New Extensions of the In-Medium Similarity Renormalization Group

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Outline

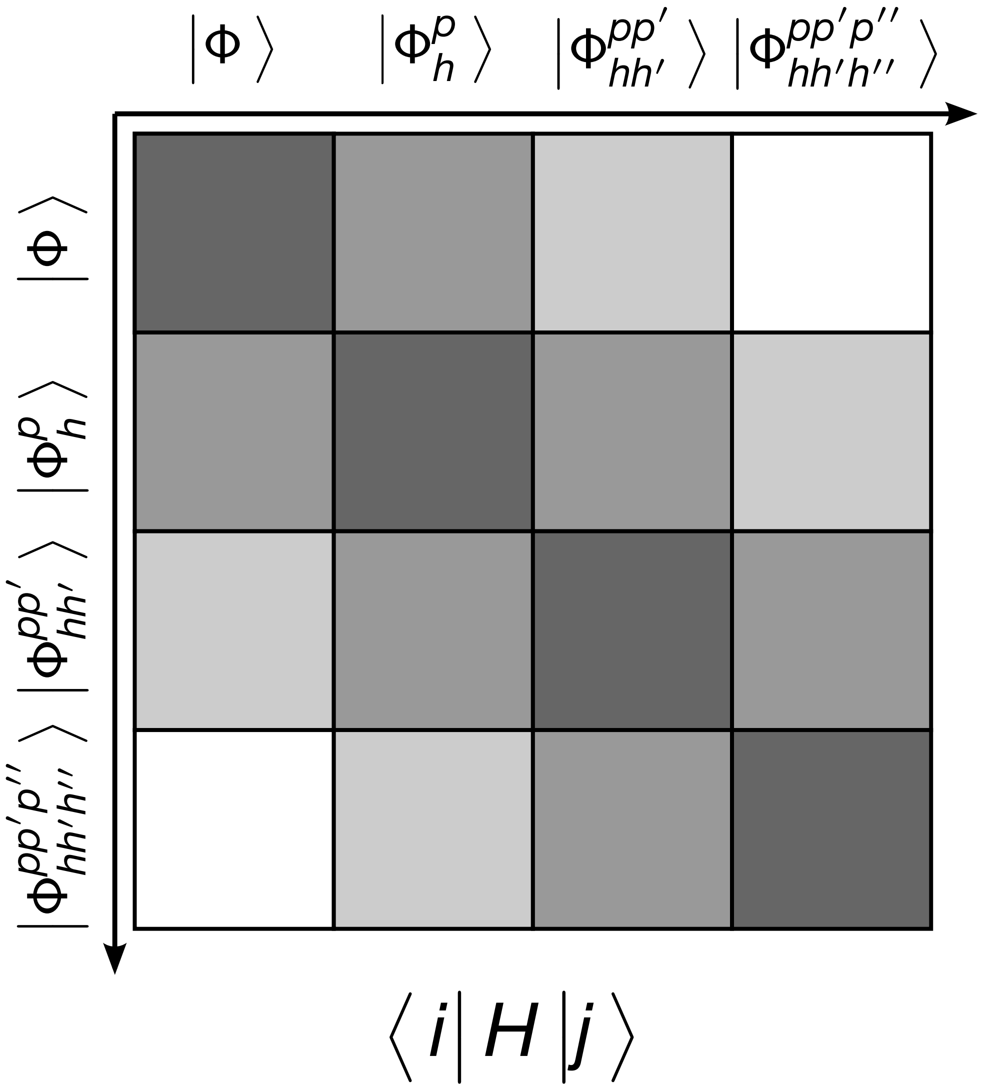
- A (Brief) Introduction to the In-Medium SRG
- Magnus Formulation of the In-Medium SRG
- IM-SRG for Excited States
- New Applications of the Multi-Reference IM-SRG
- Epilogue

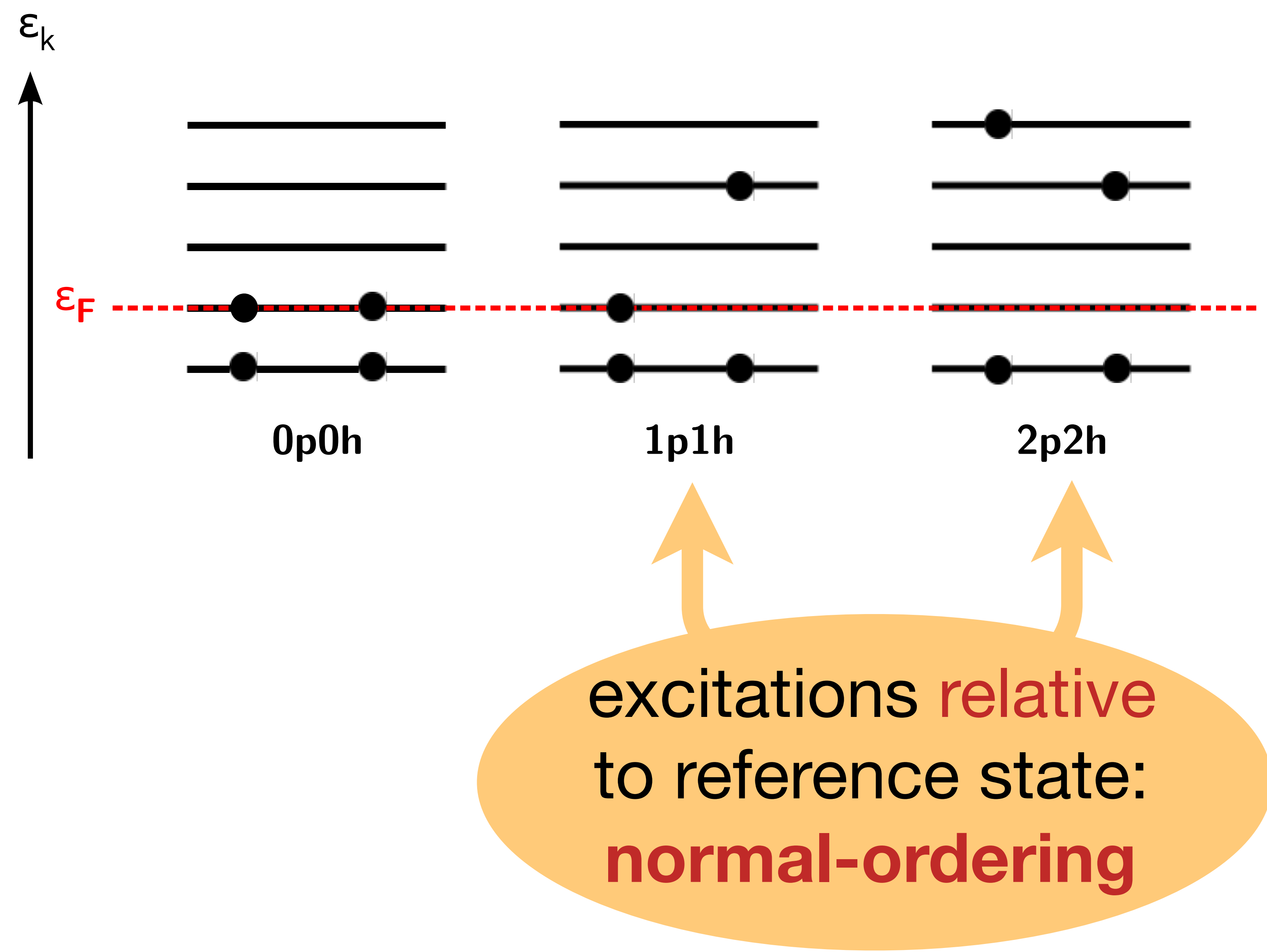
A (Brief) Introduction to the In-Medium SRG

H. H., in preparation

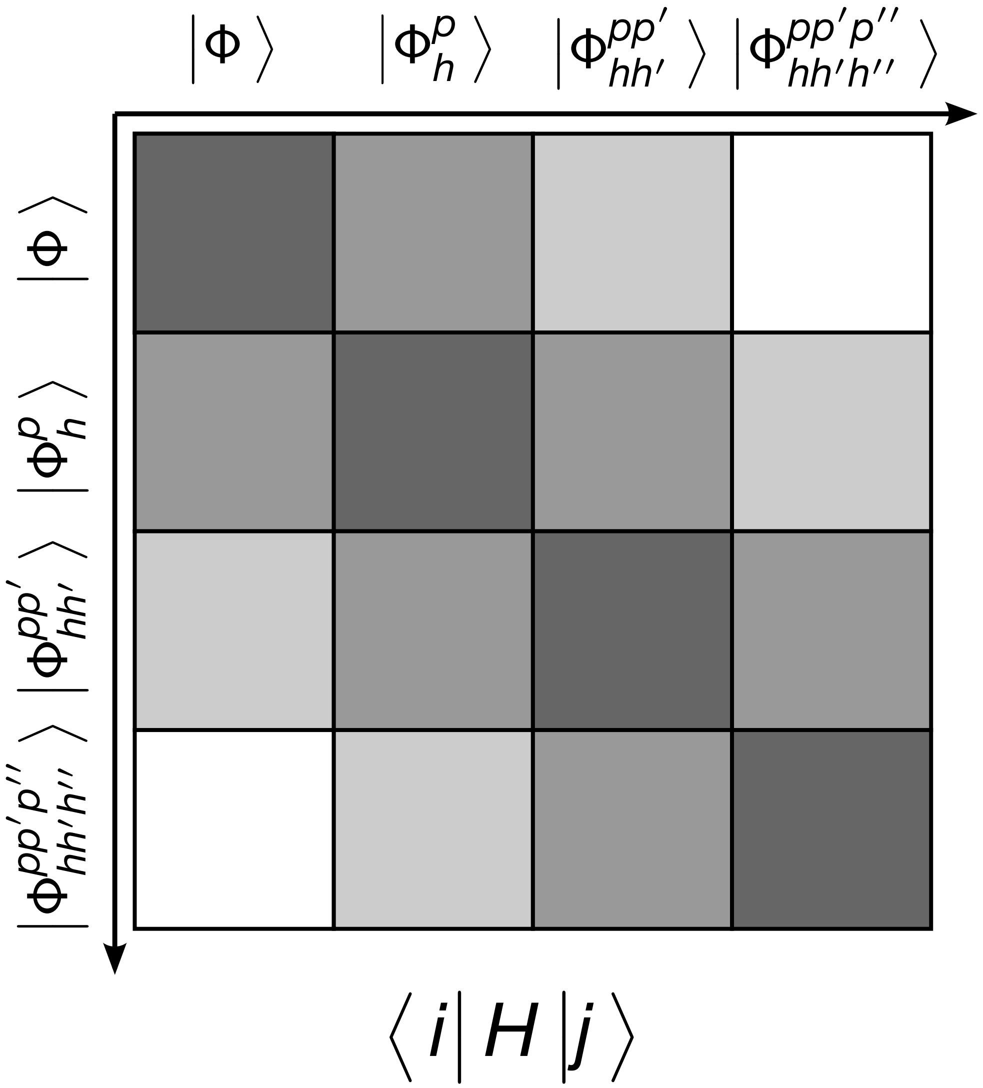
H. H., S. K. Bogner, T. D. Morris, A. Schwenk, and K. Tuskiyama, Phys. Rept. (2016) (doi:10.1016/j.physrep.2015.12.007, arXiv:1512.06956 [nucl-th])

Reference State





Single-Reference Case

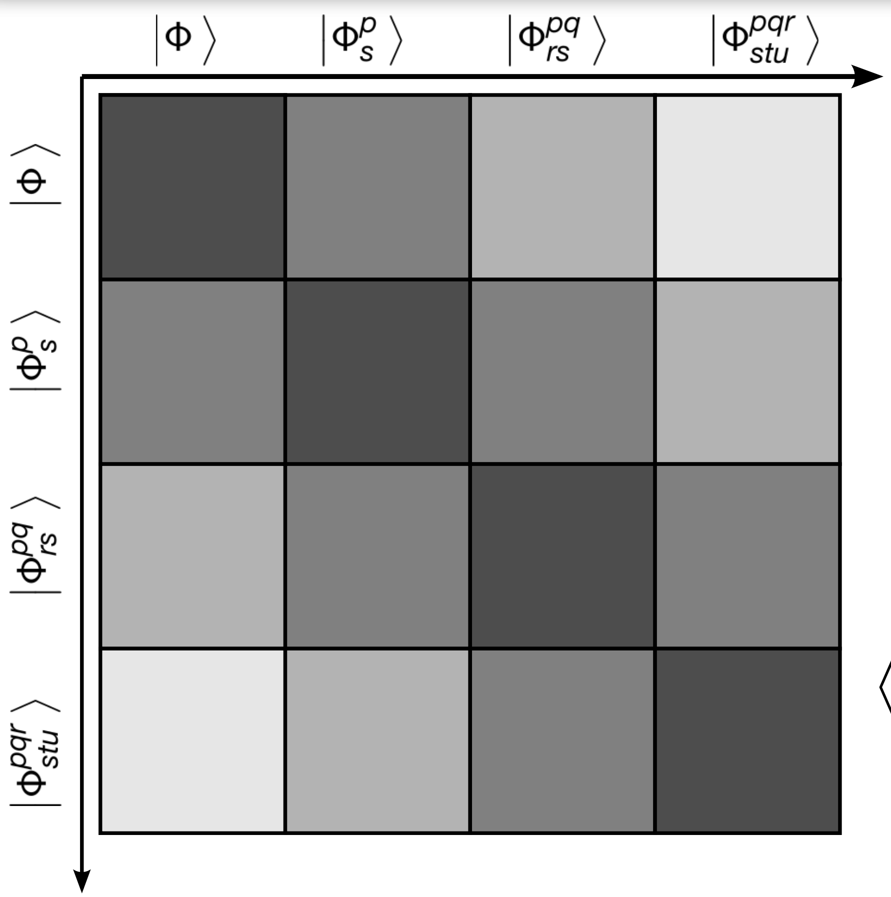


$$\langle {}^{p}_{h}|H|\Psi\rangle = \sum_{kl} f^{k}_{l} \langle\Psi| : A^{h}_{p} :: A^{k}_{l} : |\Psi\rangle = -n_h \bar{n}_p f^{p}_{h}$$

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

- reference state: **Slater determinant**
- normal-ordered operators **depend on occupation numbers (one-body density)**

Multi-Reference Case



$$\langle {}^{p}_{s} | H | \Phi \rangle \sim \bar{n}_p n_s f^p_s , \sum_{kl} f^k_l \lambda^{sk}_{pl} , \sum_{klmn} \Gamma^{kl}_{mn} \lambda^{skl}_{pmn} , \ldots$$

$$\langle {}^{pq}_{st} | H | \Phi \rangle \sim \bar{n}_p \bar{n}_q n_s n_t \Gamma^{pq}_{st} , \sum_{kl} \Gamma^{pk}_{sl} \lambda^{tk}_{ql} , \sum_{kl} f^k_l \lambda^{stk}_{pql} , \sum_{klmn} \Gamma^{kl}_{mn} \lambda^{stkl}_{pqmn} , \ldots$$

$$\langle {}^{pqr}_{stu} | H | \Phi \rangle \sim \ldots$$

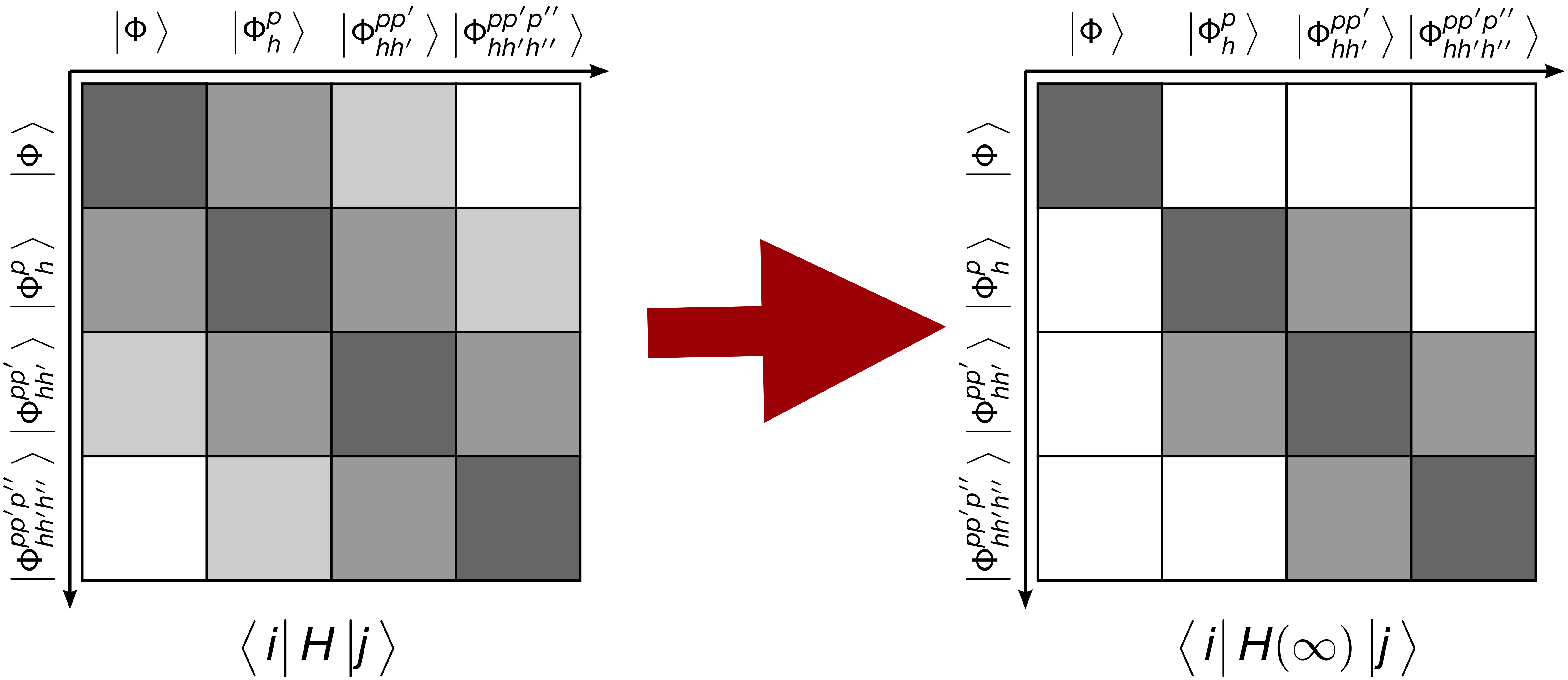
- reference state: **arbitrary**
- normal-ordered operators depend on up to **irreducible n-body density matrices** of the reference state

$$\rho^{kl}_{mn} = \lambda^{kl}_{mn} + \lambda^k_m \lambda^l_n - \lambda^k_n \lambda^l_m$$

$$\rho^{ijk}_{lmn} = \lambda^{ijk}_{lmn} + \lambda^i_l \lambda^{jk}_{mn} + \lambda^i_l \lambda^j_m \lambda^k_n + \text{permutations}$$

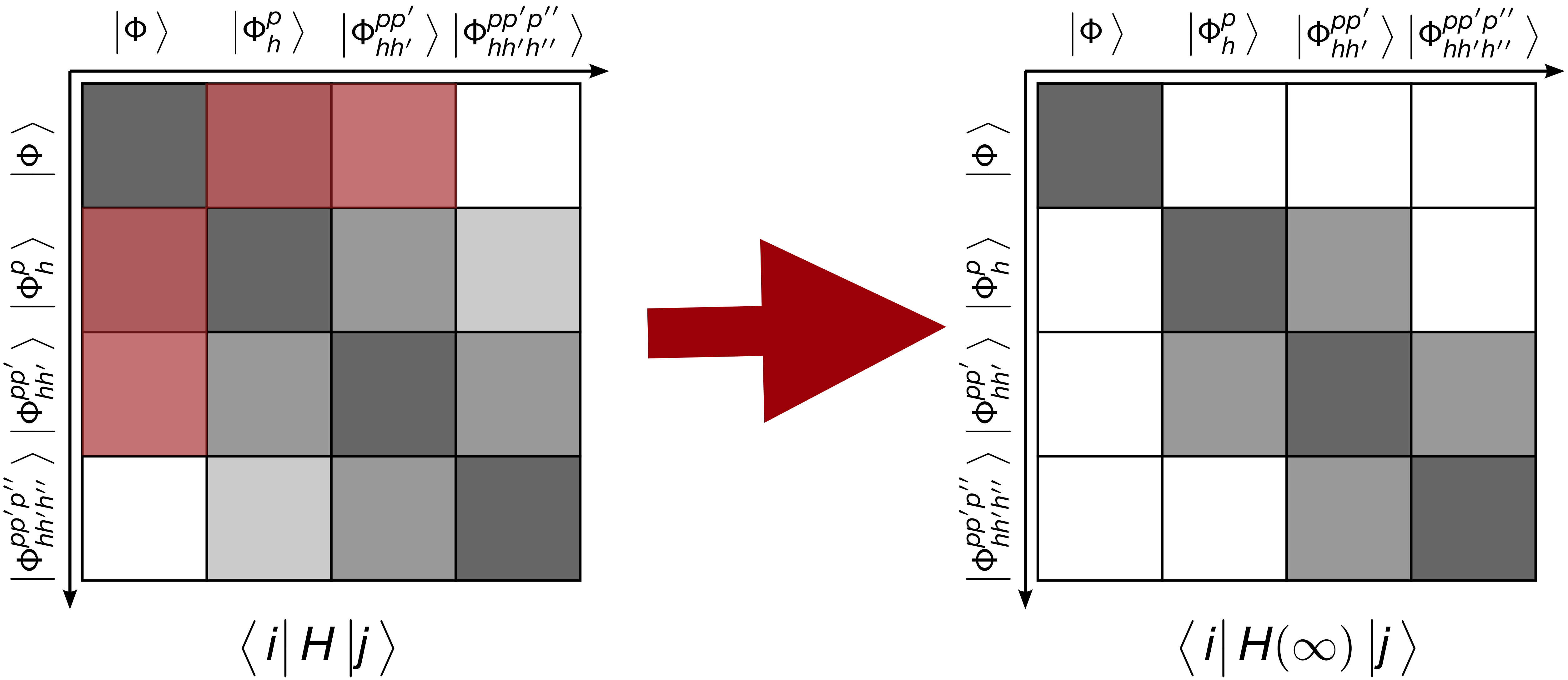
…

Decoupling in A-Body Space



aim: decouple reference state $|\Phi\rangle$ from excitations

Flow Equation



$$\frac{d}{ds}H(s) = \left[\eta(s), H(s)\right], \quad \text{e.g.,} \quad \eta(s) \equiv \left[H_d(s), H_{od}(s)\right]$$

Magnus Formulation of the In-Medium SRG

T. D. Morris, N. M. Parzuchowski, S. K. Bogner, in preparation

T. D. Morris, N. M. Parzuchowski, S. K. Bogner, PRC **92**, 034331 (2015)

W. Magnus, Comm. Pure and Appl. Math **VII**, 649-673 (1954)

Magnus Series Formulation

- explicit exponential ansatz for unitary transformation:

$$U(s) = \mathcal{S} \exp \int_0^s ds' \eta(s') \equiv \exp \Omega(s)$$

- flow equation for **Magnus** operator :

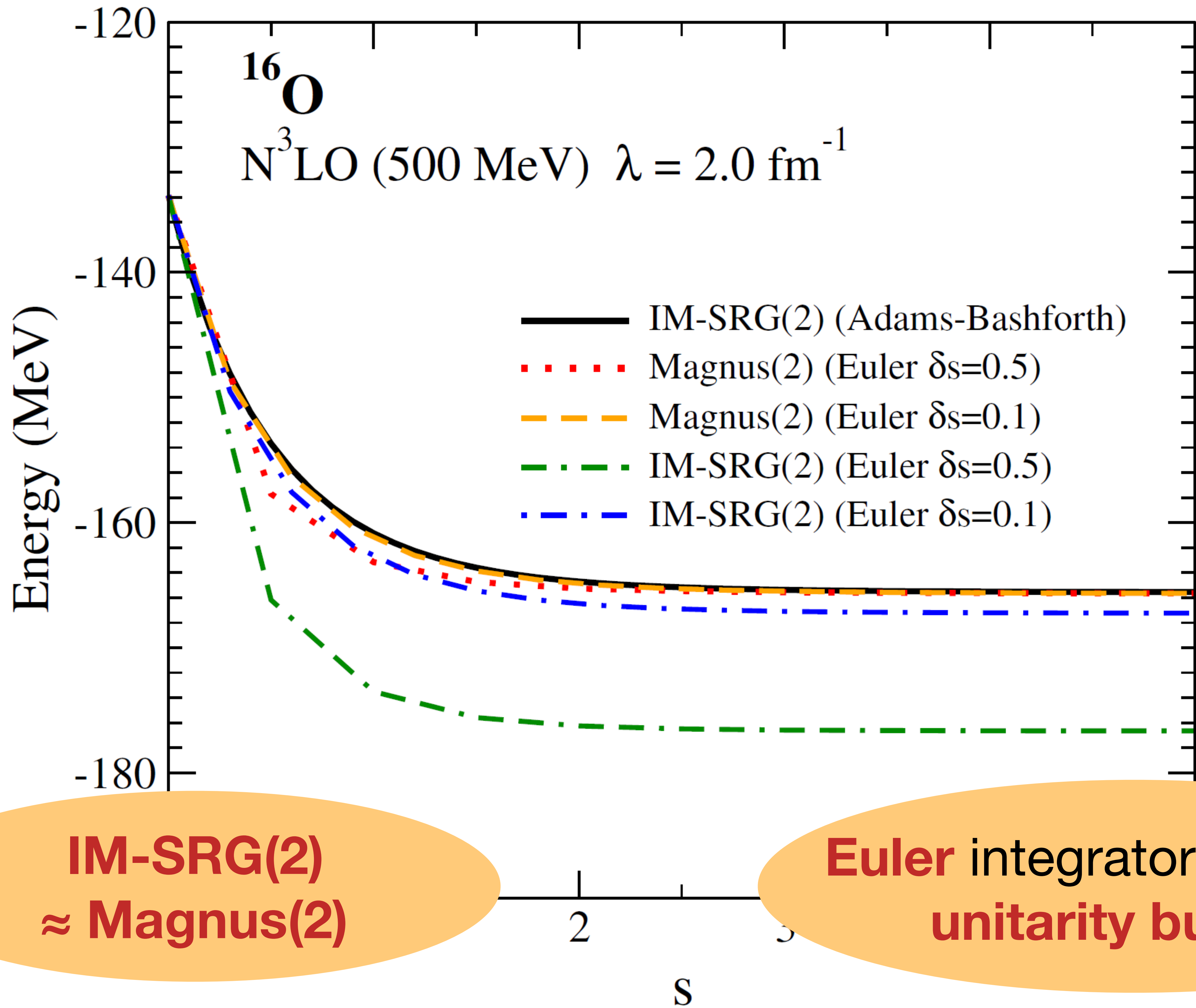
$$\frac{d}{ds}\Omega = \sum_{k=0}^{\infty} \frac{B_k}{k!} \mathrm{ad}_{\Omega}^{k}(\eta) \;, \quad \mathrm{ad}_{\Omega}(O) = [\Omega, O]$$

(B_k: Bernoulli numbers)

- construct $O(s) = U(s) O_0 U^{\dagger}(s)$ using Baker-Campbell-Hausdorff expansion (**Hamiltonian + effective operators**)

- truncate operators to **two-body level** (as in NO2B, IM-SRG(2))

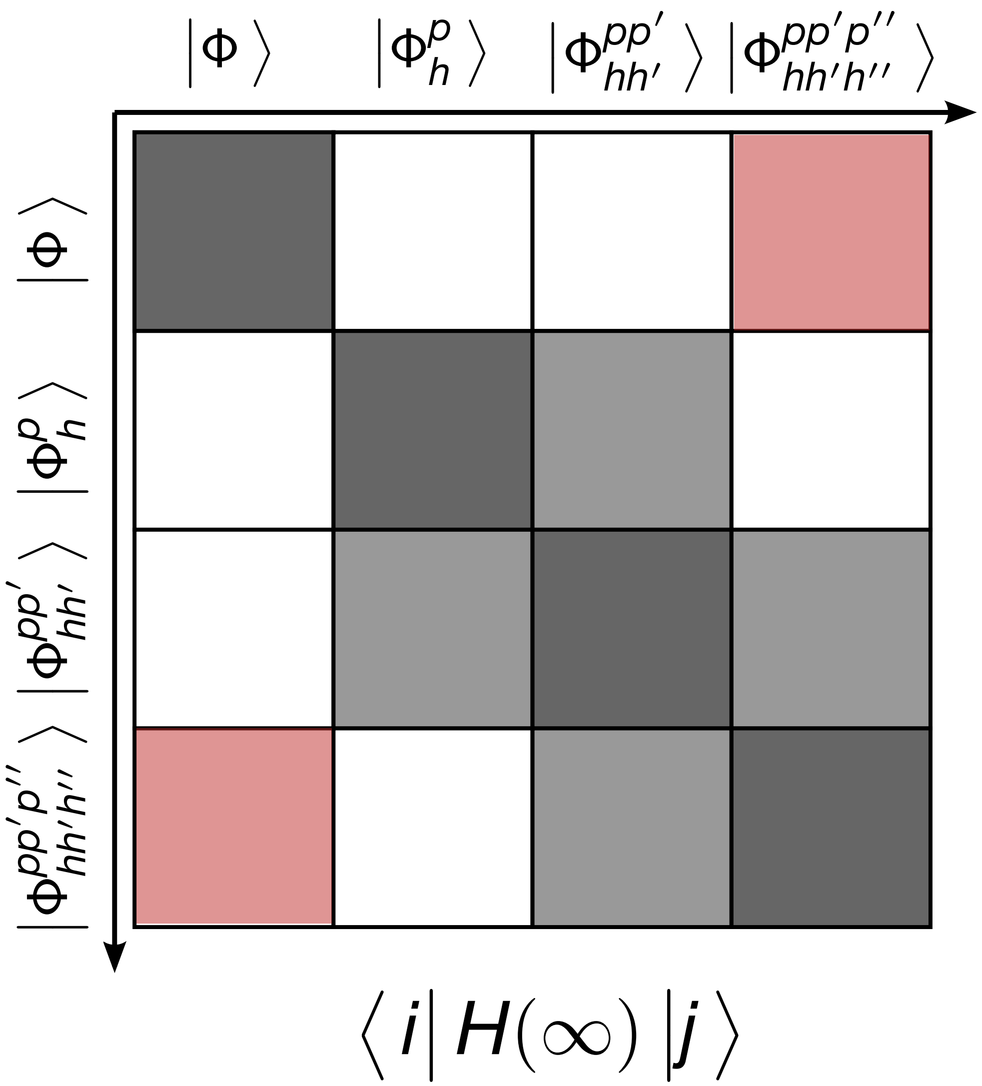
Magnus vs. Direct Integration



IM-SRG(2) ≈ Magnus(2)

Euler integrator sufficient, **unitarity built in!**

Approximate IM-SRG(3) / Magnus(3)



approximate **restoration of induced 3N terms**:

$$W(\infty) = \sum_{k=1}^{\infty} \frac{1}{k!} \mathrm{ad}_{\Omega}^{k}\left(H_0\right)_{3B}$$

$$\approx \left[\Omega, \widetilde{H}(\infty)\right]_{3B}$$

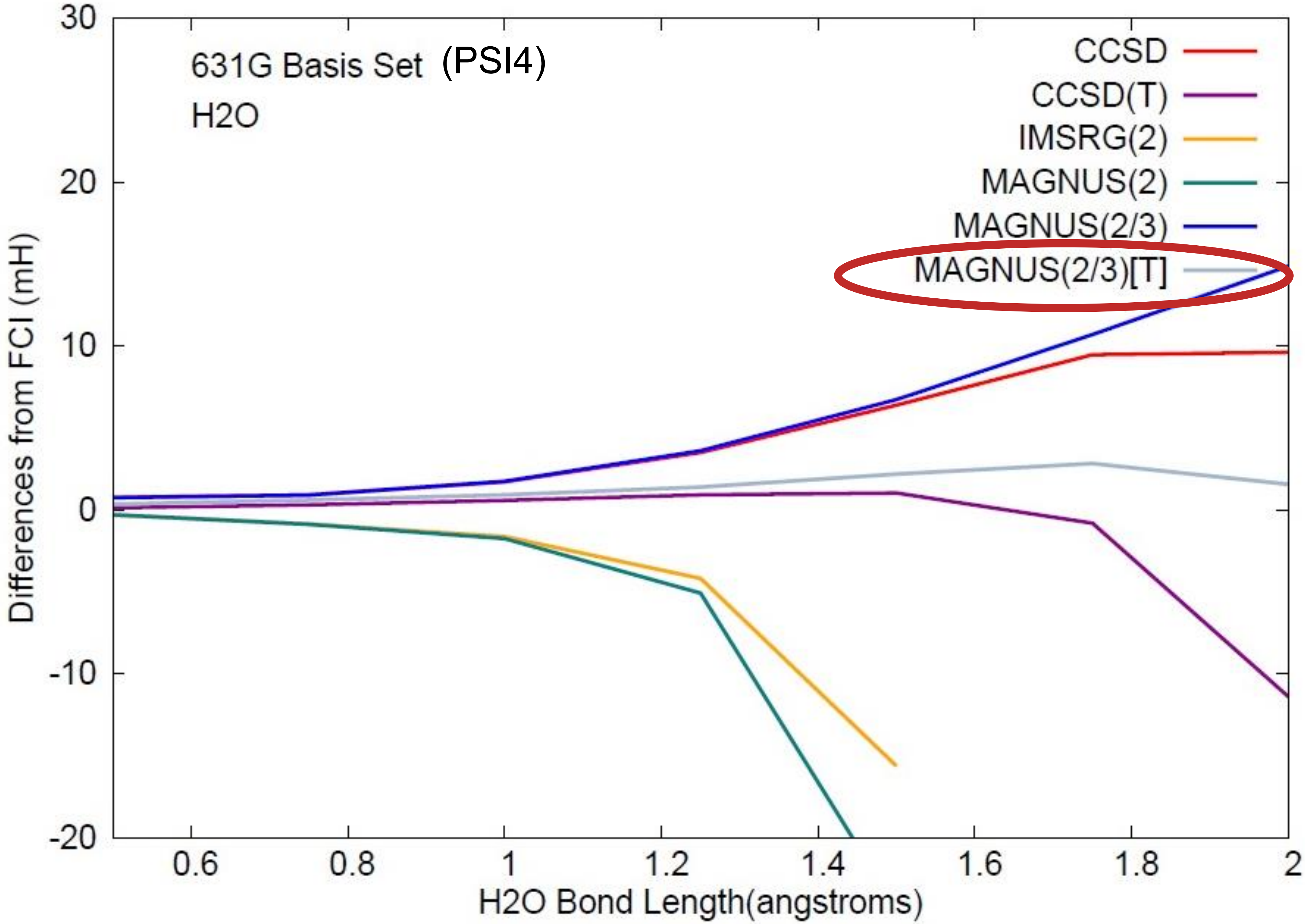
where

$$\widetilde{H}(\infty) = \sum_{k=1}^{\infty} \frac{1}{(k+1)!} \mathrm{ad}_{\Omega}^{k}\left(H_0\right)_{2B}$$

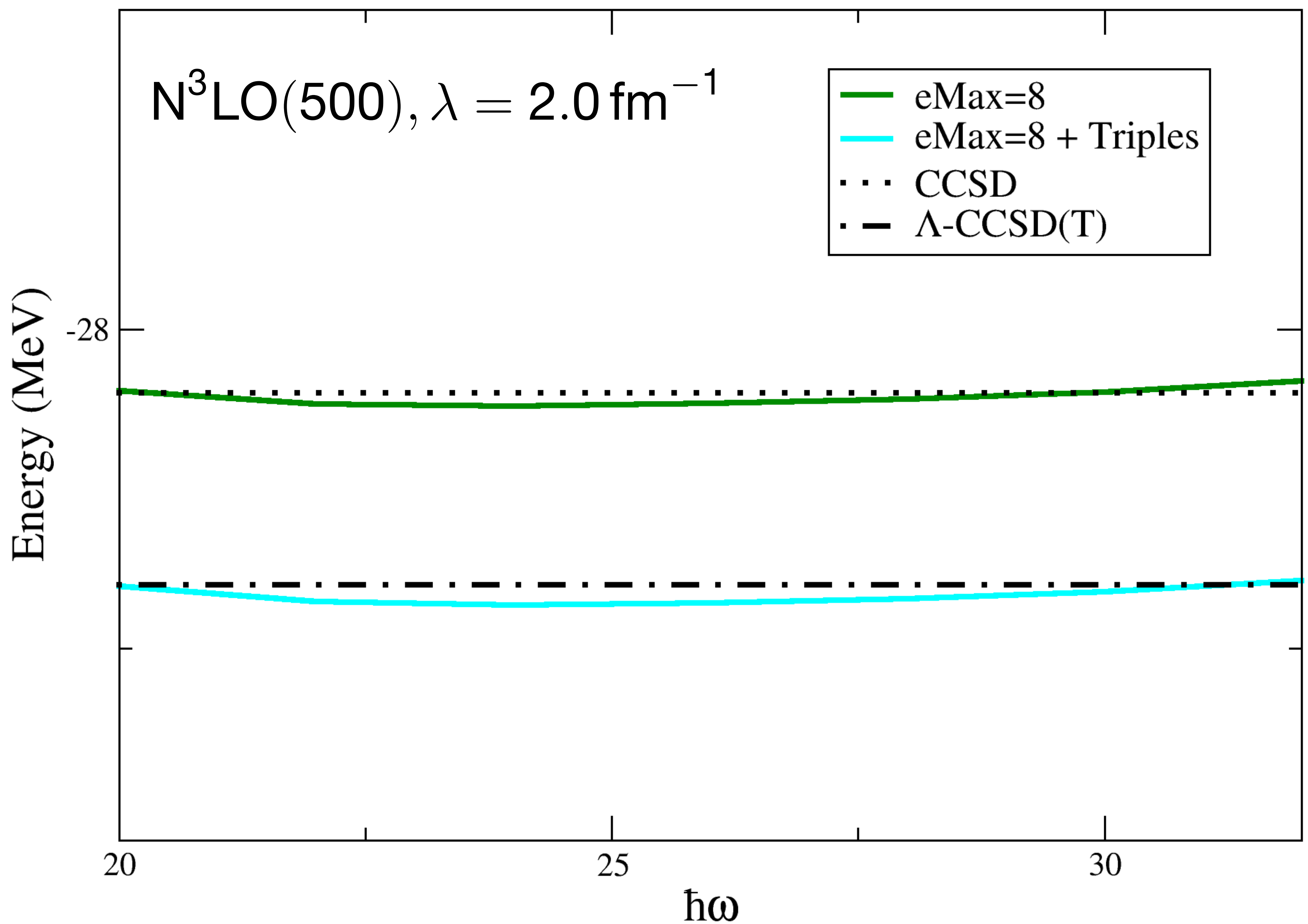
➡ **energy correction** (fully dressed ~ CR-CC(2,3)):

$$\Delta E = -\frac{1}{36} \sum_{p_1p_2p_3h_1h_2h_3} \frac{\left|W_{p_1p_2p_3h_1h_2h_3}(\infty)\right|^2}{\Delta_{p_1p_2p_3h_1h_2h_3}(\infty)}$$

Stretched Water



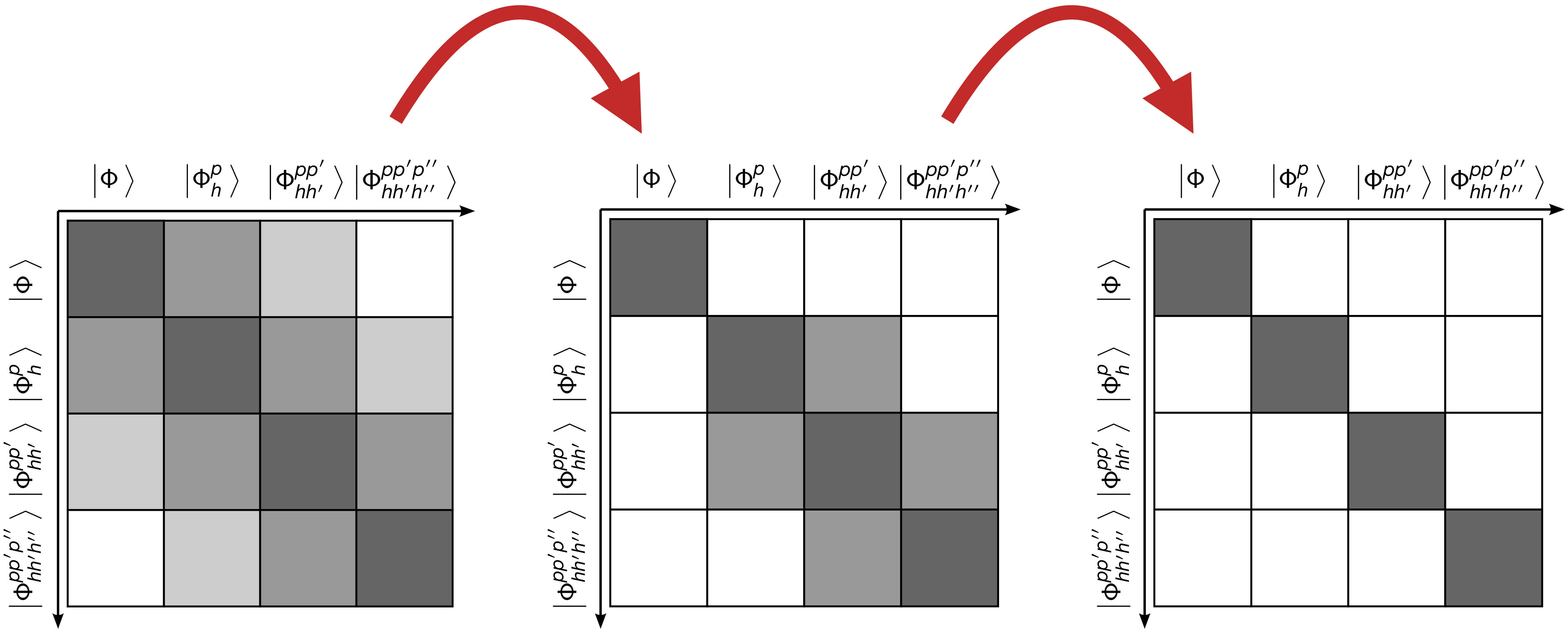
^{4}He Ground-State Energy



IM-SRG for Excited States

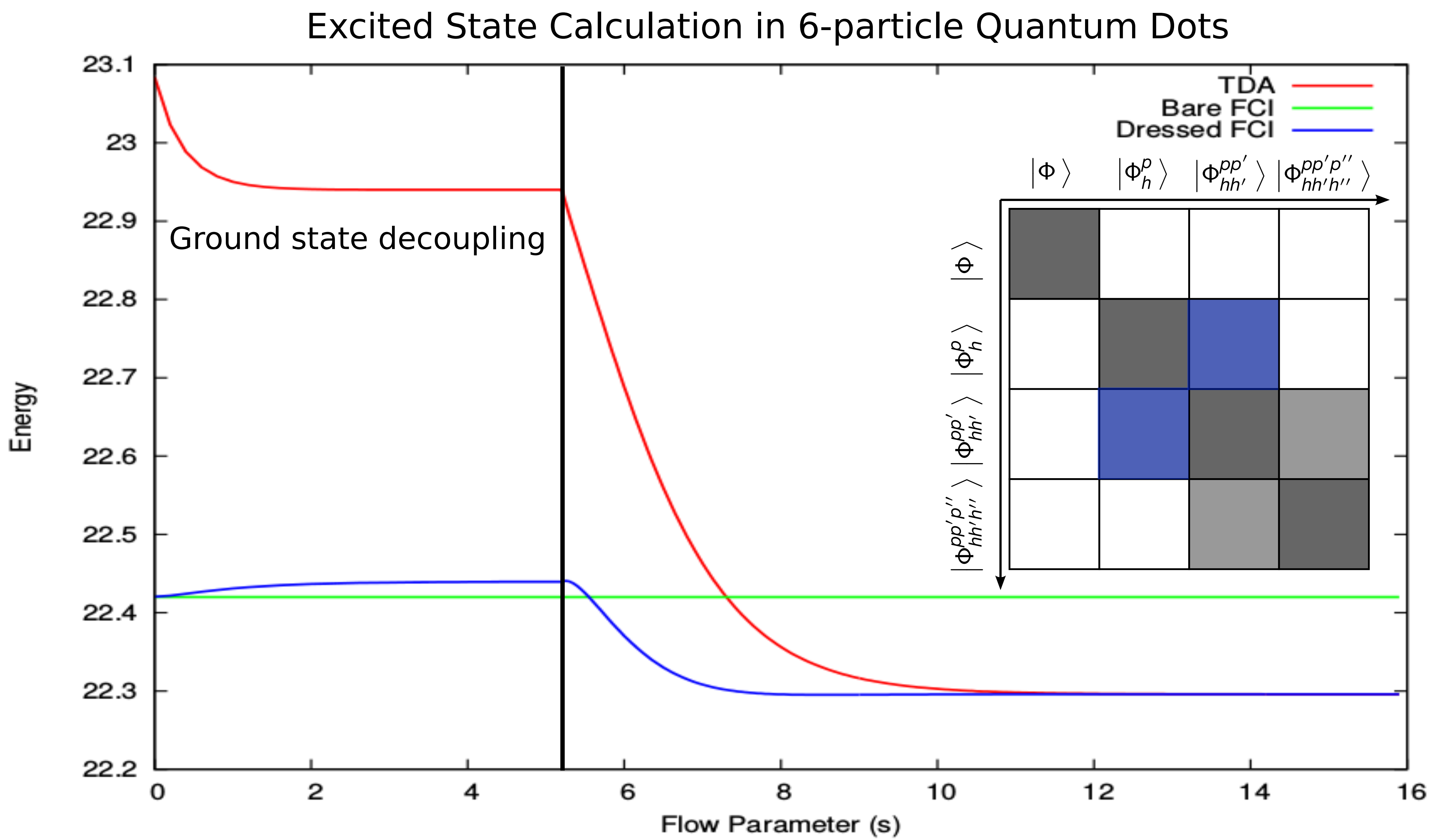
N. M. Parzuchowski, T. D. Morris, S. K. Bogner, in preparation

Excited State Decoupling



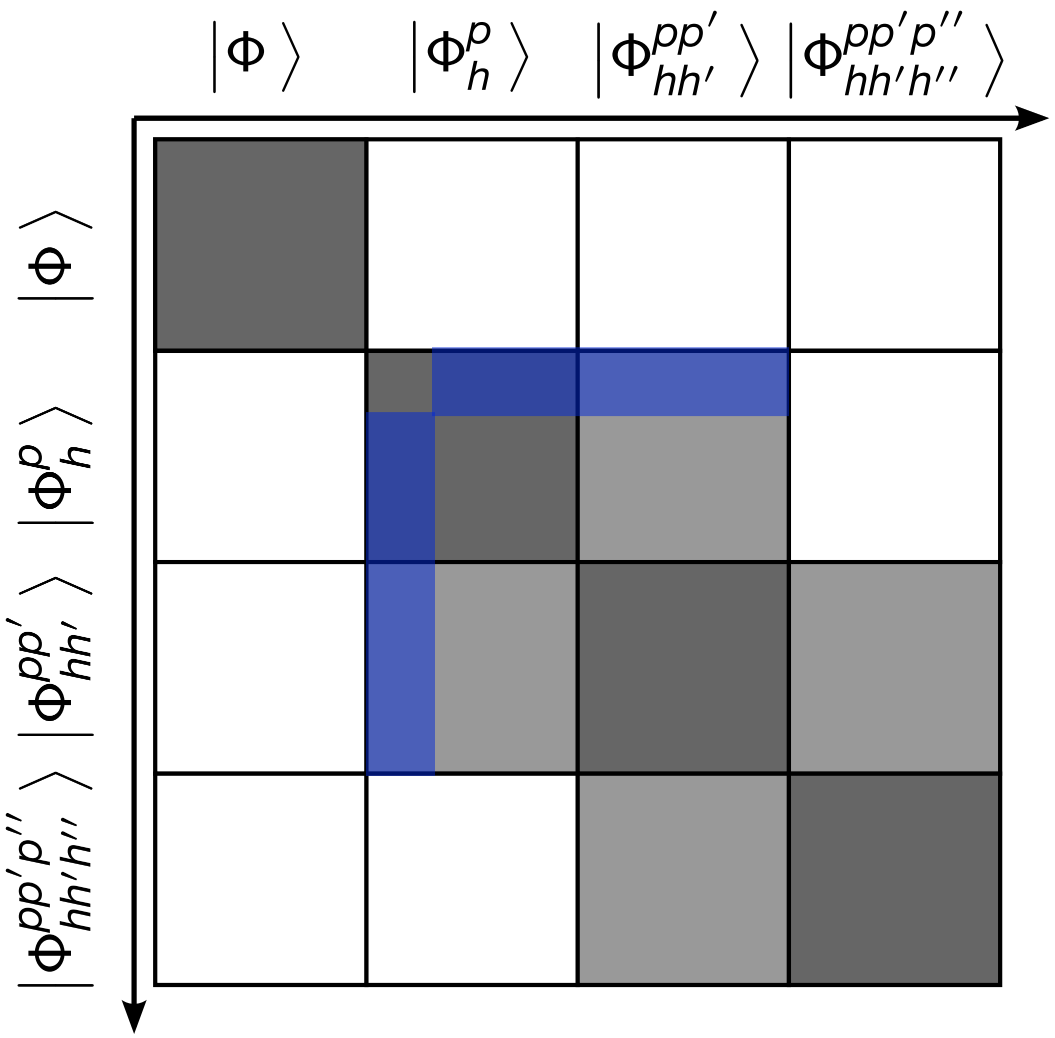
Can we decouple multiple states simultaneously?
Maybe entire blocks?

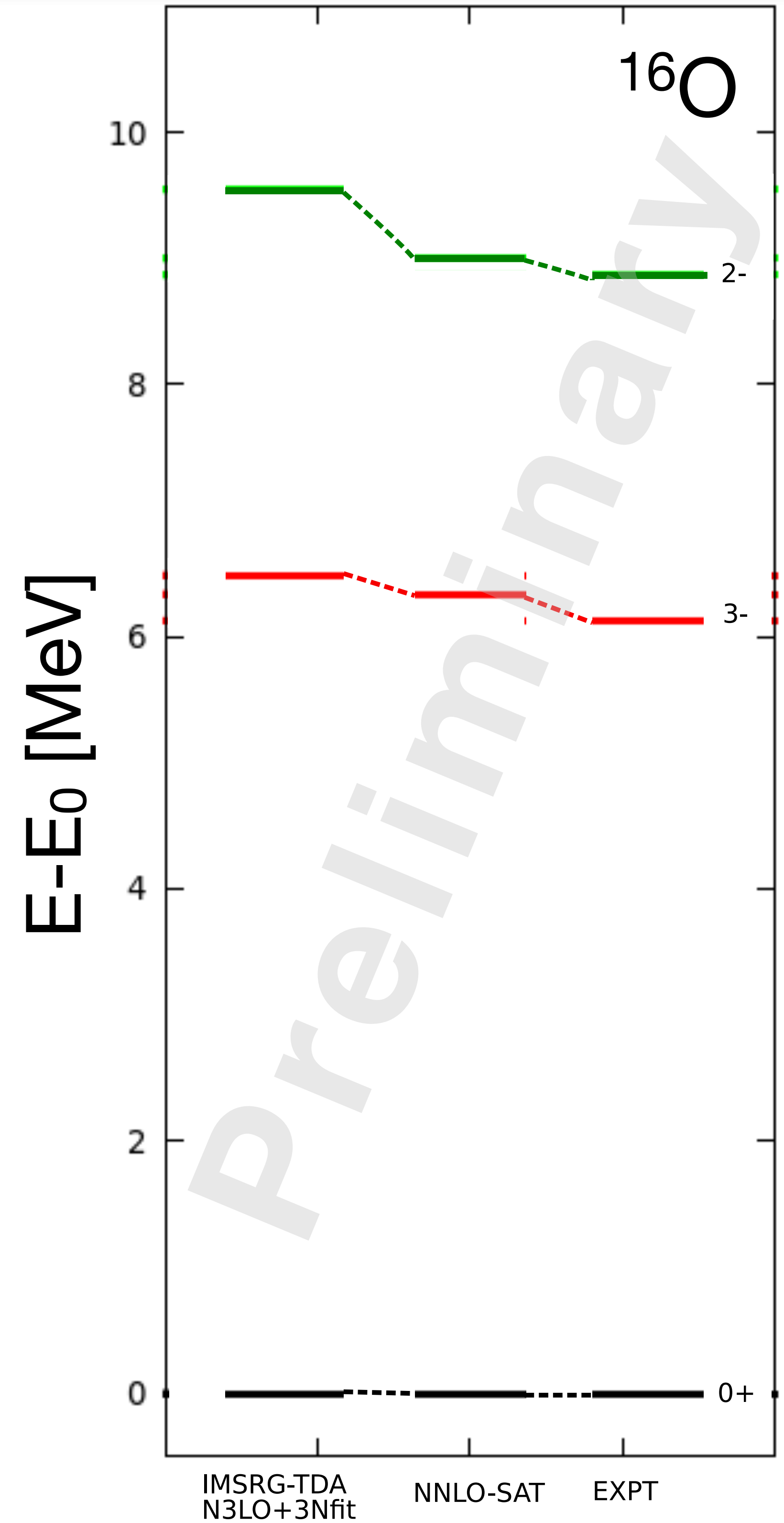
Quantum Dots



➡ **Multi-state decoupling can generate sizable induced forces…**

Sub-Block Decoupling





control induced forces by only **decoupling a 1p-1h ("valence") sub-block**

Equation-of-Motion Method

- describe "excited states" based on reference state:

$$\left|\Phi_k\right\rangle = Q_k^\dagger \left|\Phi_0\right\rangle$$

- **(MR-)IM-SRG effective Hamiltonian** in EOM approach:

$$\left[H(s), Q_k^\dagger(s)\right] = \omega_k(s) Q_k^\dagger(s), \quad \omega_k(s) = E_k(s) - E_0(s)$$

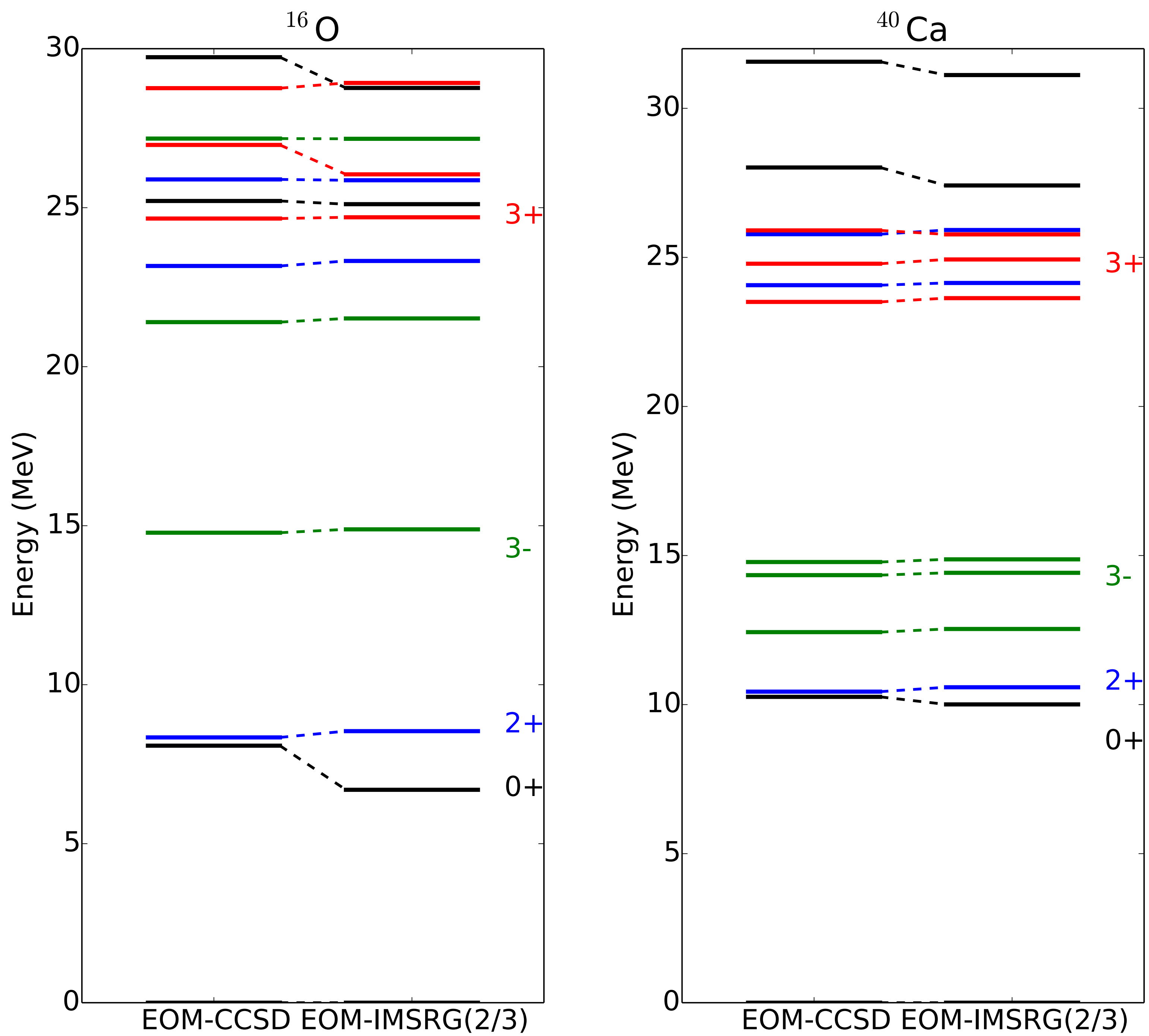
- ansatz for excitation operator (g.s. correlations built into Hamiltonian):

$$Q_k^\dagger(s) = \sum_{ph} q_h^p(s) :A_h^p: + \frac{1}{4} \sum_{pp'hh'} q_{hh'}^{pp'}(s) :A_{hh'}^{pp'}:$$

- **polynomial** effort vs. factorial scaling of Shell Model

- future: exploit multi-reference capabilities (commutator formulation identical to flow equations)

EoM Excitation Spectra



EOM-CCSD results courtesy of G. Hagen

New Applications of the MR-IM-SRG

Brillouin Generator

- consider unitary variations of the energy functional

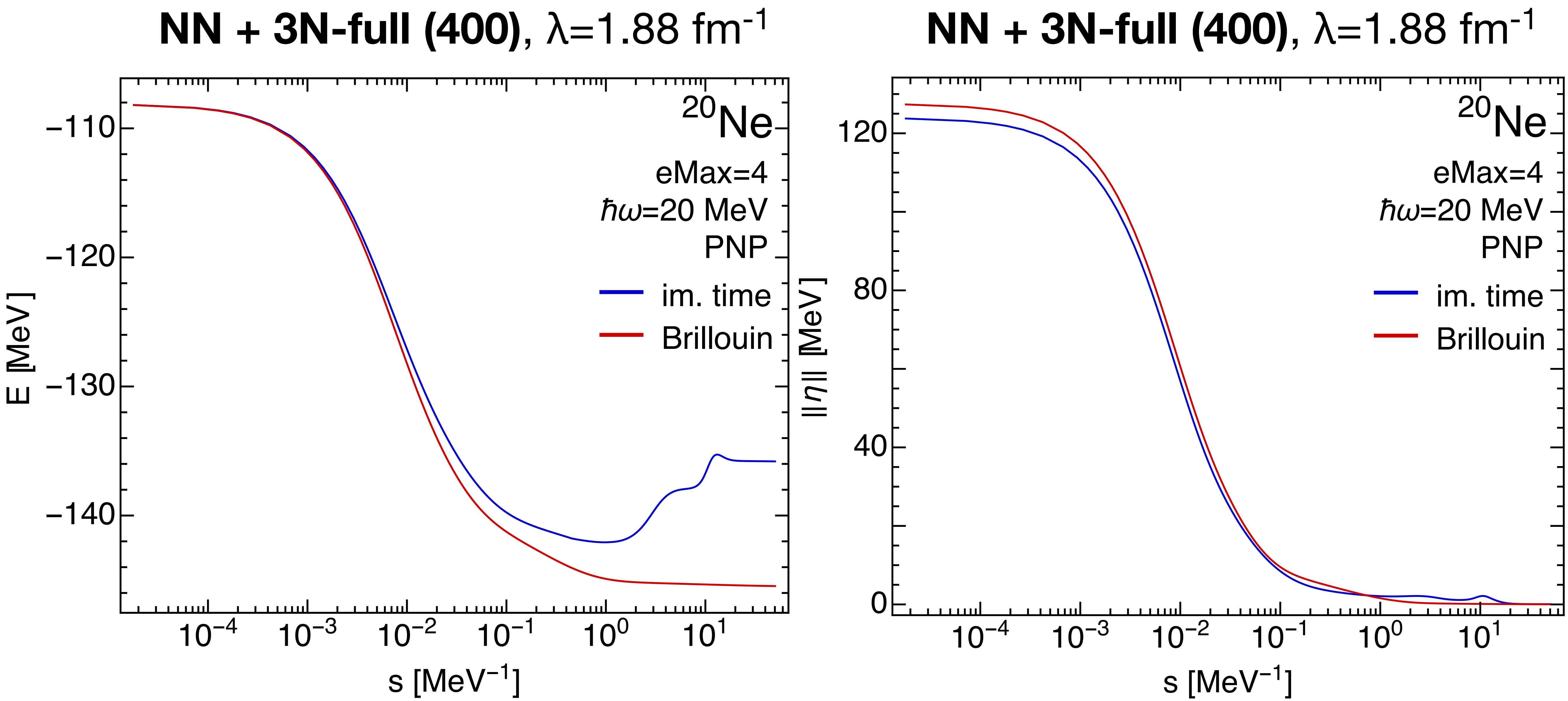
$$E(s) = \left\langle \Phi \right| H(s) \left| \Phi \right\rangle$$

- define generator as the residual of the irreducible Brillouin condition (= gradient of E)

$$\eta^p_r \equiv \left\langle \Phi \right| \left[:A^p_r:, H \right] \left| \Phi \right\rangle$$
$$\eta^{pq}_{rs} \equiv \left\langle \Phi \right| \left[:A^{pq}_{rs}:, H \right] \left| \Phi \right\rangle$$

- fixed point ($\eta = 0$) is reached when IBC is satisfied, energy stationary (cf. ACSE approach in Quantum Chemistry)
- Brillouin generator depends linearly on $\lambda^p_s, \lambda^{pq}_{st}, \lambda^{pqr}_{stu}$, higher irreducible density matrices are not required

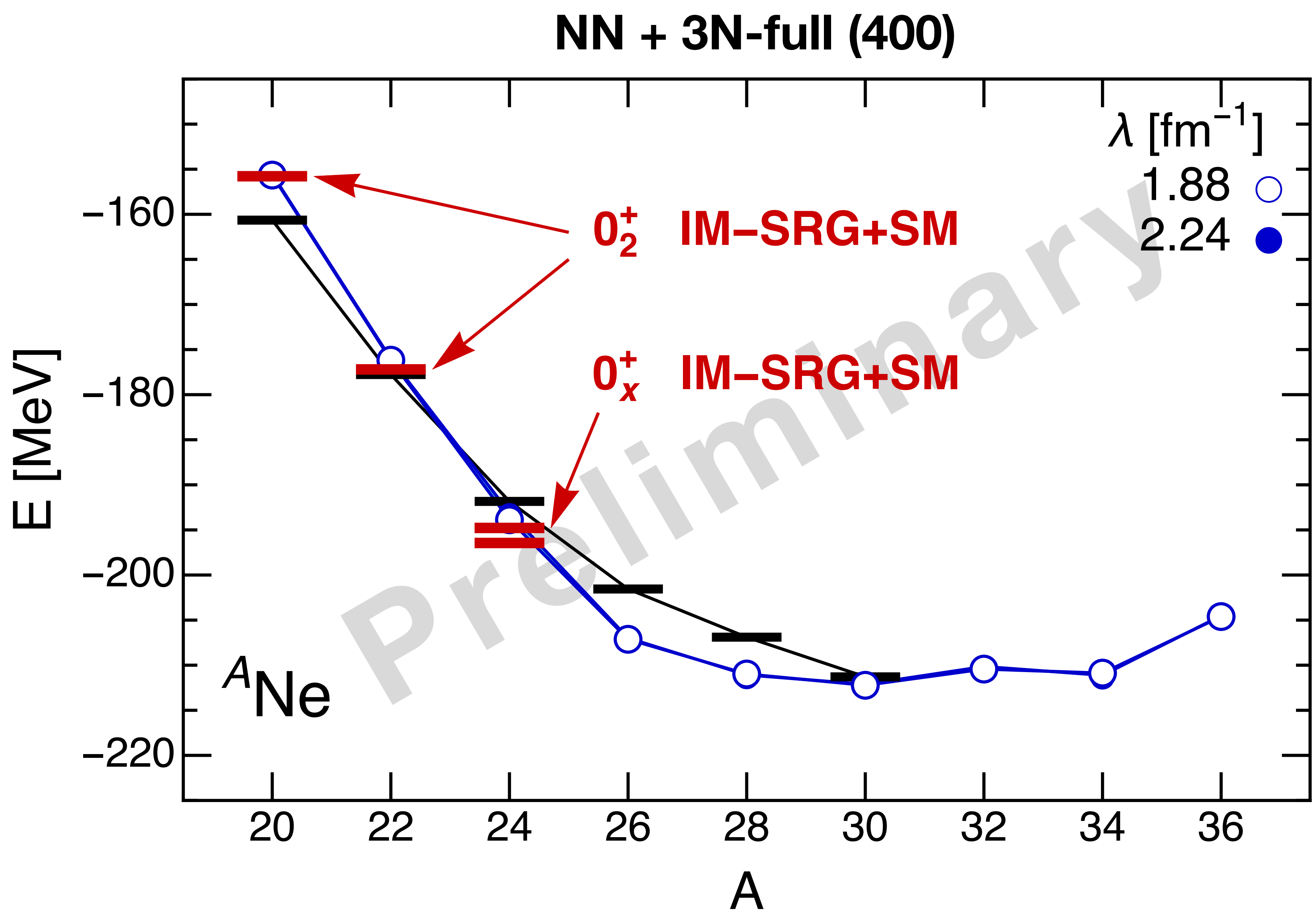
Brillouin Generator



➡ energy & norm of Brillouin generator decay monotonically

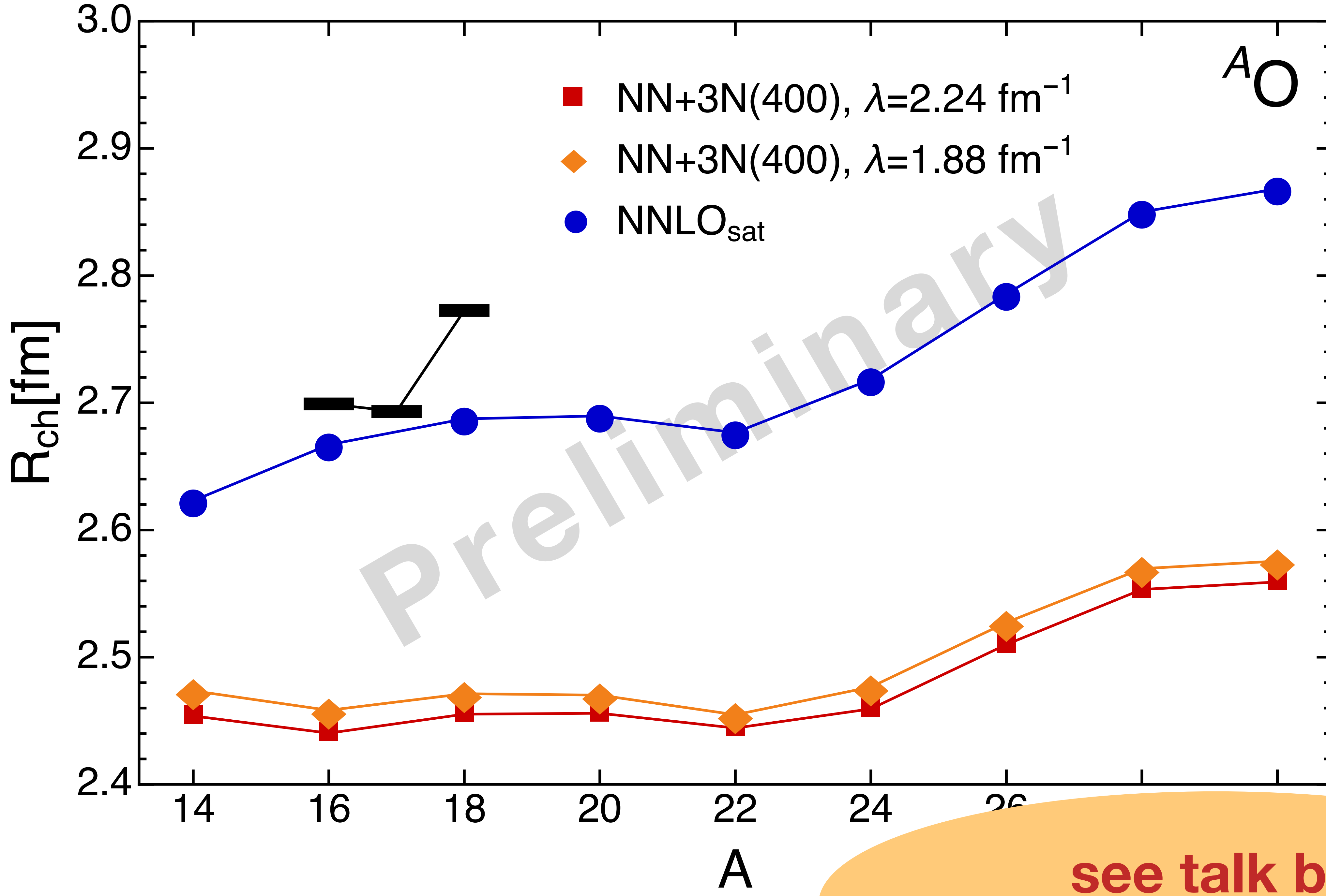
➡ Projected HFB: 3B density matrix is (quasi-)diagonal ($O(N^3)$ storage), can be fully included in generator and energy flow

Neon Isotopes



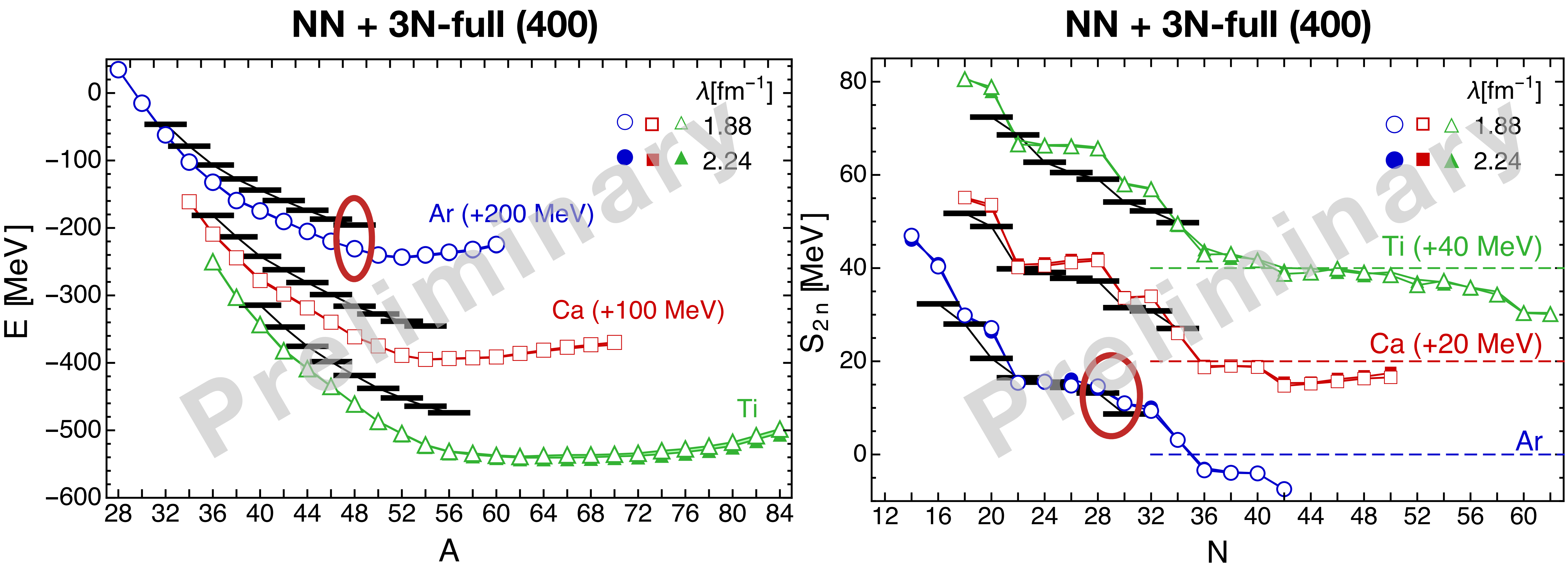
➡ MR-IM-SRG selects excited 0^+ state with spherical intrinsic structure (symmetry constrained)

Oxygen Radii



see talk by V. Somà

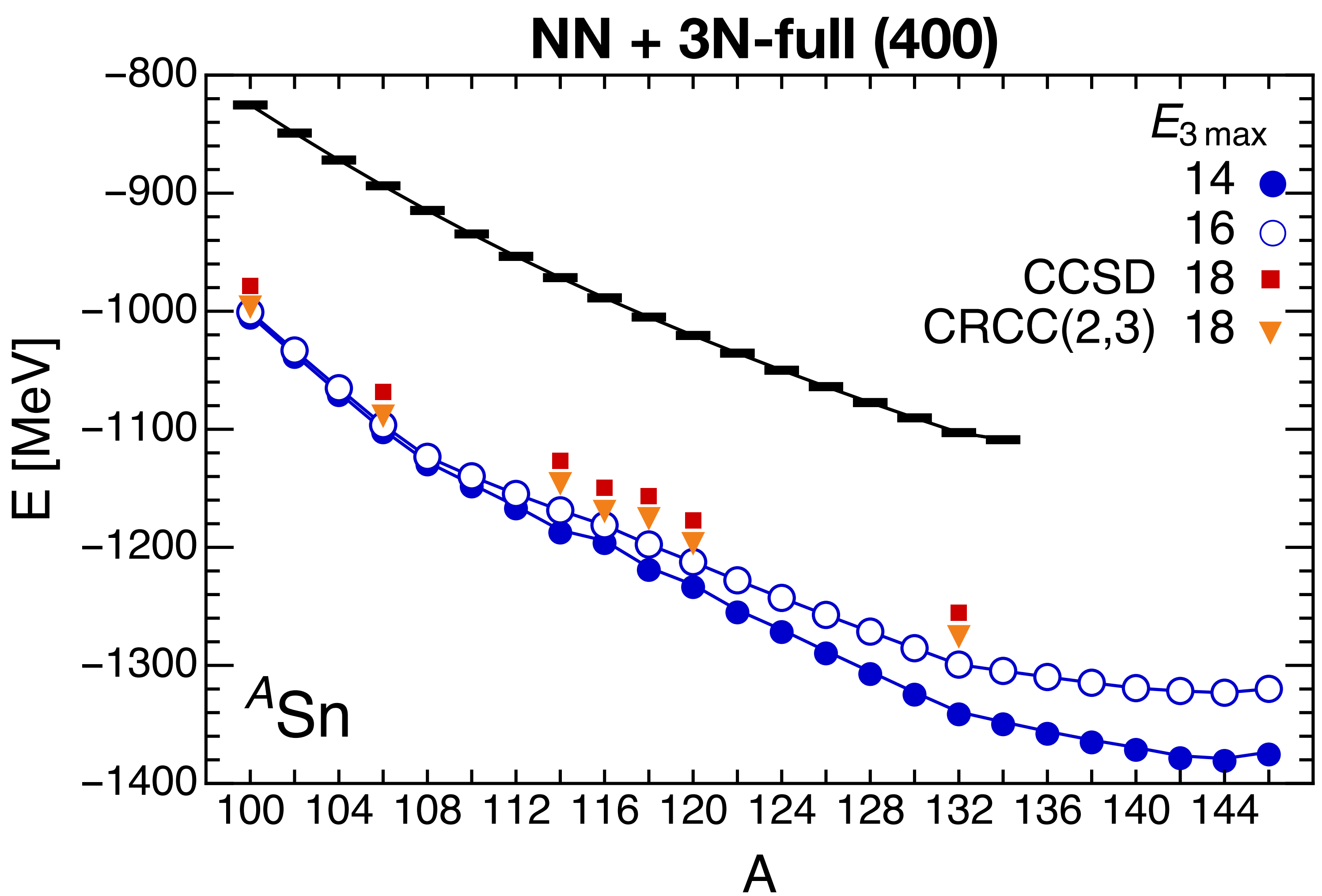
Isotopic Chains Around Ca



- S_{2n} consistent with Gor'kov GF, (weak) shell closure predicted in ^{46}Ar
  (Soma et al., PRC 89, 061301(R), 2014)

- ^{48,49}Ar masses measured at NSCL, ^{46}Ar shell closure confirmed
  (Meisel et al., PRL 114, 022501, 2015)

The Frontier: Tin



E_{3max}	memory (float) [GB]
14	5
16	~20
18	100+

- systematics of overbinding in accordance with Ca/Ni region
- not converged with respect to 3N matrix element truncation:

$$e_1 + e_2 + e_3 \leq E_{3max}$$

($e_{1,2,3}$: SHO energy quantum numbers)

- need technical improvements to go further

Epilogue

Work in Progress…

- Magnus expansion for MR-IM-SRG (incl. approximate MR-IM-SRG(3))
- **effective operators and currents** (eventually with evolution to consistent resolution scale)
- exploration of new chiral NN + 3N Hamiltonians (NNLO$_{sat}$, EKM N^{3}LO, …)
- (Multi-Reference) Equation-of-Motion methods as an alternative to Shell Model (or CI)
- new types of reference states: NCSM, Generator Coordinate Method, …
- inclusion of continuum effects

Acknowledgments

S. K. Bogner, M. Hjorth-Jensen, T. D. Morris, N. M. Parzuchowski, F. Yuan
NSCL, Michigan State University

E. Gebrerufael, K. Hebeler, R. Roth, A. Schwenk, J. Simonis, C. Stumpf, K. Vobig, K. Wendt
TU Darmstadt, Germany

A. Calci, J. D. Holt, S. R. Stroberg
TRIUMF, Canada

S. Binder
UT Knoxville & Oak Ridge National Laboratory

G. Papadimitriou
Lawrence Livermore National Laboratory

R. J. Furnstahl, S. König, S. More
The Ohio State University

P. Papakonstantinou
IBS / Rare Isotope Science Project, South Korea

T. Duguet, V. Somà
CEA Saclay, France

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More IM-SRG…

- **Applications to Medium-Mass Nuclei:**
  K. Vobig, Wednesday, 11:00
- **Excited States with IM-SRG Evolved Hamiltonians:**
  R. Trippel, Wednesday, 11:10
- **Merging NSCM and MR-IM-SRG:**
  E. Gebrerufael, Wednesday, 11:30
- **Non-Empirical Shell Model Interactions and Operators:**
  R. Stroberg, Friday, 9:30

Supplements

Similarity Renormalization Group

Basic Concept

continuous unitary transformation of the Hamiltonian to band-diagonal form w.r.t. a given "uncorrelated" many-body basis

- flow equation for Hamiltonian $H(s) = U(s)HU^\dagger(s)$:

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

- choose $\eta(s)$ to achieve desired behavior, e.g.,

$$\eta(s) = \left[H_d(s), H_{od}(s)\right]$$

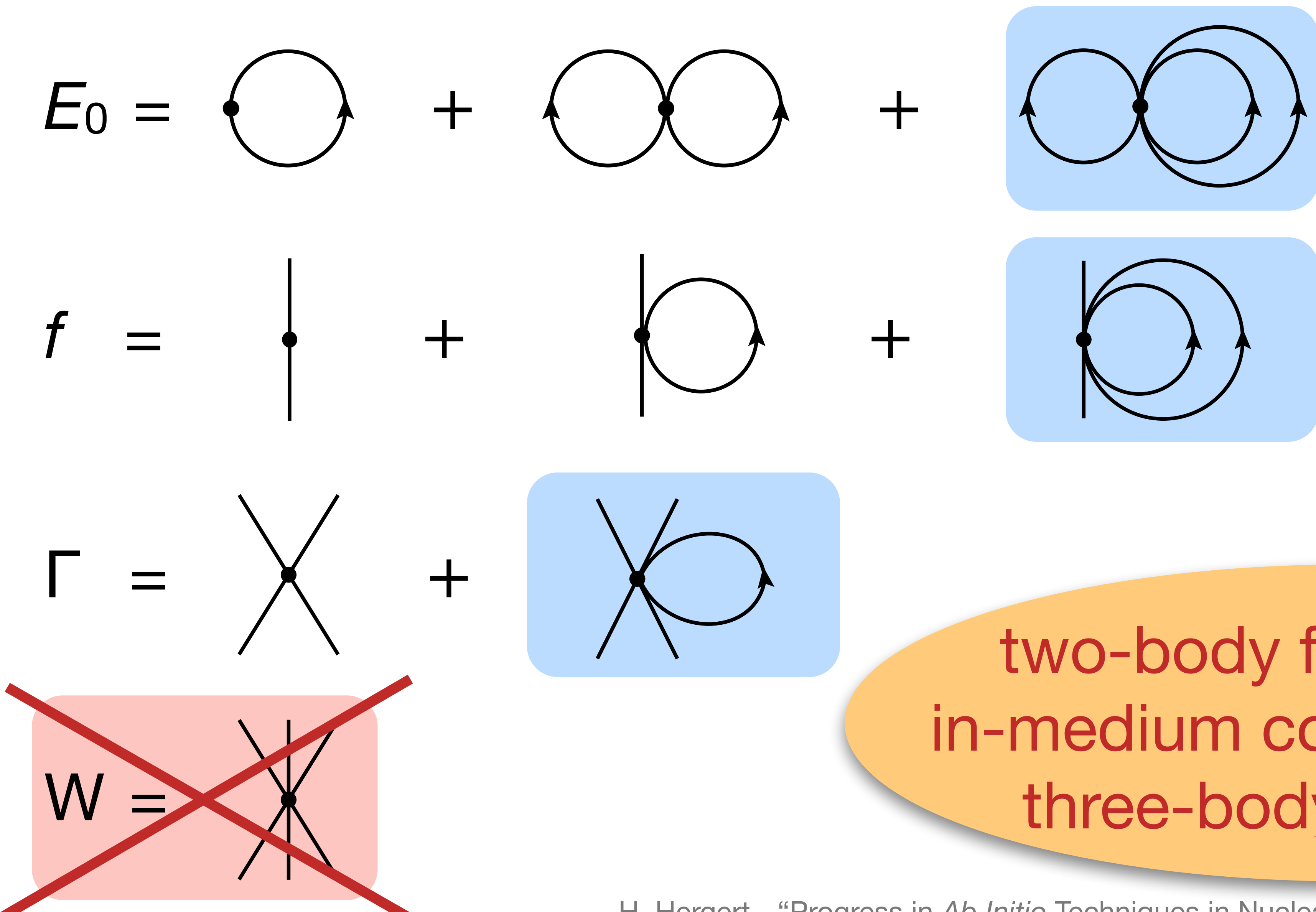
to suppress (suitably defined) off-diagonal Hamiltonian

- consistent evolution for all observables of interest

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

- 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:

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

- define normal-ordered operators recursively:

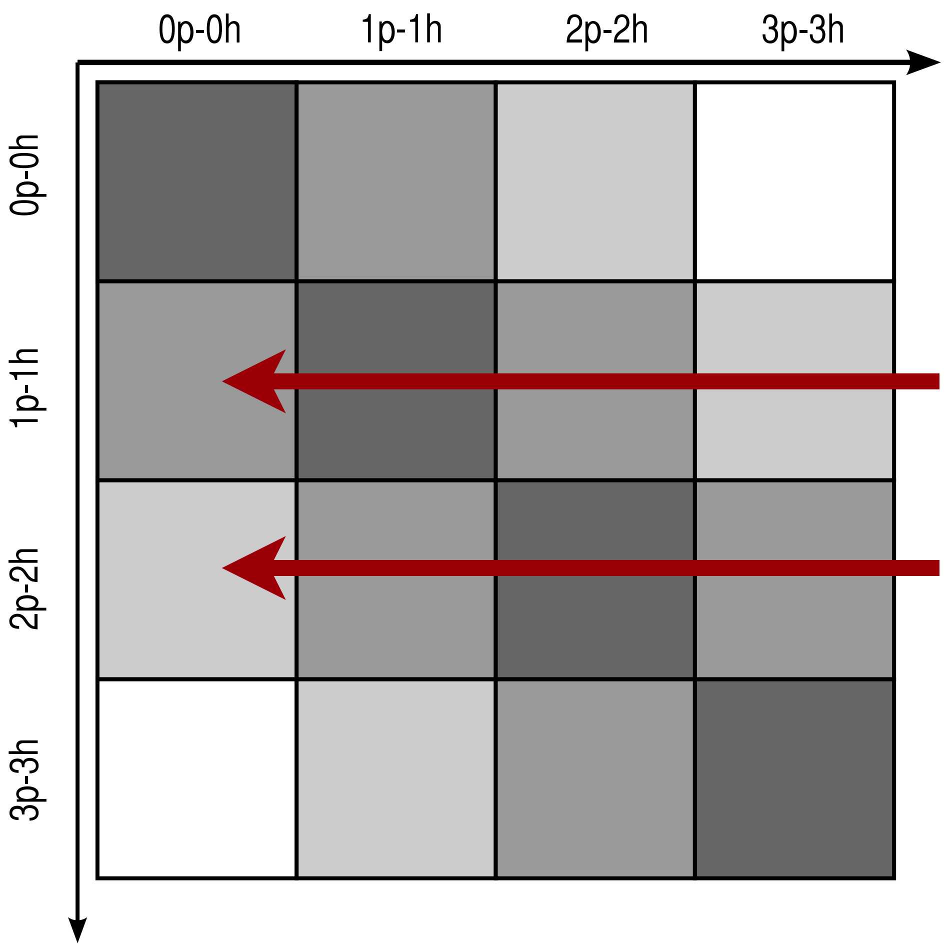
$$A^{k_1\dots k_N}_{l_1\dots l_N} = :A^{k_1\dots k_N}_{l_1\dots l_N}: + \lambda^{k_1}_{l_1} :A^{k_2\dots k_N}_{l_2\dots l_N}: + \text{singles}$$
$$+ \left(\lambda^{k_1}_{l_1}\lambda^{k_2}_{l_2} - \lambda^{k_1}_{l_2}\lambda^{k_2}_{l_1}\right) :A^{k_3\dots k_N}_{l_3\dots l_N}: + \text{doubles} + \dots$$

- algebra is simplified significantly because

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

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

Decoupling in A-Body Space



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

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

- define off-diagonal Hamiltonian (suppressed by IM-SRG flow):

$$H_{od} \equiv f_{od} + \Gamma_{od}, \quad f_{od} \equiv \sum_{ph} f^{p}_{h} :A^{p}_{h}: + \text{H.c.}, \quad \Gamma_{od} \equiv \frac{1}{4} \sum_{pp'hh'} \Gamma^{pp'}_{hh'} :A^{pp'}_{hh'}: + \text{H.c.}$$

➡ construct generator

Choice of Generator

- Wegner: $\eta^{I} = \left[H_d, H_{od}\right]$
- White: (J. Chem. Phys. 117, 7472)

$$\eta^{II} = \sum_{ph} \frac{f^p_h}{\Delta^p_h} :A^p_h: + \frac{1}{4} \sum_{pp'hh'} \frac{\Gamma^{pp'}_{hh'}}{\Delta^{pp'}_{hh'}} :A^{pp'}_{hh'}: - \text{H.c.}$$

$\Delta^p_h, \Delta^{pp'}_{hh'}$: approx. 1p1h, 2p2h excitation energies

- "imaginary time": (Morris, Bogner)

$$\eta^{III} = \sum_{ph} \text{sgn}\left(\Delta^p_h\right) f^p_h :A^p_h: + \frac{1}{4} \sum_{pp'hh'} \text{sgn}\left(\Delta^{pp'}_{hh'}\right) \Gamma^{pp'}_{hh'} :A^{pp'}_{hh'}: - \text{H.c.}$$

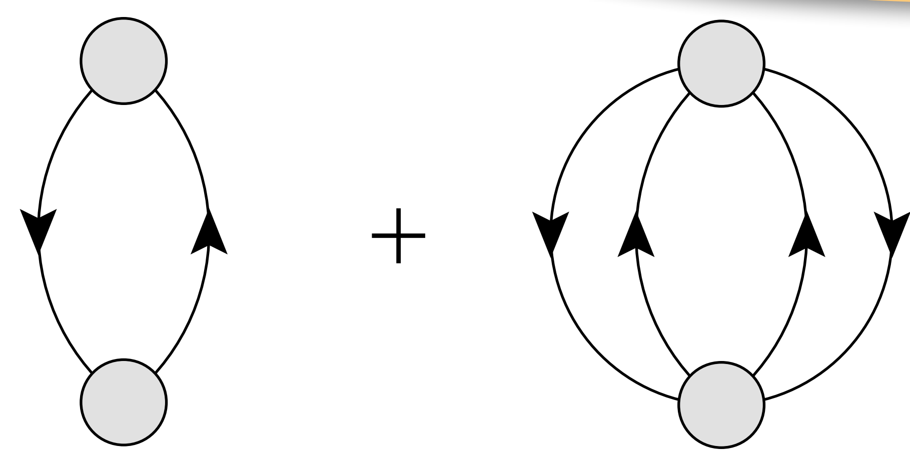
- off-diagonal matrix elements are suppressed like $e^{-\Delta^2 s}$ (Wegner), e^{-s} (White), and $e^{-|\Delta| s}$ (imaginary time)
- g.s. energies ($s \to \infty$) differ by $\ll 1\%$

IM-SRG(2) Flow Equations

0-body Flow

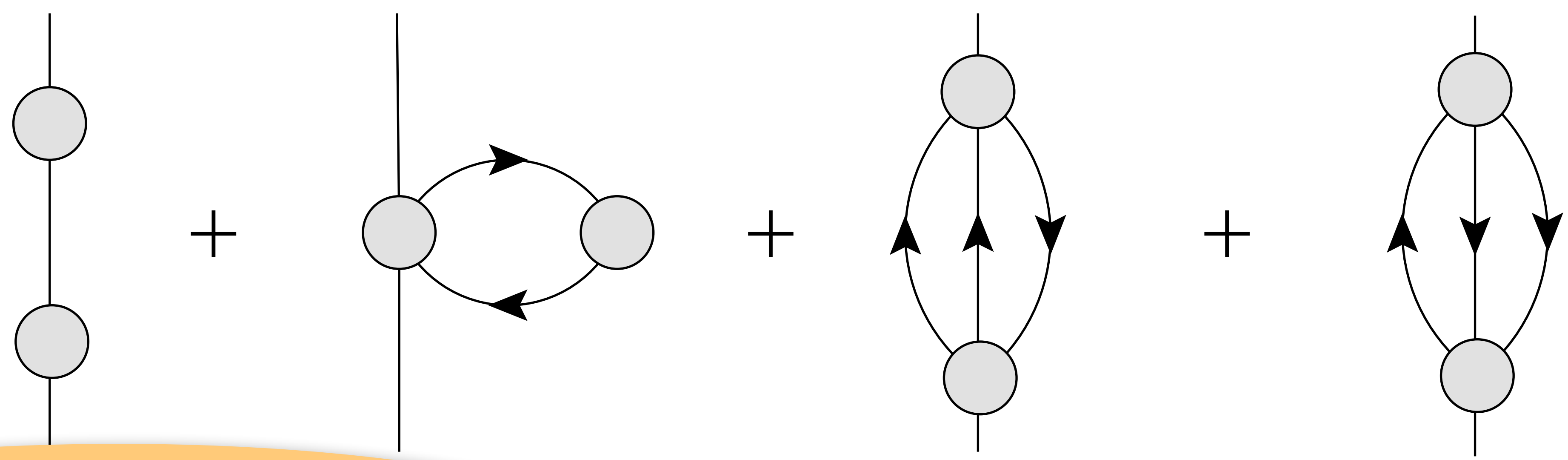
~ 2nd order MBPT for *H(s)*

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



1-body Flow

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

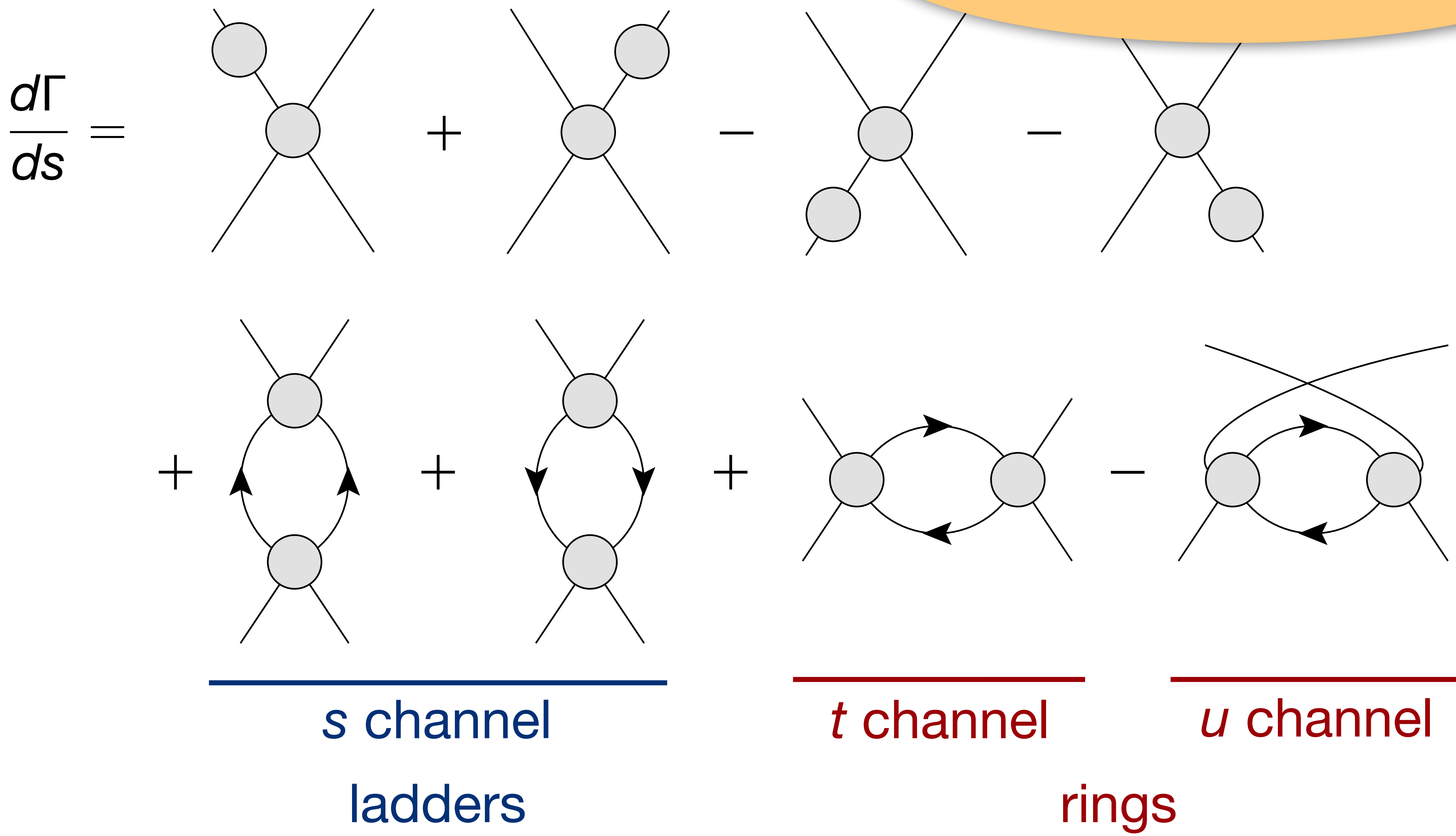


IM-SRG(2): truncate ops. at two-body level

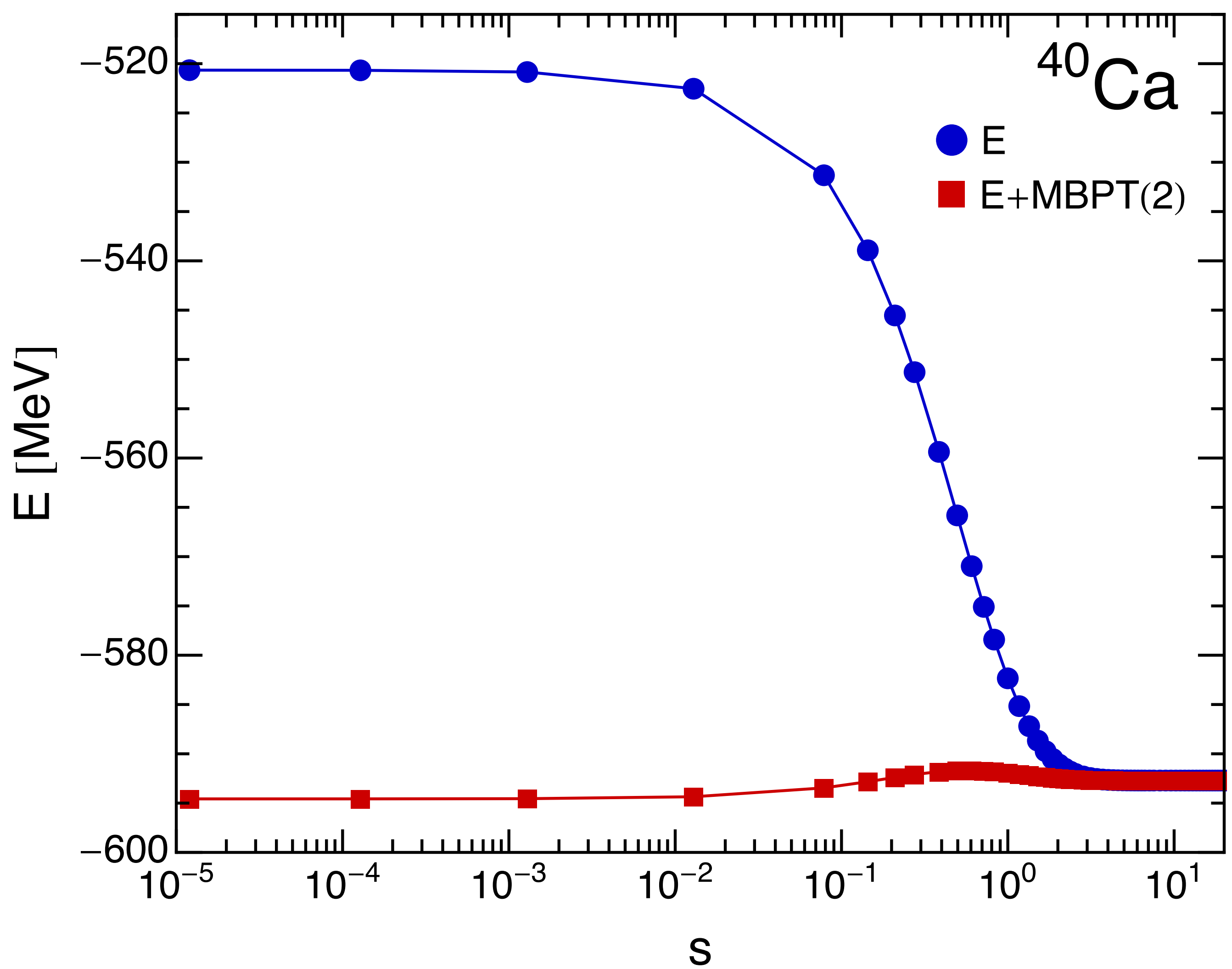
IM-SRG(2) Flow Equations

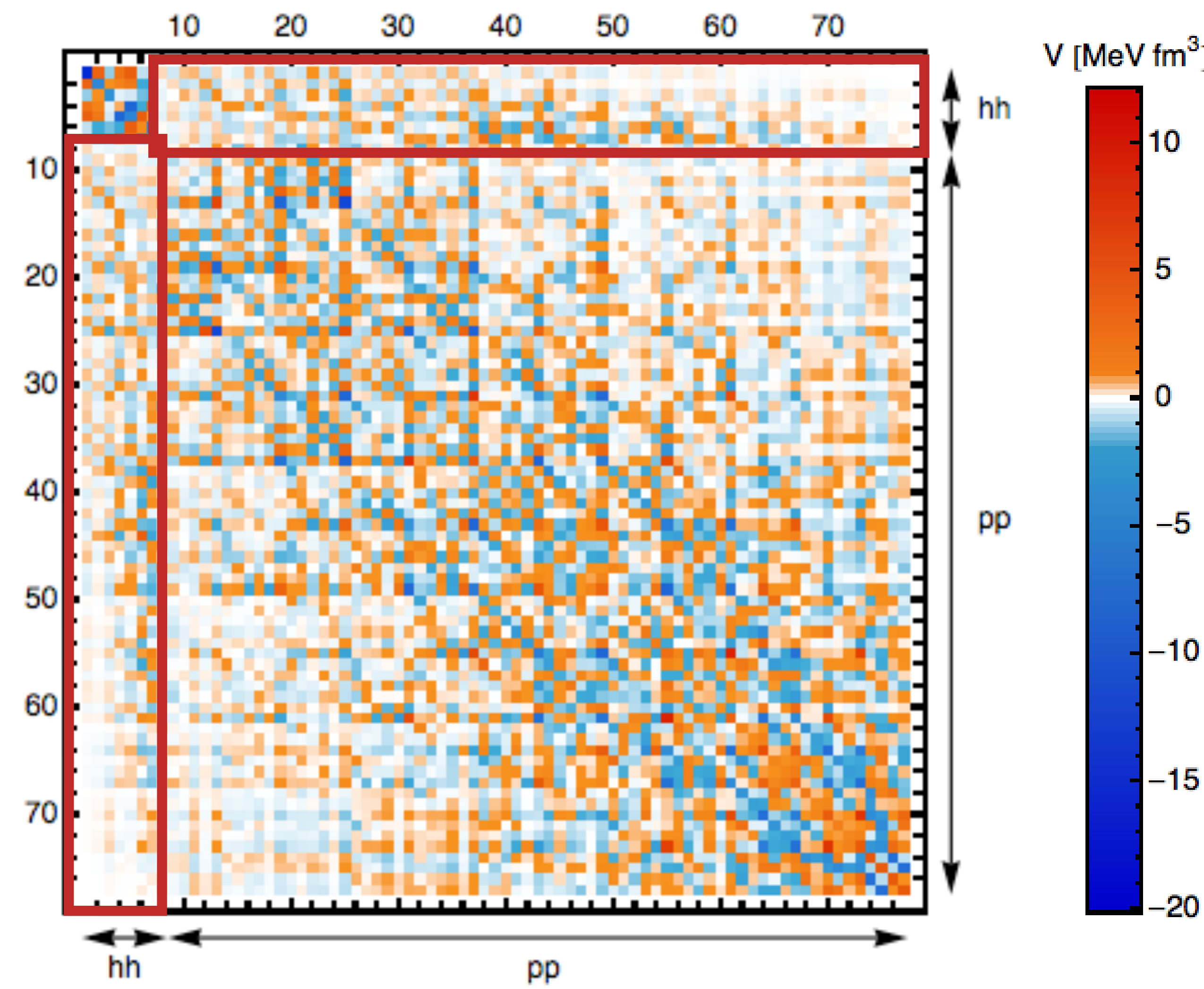
2-body Flow

O(N⁶) scaling
(before particle/hole distinction)



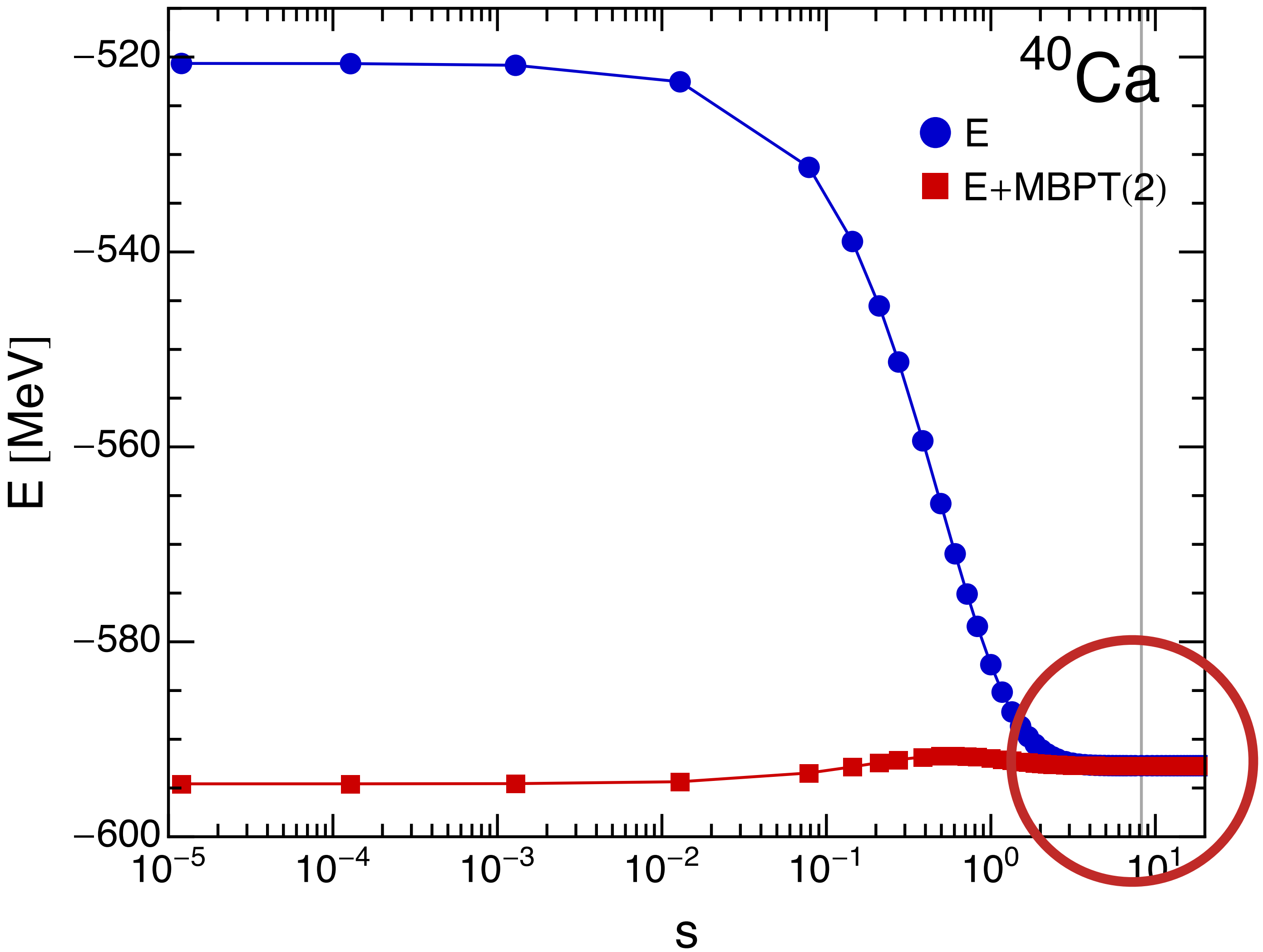
Decoupling

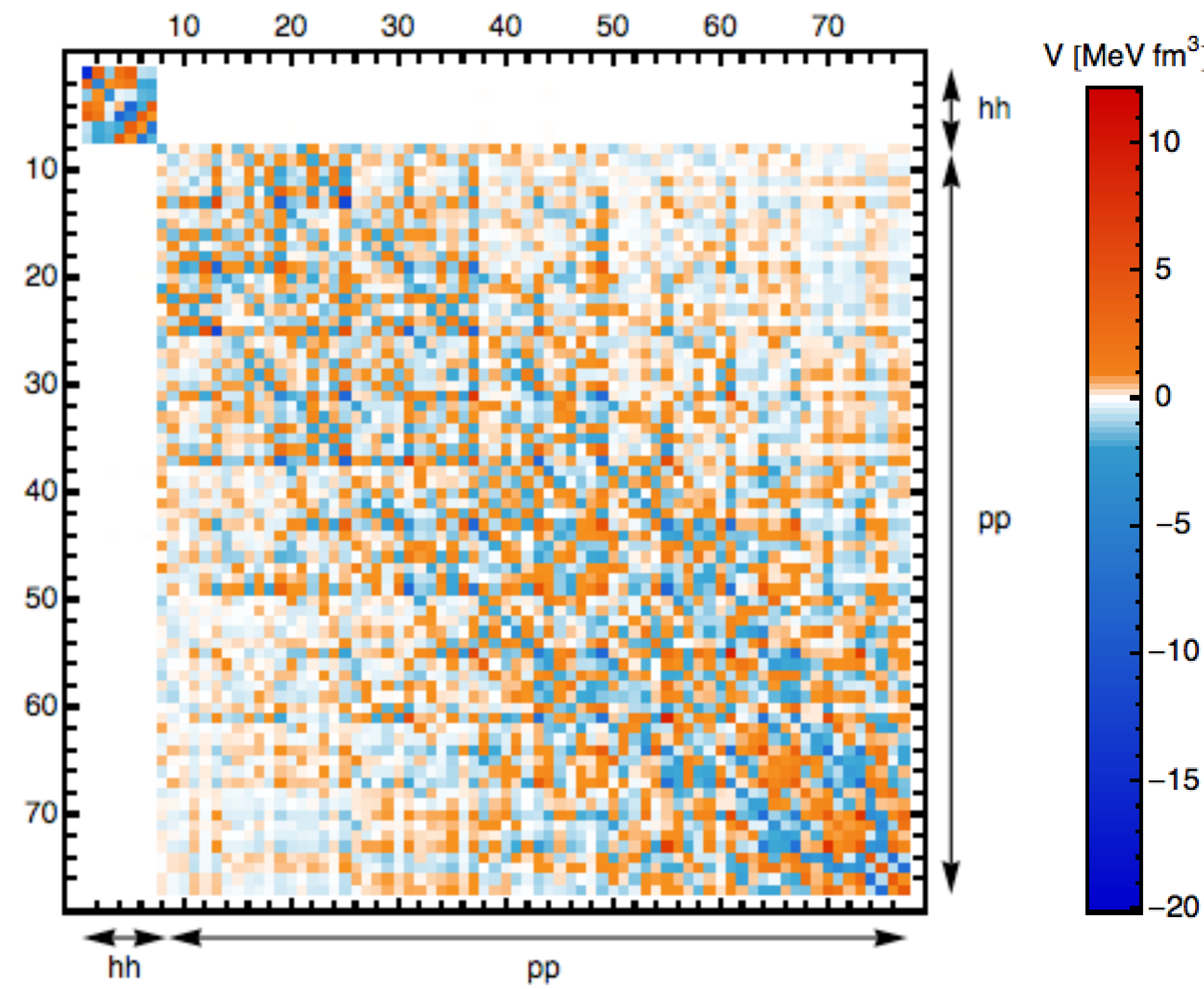




N3LO, $\lambda = 2.0\ \mathrm{fm}^{-1}, e_{\mathrm{Max}} = 8$

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

Multi-Reference IM-SRG

- generalized Wick's theorem for arbitrary reference states (Kutzelnigg & Mukherjee)

- define irreducible n-body density matrices of reference state:

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

. . .

- irreducible densities give rise to additional contractions:

$$:A^{ab\ldots}_{cd\ldots}::A^{kl\ldots}_{mn\ldots}: \quad \longrightarrow \quad \lambda^{ab}_{mn}$$
$$:A^{ab\ldots}_{cd\ldots}::A^{kl\ldots}_{mn\ldots}: \quad \longrightarrow \quad \lambda^{ab}_{cm}$$

. . .

MR-IM-SRG Flow Equations

0-body flow:

$$\frac{dE}{ds} = \sum_{ab}(n_a - n_b)\eta^a_b f^b_a + \frac{1}{2}\sum_{abcd}\eta^{ab}_{cd}\Gamma^{cd}_{ab} n_a n_b \bar{n}_c \bar{n}_d$$

O(N⁴)

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

$O(N^4)$ **$O(N^7)$**

- storage of full 3B density matrix too expensive in general

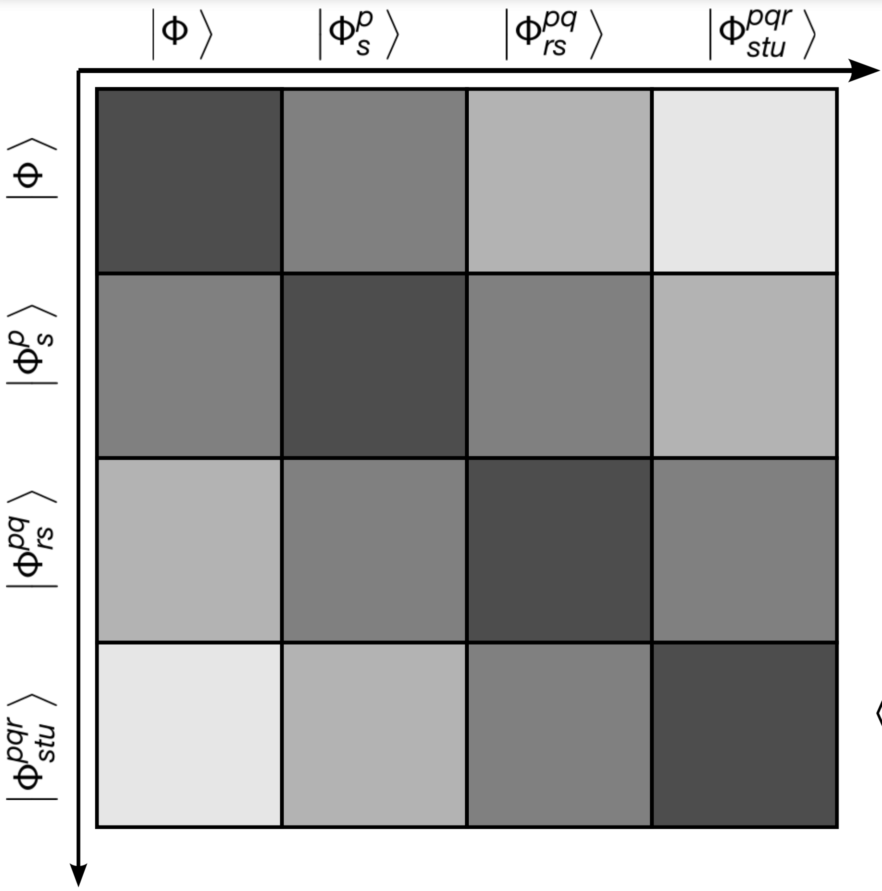
➡ exploit structure of specific reference states:

- Projected HFB: $O(N^3)$ storage, scaling reduced to $O(N^4)$

$$\lambda^{abc}_{def} = \bar{\lambda}_{abc}\,\delta^a_d\delta^b_e\delta^c_f + \tilde{\lambda}_{a|be}\,\delta^a_d\delta^{b\bar{c}}\delta_{e\bar{f}} + \text{perm.}$$

- NCSM / active-space CI: small non-zero block only

Decoupling Revisited



$$\left\langle {}^{p}_{s} \middle| H \middle| \Phi \right\rangle \sim \bar{n}_p n_s f^{p}_{s}, \sum_{kl} f^{k}_{l} \lambda^{sk}_{pl}, \sum_{klmn} \Gamma^{kl}_{mn} \lambda^{skl}_{pmn}, \ldots$$

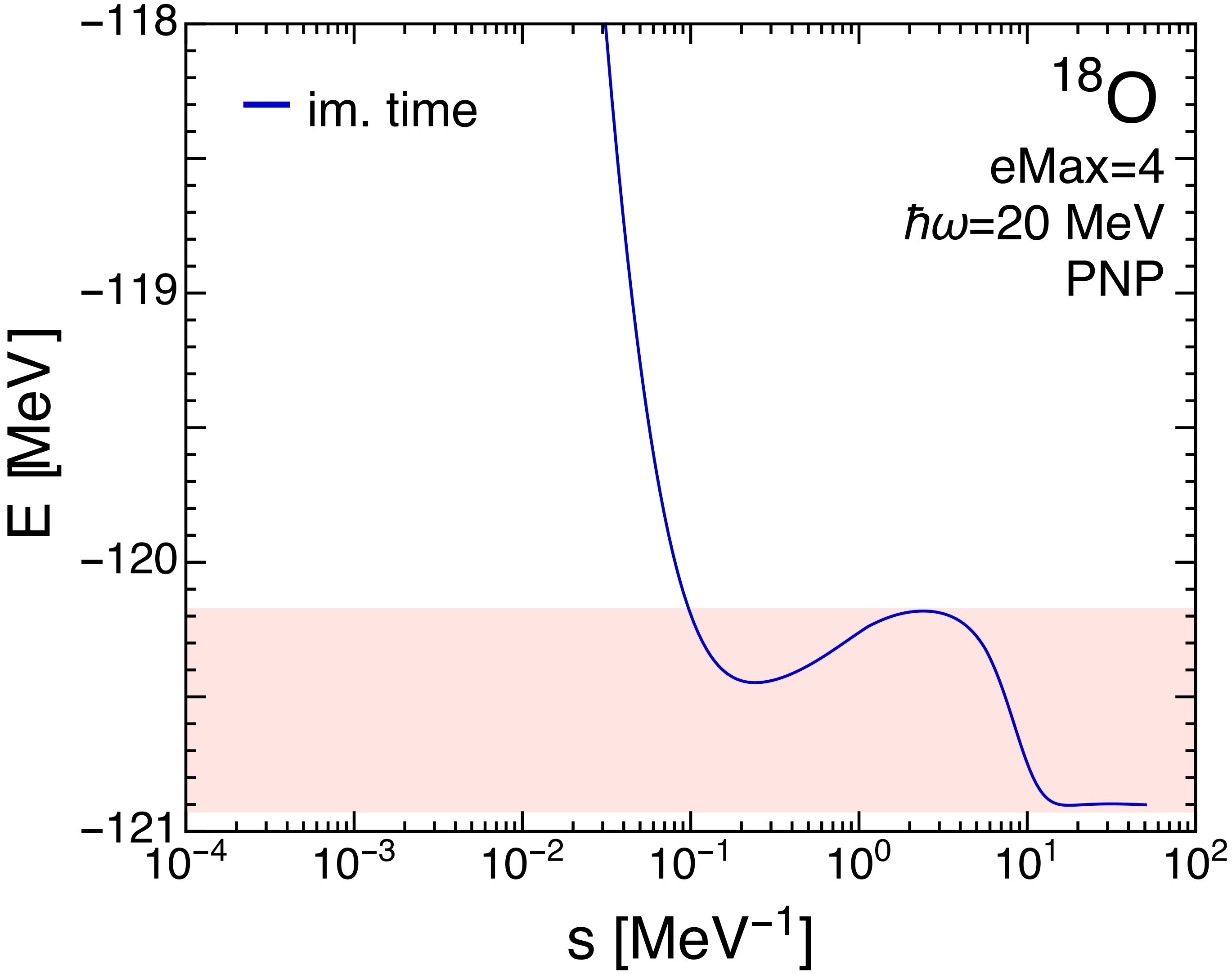
$$\left\langle {}^{pq}_{st} \middle| H \middle| \Phi \right\rangle \sim \bar{n}_p \bar{n}_q n_s n_t \Gamma^{pq}_{st}, \sum_{kl} \Gamma^{pk}_{sl} \lambda^{tk}_{ql}, \sum_{kl} f^{k}_{l} \lambda^{stk}_{pql}, \sum_{klmn} \Gamma^{kl}_{mn} \lambda^{stkl}_{pqmn}, \ldots$$

$$\left\langle {}^{pqr}_{stu} \middle| H \middle| \Phi \right\rangle \sim \ldots$$

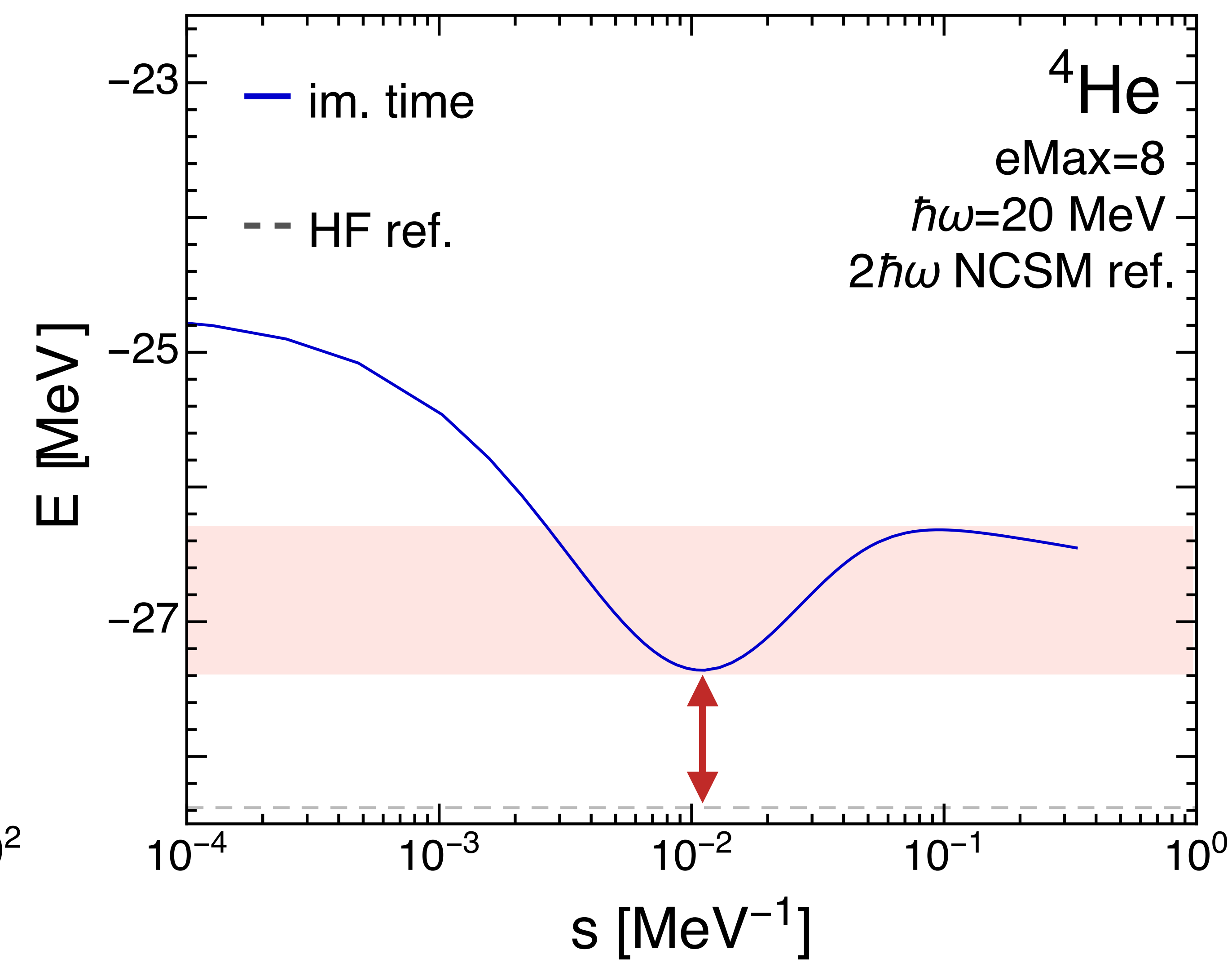
- truncation in irreducible density matrices based on, e.g.,
  - number of correlated vs. total pairs, triples, ... (caveat: highly collective reference states)
  - perturbative analysis (e.g. for shell-model like states)
- verify for chosen multi-reference state when possible

Traditional Generators

NN+3N-ind., λ=2.0 fm^{-1}



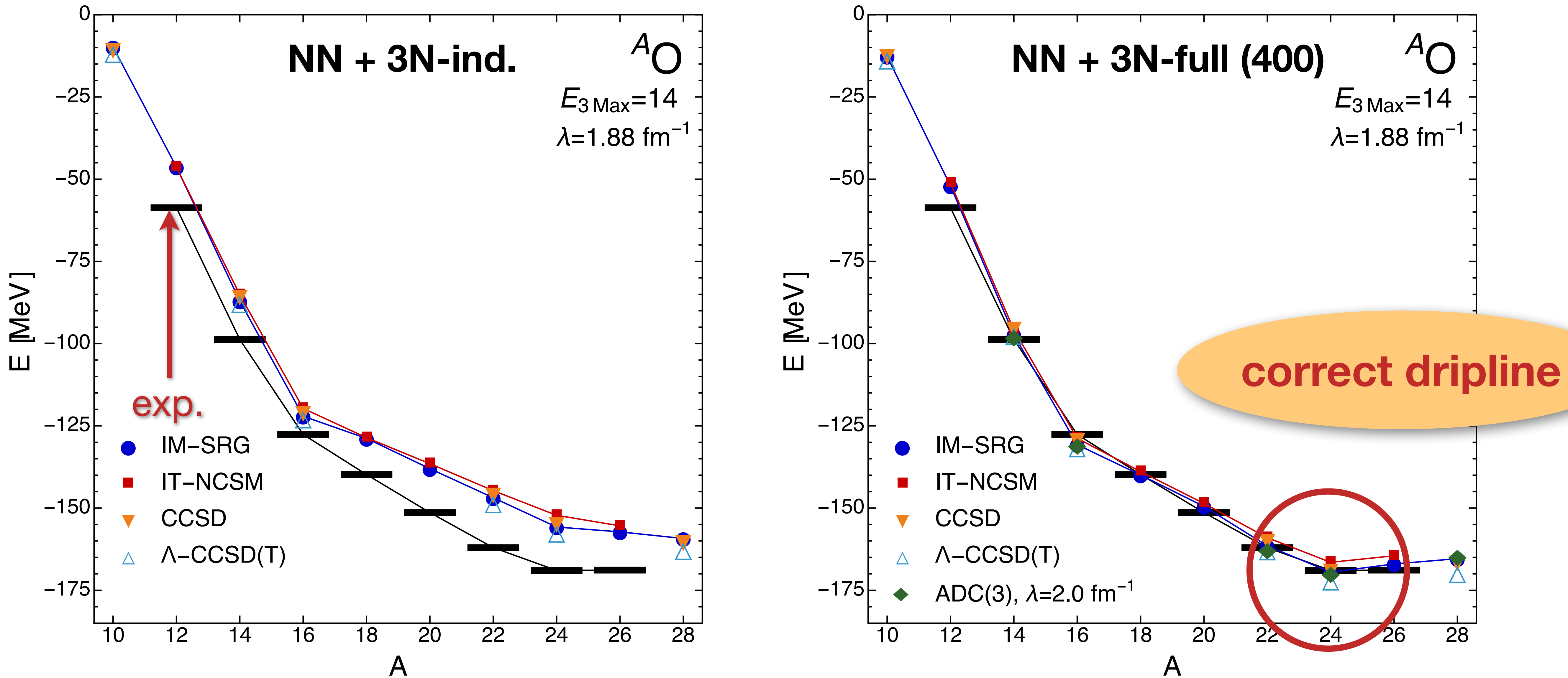
NN-only, λ=1.88 fm^{-1}



➡ approximations cause non-monotonic behavior of energy & generator norm

Results: Oxygen Chain

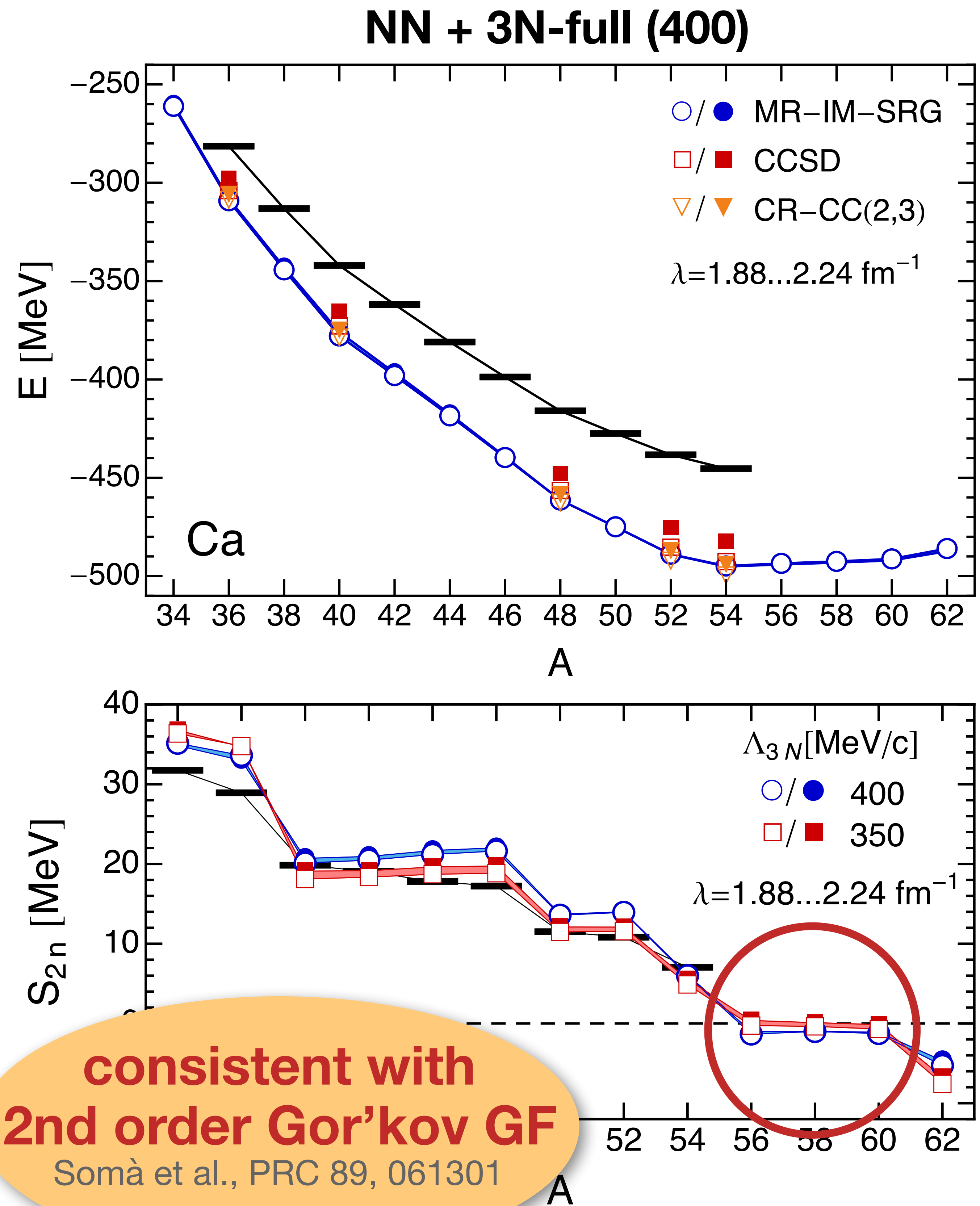
*HH et al., PRL **110**, 242501 (2013), ADC(3): A. Cipollone et al., PRL **111**, 242501 (2013)*



- Multi-Reference IM-SRG with number-projected Hartree-Fock-Bogoliubov as reference state
- consistent results from different many-body methods

Two-Neutron Separation Energies

*HH et al., PRC **90**, 041302(R) (2014)*



consistent with 2nd order Gor'kov GF

Somà et al., PRC 89, 061301

- differential observables (S_{2n}, spectra,...) filter out interaction components that cause overbinding
- predict flat trends for g.s. energies/S_{2n} beyond ^{54}Ca - await experimental data
- ^{52}Ca, ^{54}Ca robustly magic due to 3N interaction
- no continuum coupling yet, other S_{2n} uncertainties < 1MeV