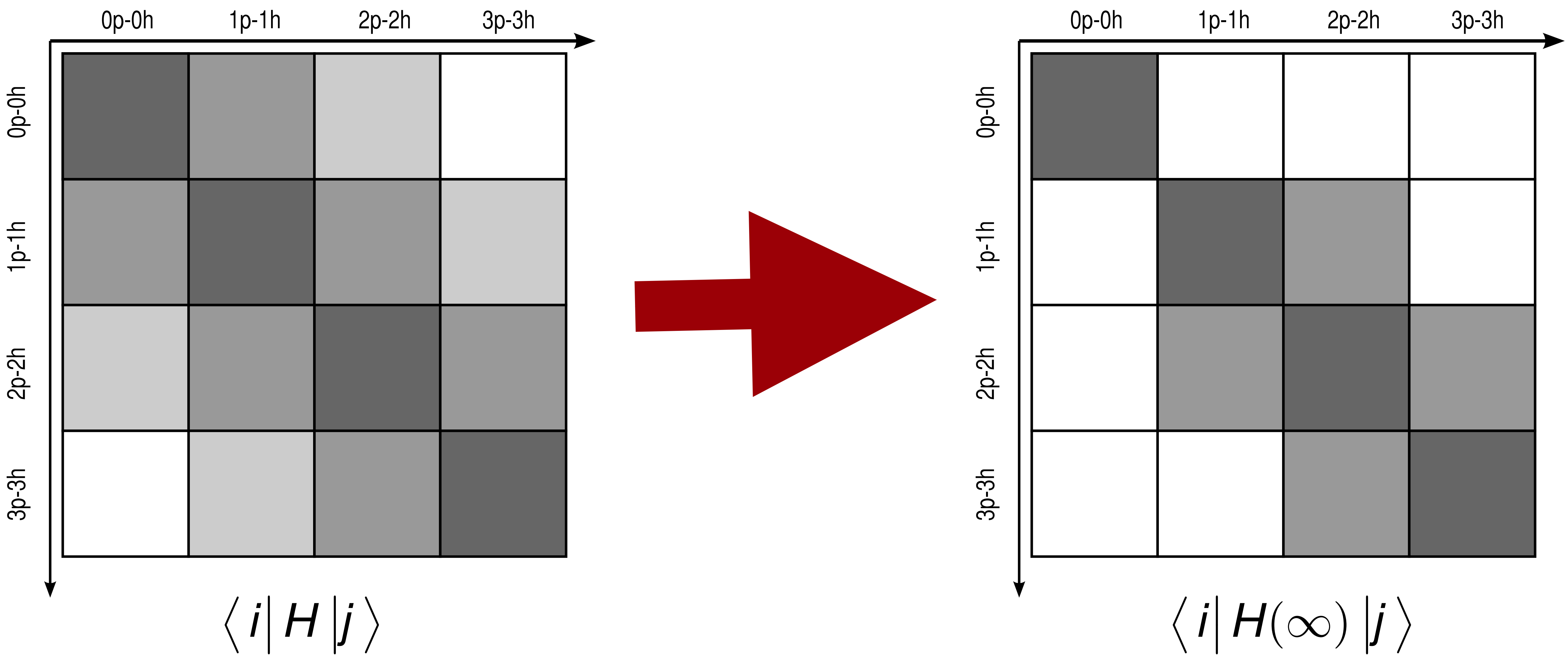
K. Tsukiyama, S. K. Bogner, and A. Schwenk, Phys. Rev. Lett. **106** (2011), 222502

Decoupling in A-Body Space





Decoupling in A-Body Space



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

Normal-Ordering & Wick's Theorem

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

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

- 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

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

Normal-Ordered Hamiltonian

Normal-Ordered Hamiltonian

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

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

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

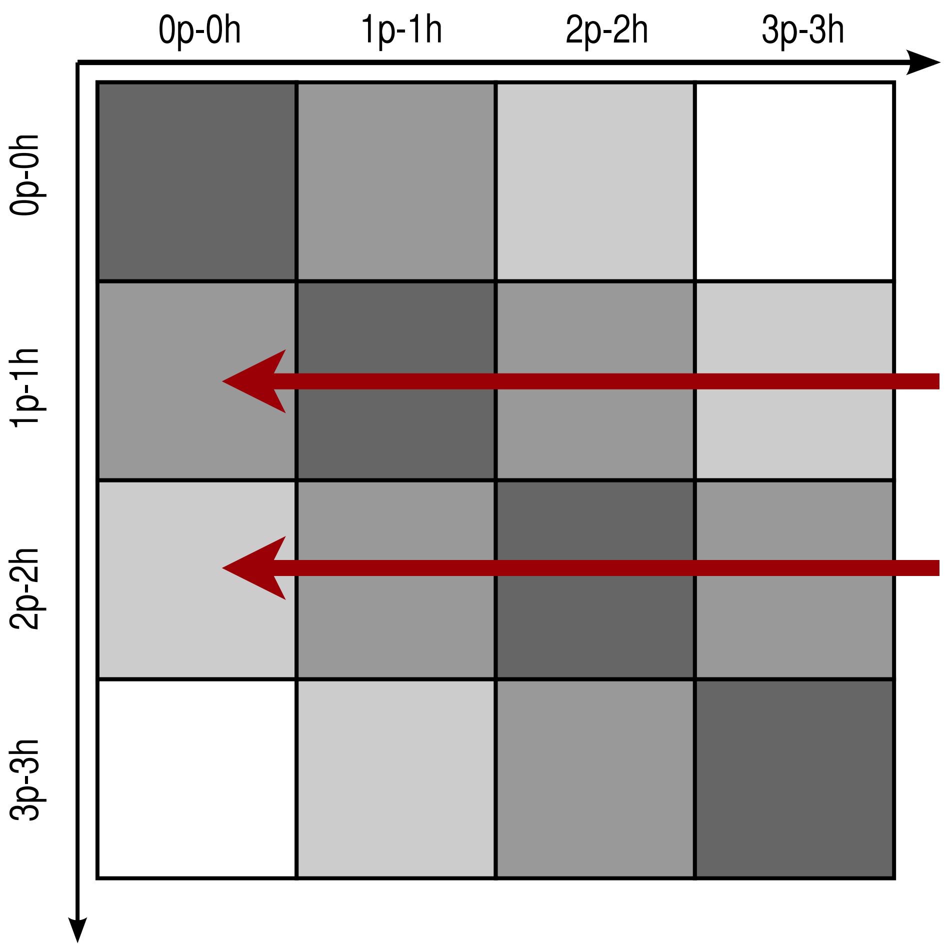
$$\Gamma^{kl}_{mn} = \langle kl | V_2 + T_2 | mn \rangle + \sum_h \langle klh | V_3 | mnh \rangle n_h$$

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

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



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

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

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

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

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

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

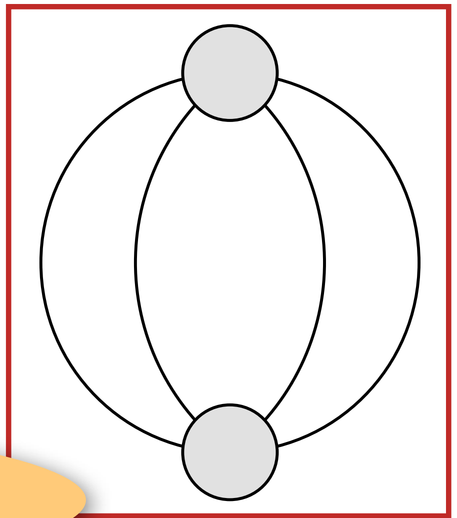
$$E_{p} - E_{h}, E_{pp'} - E_{hh'} : \quad \text{approx. 1p1h, 2p2h excitation energies}$$

- 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

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

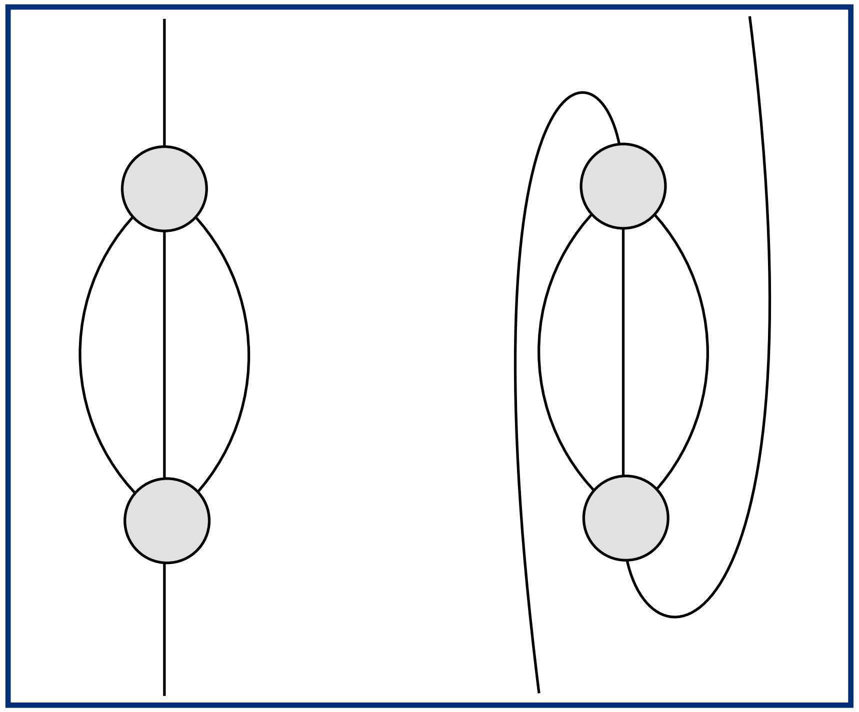


~ 2nd order MBPT for *H(s)*

1-body Flow

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

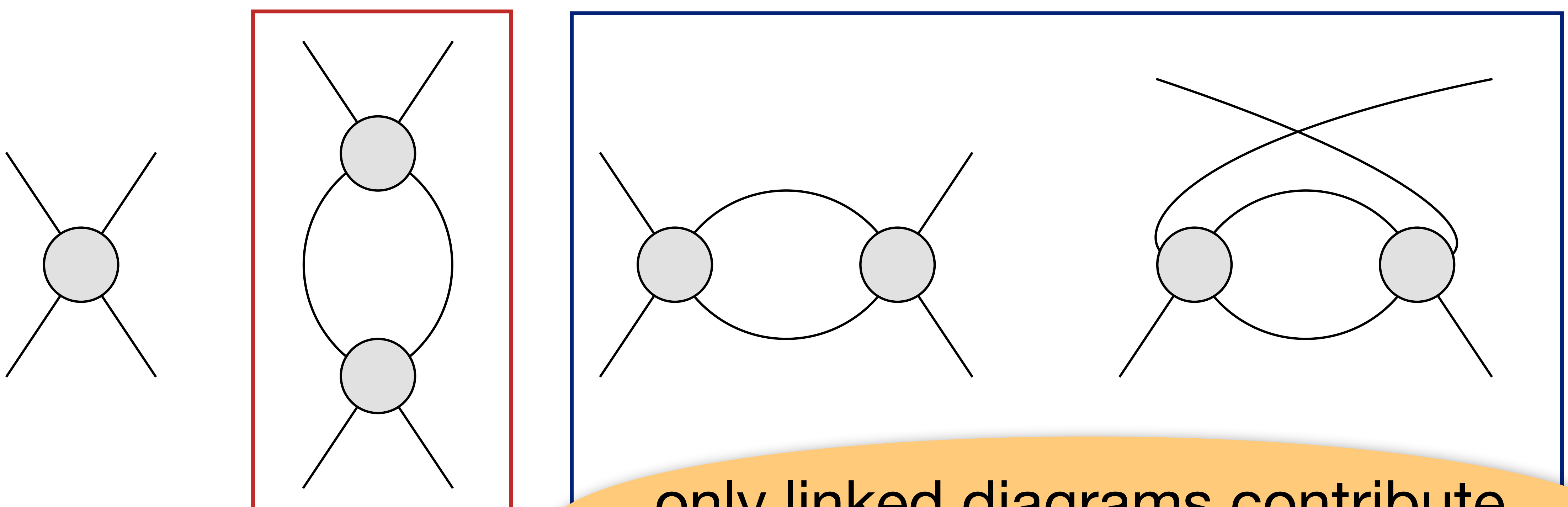
$$+ \frac{1}{2} \sum_{abcdef} \left(\eta^{1a}_{bc} \Gamma^{bc}_{2a} - \Gamma^{1a}_{bc} \eta^{bc}_{2a} \right) (n_a \bar{n}_b \bar{n}_c + \bar{n}_a n_b n_c)$$



In-Medium SRG Flow Equations

2-body Flow

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

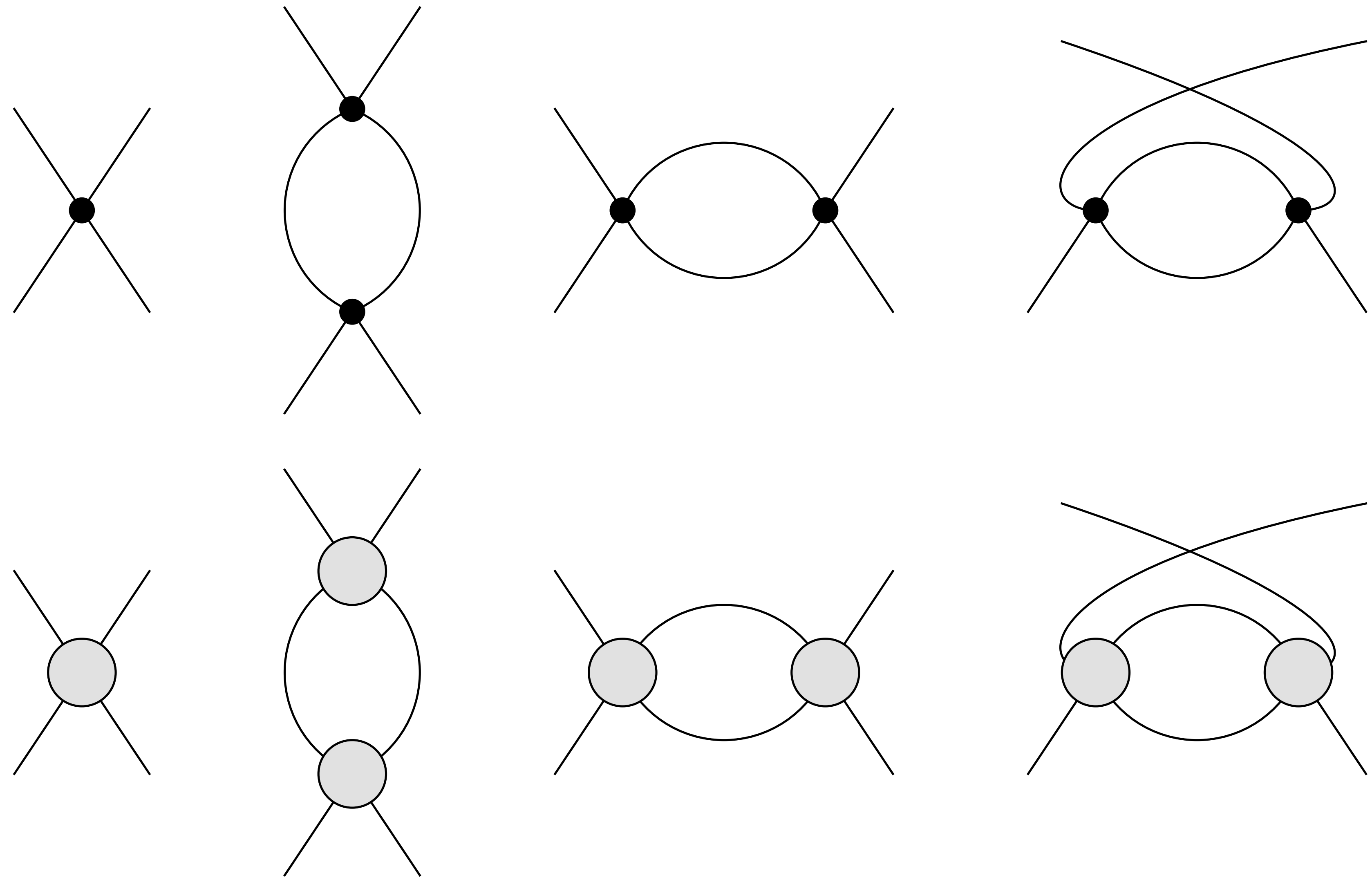


only linked diagrams contribute, IM-SRG size-extensive

In-Medium SRG Flow: Diagrams

$\Gamma(\delta s) \sim$

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



In-Medium SRG Flow: Diagrams

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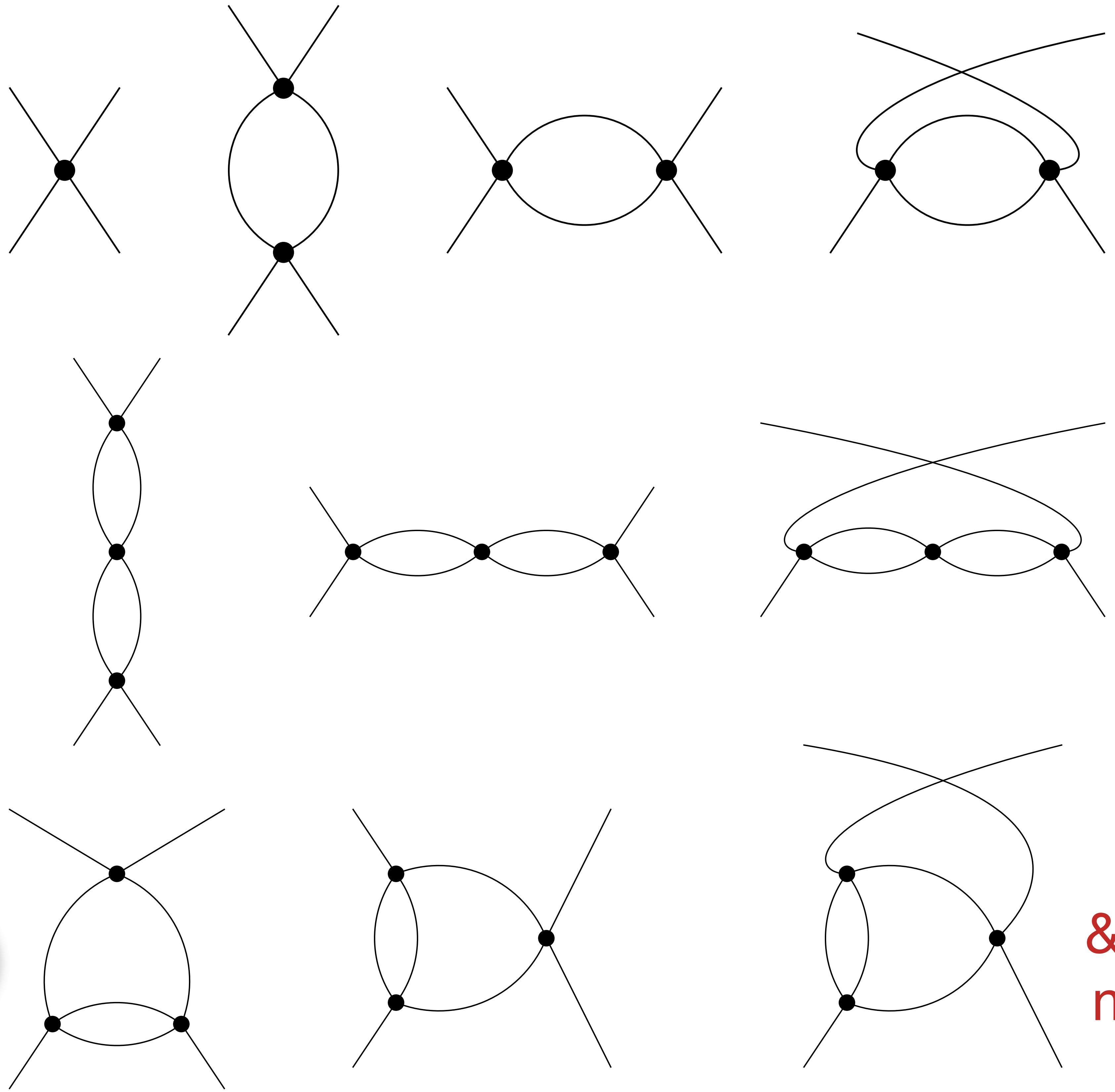
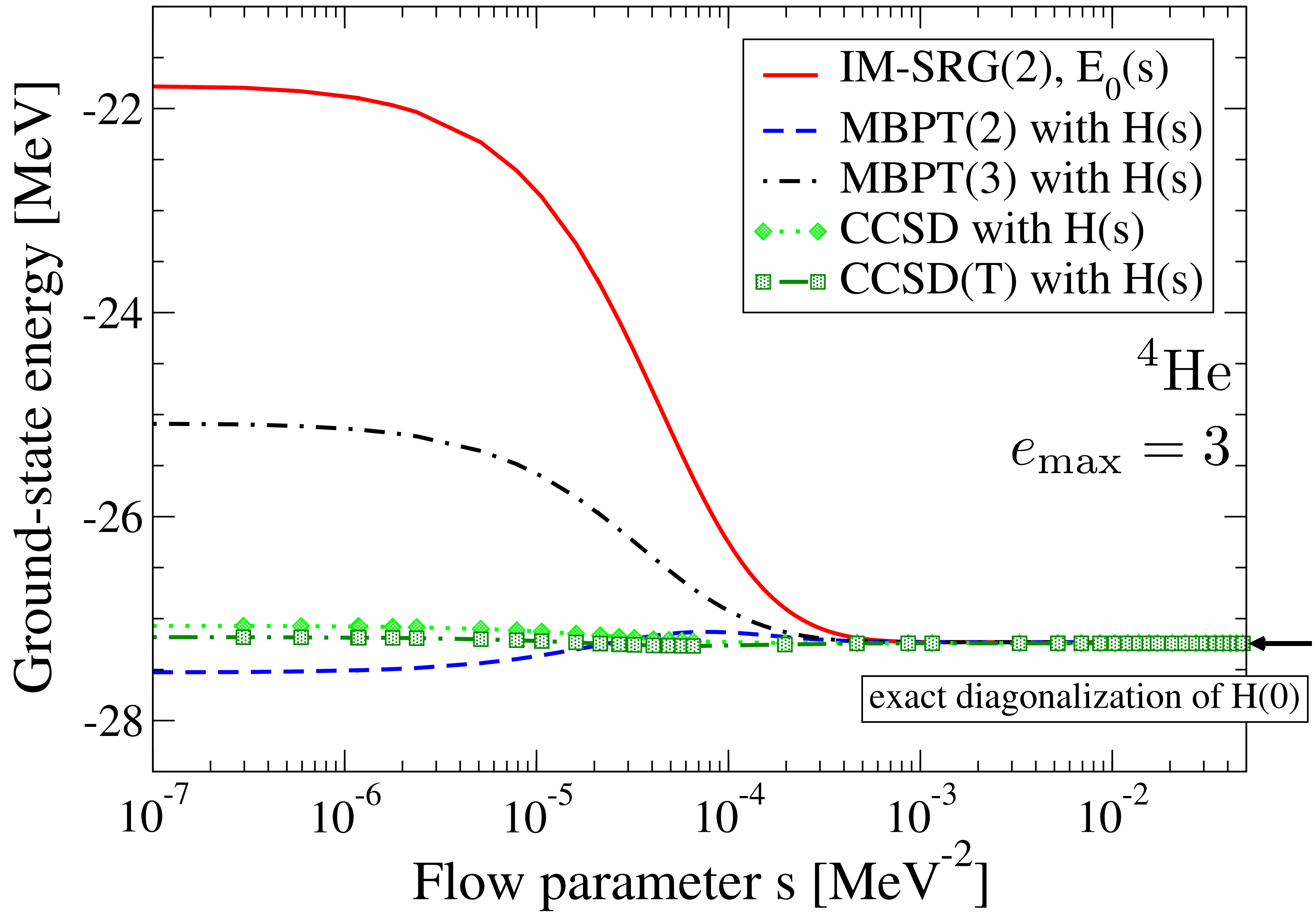


non-perturbative resummation

& many more...

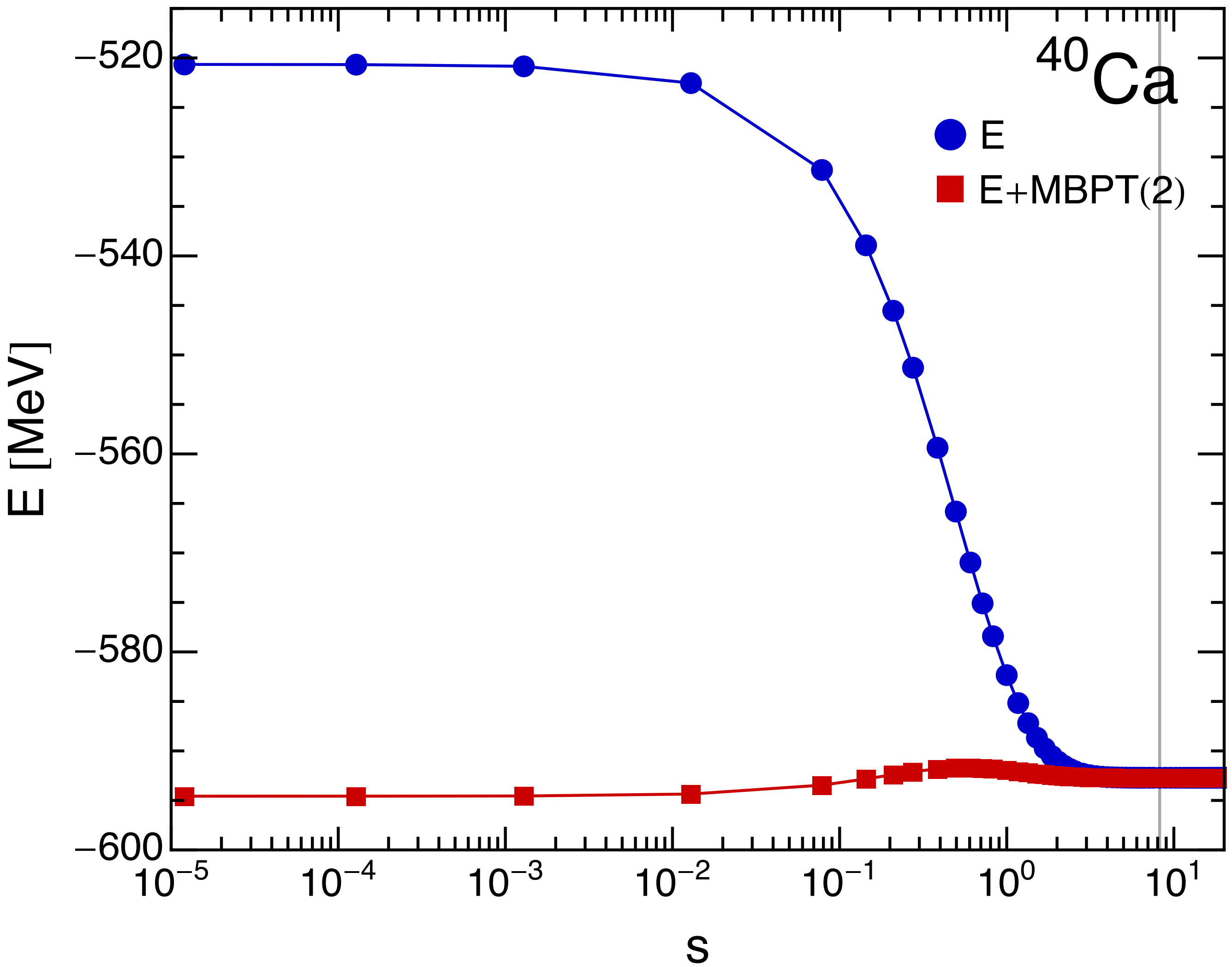
Resummation

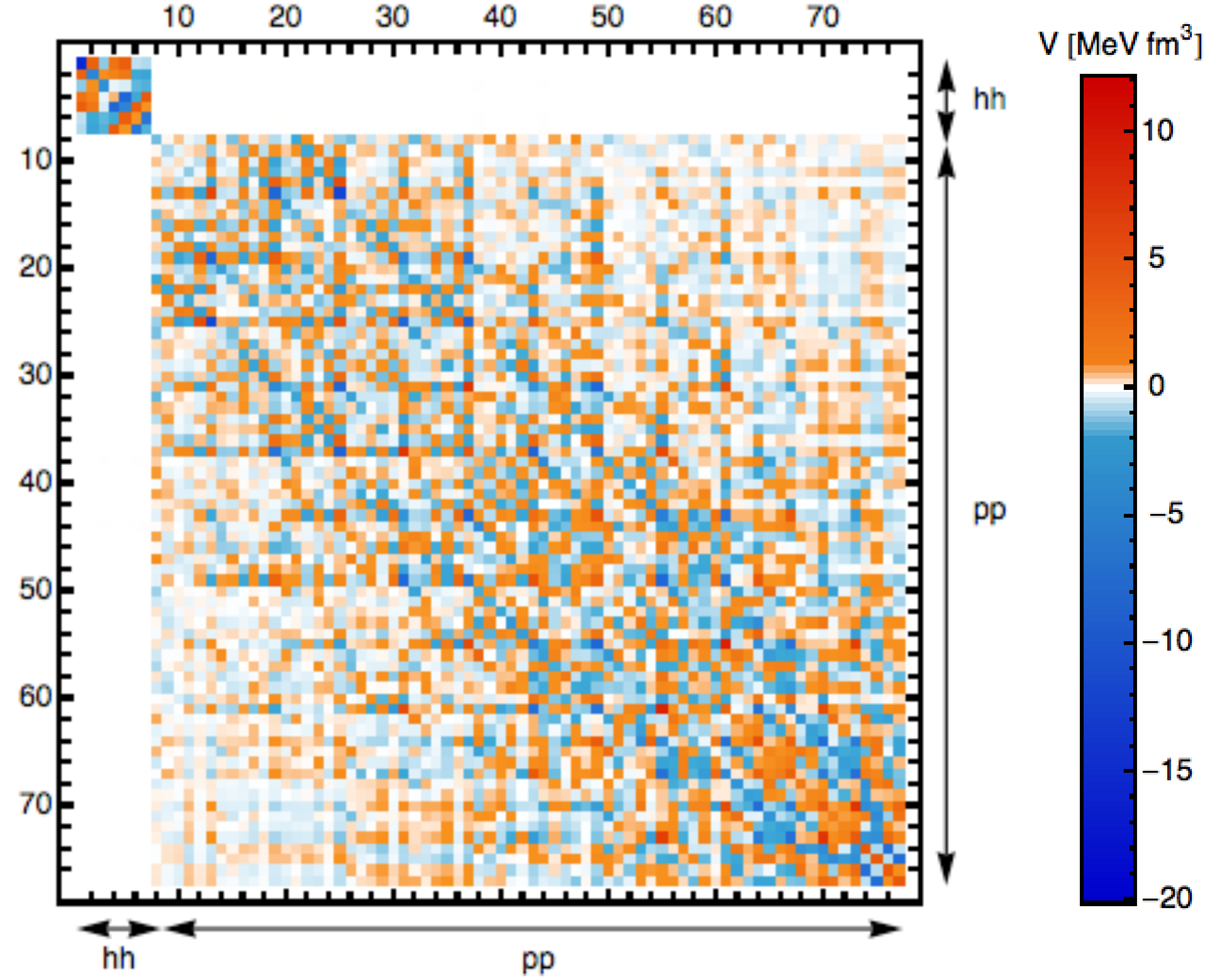


[K. Tsukiyama, S. K. Bogner & A. Schwenk, Phys. Rev. Lett. 106 (2011), 222502

E_0 rapidly approaches perturbation theory & quasi-exact results

Decoupling

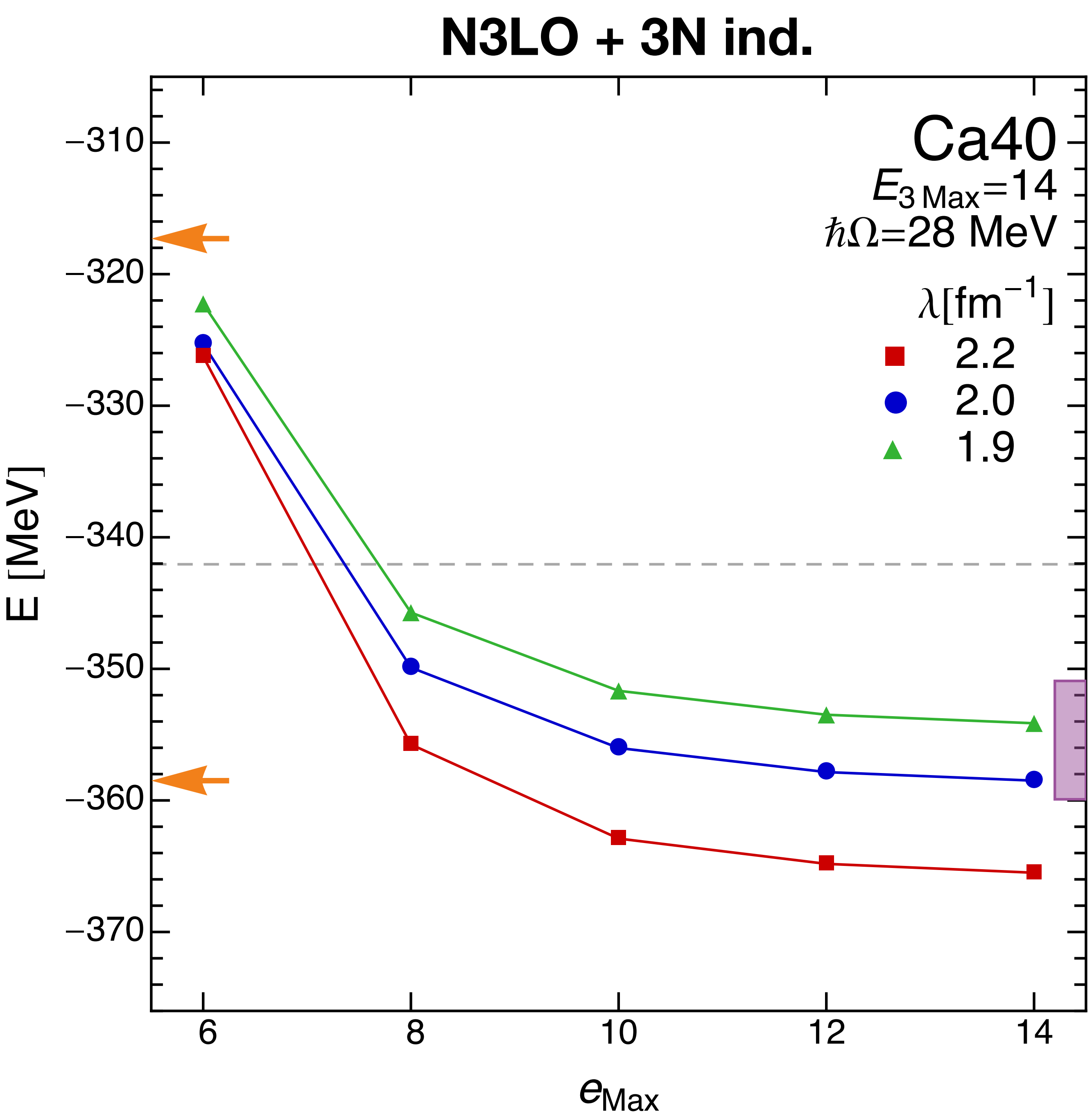




$V_{\text{SRG}}(\text{N3LO}), \lambda = 2.0\ \text{fm}^{-1}, e_{\text{Max}} = 8$

off-diagonal couplings are rapidly driven to zero

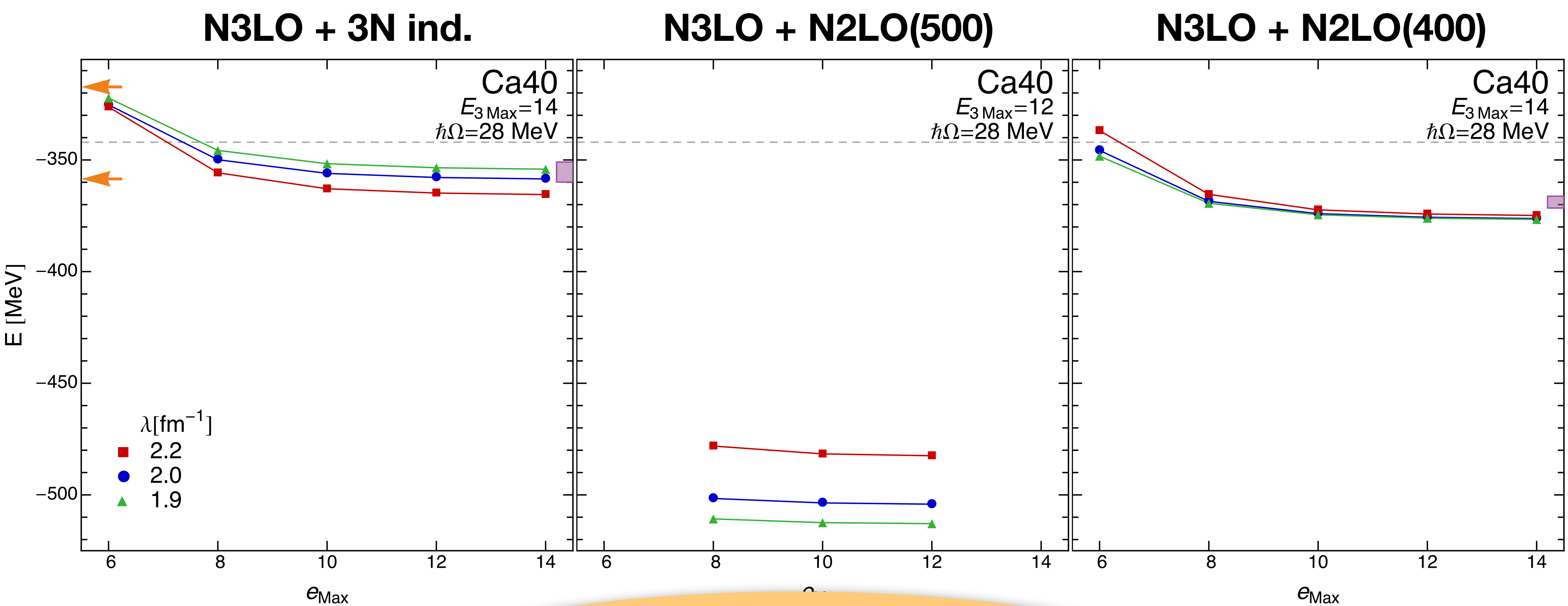
Results



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

CCSD, $\lambda = 1.9 - 2.2$ fm^{-1} , S.Binder, R.Roth et al., in preparation & PRL 109, 052501 (2012)

Results



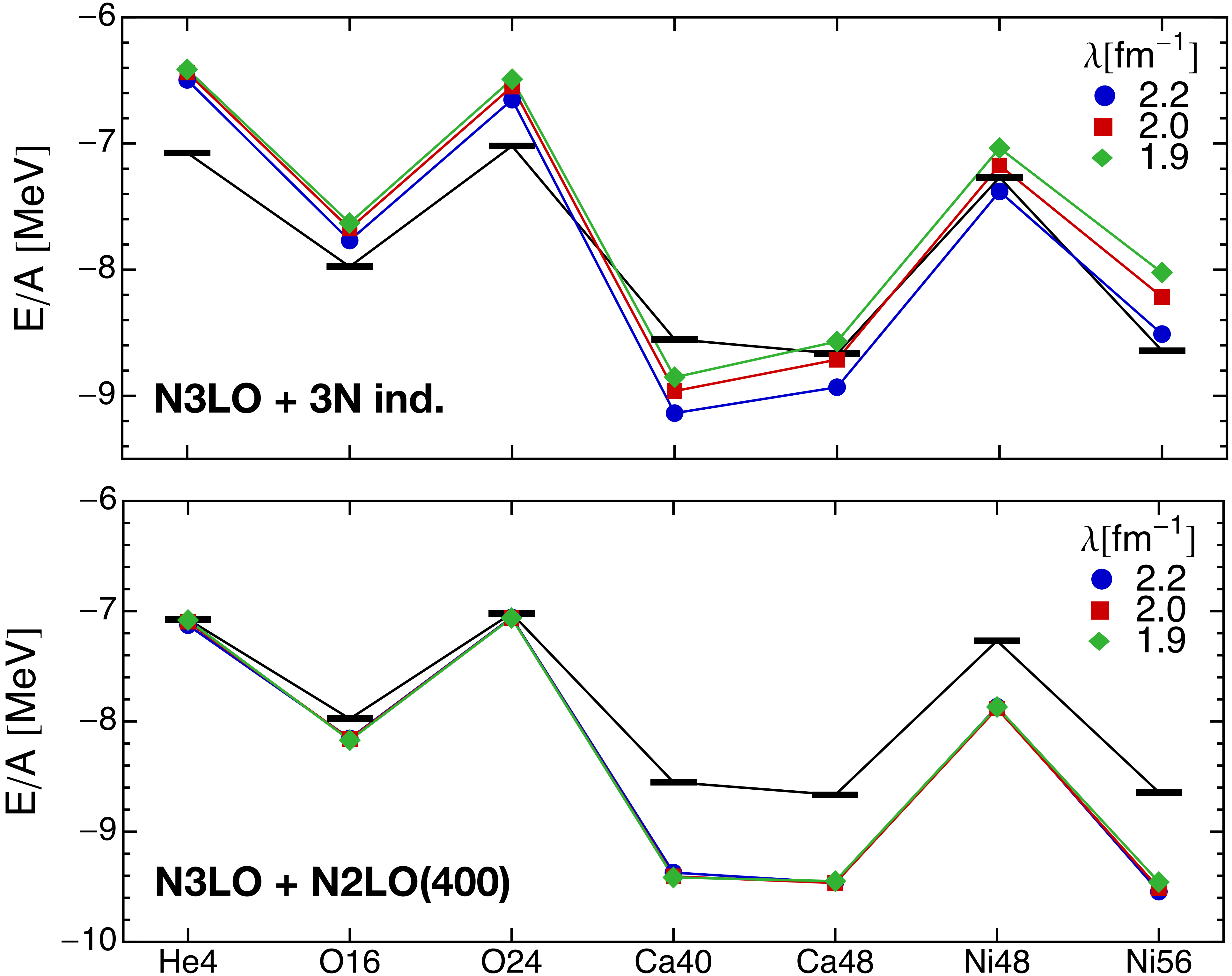
constraints & diagnostics for chiral Hamiltonians

(cf. talk by R. Roth)

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

CCSD, $\lambda = 1.9 - 2.2\ \mathrm{fm}^{-1}$, S.Binder, R.Roth et al., in preparation & PRL 109, 052501 (2012)

Results



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

Multi-Reference
In-Medium SRG

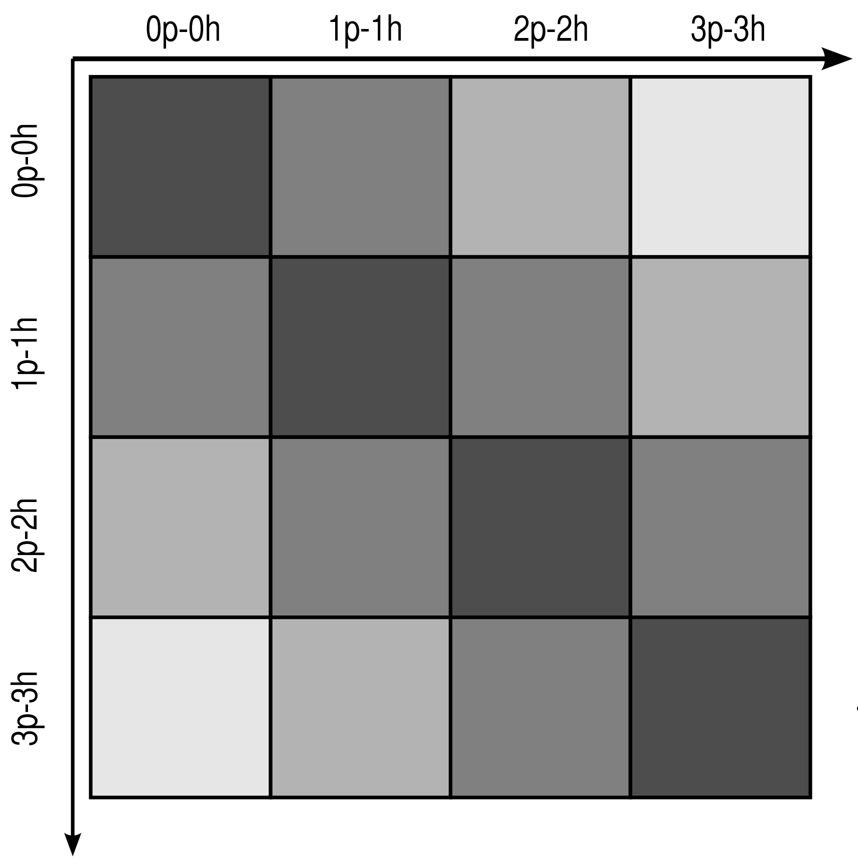
Generalized Normal Ordering

- 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



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

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

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

- 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:

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

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

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

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

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

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

Particle-Number Projection

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

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

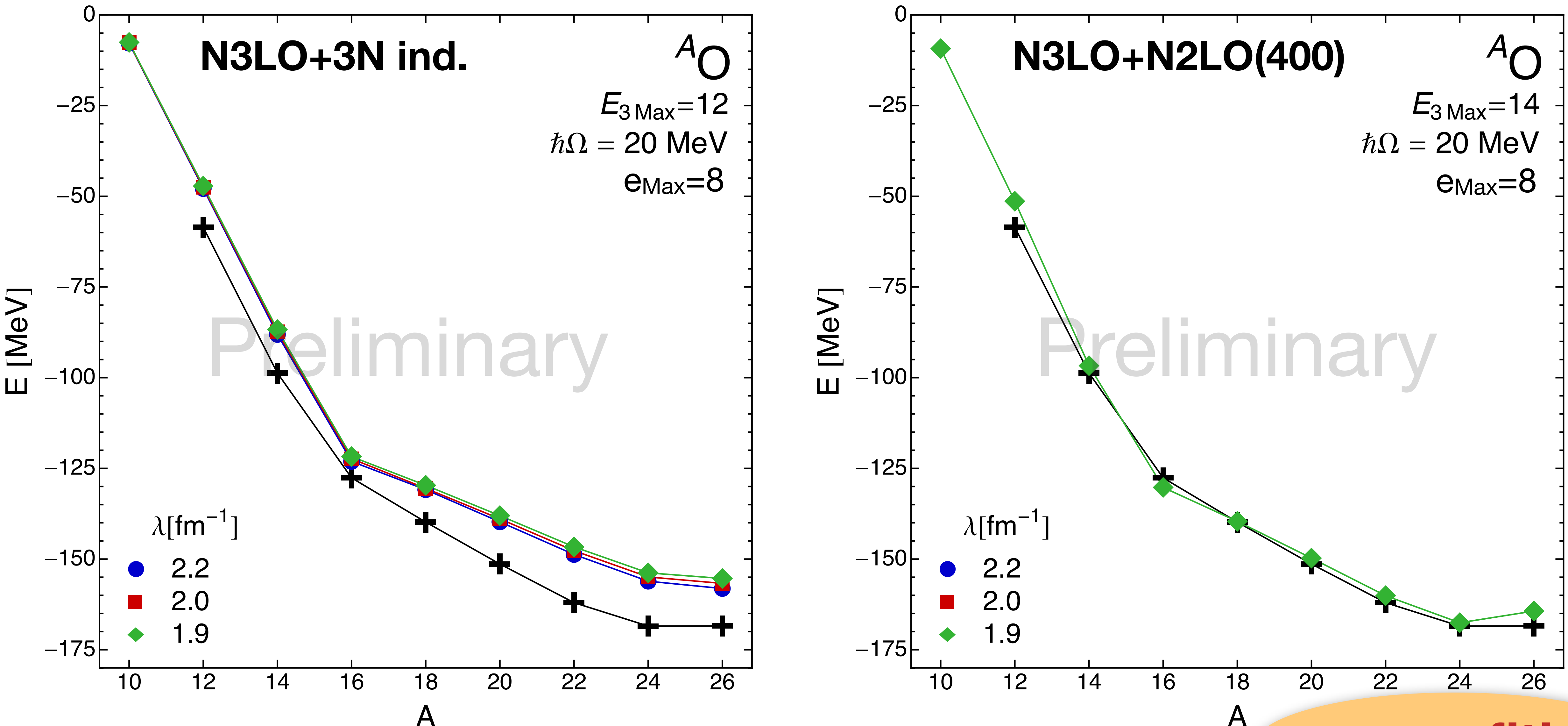
- calculate one- and two-body densities (project only once):

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

- 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



no refit!

- results insensitive to choice of generator for same H^{od}
- manageable increase in effort (stiff ODE)

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

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

➡ efficient evolution of observables (density matrices)?

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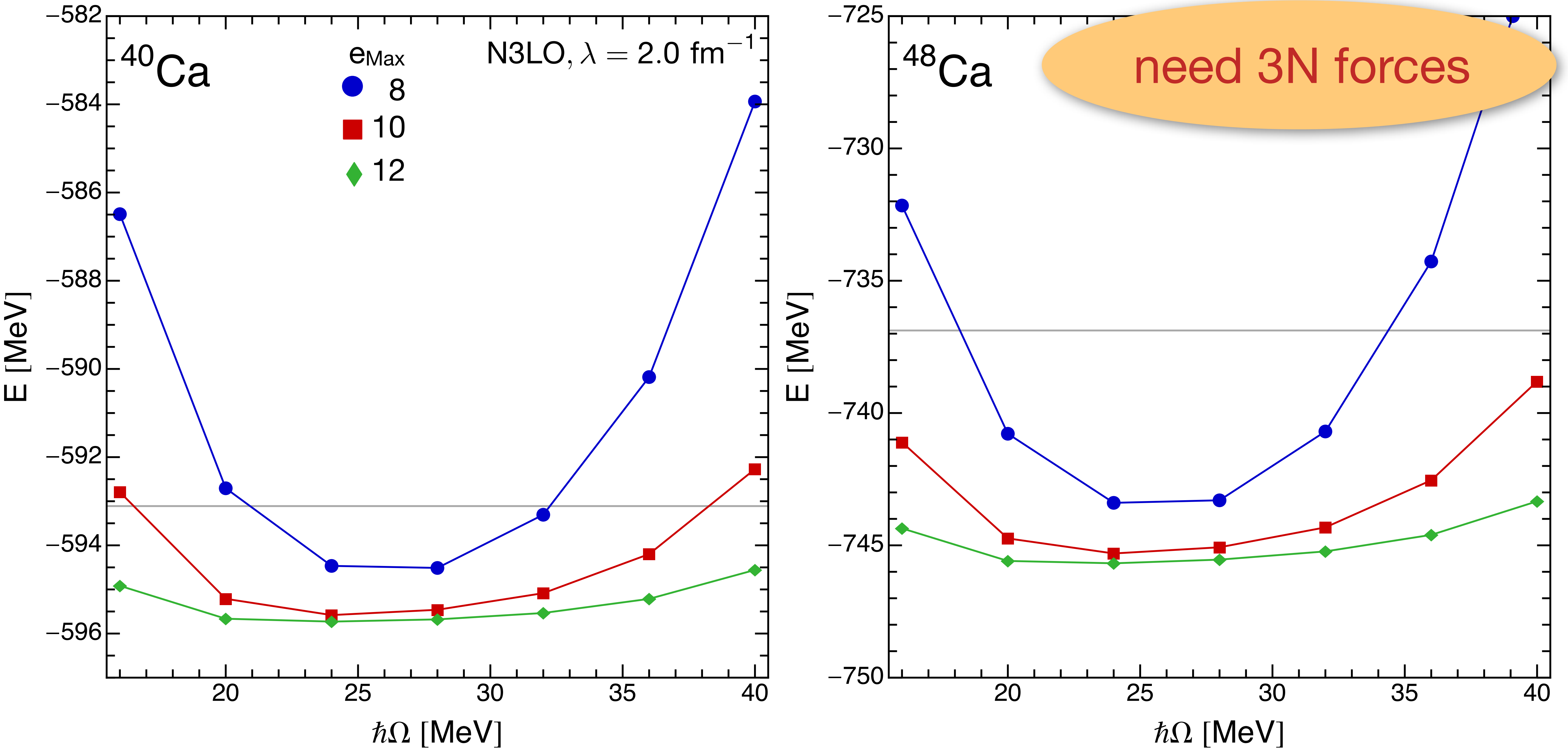
E. R. Anderson, R. J. Furnstahl, K. Hebeler, R. J. Perry, K. A. Wendt
Ohio State University

P. Papakonstantinou
IPN Orsay, France

Supplements

Results

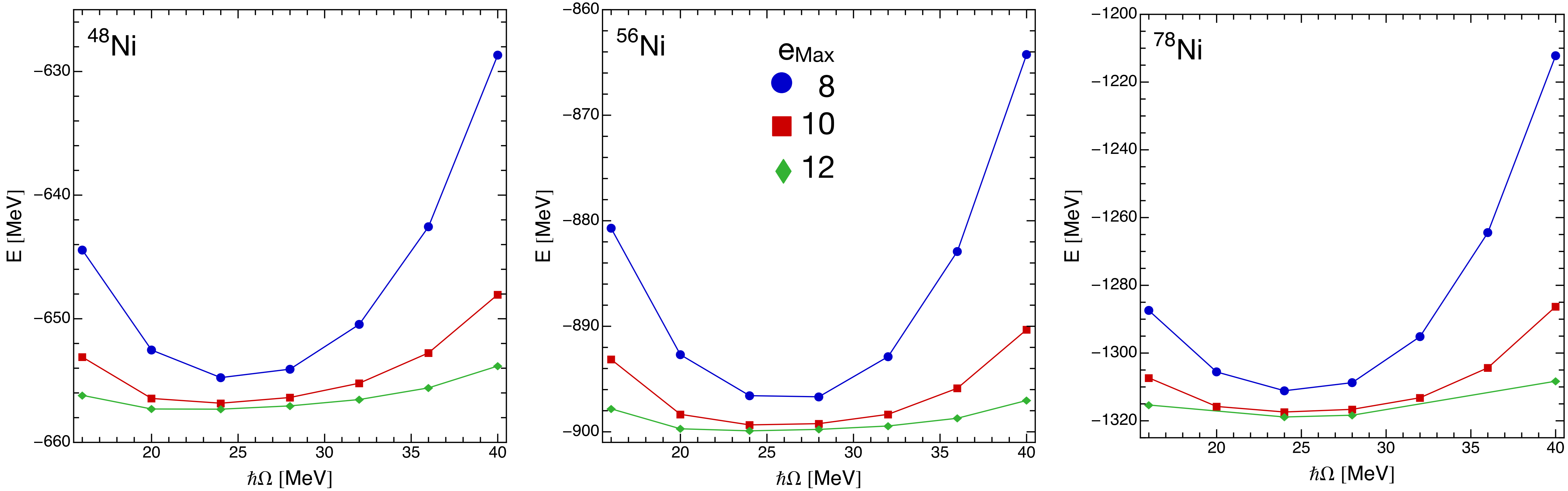


[gray lines: CCSD by S. Binder, $e_{Max} = 12, \hbar\Omega = 20$ MeV]

converged g.s. energies between CCSD and Λ-CCSD(T)

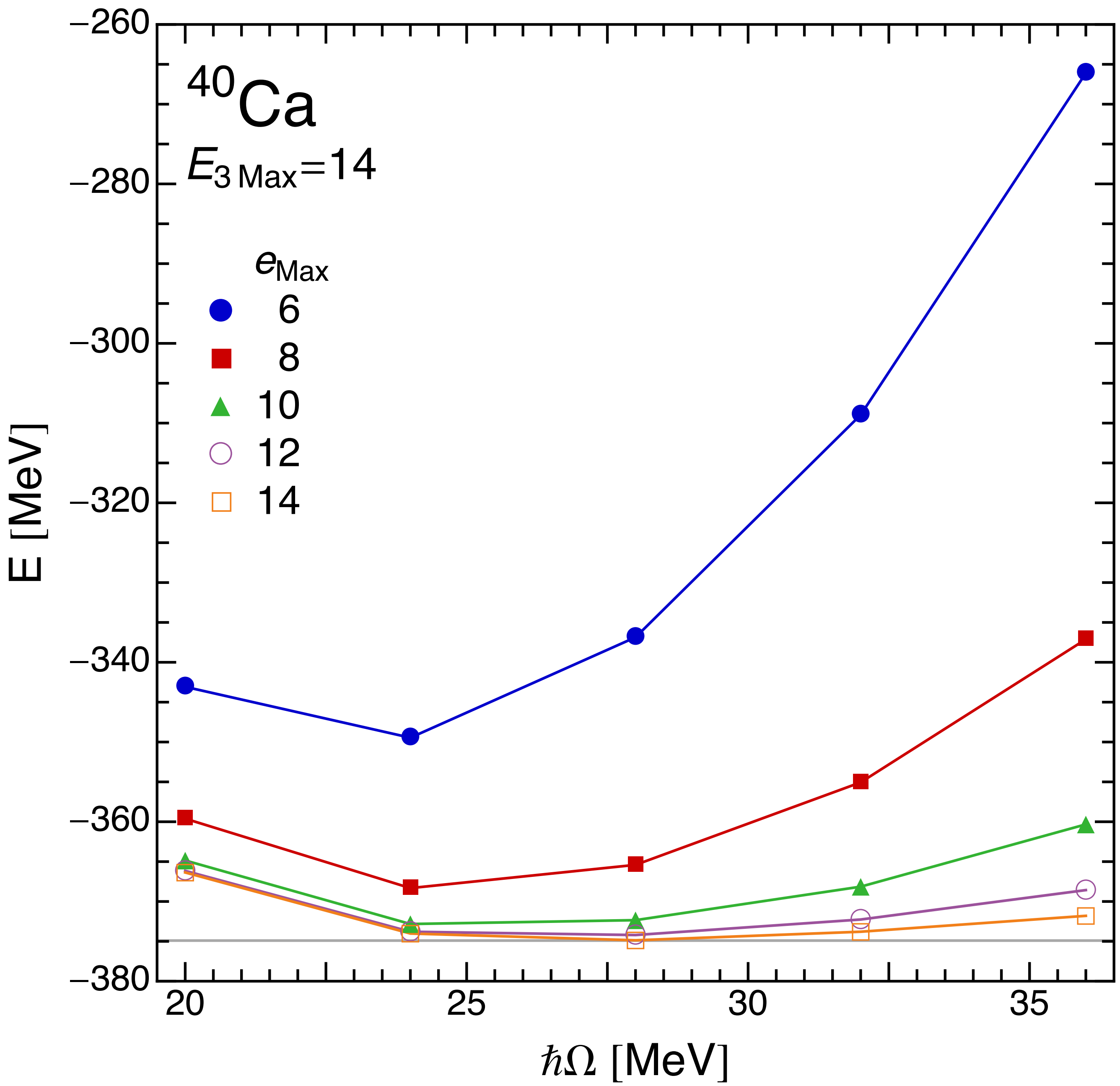
Isotopic “Chains”

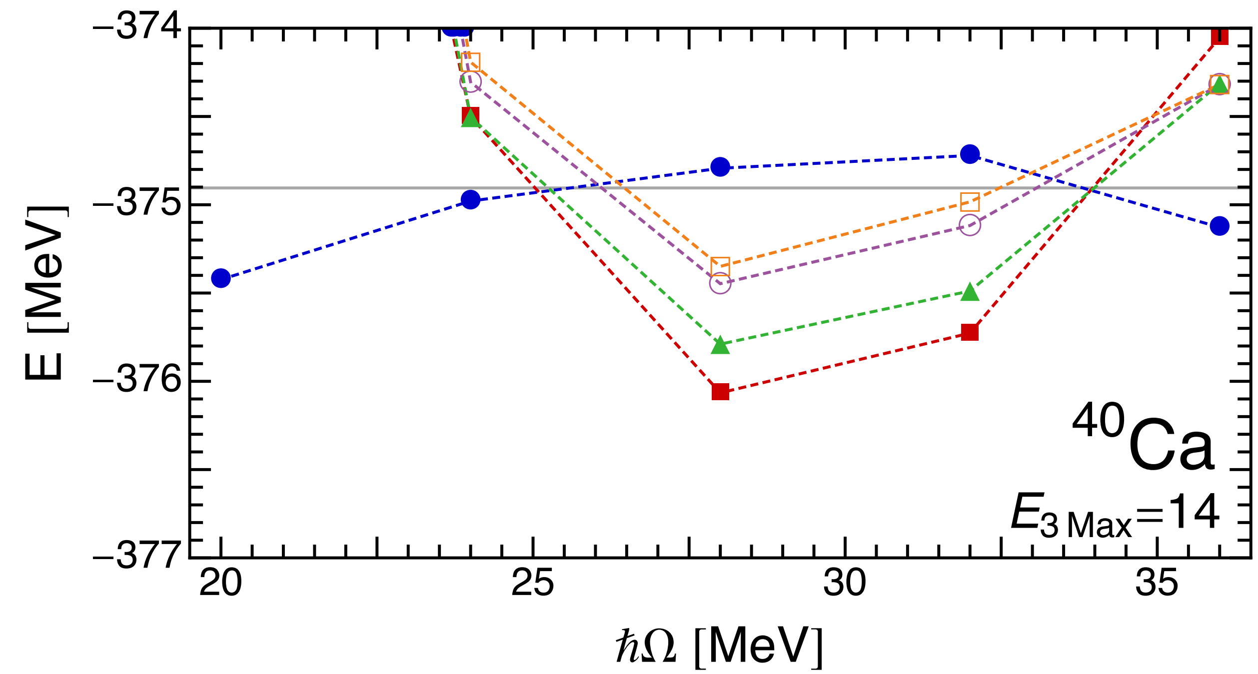
N3LO, $\lambda = 2.0\ \text{fm}^{-1}$, NN only



- “closed-shell” Ni and Sn isotopes can give insight into isovector interaction...
- ... but complete isotopic chains would be preferable, i.e., devise an approach to open-shell nuclei

Extrapolation





max./UV momentum:

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

radial extent:

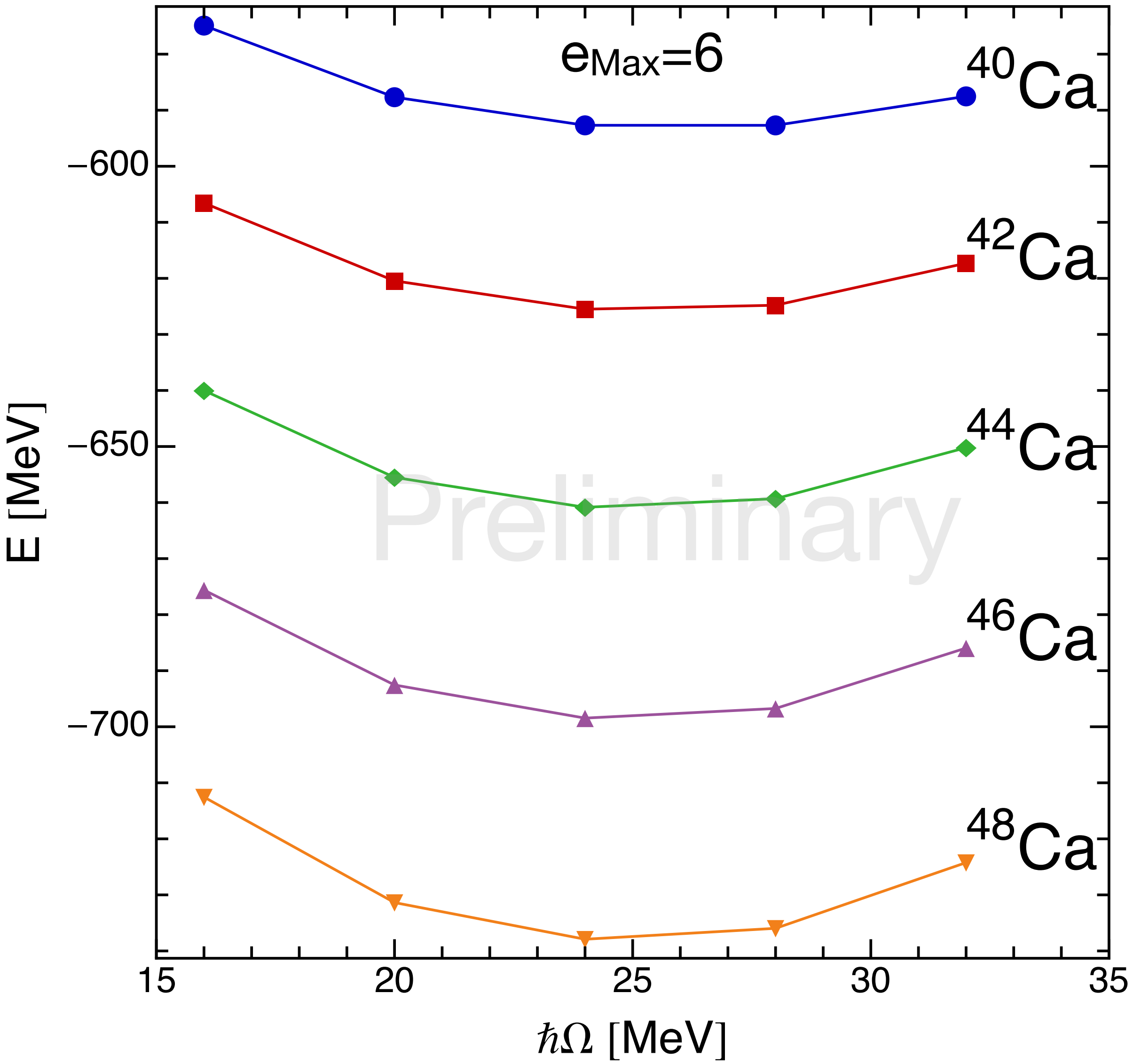
$$L = \sqrt{2(e_{\mathrm{Max}} + 3/2)\hbar/m\Omega}$$

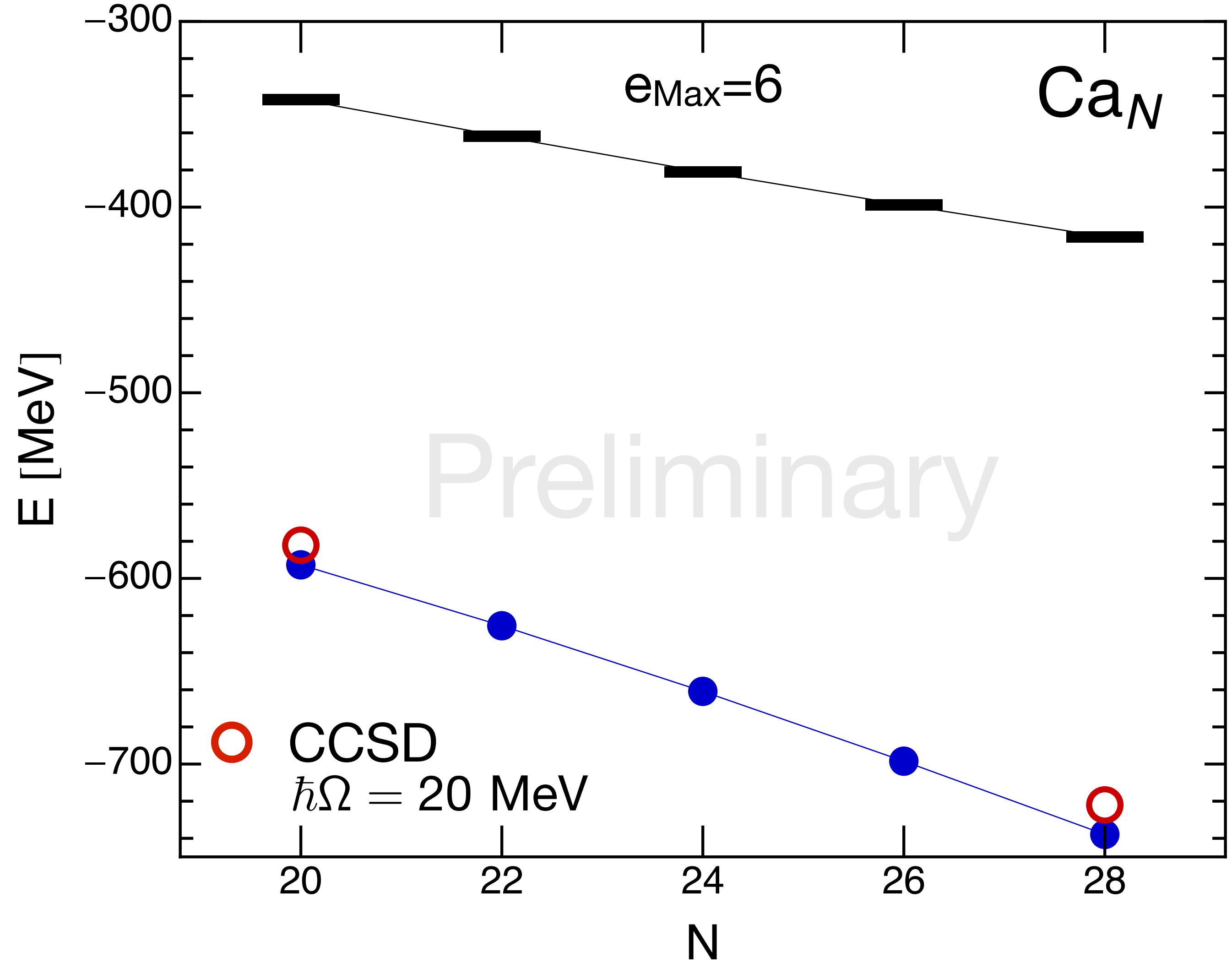
simultaneous ultraviolet & infrared extrapolation:

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

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

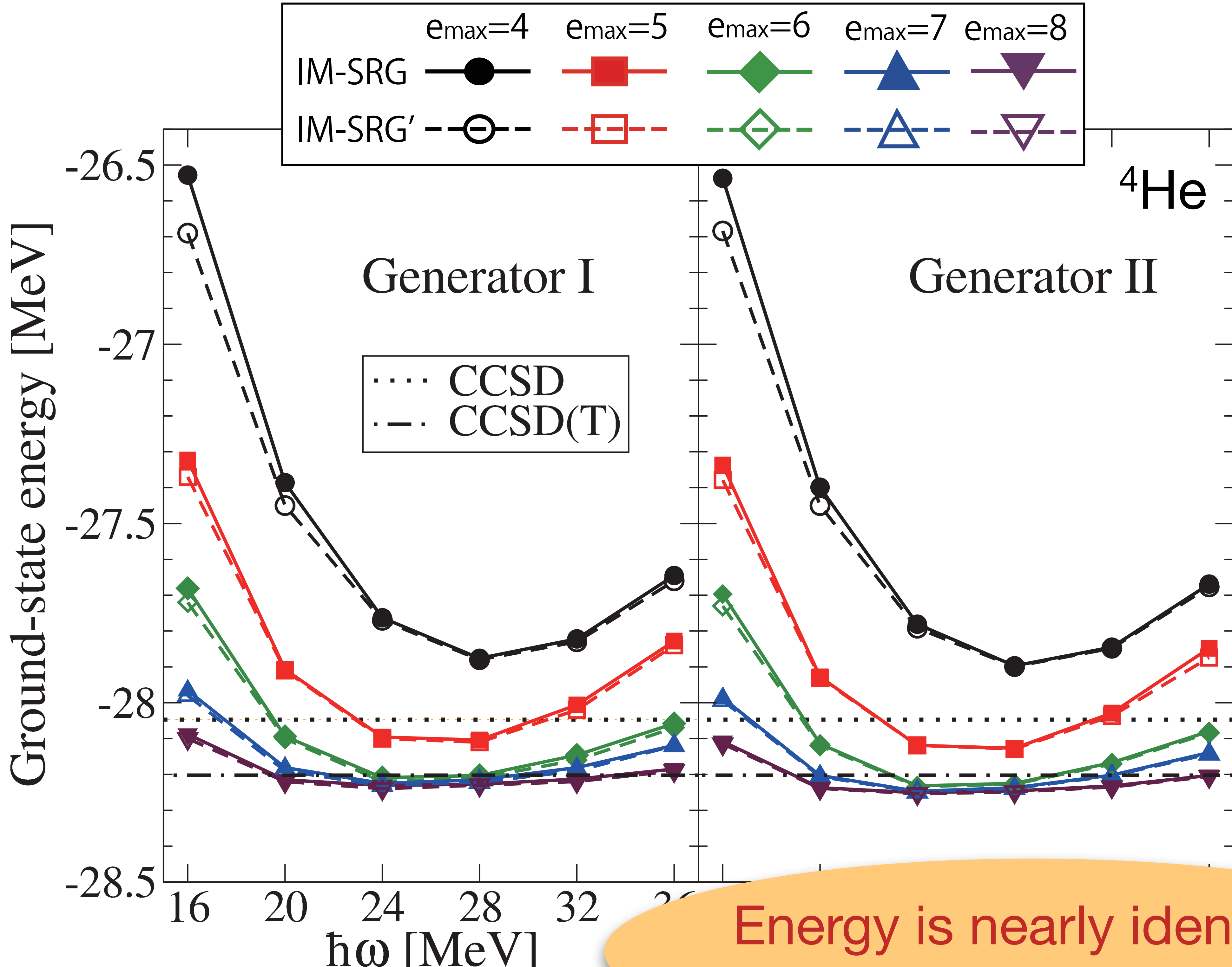
Results





- preliminary results reasonable for *NN*-only calculation
- multiple generators give similar results
- BUT: evolution takes much longer (stiffness issue?)

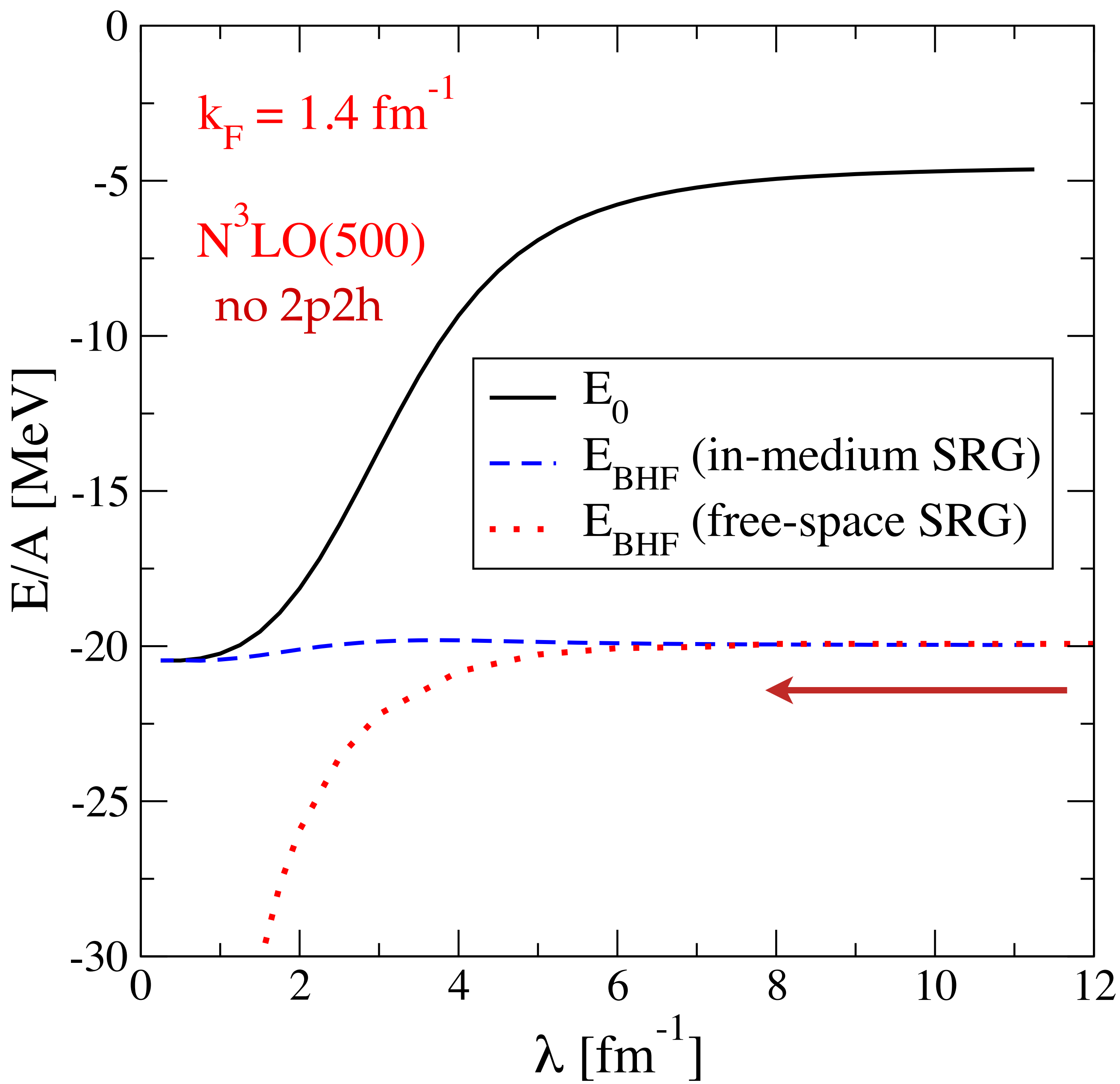
Results



Energy is nearly identical for both generators!

[K. Tsukiyama, S. K. Bogner & A. Schwenk, Phys...

Symmetric Nuclear Matter



[S. Bogner et al., Prog. Part. Nucl. Phys. 65, 97 (2010)]

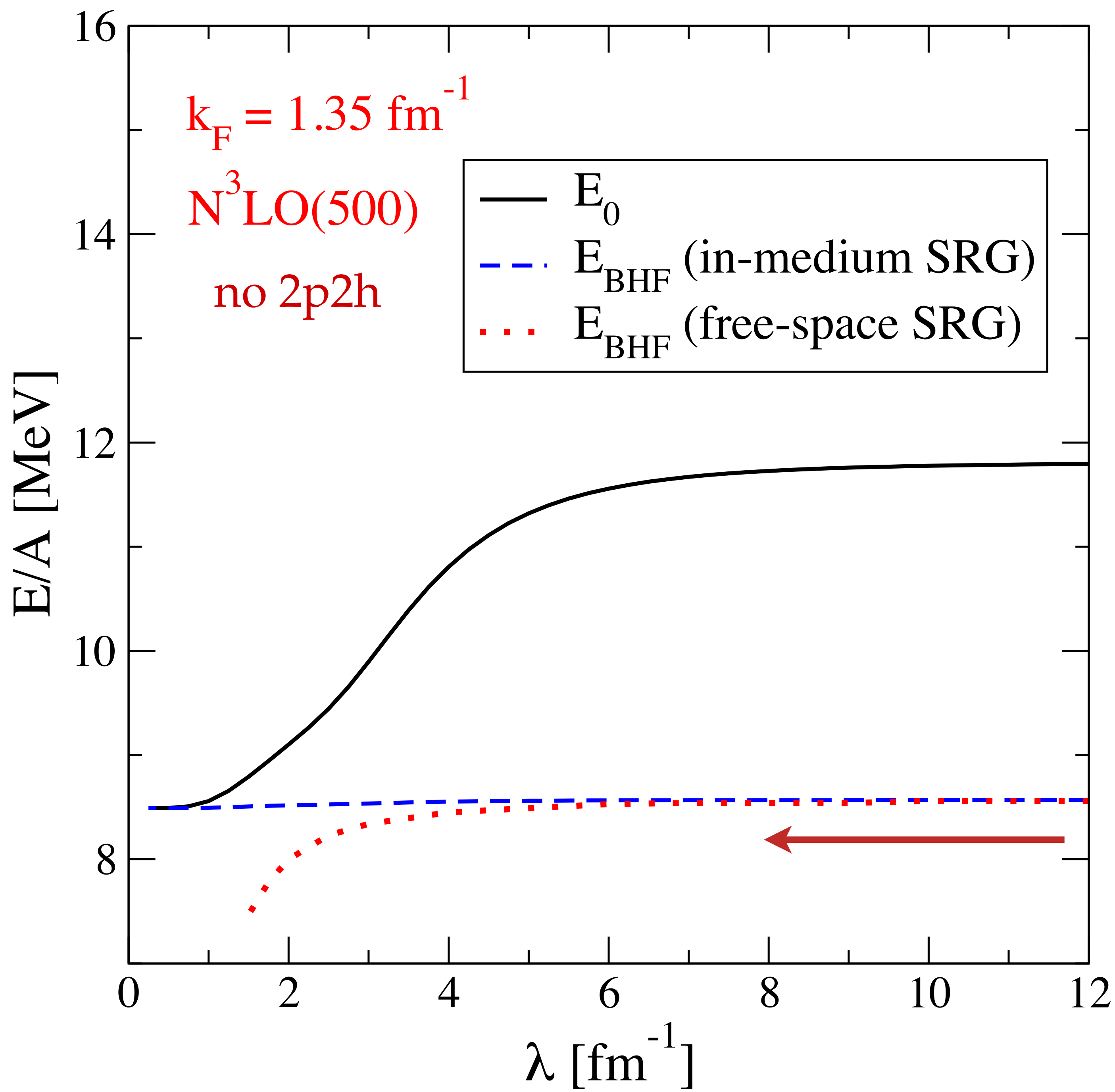
Free-Space SRG

- E_{BHF} (pp ladder sum) is strongly λ-dependent (NN interaction only!)

In-Medium SRG

- λ-dependence weak: dominant many-body forces included through normal ordering
- E_0 (= HF exp. value) approaches ladder sum: correlations are weakened

Neutron Matter



[S. Bogner et al., Prog. Part. Nucl. Phys. 65, 97 (2010)]

Free-Space SRG

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