

# In-Medium SRG for Finite Nuclei

Heiko Hergert

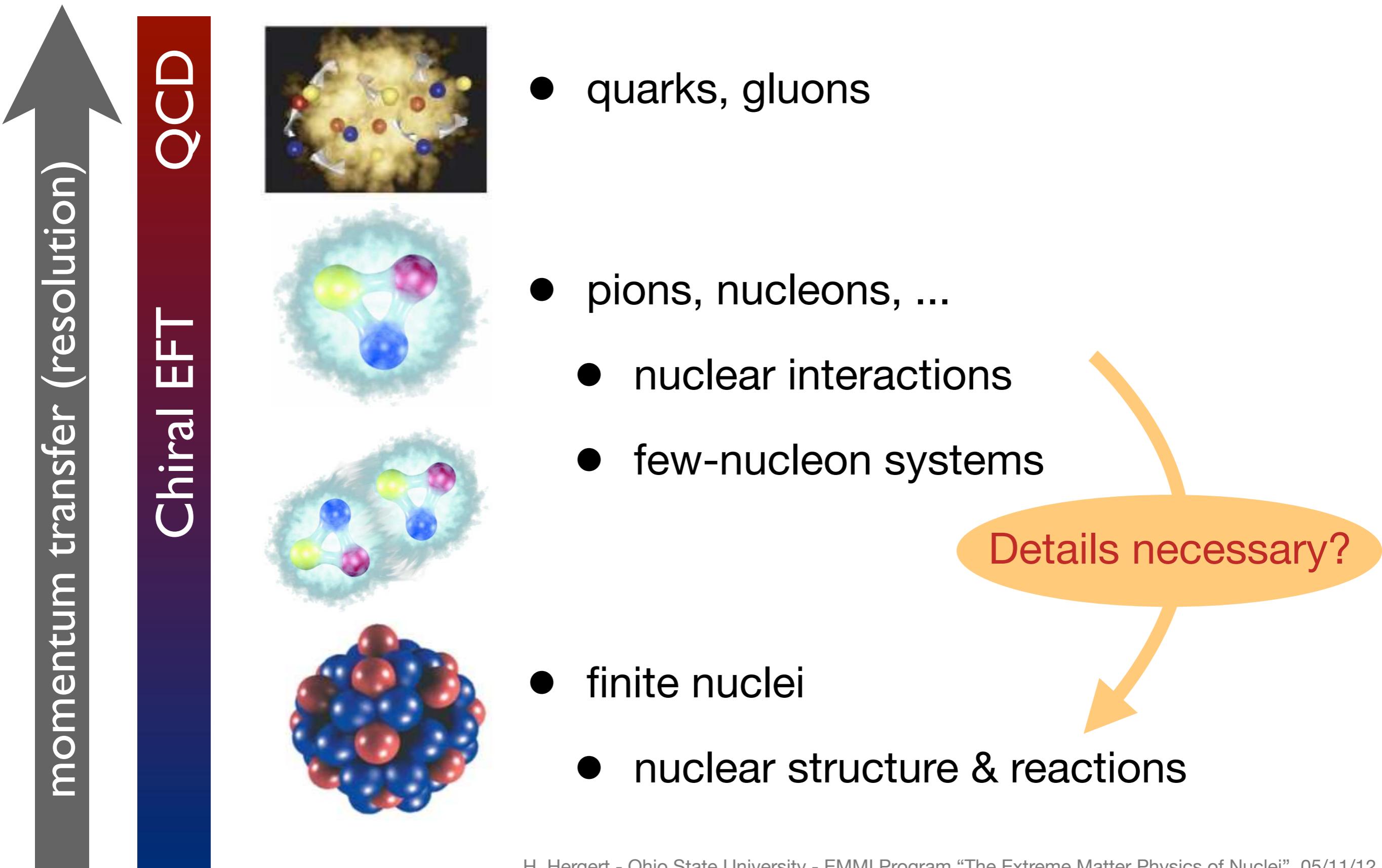
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# Outline

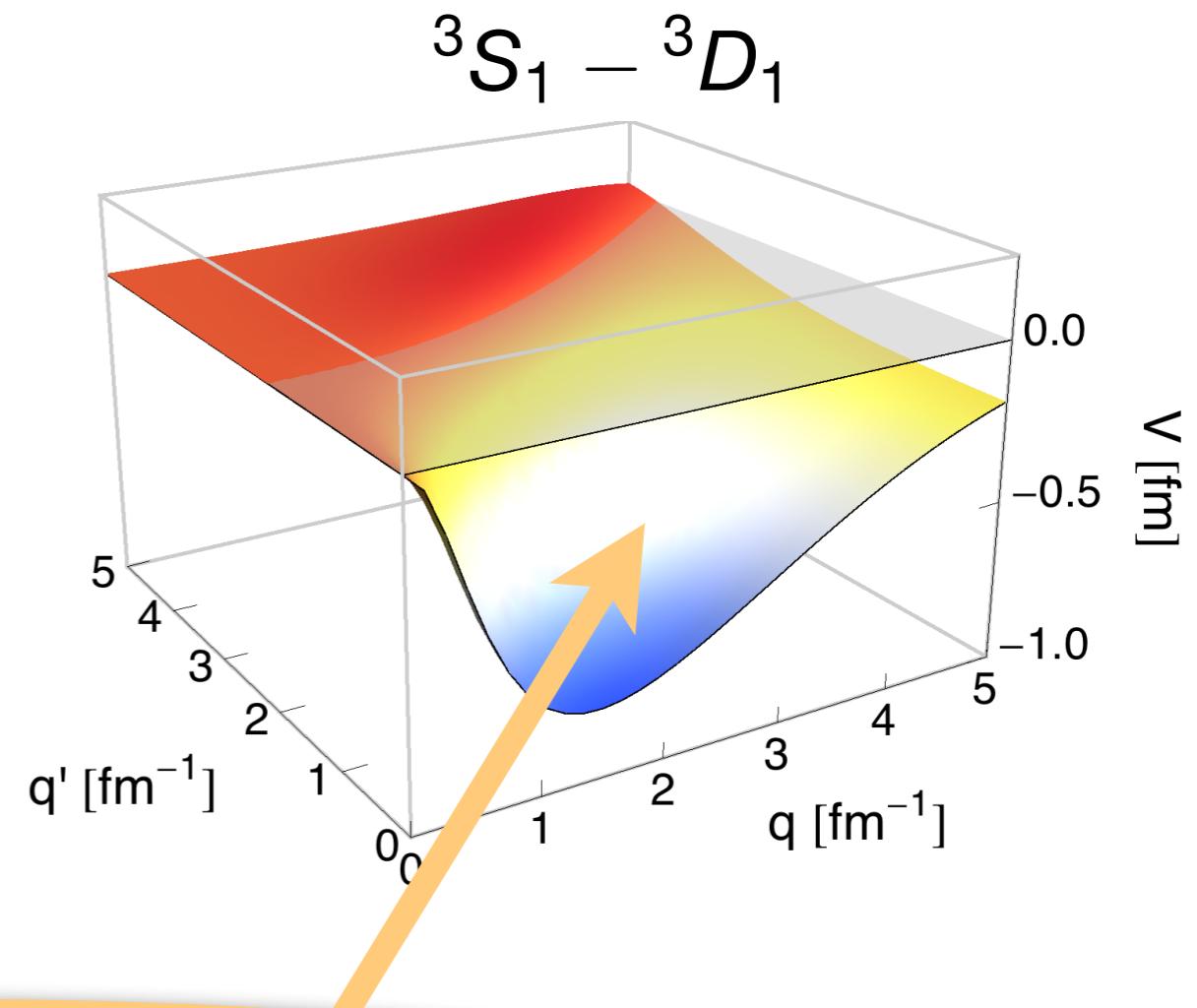
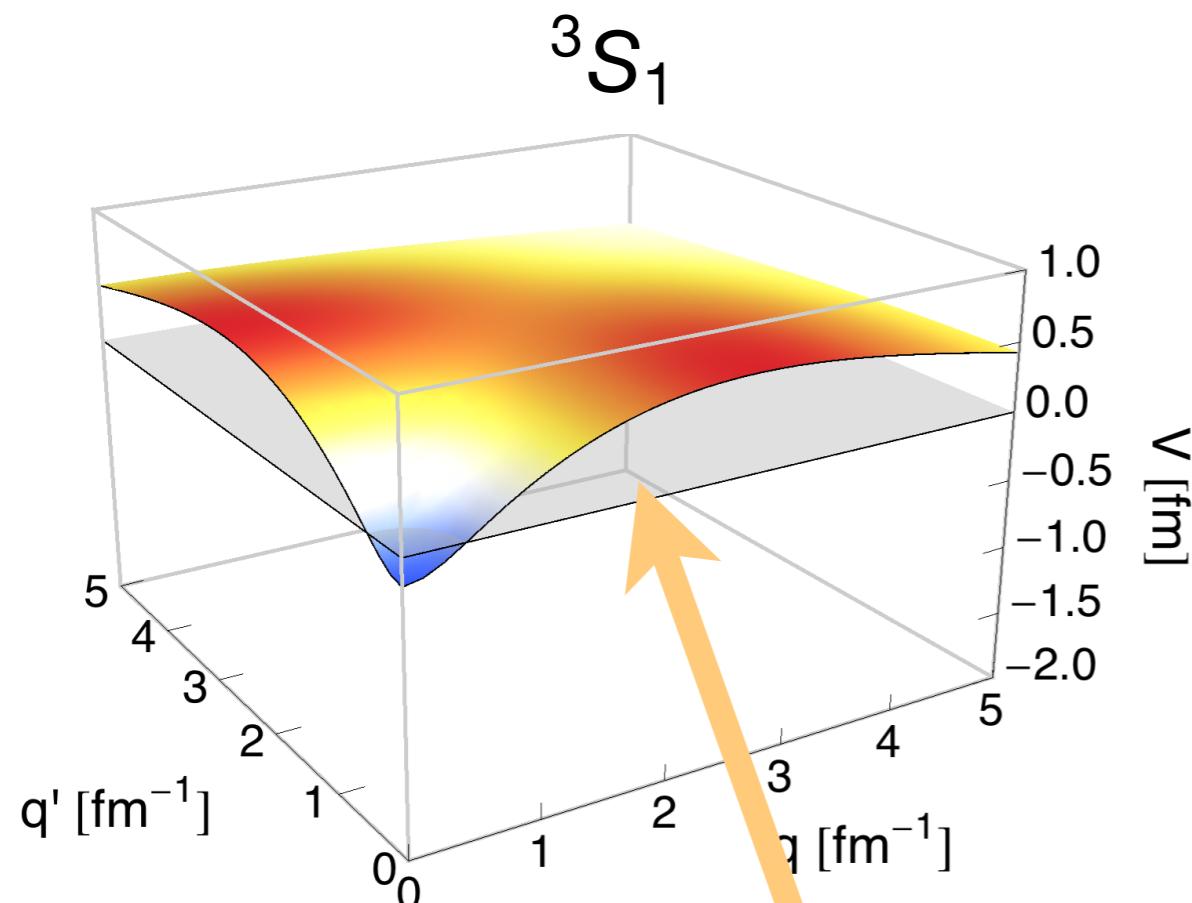
- Similarity Renormalization Group in Nuclear Physics
- In-Medium SRG for Closed Shell-Nuclei
- Multi-Reference In-Medium SRG
- Open-Shell Nuclei
- Outlook

# Scales of the Strong Interaction



# Correlations in the NN System

Argonne V18



strong short-range correlations  
 $\iff$  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

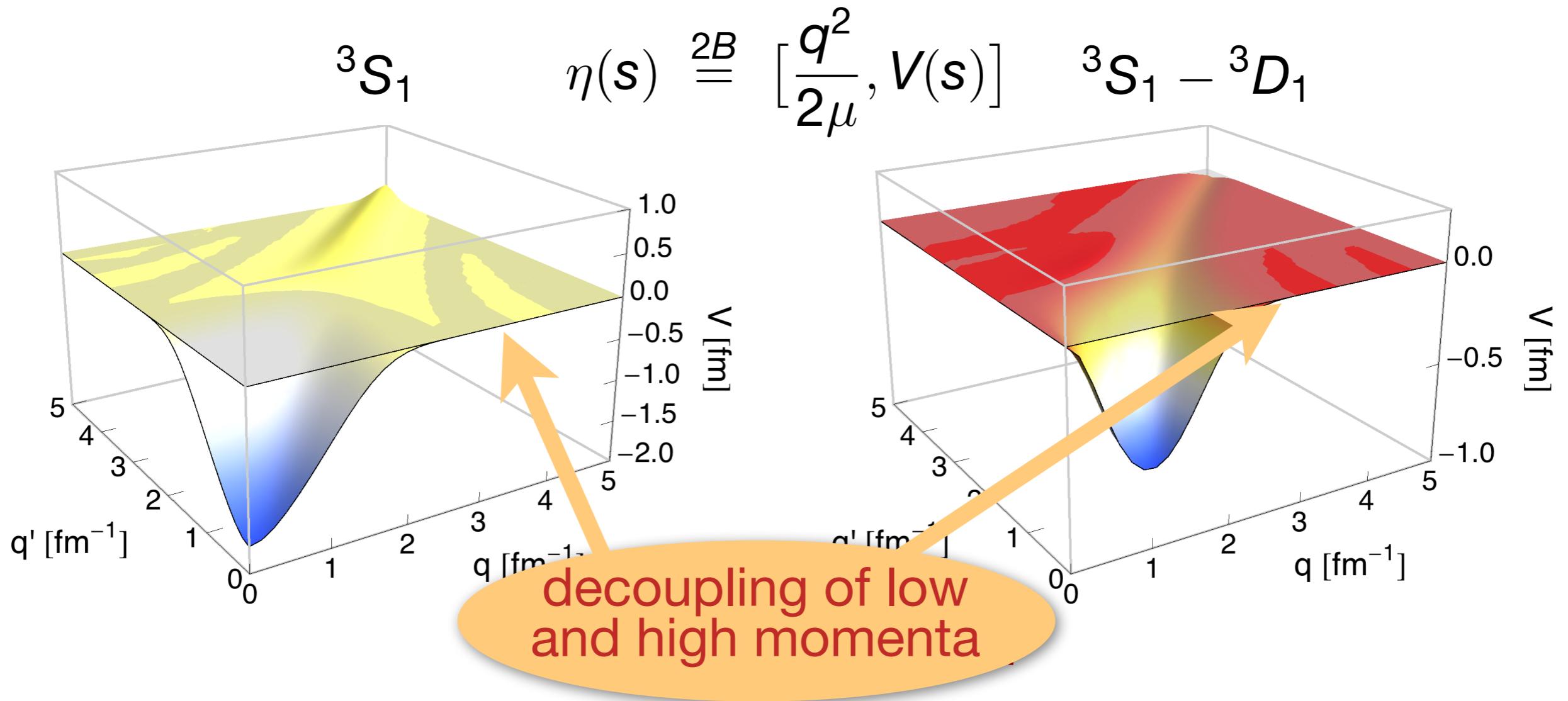
$$H(s) = U(s) H U^\dagger(s) \equiv T + V(s)$$

- flow equation:

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

- 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

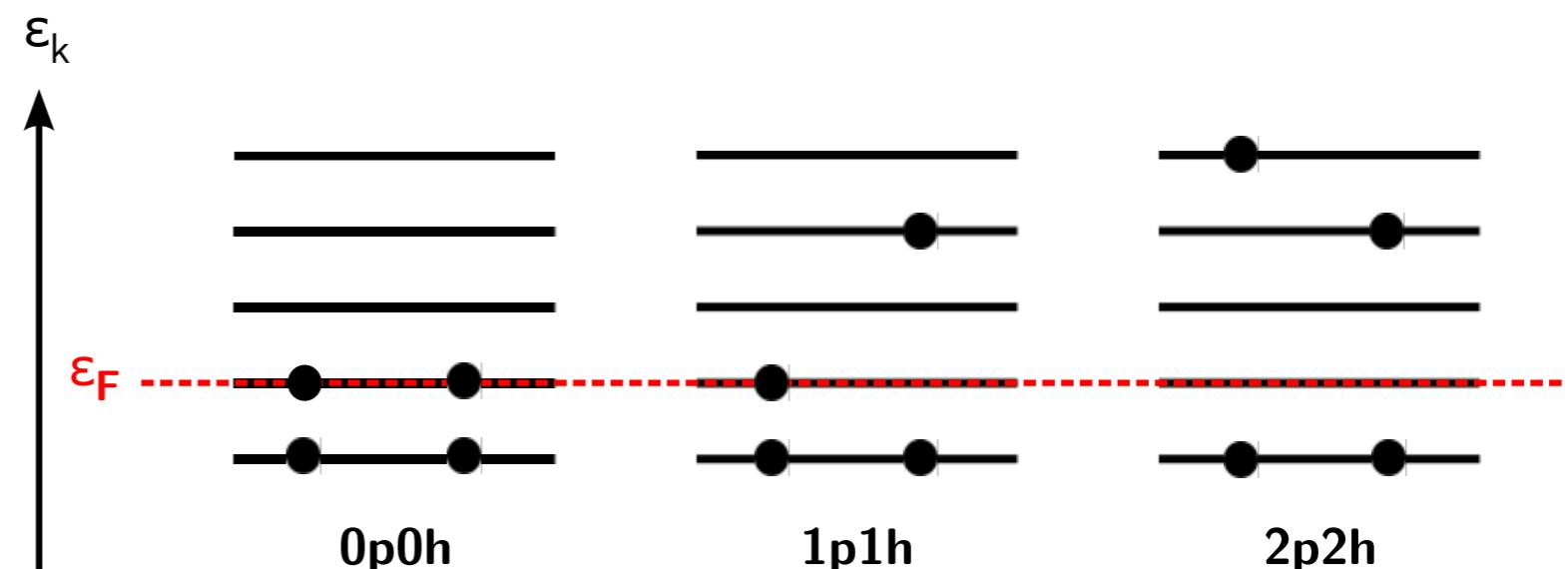
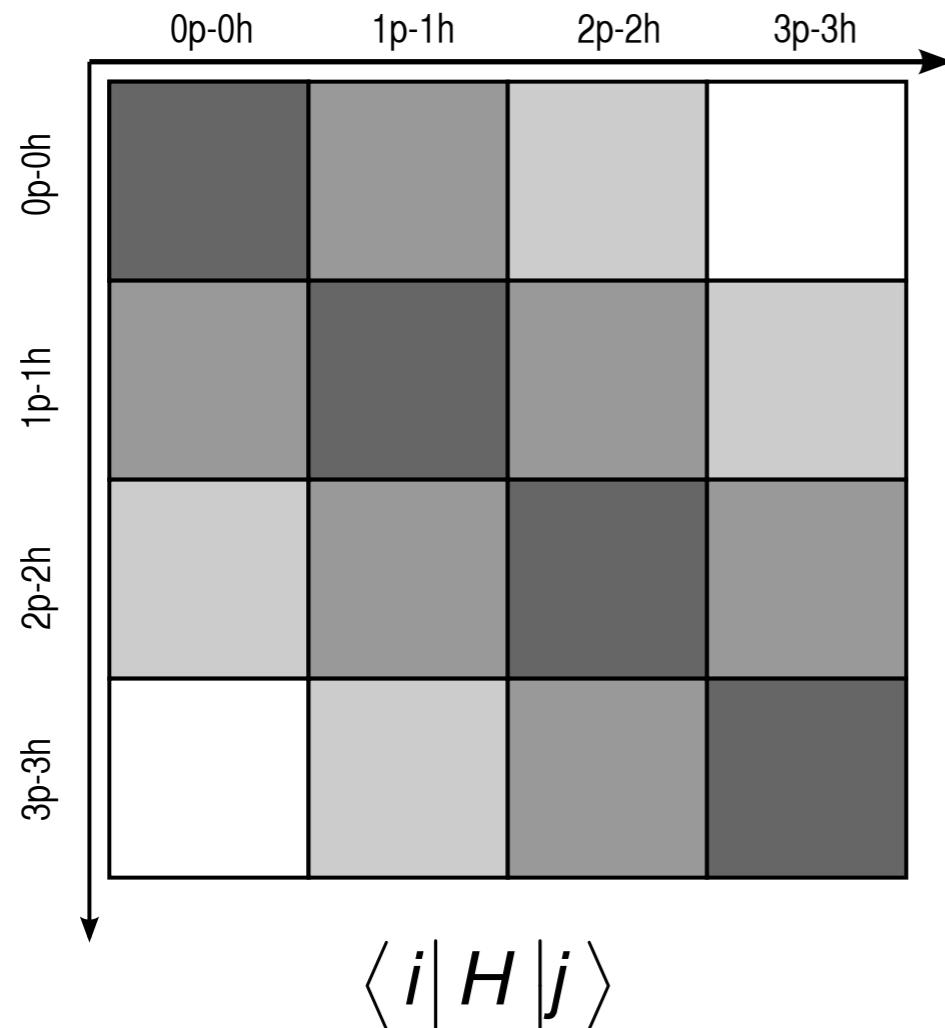


- decoupling drastically improves convergence
- SRG evolution induces many-body forces: inclusion of three-body sector has been achieved  
(Jurgenson, Furnstahl, Navratil, PRL 103, 082501; Hebeler, PRC 85, 021002 )

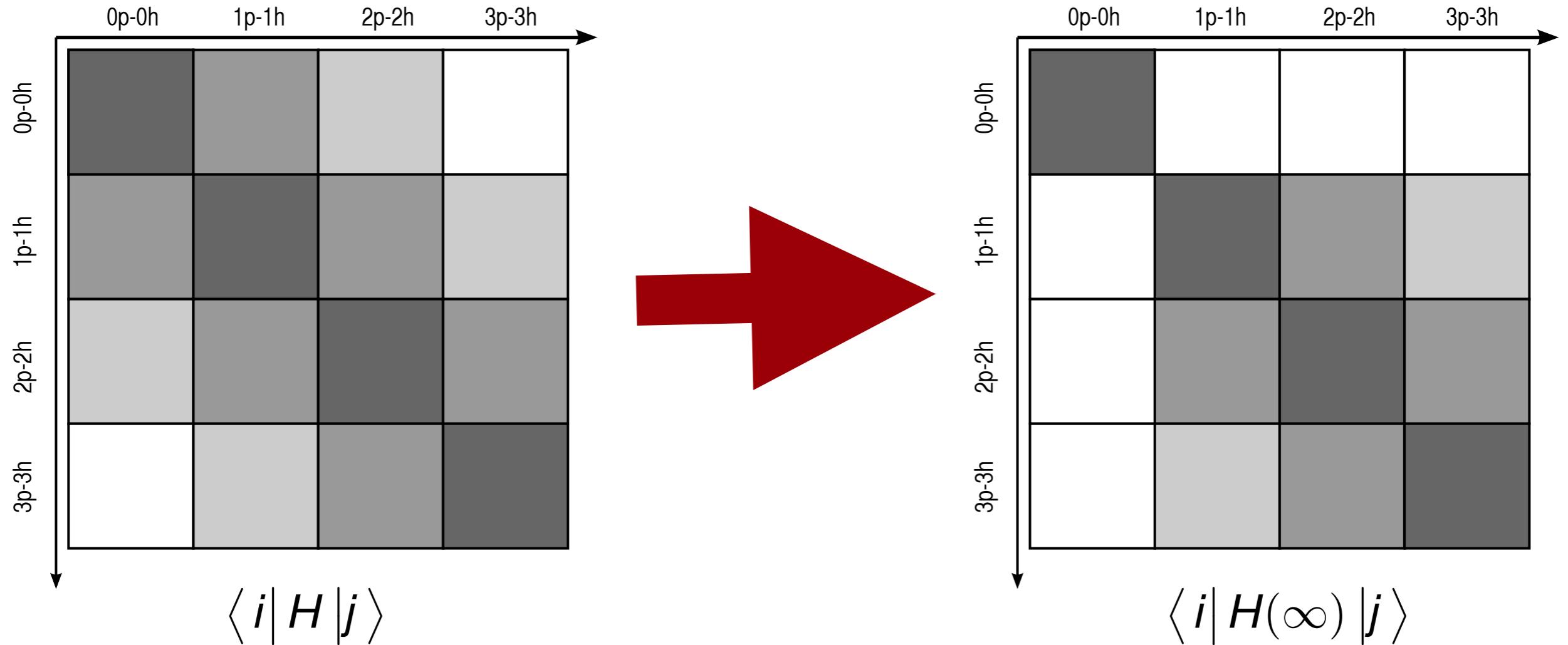
# In-Medium SRG for Closed-Shell Nuclei

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

$$A_I^k \equiv a_k^\dagger a_I, \quad \lambda_I^k \equiv \langle \Psi | A_I^k | \Psi \rangle, \quad \xi_I^k \equiv \lambda_I^k - \delta_I^k$$

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

$$\begin{aligned} A_{I_1 \dots I_N}^{k_1 \dots k_N} = & : A_{I_1 \dots I_N}^{k_1 \dots k_N} : + \lambda_{I_1}^{k_1} : A_{I_2 \dots I_N}^{k_2 \dots k_N} : + \text{singles} \\ & + \left( \lambda_{I_1}^{k_1} \lambda_{I_2}^{k_2} - \lambda_{I_2}^{k_1} \lambda_{I_1}^{k_2} \right) : A_{I_3 \dots I_N}^{k_3 \dots k_N} : + \text{doubles} + \dots \end{aligned}$$

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

$$\begin{aligned} : A_{m_1 \dots m_N}^{k_1 \dots k_N} :: A_{n_1 \dots n_N}^{l_1 \dots l_N} : = & (-1)^{N-1} \lambda_{n_1}^{k_1} : A_{m_1 \dots m_N n_2 \dots n_N}^{k_2 \dots k_N l_1 \dots l_N} : \\ & + (-1)^{N-1} \xi_{m_1}^{l_1} : A_{m_2 \dots m_N n_1 \dots n_N}^{k_1 \dots k_N l_2 \dots l_N} : + \dots \end{aligned}$$

# Normal-Ordered Hamiltonian

## Normal-Ordered Hamiltonian

$$H = E_0 + \sum_{kl} f_I^k : A_I^k : + \frac{1}{4} \sum_{klmn} \Gamma_{mn}^{kl} : A_{mn}^{kl} : + \frac{1}{36} \sum_{ijklmn} W_{lmn}^{ijk} : A_{lmn}^{ijk} :$$

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

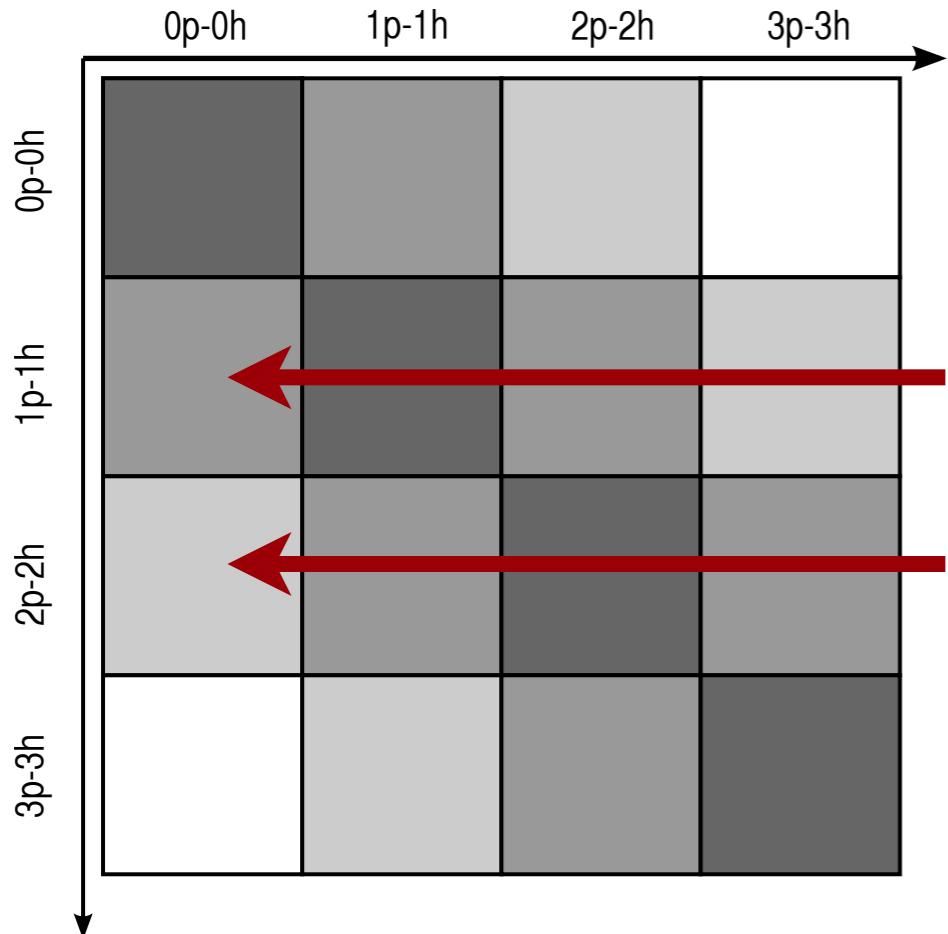
$$f_I^k = \left(1 - \frac{1}{A}\right) t_{kl} + \frac{1}{2} \sum_h \langle kh | V_2 + T_2 | lh \rangle n_h + \frac{1}{2} \sum_{hh'} \langle khh' | V_3 | lhh' \rangle n_h n_{h'}$$

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

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

two-body formalism includes  
(some) three-body interactions

# Choice of Generator



$$\langle \frac{p}{h} | H | \Psi \rangle = \sum_{kl} f_l^k \langle \Psi | : A_p^h :: A_l^k : | \Psi \rangle = -n_h \bar{n}_p f_h^p$$

$$\langle \frac{pp'}{hh'} | H | \Psi \rangle = \sum_{klmn} \Gamma_{mn}^{kl} \langle \Psi | : A_{pp'}^{hh'} :: A_{mn}^{kl} : | \Psi \rangle \sim \Gamma_{hh'}^{pp'}$$

## Off-Diagonal Hamiltonian

$$H^{od} \equiv f^{od} + \Gamma^{od}, \quad f^{od} \equiv \sum_{ph} f_h^p : A_h^p : + \text{H.c.}, \quad \Gamma^{od} \equiv \sum_{pp'hh'} \Gamma_{hh'}^{pp'} : A_{hh'}^{pp'} : + \text{H.c.}$$

# Choice of Generator

- Wegner

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

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

$$\eta^{II} = \sum_{ph} \frac{f_h^p}{E_p - E_h} : A_h^p : + \sum_{pp'hh'} \frac{\Gamma_{hh'}^{pp'}}{E_{pp'} - E_{hh'}} : A_{hh'}^{pp'} : + \text{H.c.}$$

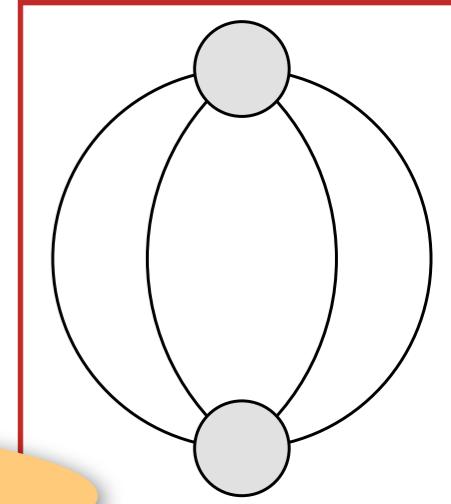
$E_p - E_h, E_{pp'} - E_{hh'}$  : approx. 1p1h, 2p2h excitation energies

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

# In-Medium SRG Flow Equations

## 0-body Flow

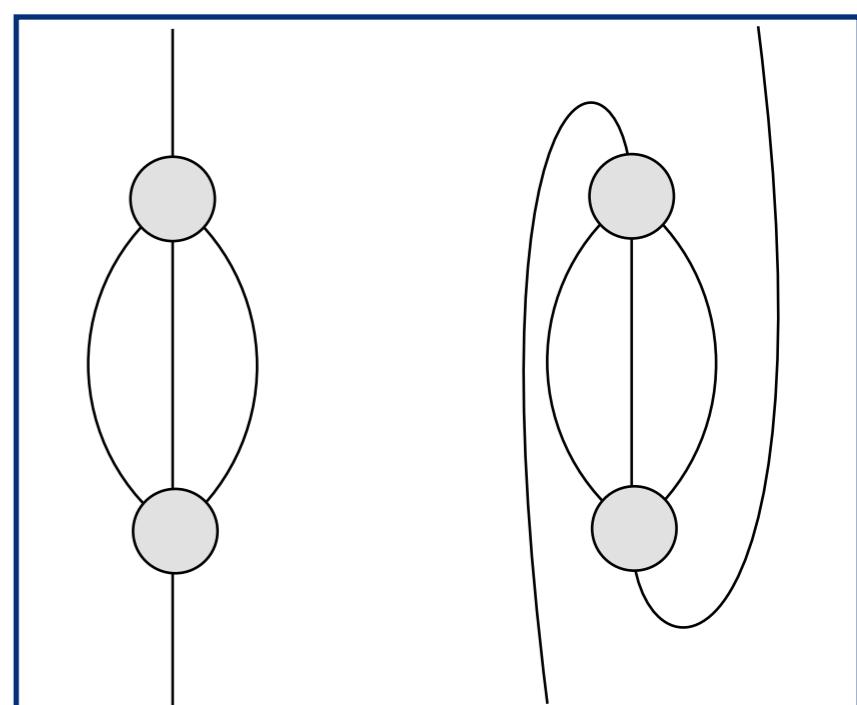
$$\frac{dE}{ds} = \sum_{ab} (n_a - n_b) \left( \eta_b^a f_a^b - f_b^a \eta_a^b \right) + \frac{1}{4} \sum_{abcd} \underbrace{\left( \eta_{cd}^{ab} \Gamma_{ab}^{cd} - \Gamma_{cd}^{ab} \eta_{ab}^{cd} \right)}_{\sim 2nd \text{ order MBPT for } H(s)} n_a n_b \bar{n}_c \bar{n}_d$$



$\sim$  2nd order MBPT for  $H(s)$

## 1-body Flow

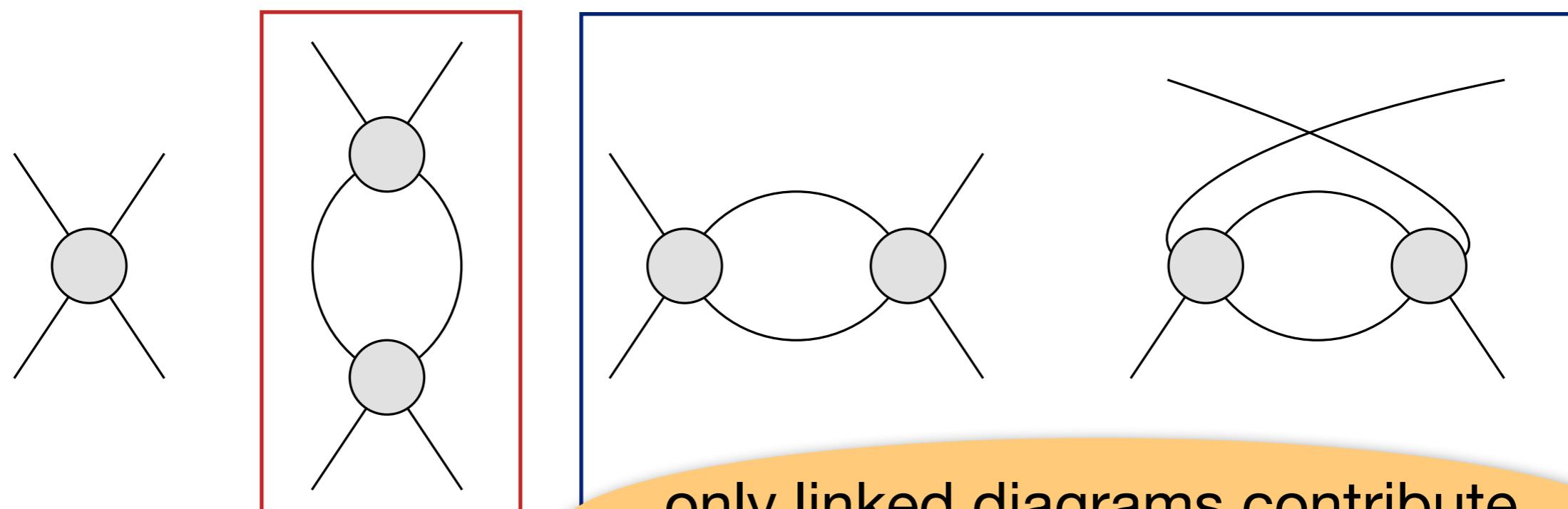
$$\begin{aligned} \frac{d}{ds} f_2^1 &= \sum_a \left( \eta_a^1 f_2^a - f_a^1 \eta_2^a \right) + \sum_{ab} \left( \eta_b^a \Gamma_{a2}^{b1} - f_b^a \eta_{a2}^{b1} \right) (n_a - n_b) \\ &\quad + \frac{1}{2} \sum_{abcdef} \underbrace{\left( \eta_{bc}^{1a} \Gamma_{2a}^{bc} - \Gamma_{bc}^{1a} \eta_{2a}^{bc} \right)}_{\sim 2nd \text{ order MBPT for } H(s)} (n_a \bar{n}_b \bar{n}_c + \bar{n}_a n_b n_c) \end{aligned}$$



# In-Medium SRG Flow Equations

## 2-body Flow

$$\begin{aligned}\frac{d}{ds} \Gamma_{34}^{12} = & \sum_a \left( \eta_a^1 \Gamma_{34}^{a2} + \eta_a^2 \Gamma_{34}^{1a} - \eta_3^a \Gamma_{a4}^{12} - \eta_4^a \Gamma_{3a}^{12} - f_a^1 \eta_{34}^{a2} - f_a^2 \eta_{34}^{1a} + f_3^a \eta_{a4}^{12} + f_4^a \eta_{3a}^{12} \right) \\ & + \frac{1}{2} \sum_{ab} \underbrace{\left( \eta_{ab}^{12} \Gamma_{34}^{ab} - \Gamma_{ab}^{12} \eta_{34}^{ab} \right) (1 - n_a - n_b)}_{\text{linked diagrams}} \\ & + \sum_{ab} \underbrace{(n_a - n_b) \left( \left( \eta_{3b}^{1a} \Gamma_{4a}^{2b} - \Gamma_{3b}^{1a} \eta_{4a}^{2b} \right) - \left( \eta_{3b}^{2a} \Gamma_{4a}^{1b} - \Gamma_{3b}^{2a} \eta_{4a}^{1b} \right) \right)}_{\text{linked diagrams}}\end{aligned}$$



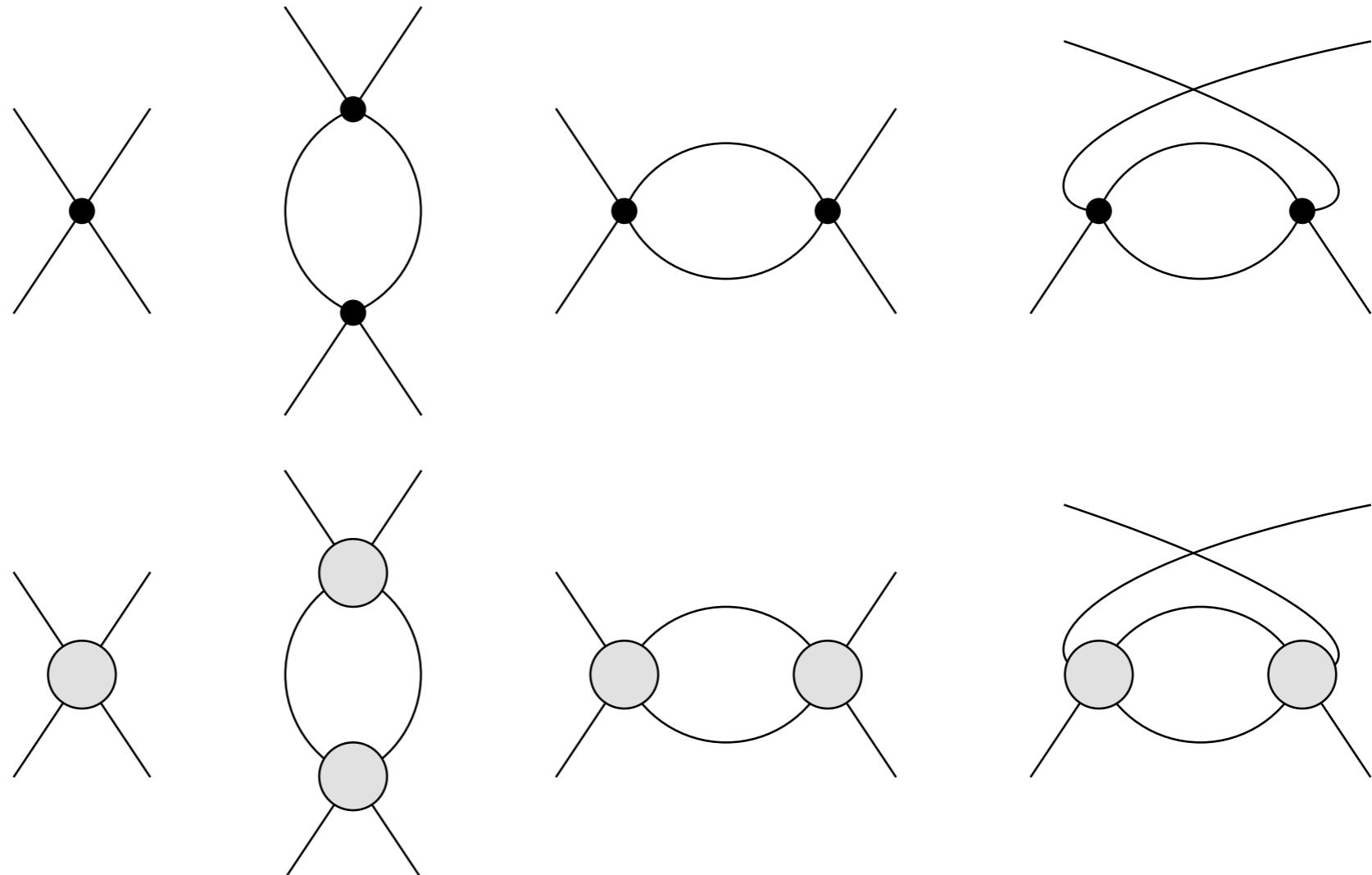
only linked diagrams contribute,  
IM-SRG size-extensive

# In-Medium SRG Flow: Diagrams

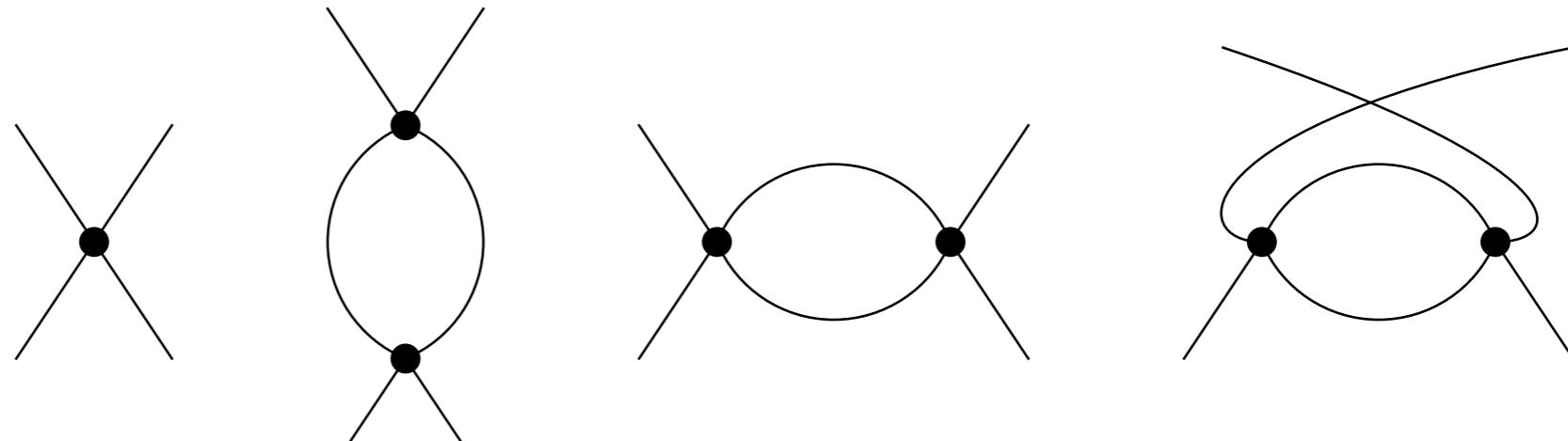
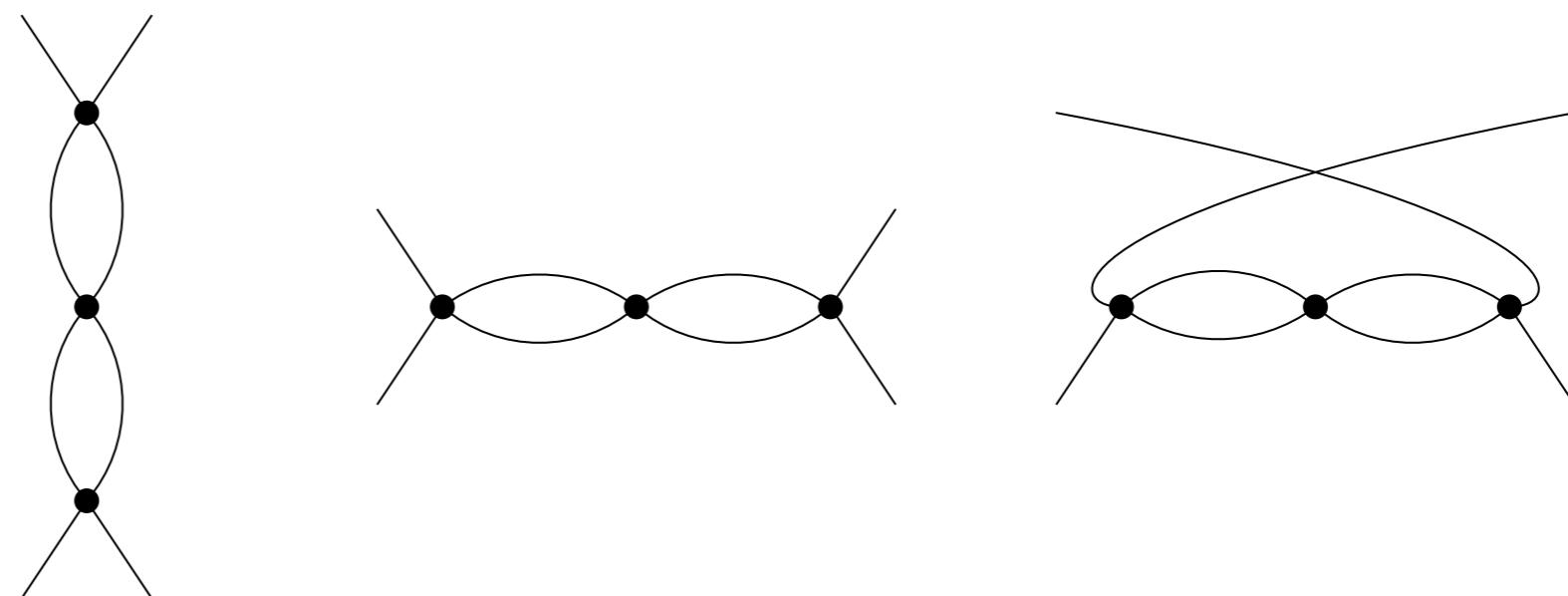
$$\Gamma(\delta s) \sim$$



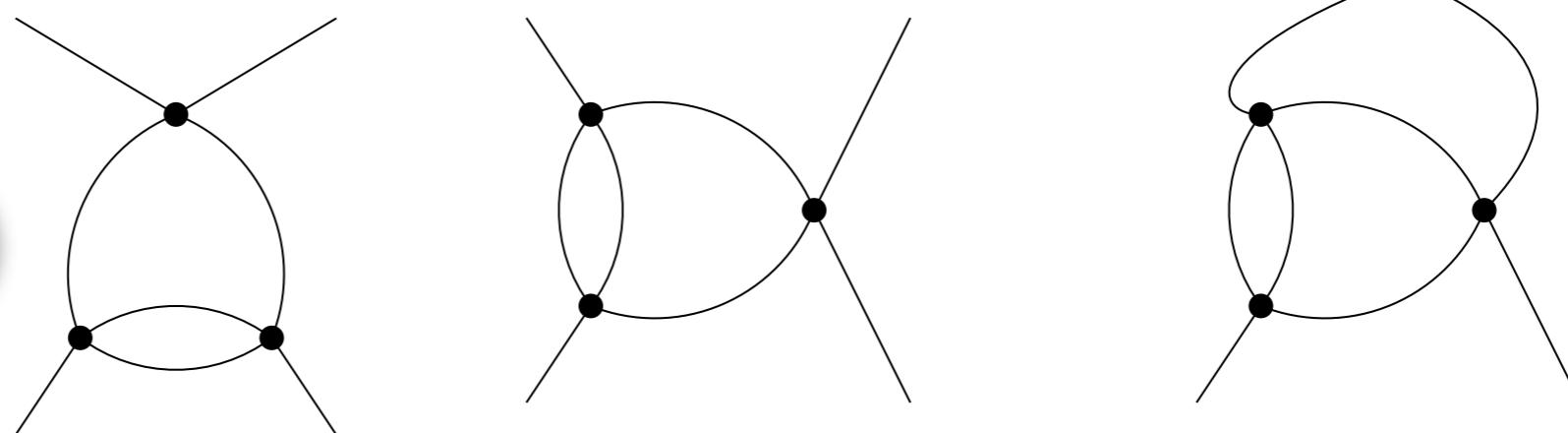
$$\Gamma(2\delta s) \sim$$



# In-Medium SRG Flow: Diagrams

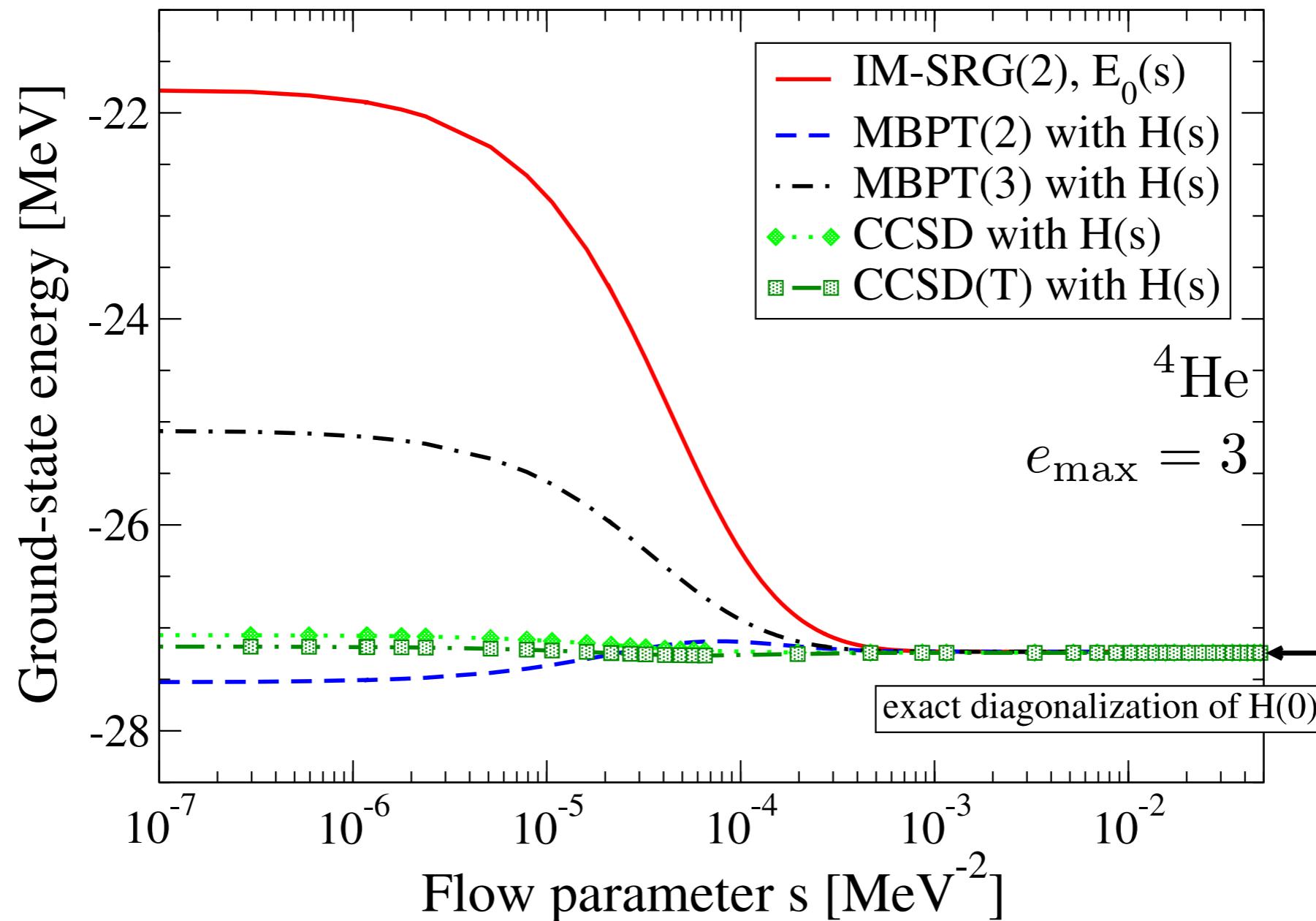
 $\Gamma(\delta s) \sim$  $\Gamma(2\delta s) \sim$ 

non-  
perturbative  
resummation



& many  
more...

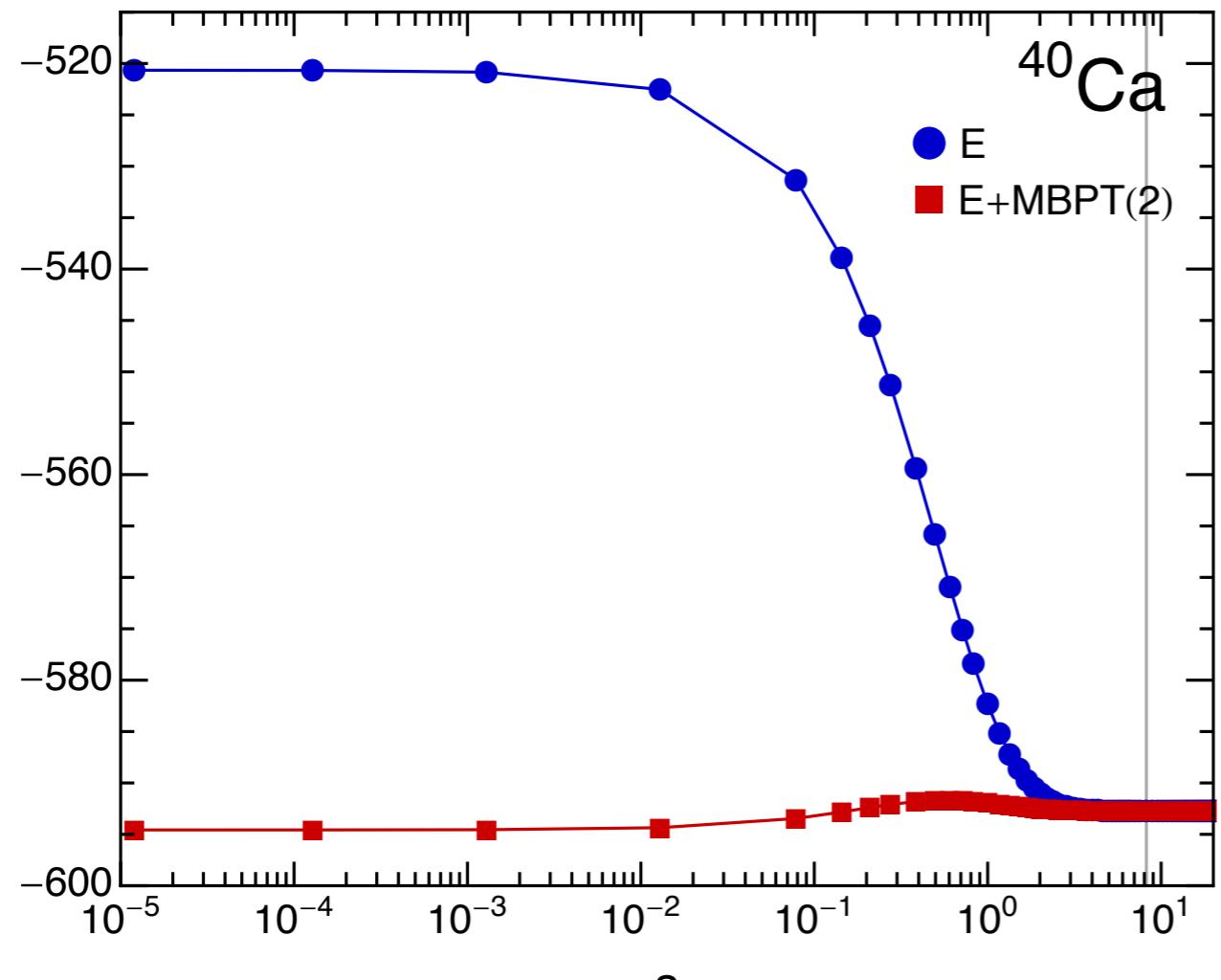
# Resummation



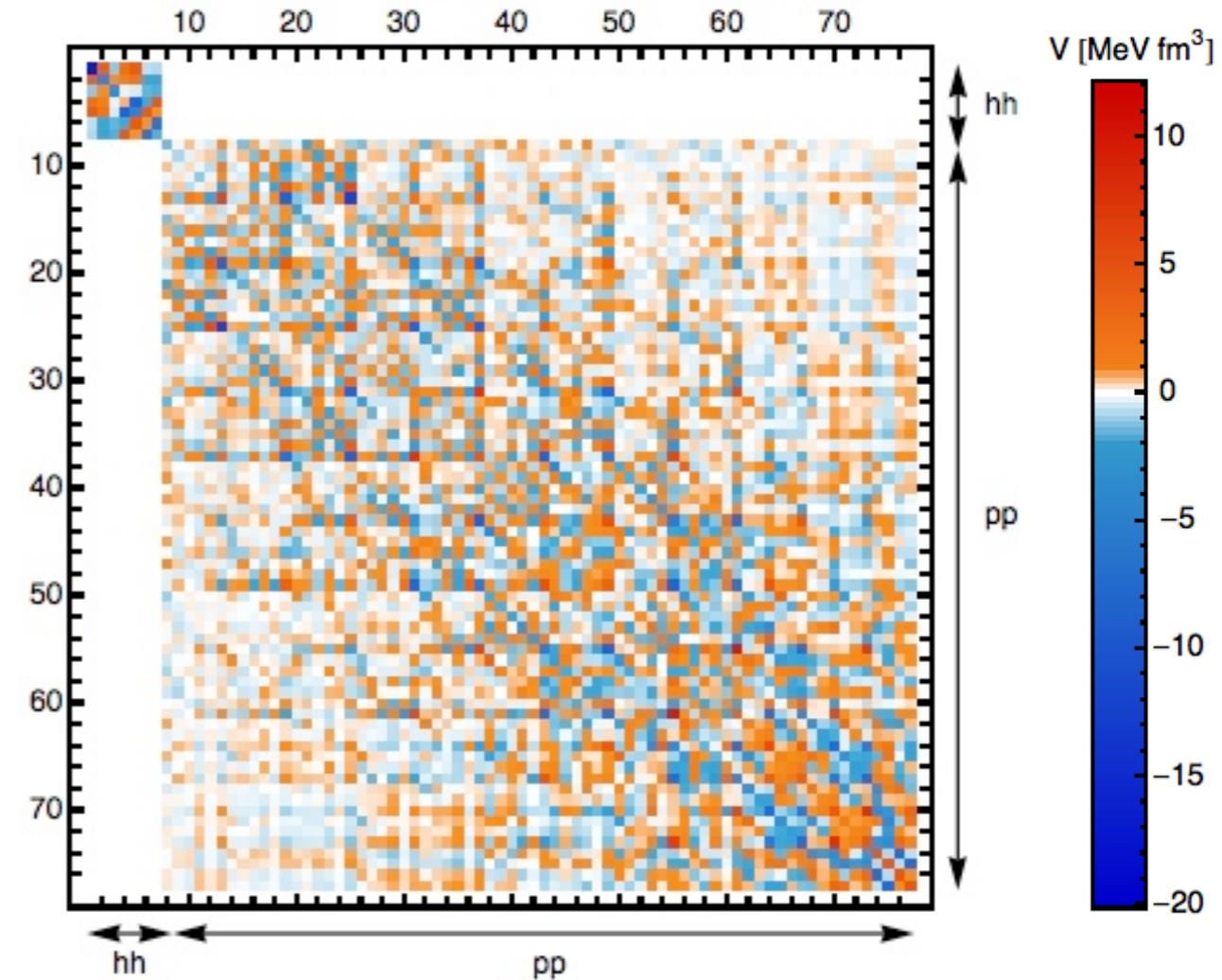
[K. Tsukiyama, S. K. Bogner & A. Schwenk, Phys. Rev. Lett. 106 (2011), 222502]

$E_0$  rapidly approaches perturbation theory & quasi-exact results

# Decoupling

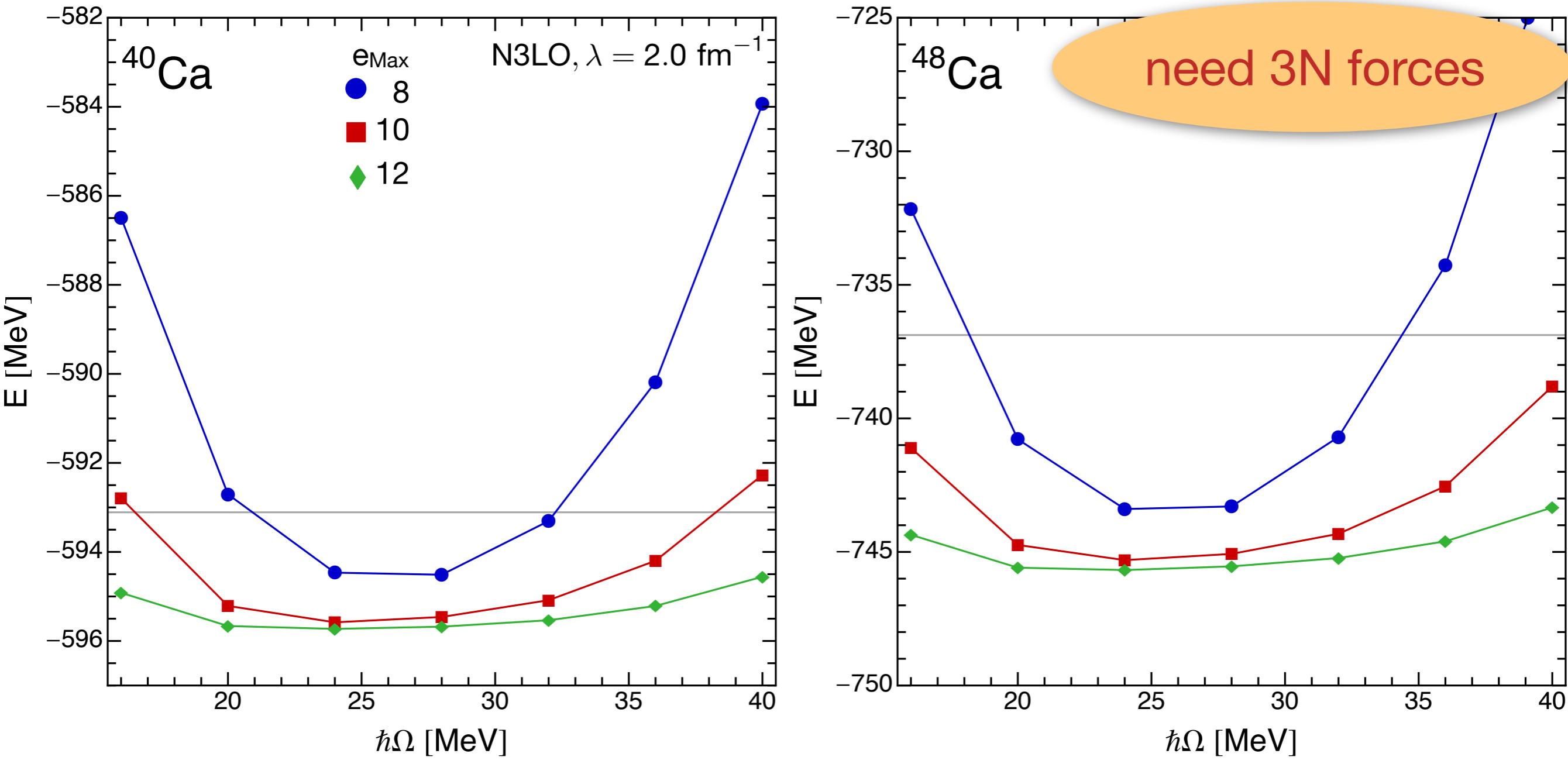


$$V_{\text{SRG}}(\text{N3LO}), \lambda = 2.0 \text{ fm}^{-1}, e_{\text{Max}} = 8$$



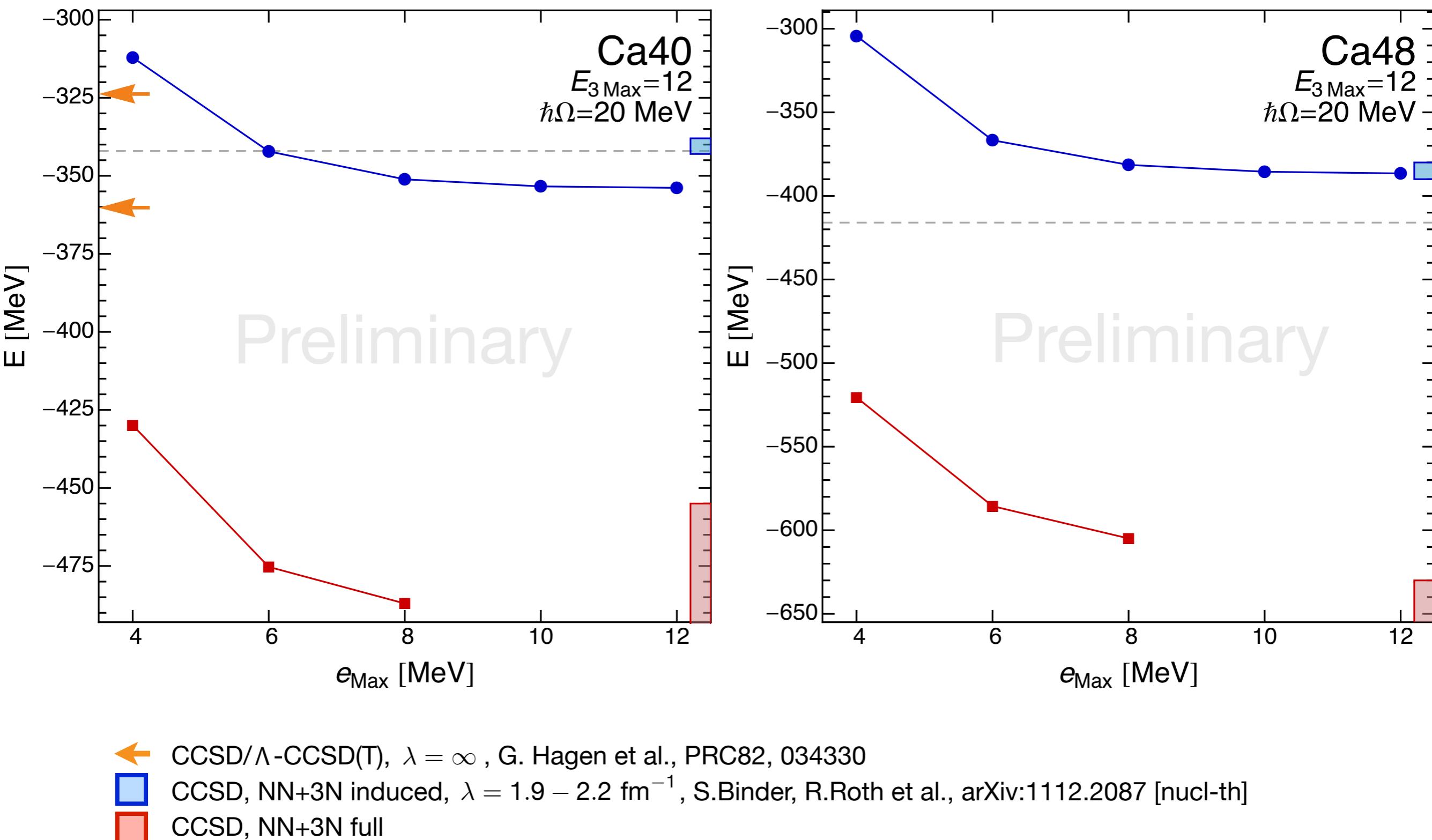
off-diagonal couplings are  
rapidly driven to zero

# Results



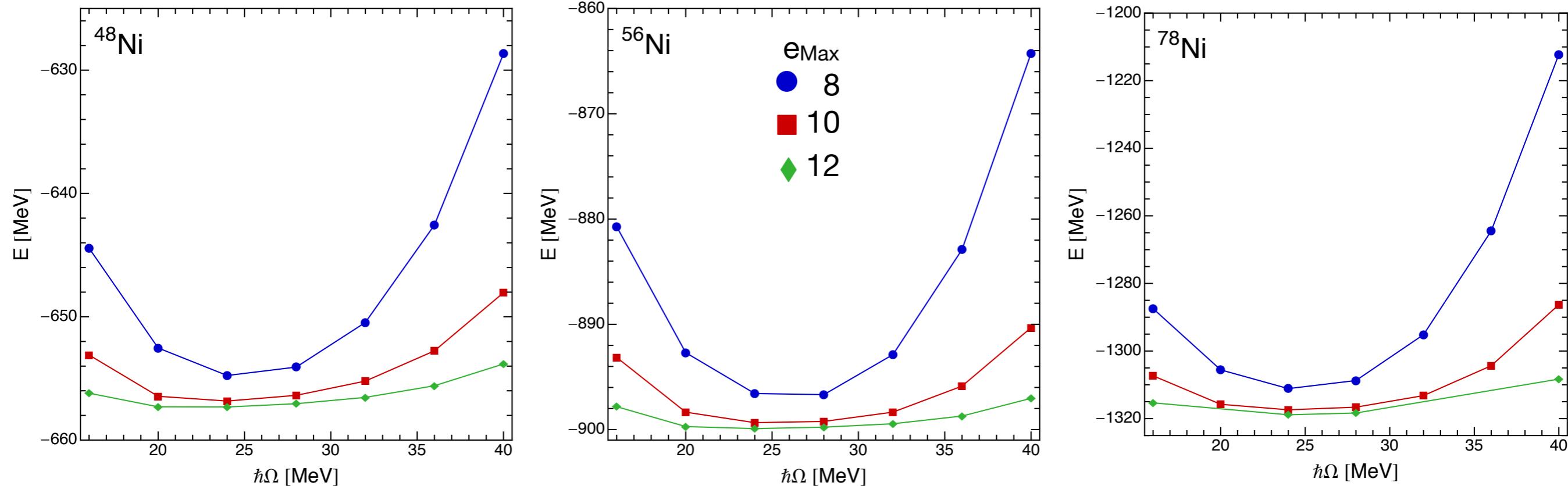
converged g.s. energies between CCSD and  $\Lambda$ -CCSD(T)

# Results: 3N Forces



# 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

# Multi-Reference In-Medium SRG

# Generalized Normal Ordering

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

$$\rho_{mn}^{kl} = \lambda_{mn}^{kl} + \lambda_m^k \lambda_n^l - \lambda_n^k \lambda_m^l$$

$$\rho_{lmn}^{ijk} = \lambda_{lmn}^{ijk} + \lambda_l^i \lambda_{mn}^{jk} + \lambda_l^i \lambda_m^j \lambda_n^k + \text{permutations}$$

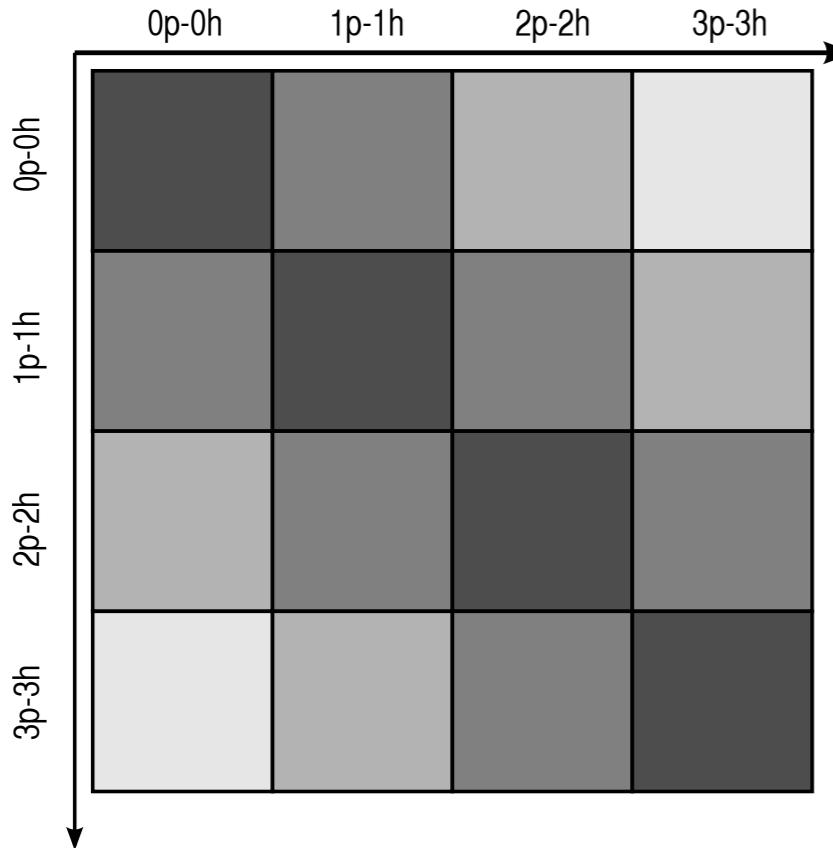
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$: A_m^k \dots : A_n^l \dots :$	$\lambda_n^k$
$: A_m^k \dots : A_n^l \dots :$	$\xi_m^l$
$: A_{cd}^{ab} \dots : A_{mn}^{kl} \dots : , : A_{cd}^{ab} \dots : A_{mn}^{kl} \dots : , \text{etc.}$	$\lambda_{mn}^{ab}, \lambda_{cm}^{ab}, \text{etc.}$
$: A_{def}^{abc} \dots : A_{nop}^{klm} \dots : , : A_{def}^{abc} \dots : A_{nop}^{klm} \dots : , \text{etc.}$	$\lambda_{nop}^{abc}, \lambda_{nop}^{abk}, \text{etc.}$

...

...

# Decoupling



$$\langle \frac{p}{h} | H | \Psi \rangle \sim f_h^p, \sum_{kl} f_l^k \lambda_{pl}^{hk}, \sum_{klmn} \Gamma_{mn}^{kl} \lambda_{pmn}^{hkl}, \dots$$

$$\langle \frac{pp'}{hh'} | H | \Psi \rangle \sim \Gamma_{hh'}^{pp'}, \sum_{km} \Gamma_{hm}^{pk} \lambda_{p'm}^{h'k}, \sum_{kl} f_l^k \lambda_{pp'l}^{hh'k}, \sum_{klmn} \Gamma_{mn}^{kl} \lambda_{pp'mn}^{hh'kl}, \dots$$

$$\langle \frac{pp'p''}{hh'h'} | H | \Psi \rangle \sim \dots$$

- 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:

$$\begin{aligned} \frac{dE}{ds} = & \sum_{ab} (n_a - n_b) \left( \eta_b^a f_a^b - f_b^a \eta_a^b \right) + \frac{1}{4} \sum_{abcd} \left( \eta_{cd}^{ab} \Gamma_{ab}^{cd} - \Gamma_{cd}^{ab} \eta_{ab}^{cd} \right) n_a n_b \bar{n}_c \bar{n}_d \\ & + \frac{1}{4} \sum_{abcd} \left( \frac{d}{ds} \Gamma_{cd}^{ab} \right) \lambda_{cd}^{ab} + \frac{1}{4} \sum_{abcdklm} \left( \eta_{cd}^{ab} \Gamma_{am}^{kl} - \Gamma_{cd}^{ab} \eta_{am}^{kl} \right) \lambda_{cdm}^{bkl} \end{aligned}$$

1-body flow:

$$\begin{aligned} \frac{d}{ds} f_2^1 = & \sum_a \left( \eta_a^1 f_2^a - f_a^1 \eta_2^a \right) + \sum_{ab} \left( \eta_b^a \Gamma_{a2}^{b1} - f_b^a \eta_{a2}^{b1} \right) (n_a - n_b) \\ & + \frac{1}{2} \sum_{abcdef} \left( \eta_{bc}^{1a} \Gamma_{2a}^{bc} - \Gamma_{bc}^{1a} \eta_{2a}^{bc} \right) (n_a \bar{n}_b \bar{n}_c + \bar{n}_a n_b n_c) \\ & + \frac{1}{4} \sum_{abcde} \left( \eta_{bc}^{1a} \Gamma_{2a}^{de} - \Gamma_{bc}^{1a} \eta_{2a}^{de} \right) \lambda_{bc}^{de} + \sum_{abcde} \left( \eta_{bc}^{1a} \Gamma_{2d}^{be} - \Gamma_{bc}^{1a} \eta_{2d}^{be} \right) \lambda_{cd}^{ae} \\ & - \frac{1}{2} \sum_{abcde} \left( \eta_{2b}^{1a} \Gamma_{ae}^{cd} - \Gamma_{2b}^{1a} \eta_{ae}^{cd} \right) \lambda_{be}^{cd} + \frac{1}{2} \sum_{abcde} \left( \eta_{2b}^{1a} \Gamma_{de}^{bc} - \Gamma_{2b}^{1a} \eta_{de}^{bc} \right) \lambda_{de}^{ac} \end{aligned}$$

# Multi-Reference Flow Equations

2-body flow:

$$\begin{aligned}\frac{d}{ds} \Gamma_{34}^{12} = & \sum_a \left( \eta_a^1 \Gamma_{34}^{a2} + \eta_a^2 \Gamma_{34}^{1a} - \eta_3^a \Gamma_{a4}^{12} - \eta_4^a \Gamma_{3a}^{12} - f_a^1 \eta_{34}^{a2} - f_a^2 \eta_{34}^{1a} + f_3^a \eta_{a4}^{12} + f_4^a \eta_{3a}^{12} \right) \\ & + \frac{1}{2} \sum_{ab} \left( \eta_{ab}^{12} \Gamma_{34}^{ab} - \Gamma_{ab}^{12} \eta_{34}^{ab} \right) (1 - n_a - n_b) \\ & + \sum_{ab} (n_a - n_b) \left( \left( \eta_{3b}^{1a} \Gamma_{4a}^{2b} - \Gamma_{3b}^{1a} \eta_{4a}^{2b} \right) - \left( \eta_{3b}^{2a} \Gamma_{4a}^{1b} - \Gamma_{3b}^{2a} \eta_{4a}^{1b} \right) \right)\end{aligned}$$

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, arXiv:1203.2515 [nucl-th])
- 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**:

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

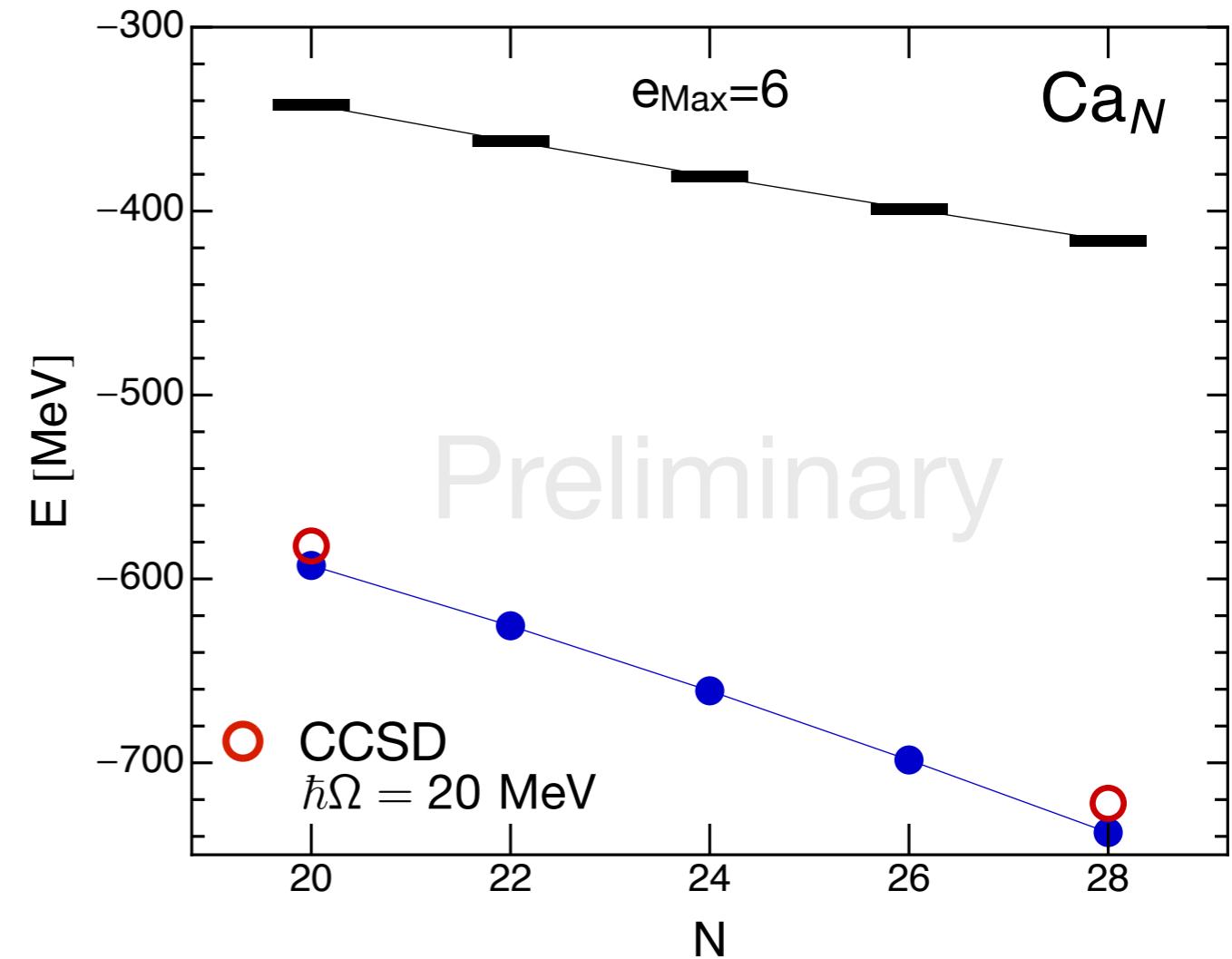
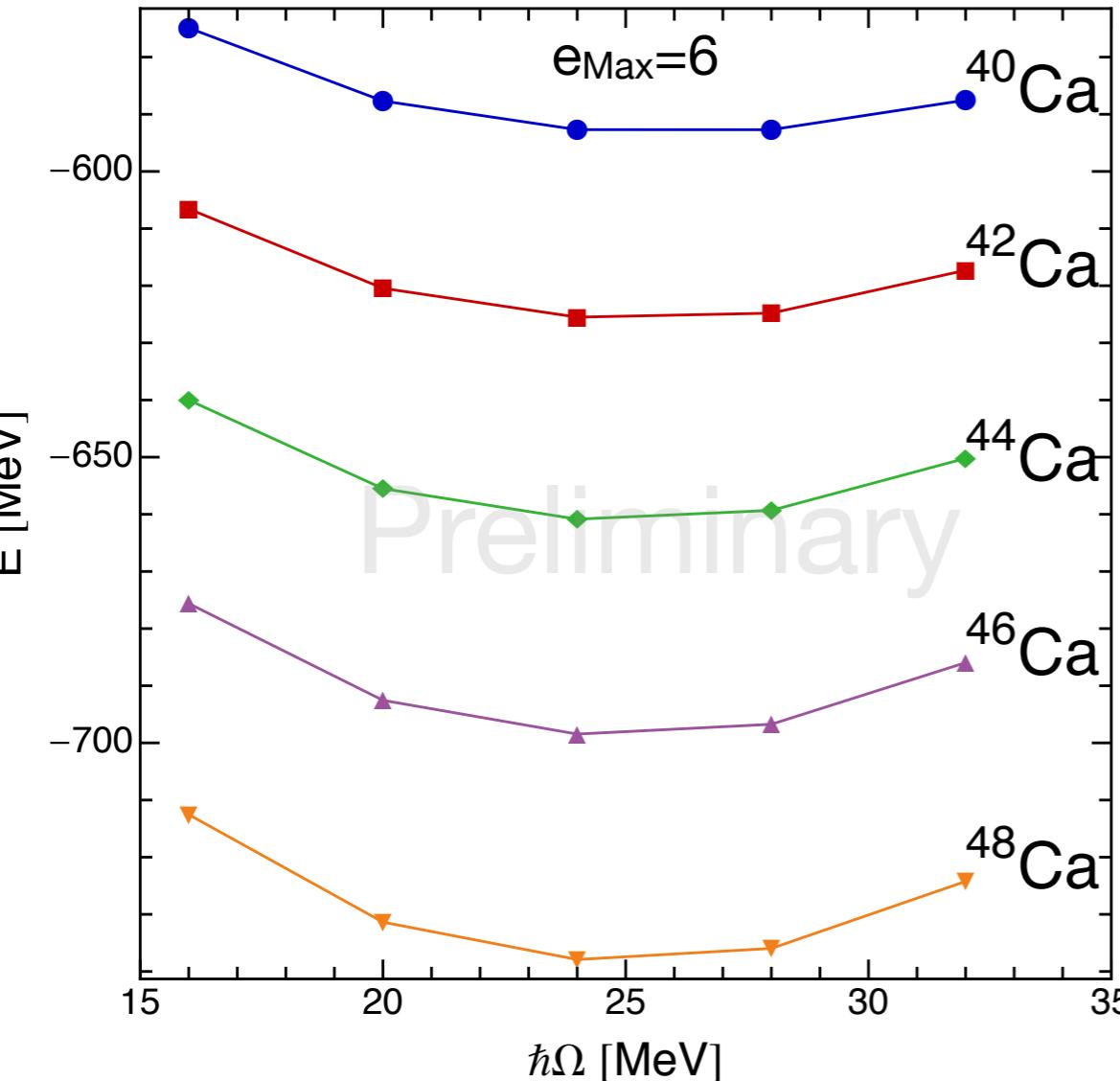
- calculate one- and two-body densities (**project only once**):

$$\lambda_I^k = \frac{\langle \Psi | A_I^k P_N | \Psi \rangle}{\langle \Psi | \Psi \rangle}, \quad \lambda_{mn}^{kl} = \frac{\langle \Psi | A_{mn}^{kl} P_N | \Psi \rangle}{\langle \Psi | \Psi \rangle} - \lambda_m^k \lambda_m^l + \lambda_n^k \lambda_m^l$$

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

$$\lambda_I^k = n_k \delta_I^k \left(= v_k^2 \delta_I^k\right), \quad 0 \leq n_k \leq 1$$

# Results



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

# 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)
- ✓ 3N forces implemented, systematic calculations for closed-shell nuclei in progress
- optimal choice of generator for open-shell nucleus?
- efficient evolution of observables (density matrices)?

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TU Darmstadt, Germany

**E. R. Anderson, R. J. Furnstahl, K. Hebeler, R. J. Perry, K. A. Wendt**

Ohio State University

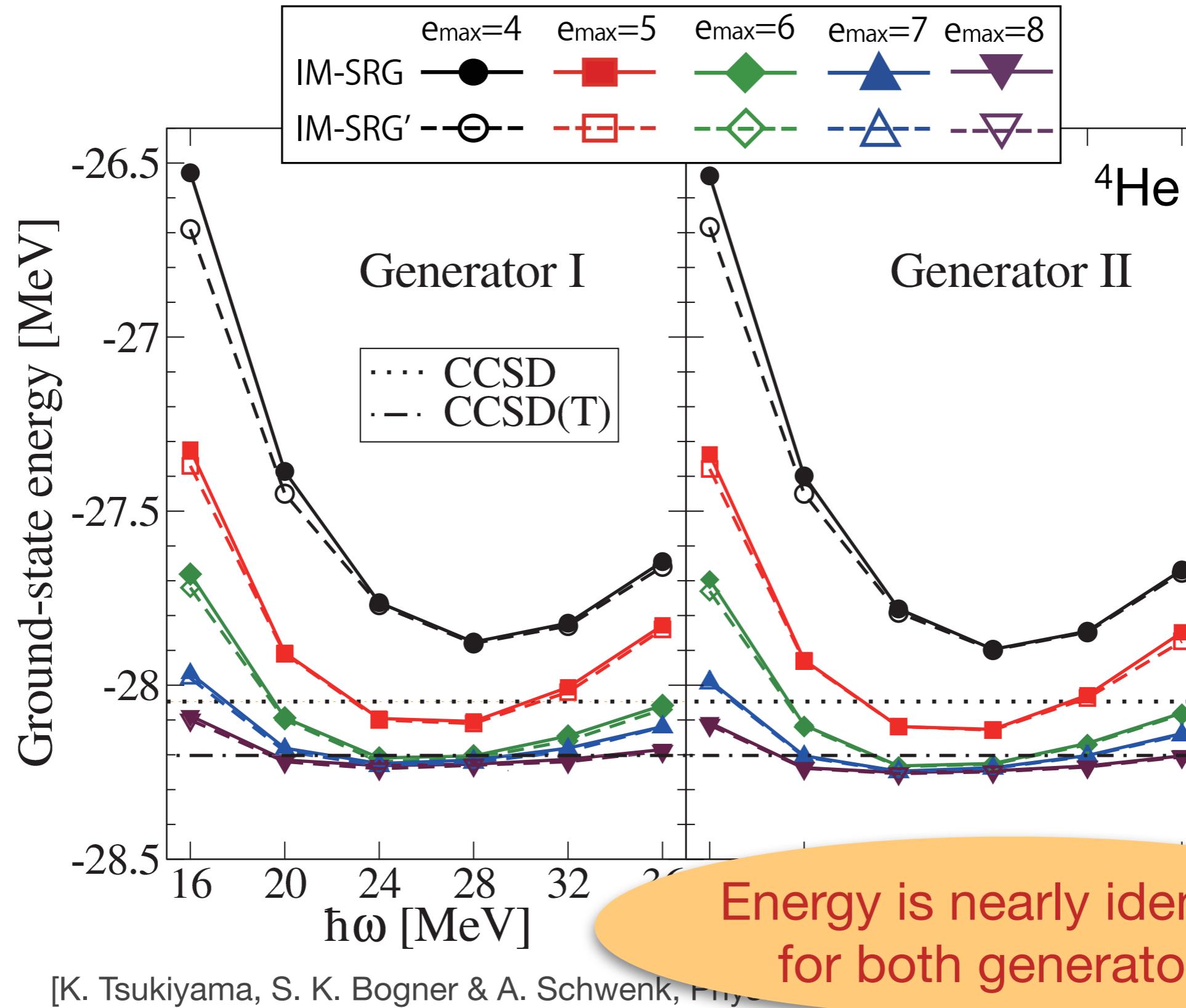
**P. Papakonstantinou**

IPN Orsay, France

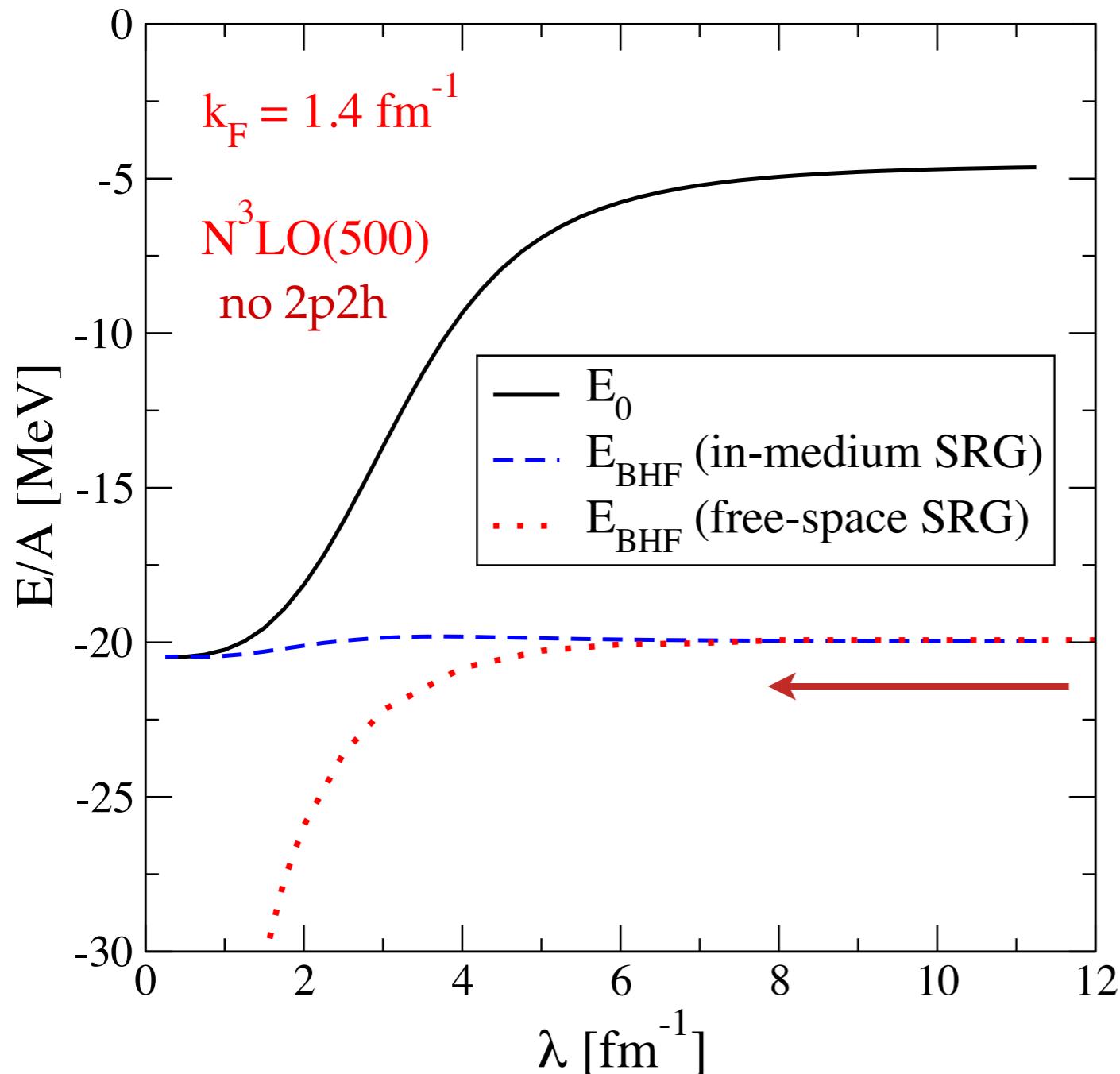


# Supplements

# Results



# Symmetric Nuclear Matter



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

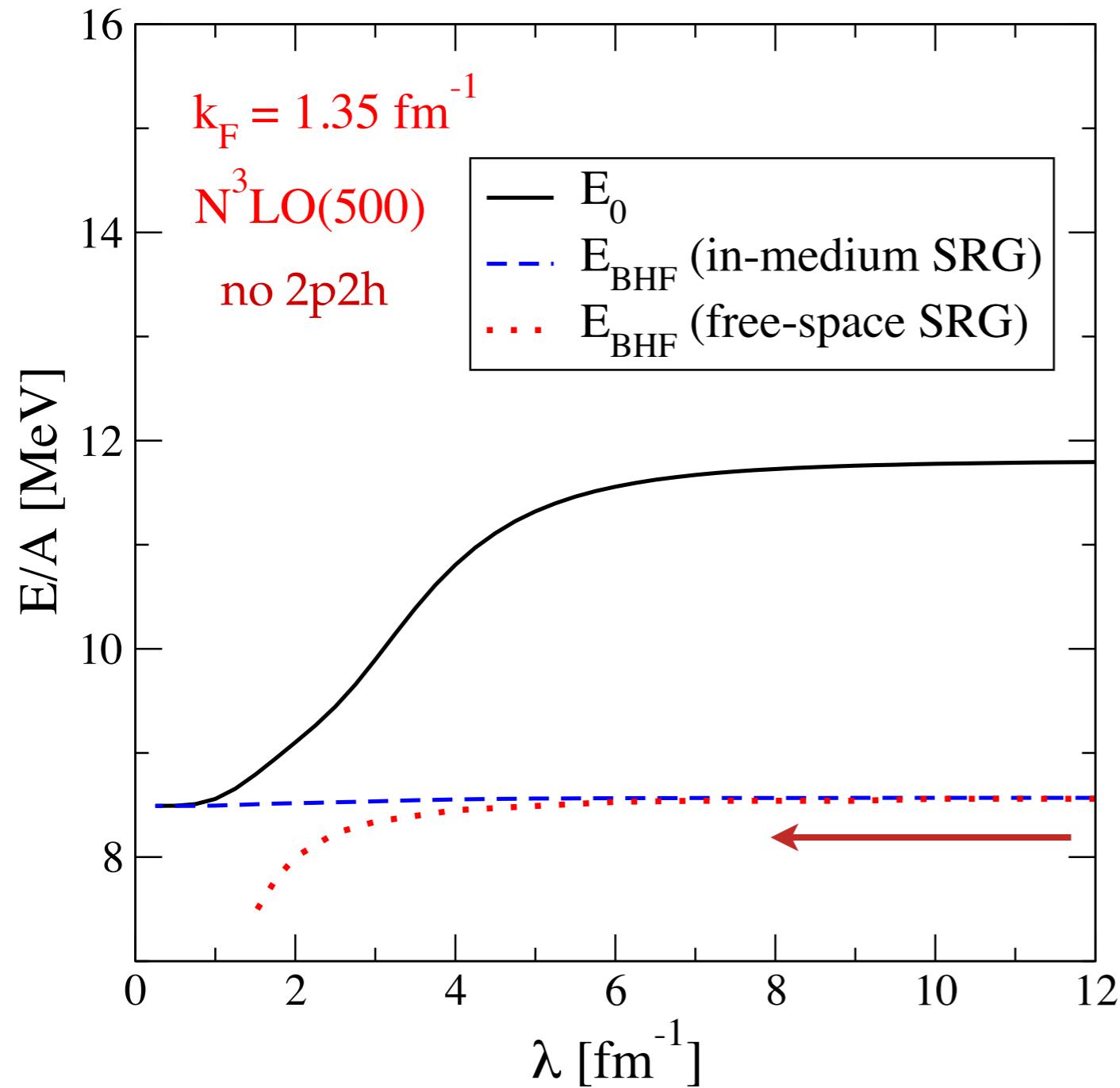
## Free-Space SRG

- $E_{\text{BHF}}$  (pp ladder sum) is strongly  $\lambda$ -dependent (NN interaction only!)

## In-Medium SRG

- $\lambda$ -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

- $E_{\text{BHF}}$  (pp ladder sum) is strongly  $\lambda$ -dependent (NN interaction only!)

## In-Medium SRG

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