Introduction to In-Medium Similarity Renormalization Group Methods

Text

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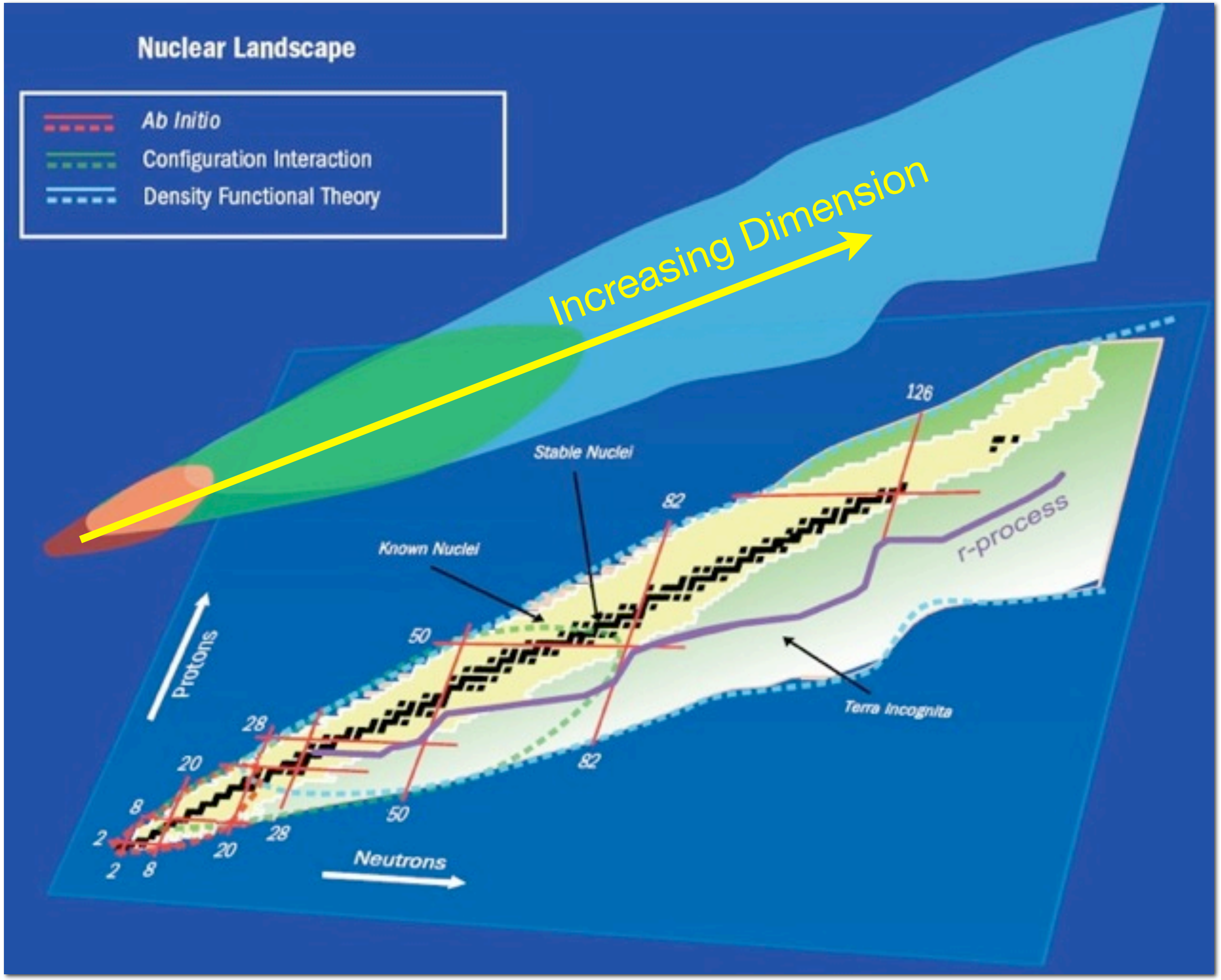
The nuclear many-body landscape



Calculate the properties of thousands of strongly-interacting nuclei from underlying forces

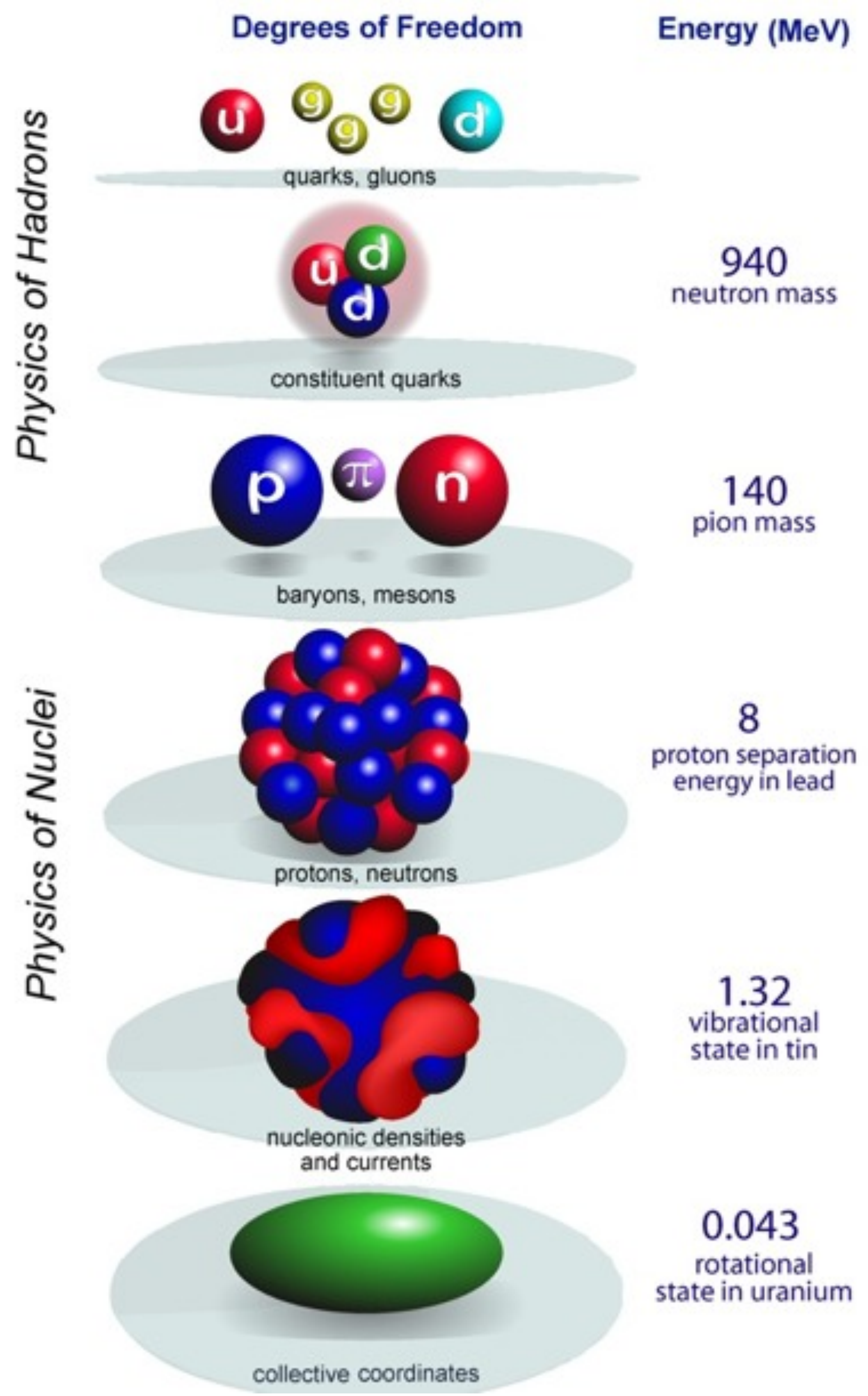
Challenges

- Multi-scale

$$V(\Lambda) = V_{2N}(\Lambda) + V_{3N}(\Lambda) + \cdots$$

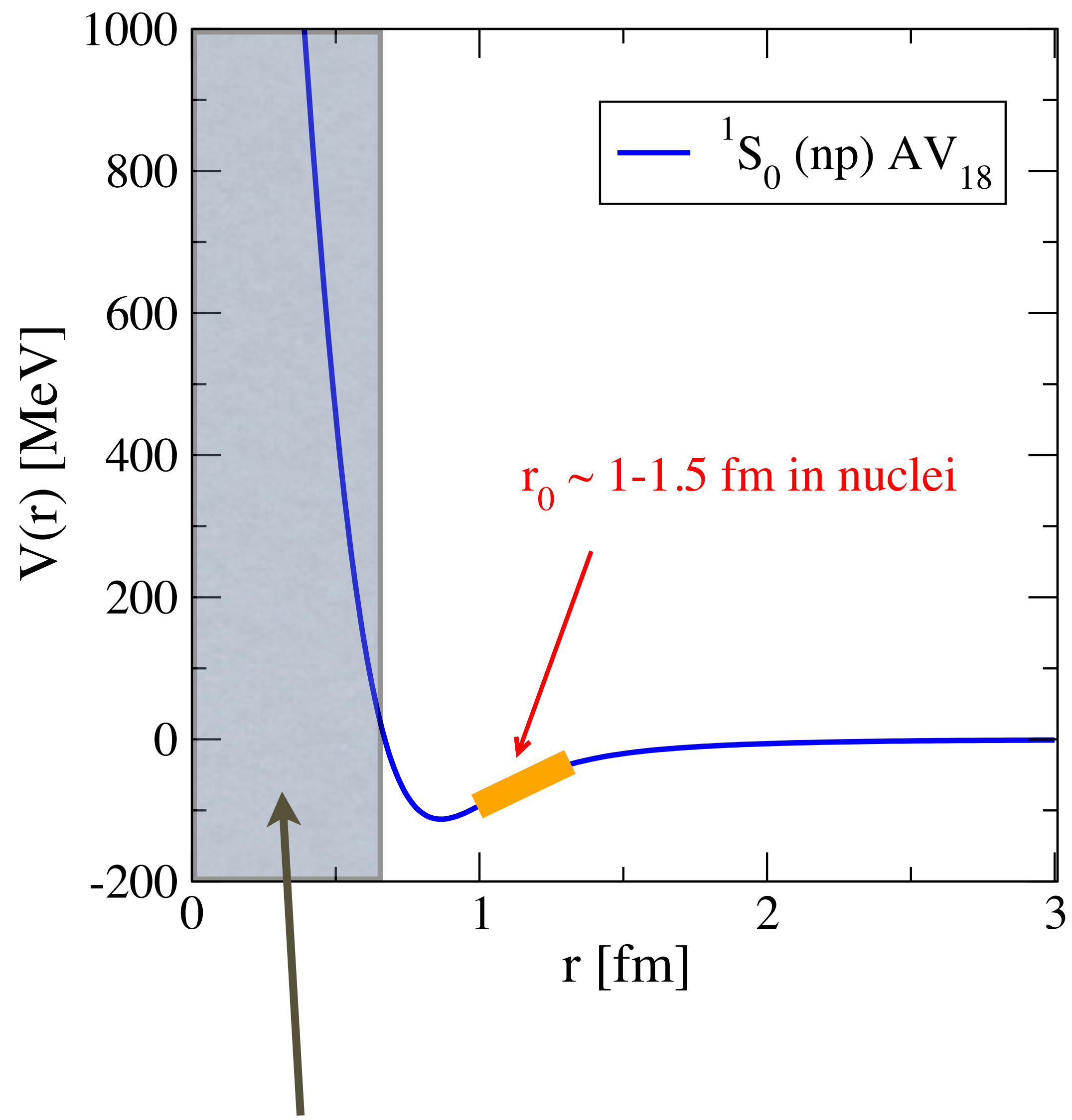
- Effective theories at each scale connected by renormalization group

Use RG to pick a convenient Λ "resolution scale"

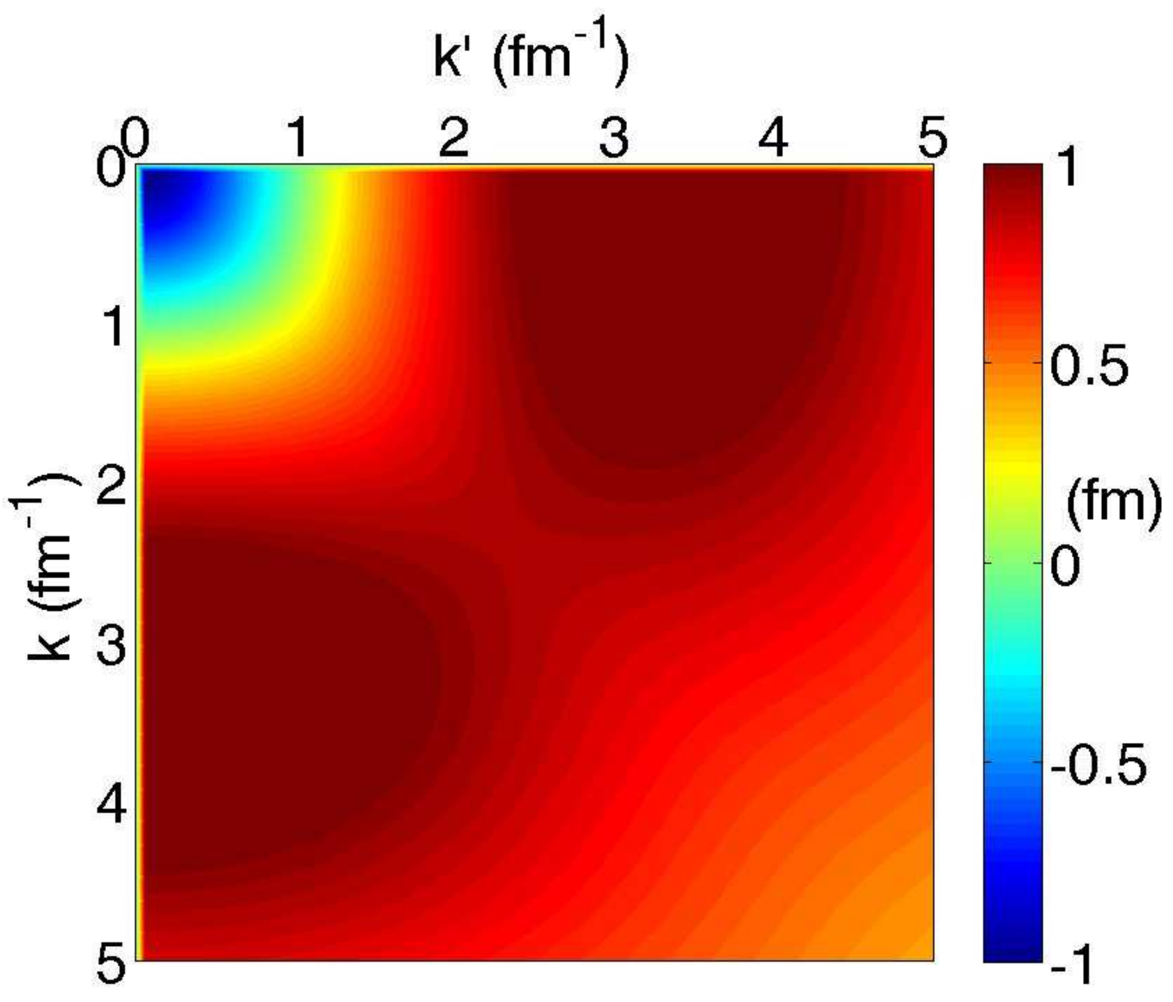


Challenges

- Multi-scale
- strong interactions



“hard-core” of V(r) =>
strong offdiagonal V(k,k’)



$$V_{l=0}(k,k') = \int d^3r\, j_0(kr)\, V(r)\, j_0(k'r')$$

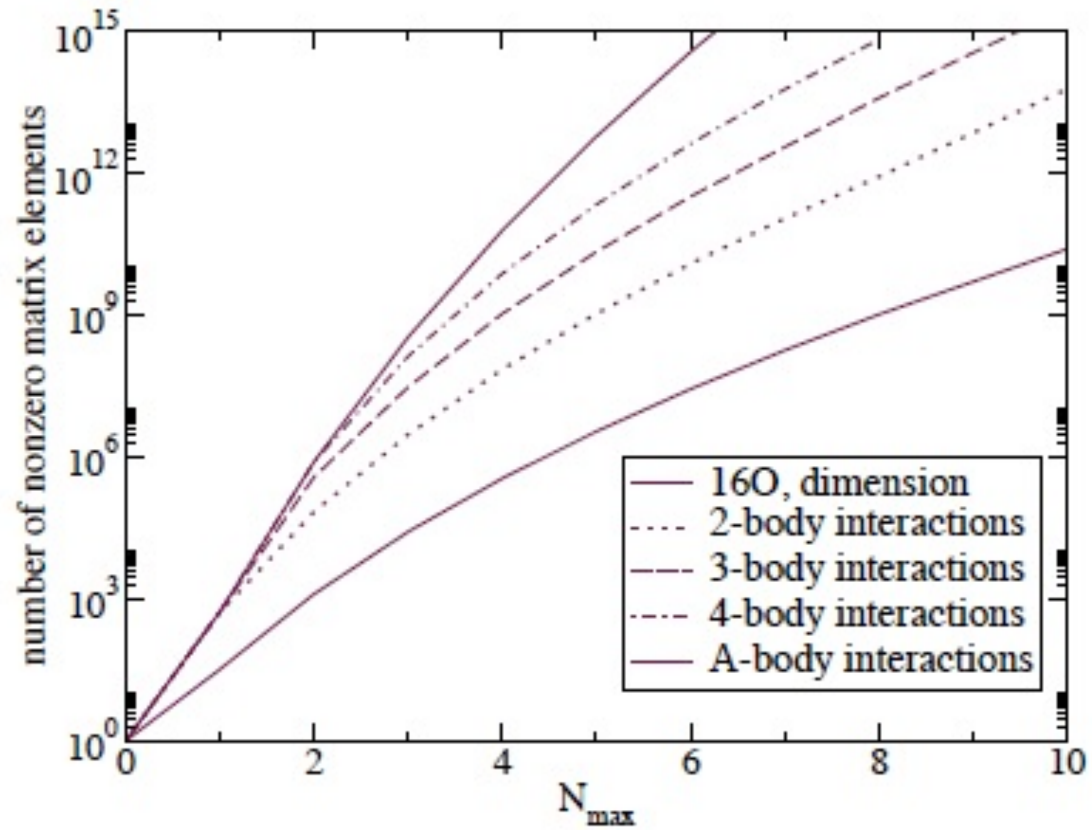
Challenges

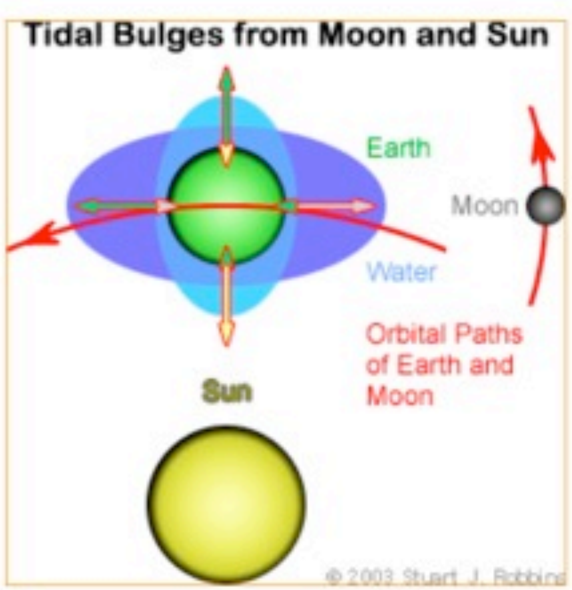
- Multi-scale
- strong interactions
- 3-body forces

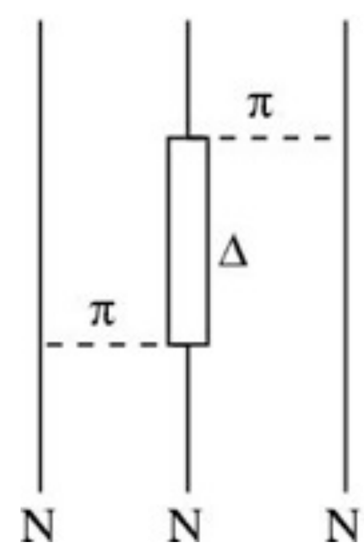
Three-body force

From Wikipedia, the free encyclopedia

A **three-body force** is a force that does not exist in a system of two objects but appears in a three-body system. In general, if the behaviour of a system of more than two objects cannot be described by the two-body interactions between all possible pairs, as a first approximation, the deviation is mainly due to a three-body force.



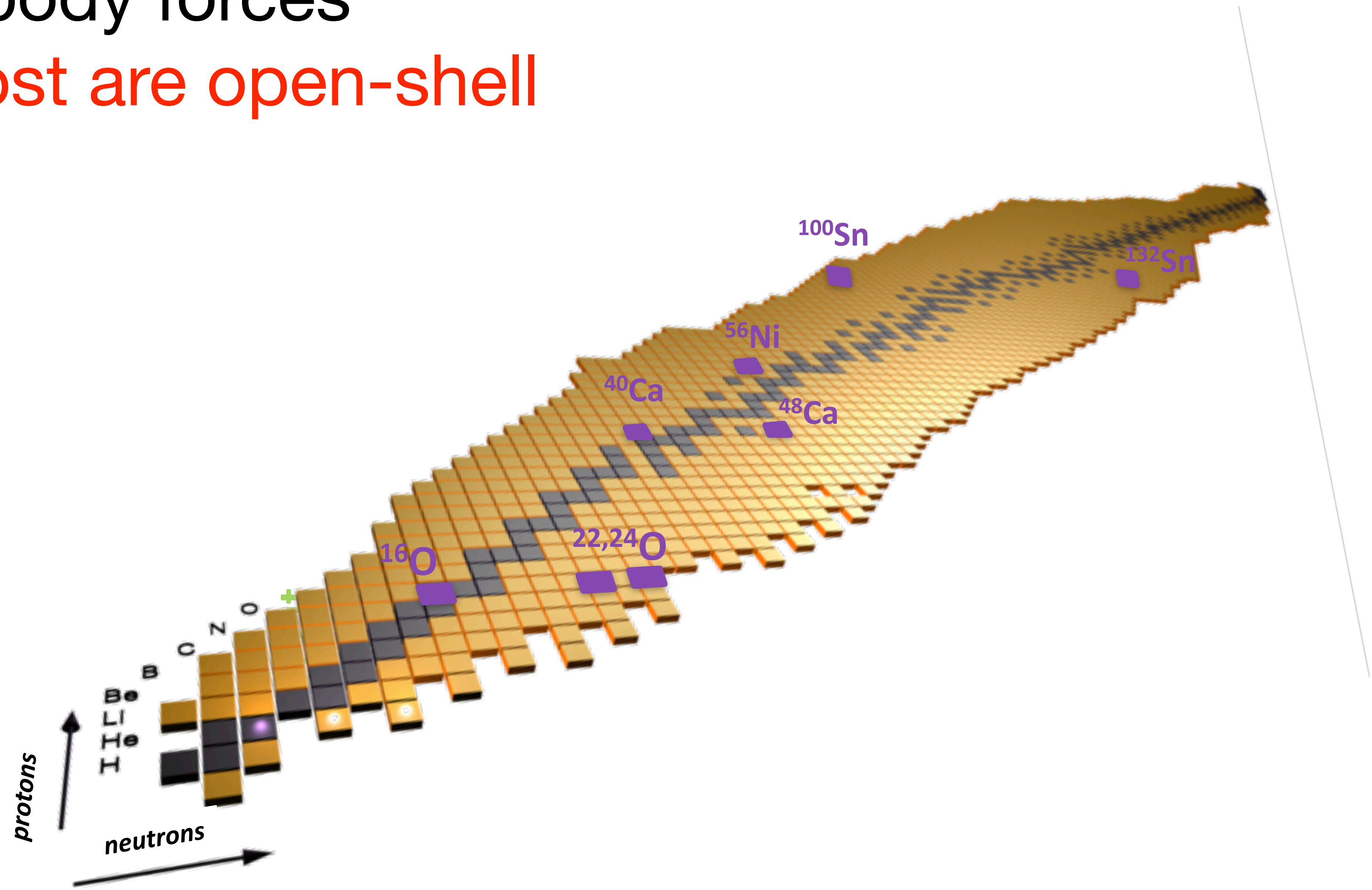




Polarization effect a-la Axilrod-Teller

Challenges

- Multi-scale
- strong interactions
- 3-body forces
- Most are open-shell



In-Medium SRG for Closed-Shell Systems

H. Hergert, S. K. Bogner, S. Binder, A. Calci, J. Langhammer, R. Roth, and A. Schwenk, Phys. Rev. C **87**, 034307 (2013)
K. Tsukiyama, S. K. Bogner, and A. Schwenk, Phys. Rev. Lett. **106**, 222502 (2011)
S.K. Bogner, R. Furnstahl, and A. Schwenk, Prog. Part. Nucl. Phys. **65** (2010), 94
S. Reimann, S.K. Bogner and M. Hjorth-Jensen, in preparation

Similarity Renormalization Group

The SRG Tower of Babel

1) Hamiltonian Flow
2) Continuous Unitary Transformations (CUTs)
3) Numerical Canonical Diagonalization
4) Isospectral Flow
5) ...

Similarity Renormalization Group

Basic Concept

continuous unitary transformation to drive Hamiltonian to band- or block diagonal form (Glazek and Wilson, Wegner)

- evolved Hamiltonian

$$H(s) = U(s) H U^{\dagger}(s) \equiv H_d(s) + H_{od}(s)$$

s = continuous flow parameter

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$$H(s) = U(s)HU^\dagger(s) \equiv H_d(s) + H_{od}(s)$$

- flow equation:

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

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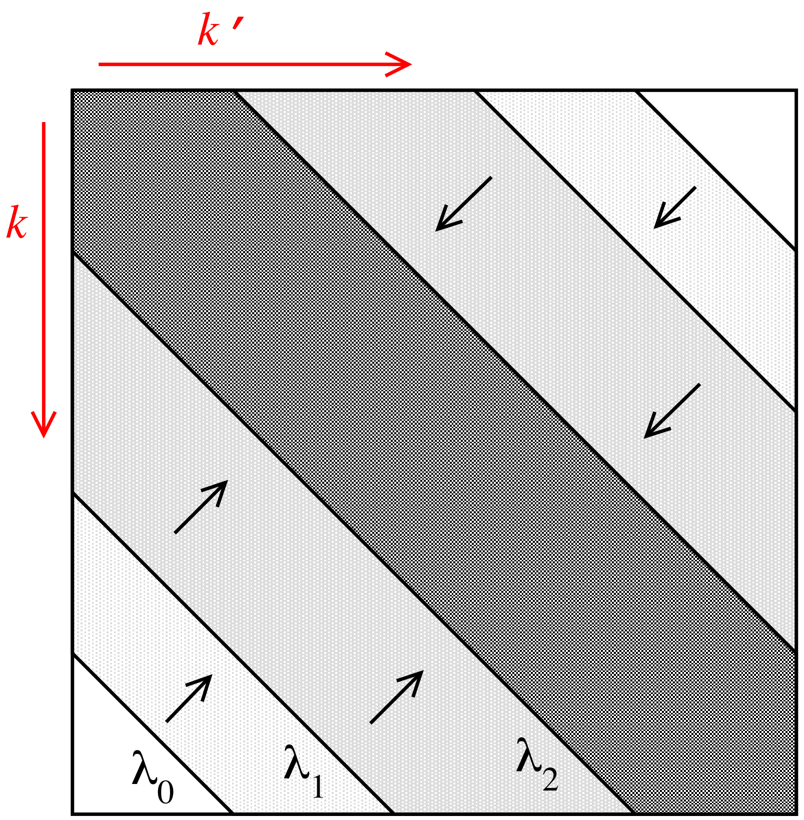
$$\frac{d}{ds}H(s) = \left[\eta(s), H(s)\right], \quad \eta(s) = \frac{dU(s)}{ds}U^{\dagger}(s) = -\eta^{\dagger}(s)$$

- choose $\eta(s)$ to drive *H(s)* to desired form

E.g. $\eta(s) = [H_d(s), H_{od}(s)] \quad \Rightarrow \quad \lim_{s\to\infty} H_{od}(s) = 0$

Similarity Renormalization Group

Original Motivation: Decouple low- high-momentum modes to “soften” nuclear interactions (Free-space SRG)



$$\eta(s) = [T, H(s)]$$

Drives H towards diagonal in k-space

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

like a floating UV cutoff

Similarity Renormalization Group

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Exercise:

Estimate how the size of the s.p. basis scales with Λ. Given this, estimate the size of the Hamiltonian matrix for ^{16}O.

Hints:

1) The basis must be sufficiently extended in space to capture the size of the nucleus ($R \sim 1.2A^{1/3}$ fm).

2) The basis must be sufficiently extended in momentum to capture the size of the cutoff Λ in the Hamiltonian.

3) Use a phase space argument to get # of sp states

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Estimate how the size of the s.p. basis scales with Λ. Given this, estimate the size of the Hamiltonian matrix for ^{16}O.

Answer: # of s.p. states D ~ $\Lambda^3 A$

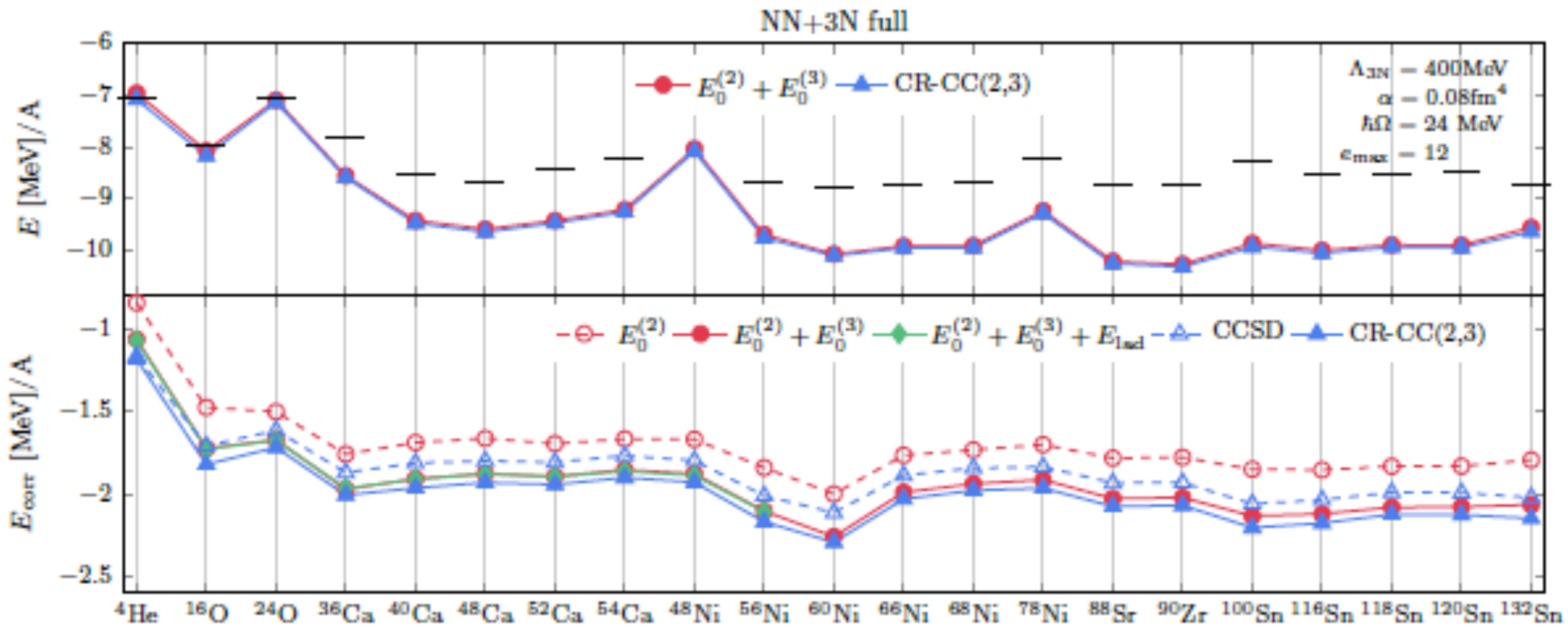
Dim(H) = # of A-body Slater determinants
= D!/(D-A)!/A!

e.g., for Λ = 4.0 fm^{-1} Dim(H) ~ 10^{14}

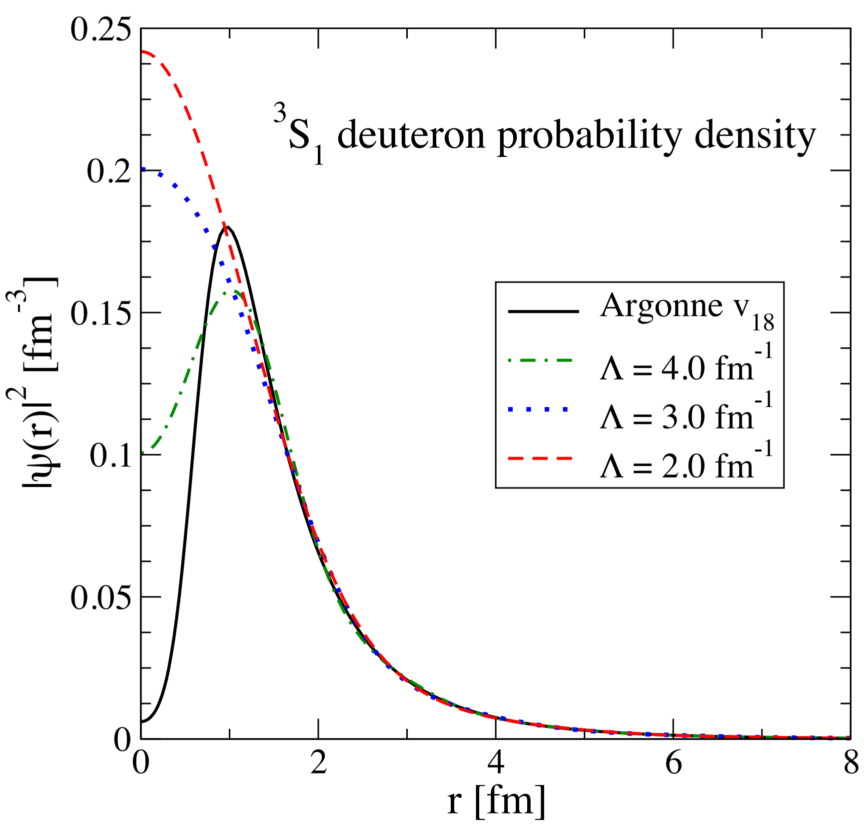
Strong incentive to lower Λ!

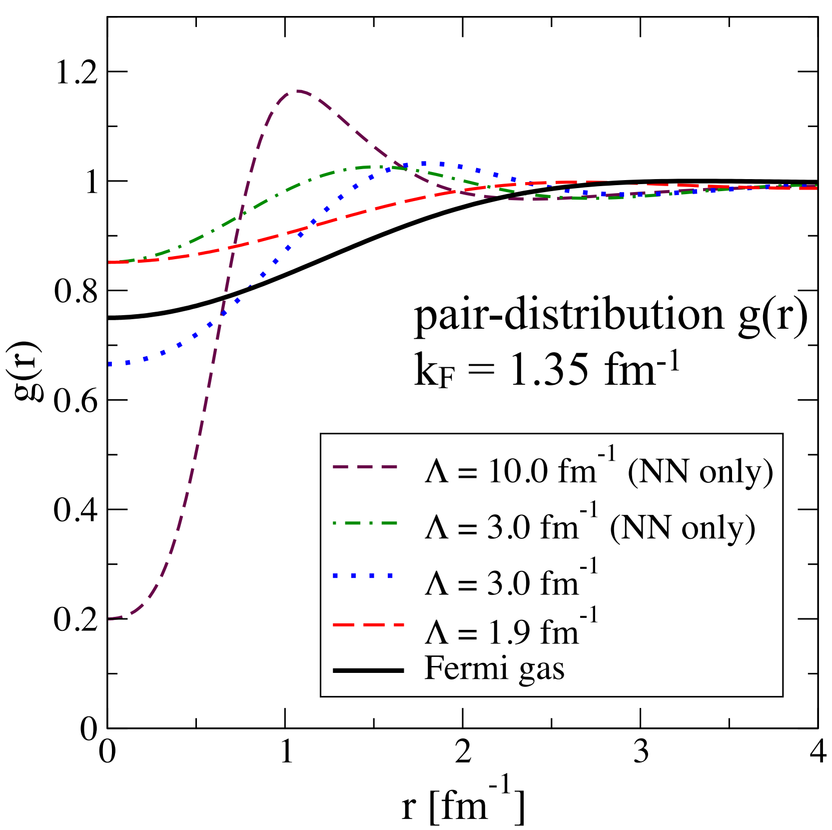
Simplifications with SRG interactions

A. Tichai et al.



Good agreement of MBPT(3) and CR-CC(2,3) with SRG-softened interactions





Weaker correlations, faster convergence, etc.

Price Paid: Induced Interactions

- SRG is a unitary transformation in A-body space

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- SRG is a unitary transformation in A-body space
- up to A-body interactions are induced during the flow

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

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- 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; Roth et al., PRL 109, 052501)

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Need to go (at least) to 3-body level to get λ independent results, in some cases even this is not enough (Roth et al., PRL 109, 052501)

Free space versus in-medium evolution

Free space SRG: $V(\lambda)_{2N}$ fixed in 2N system
$V(\lambda)_{3N}$ fixed in 3N system

$V(\lambda)_{aN}$ fixed in aN system

Use $T + V(\lambda)_{2N} + V(\lambda)_{3N} + \ldots + V(\lambda)_{aN}$ in A-body system

In-medium SRG:
evolution done at directly in A-body system.

Different mass regions => different SRG evolutions

inconvenience outweighed (?) by simplifications allowed by normal-ordering

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:

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

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- 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

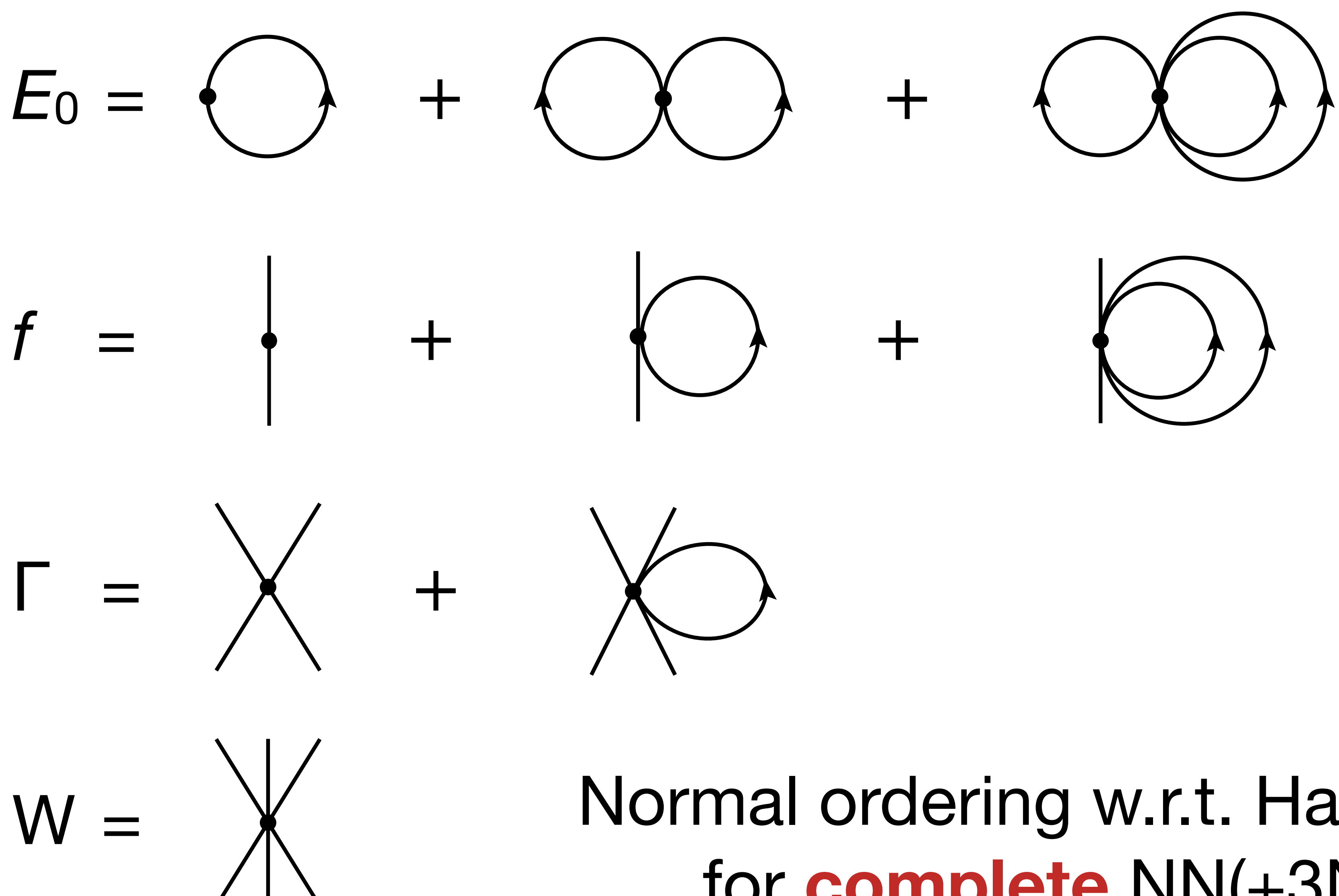
$$\left\langle \Phi \right| : A^{k_1 \dots k_N}_{l_1 \dots l_N} : \left| \Phi \right\rangle = 0$$

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

Normal-Ordered Hamiltonian

Normal-Ordered Hamiltonian

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



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

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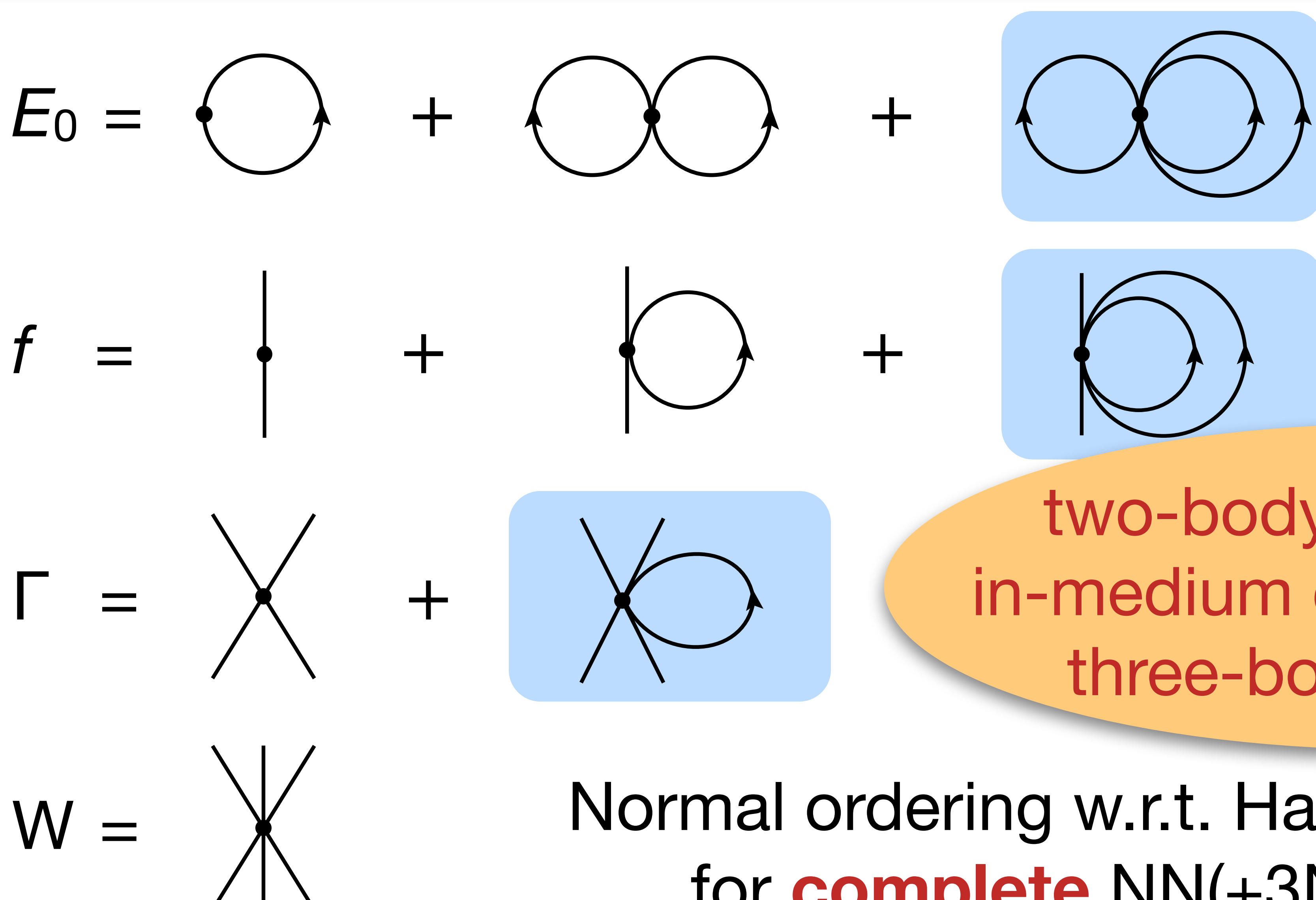

two-body formalism with in-medium contributions from three-body interactions

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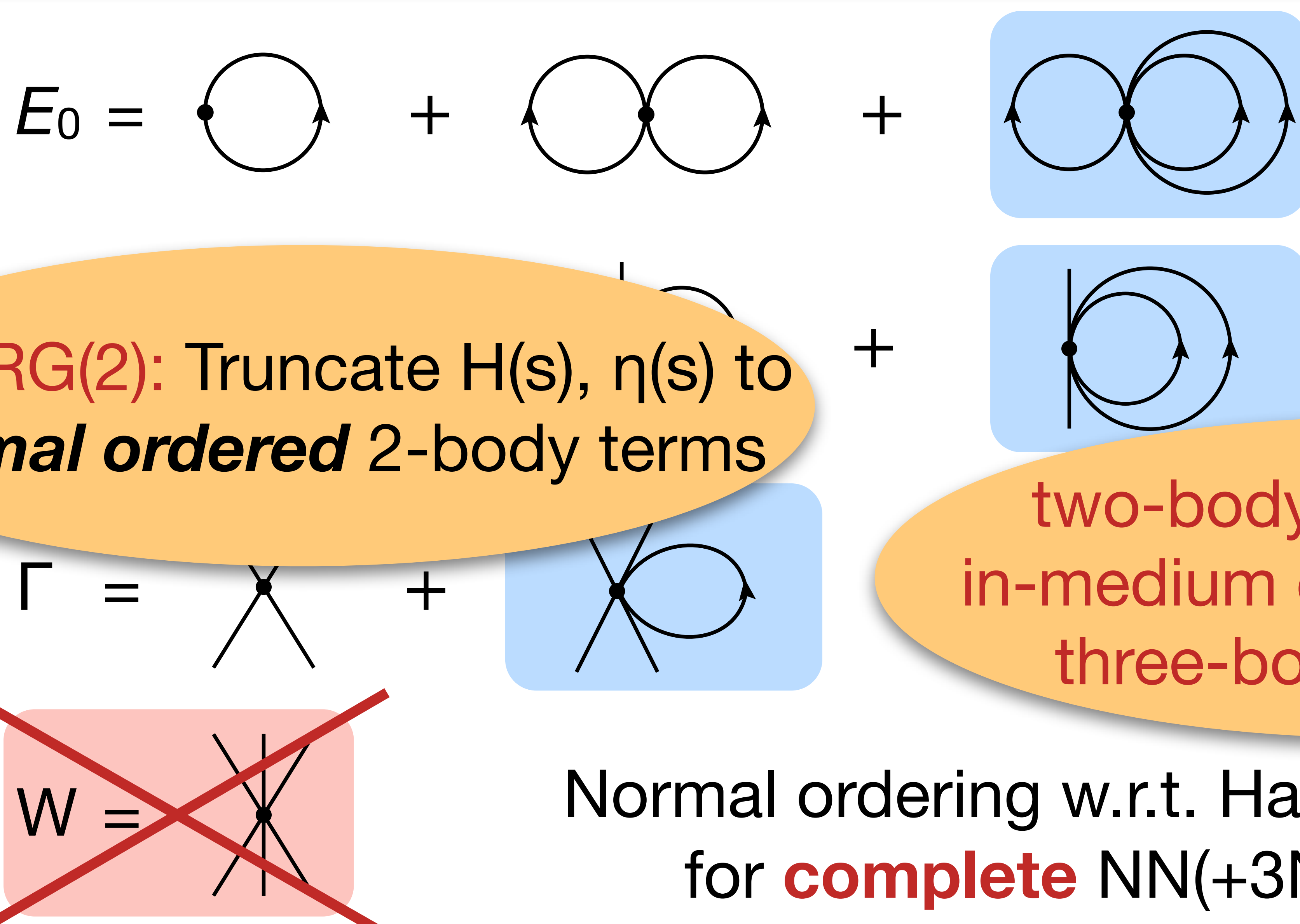
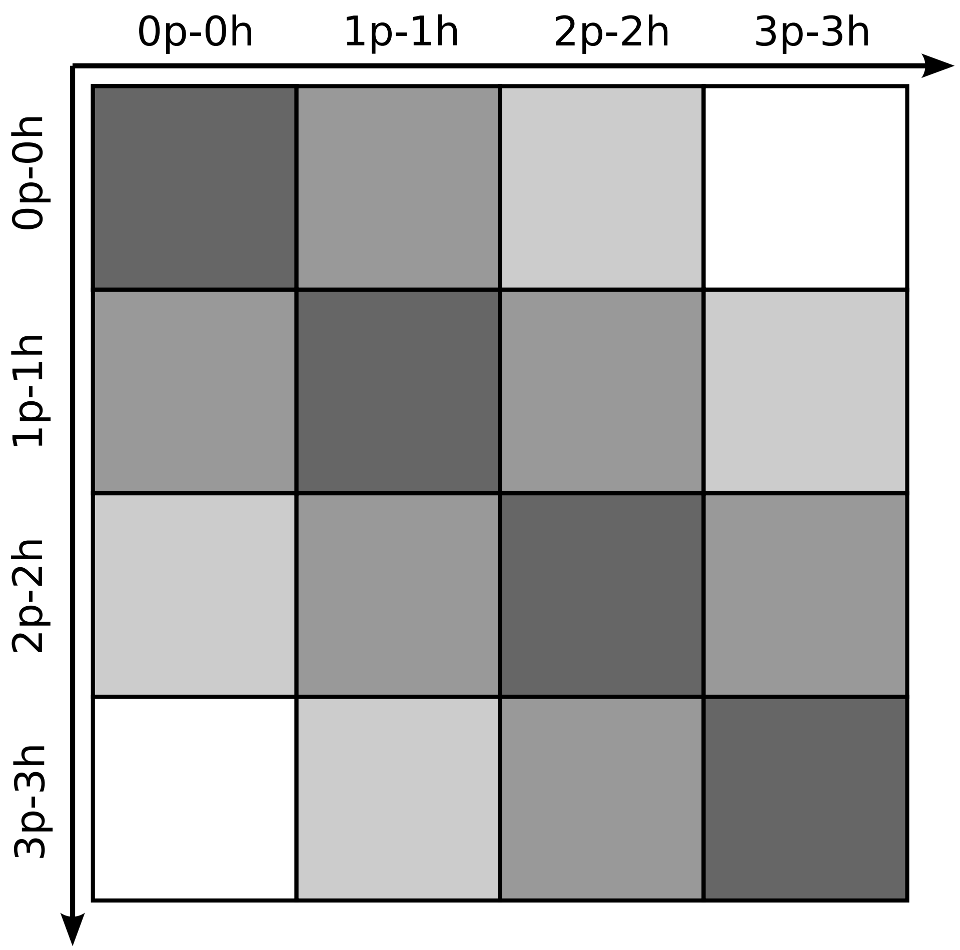


IM-SRG(2): Truncate H(s), η(s) to ***normal ordered*** 2-body terms

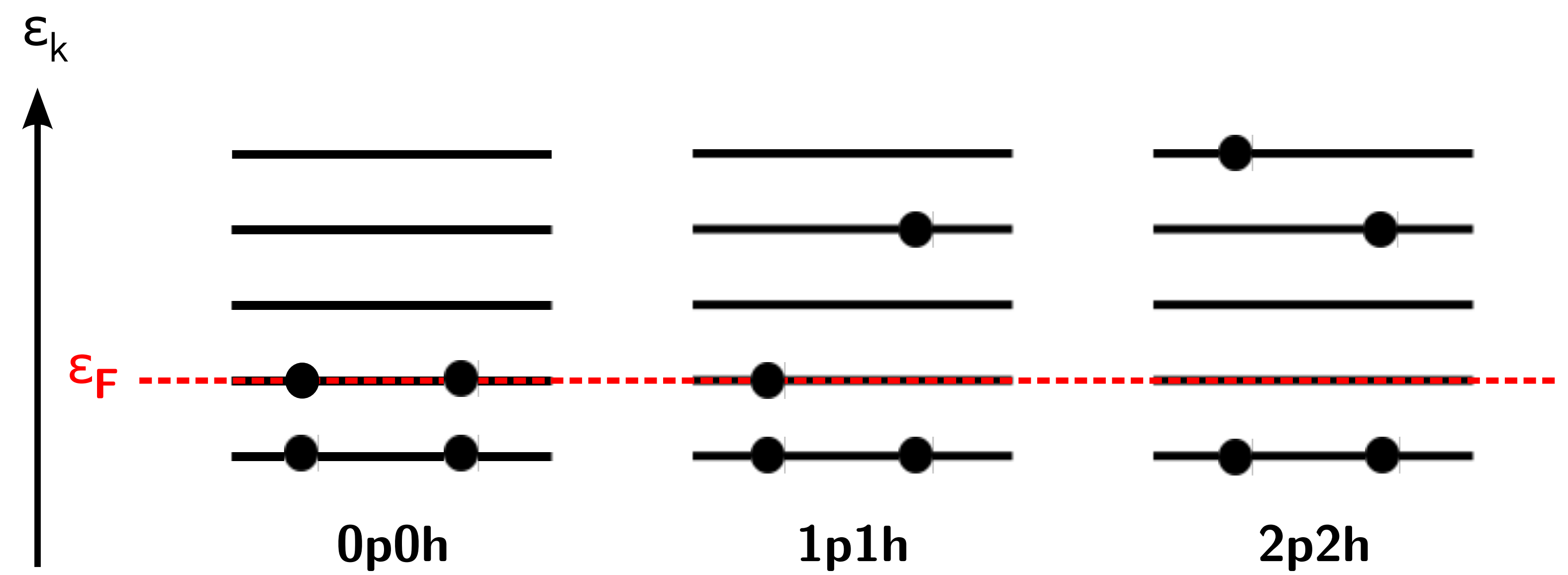
two-body formalism with in-medium contributions from three-body interactions

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

Decoupling in A-Body Space



$\langle i | H | j \rangle$



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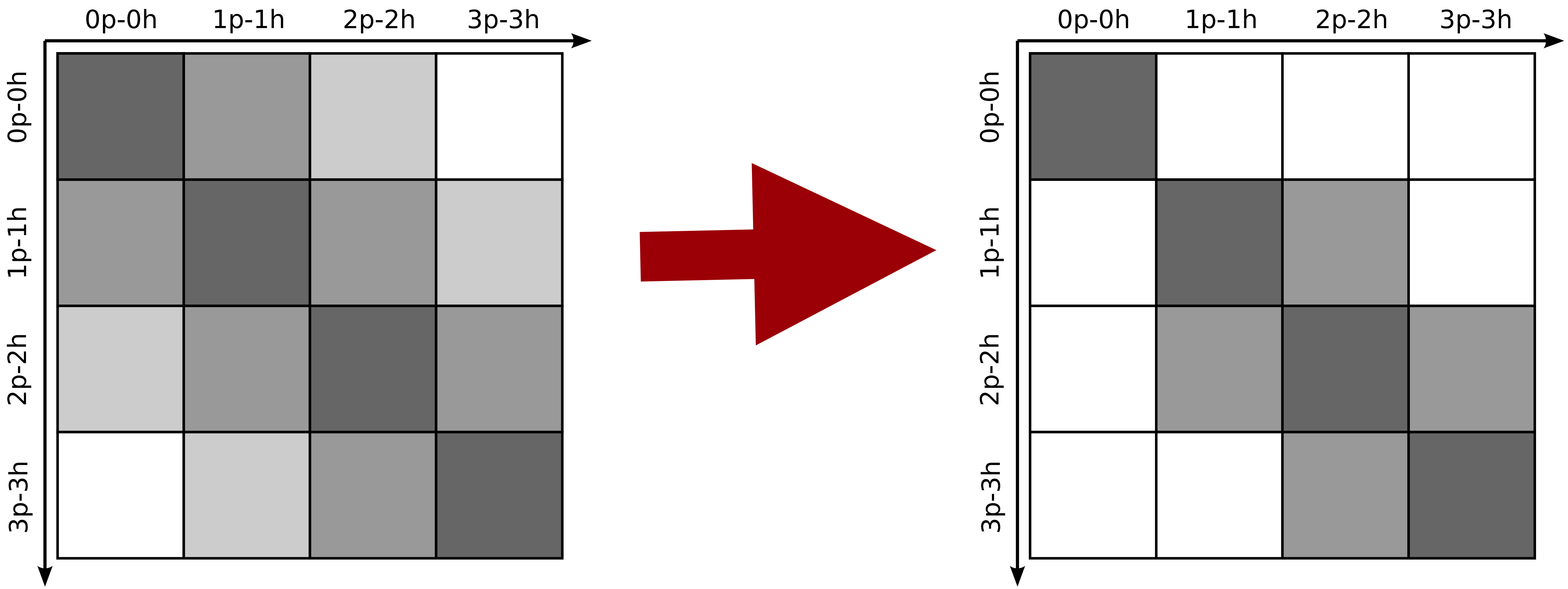
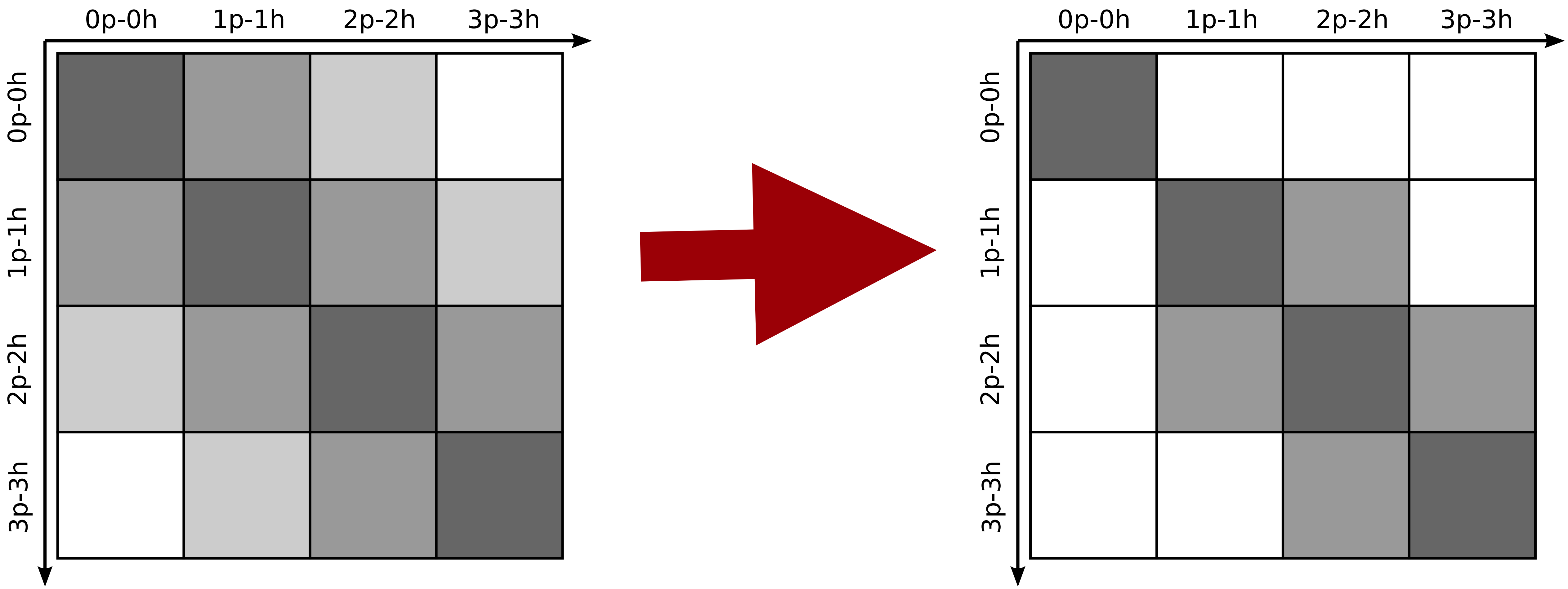


$\langle i | H | j \rangle$ $\langle i | H(\infty) | j \rangle$

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

$$H_{od} = \left\{ f_h^p \,,\, f_p^h \,,\, \Gamma_{hh'}^{pp'} \,,\, \Gamma_{pp'}^{hh'} \right\}$$

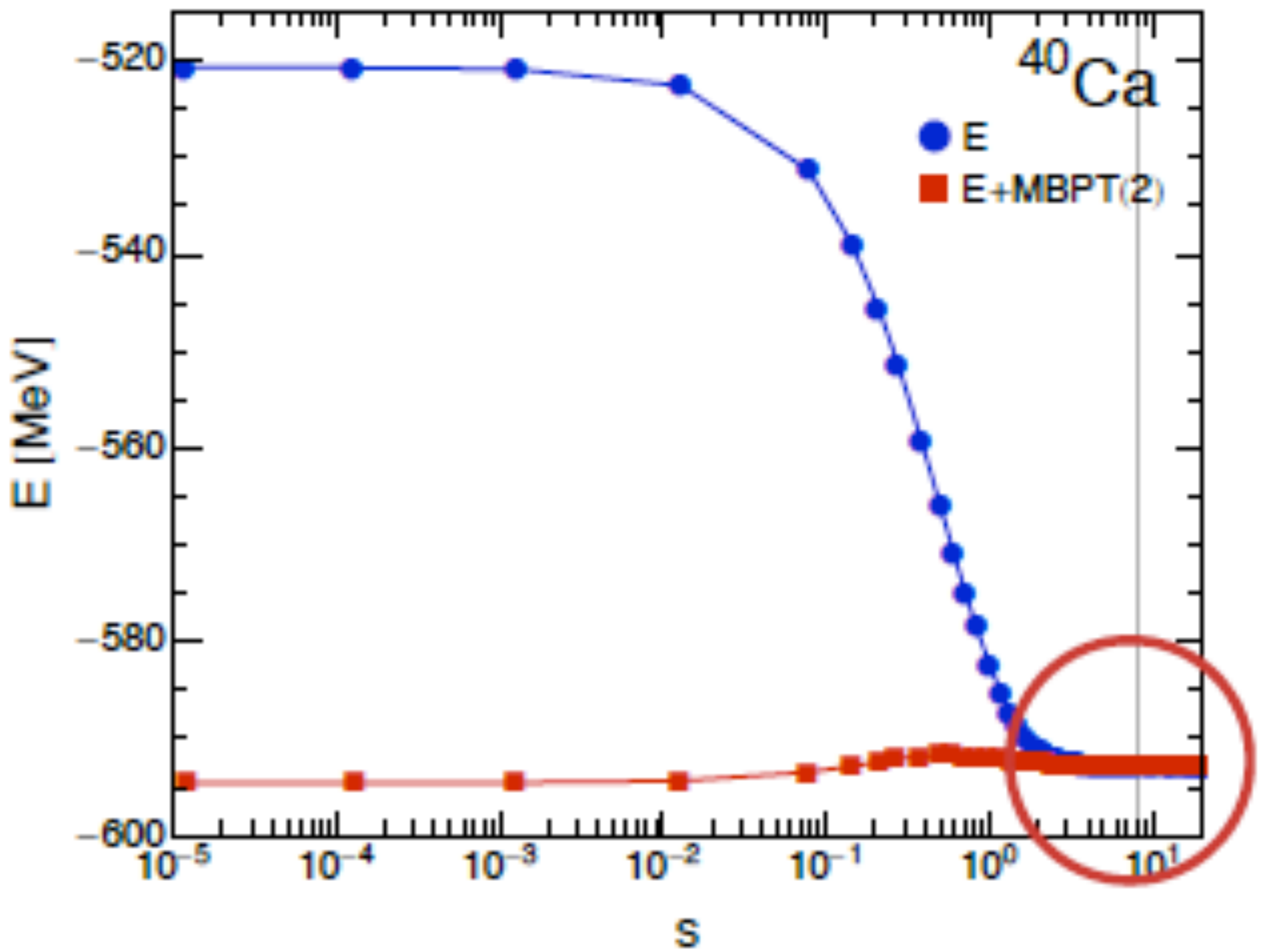
Decoupling in A-Body Space

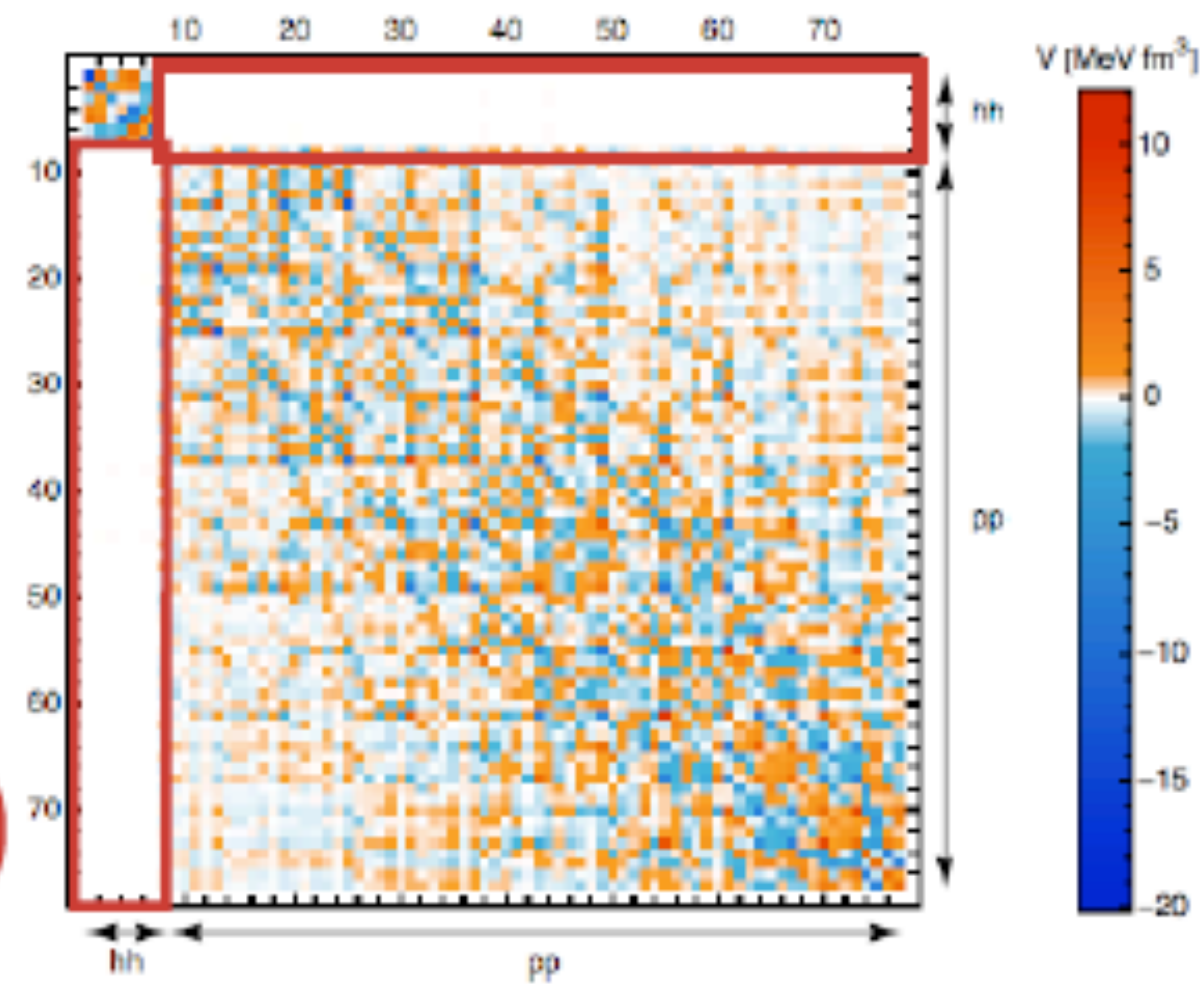


$\langle i | H | j \rangle$ $\langle i | H(\infty) | j \rangle$

$$E_{gs} = \langle 0p0h | H(\infty) | 0p0h \rangle$$

Decoupling in A-Body Space





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

non-perturbative resummation of MBPT series (correlations)

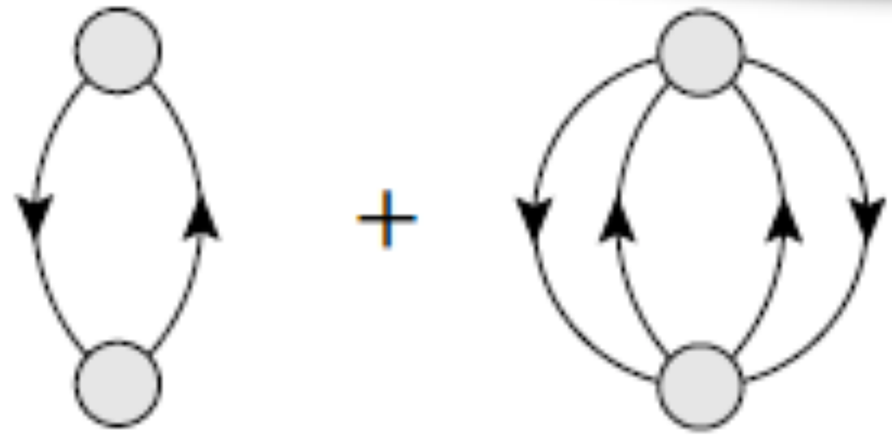
off-diagonal couplings are rapidly driven to zero

In-medium SRG flow equations

0-body Flow

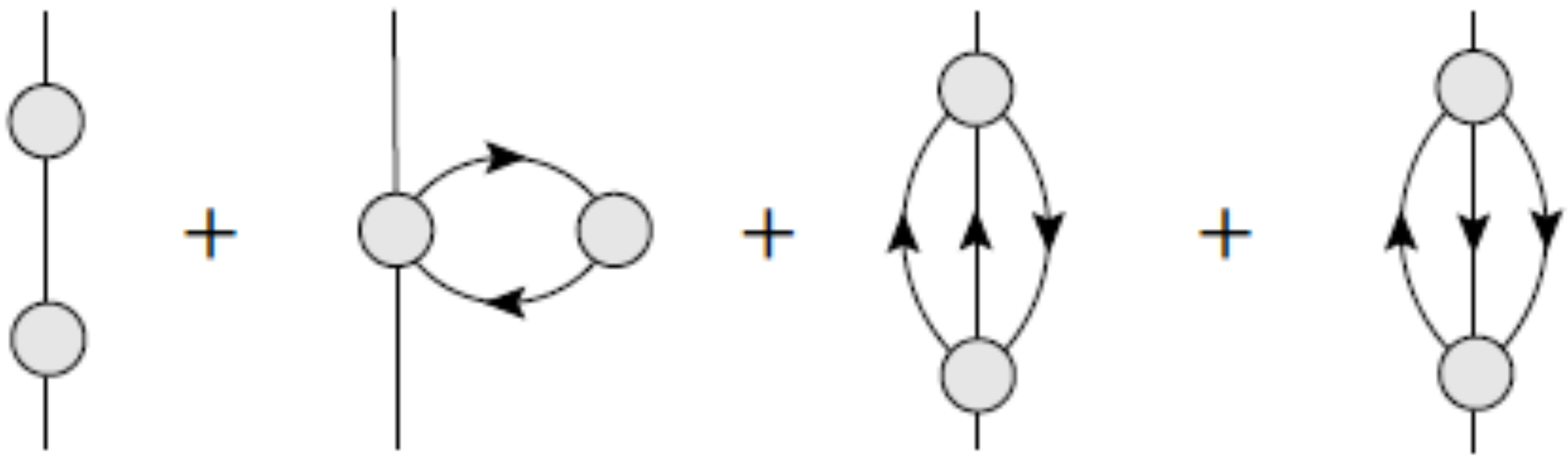
~ 2nd order MBPT for *H(s)*

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



1-body Flow

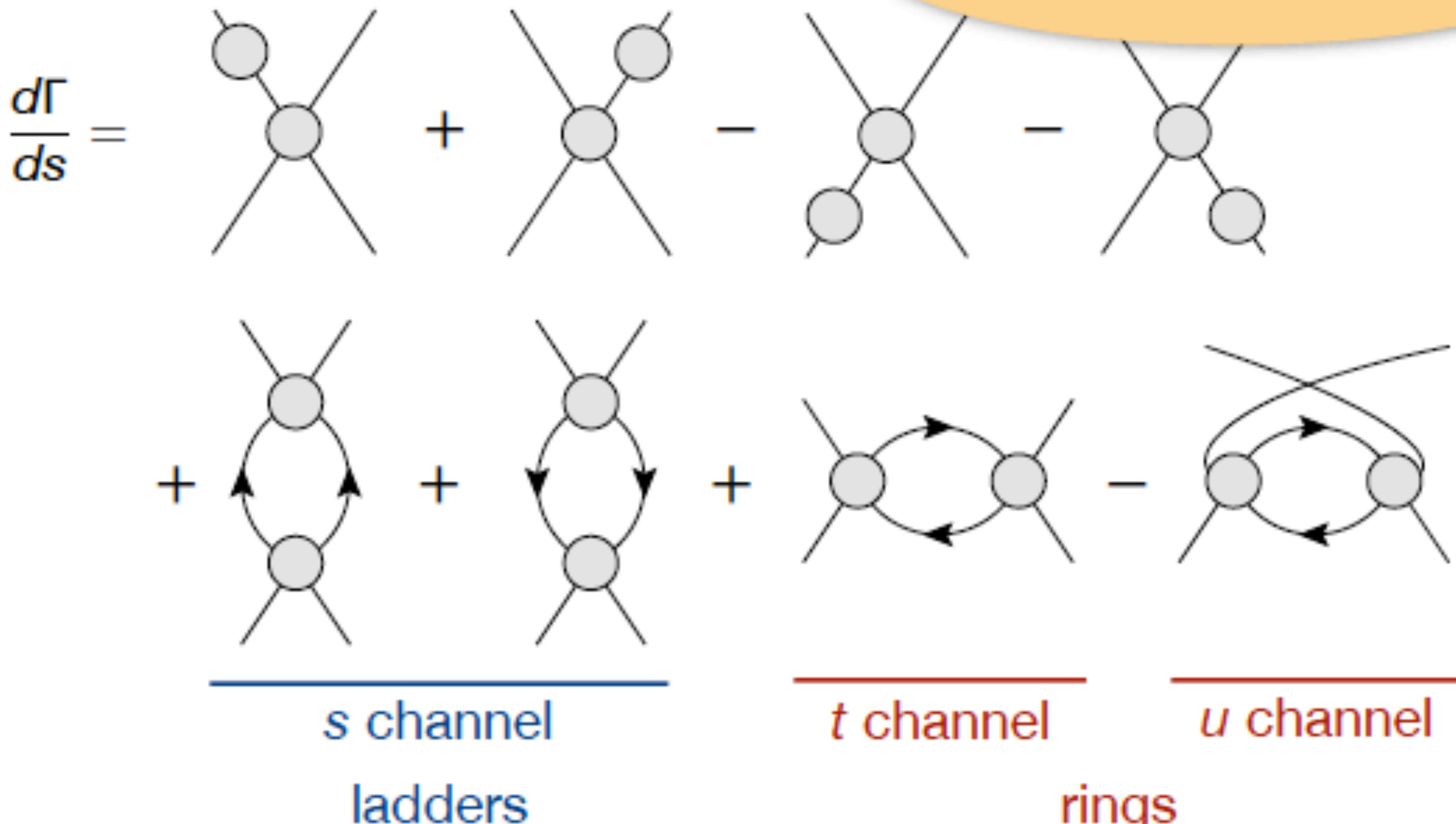
$$\frac{df}{ds} =$$



In-medium SRG flow equations

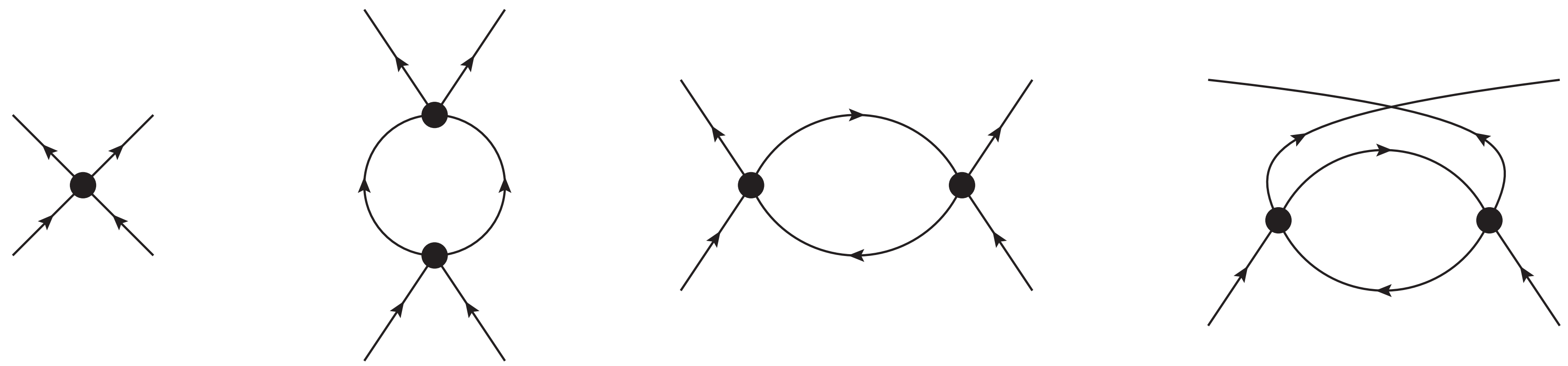
2-body Flow

O(N^6) scaling
(before particle/hole distinction)



Non-perturbative summation

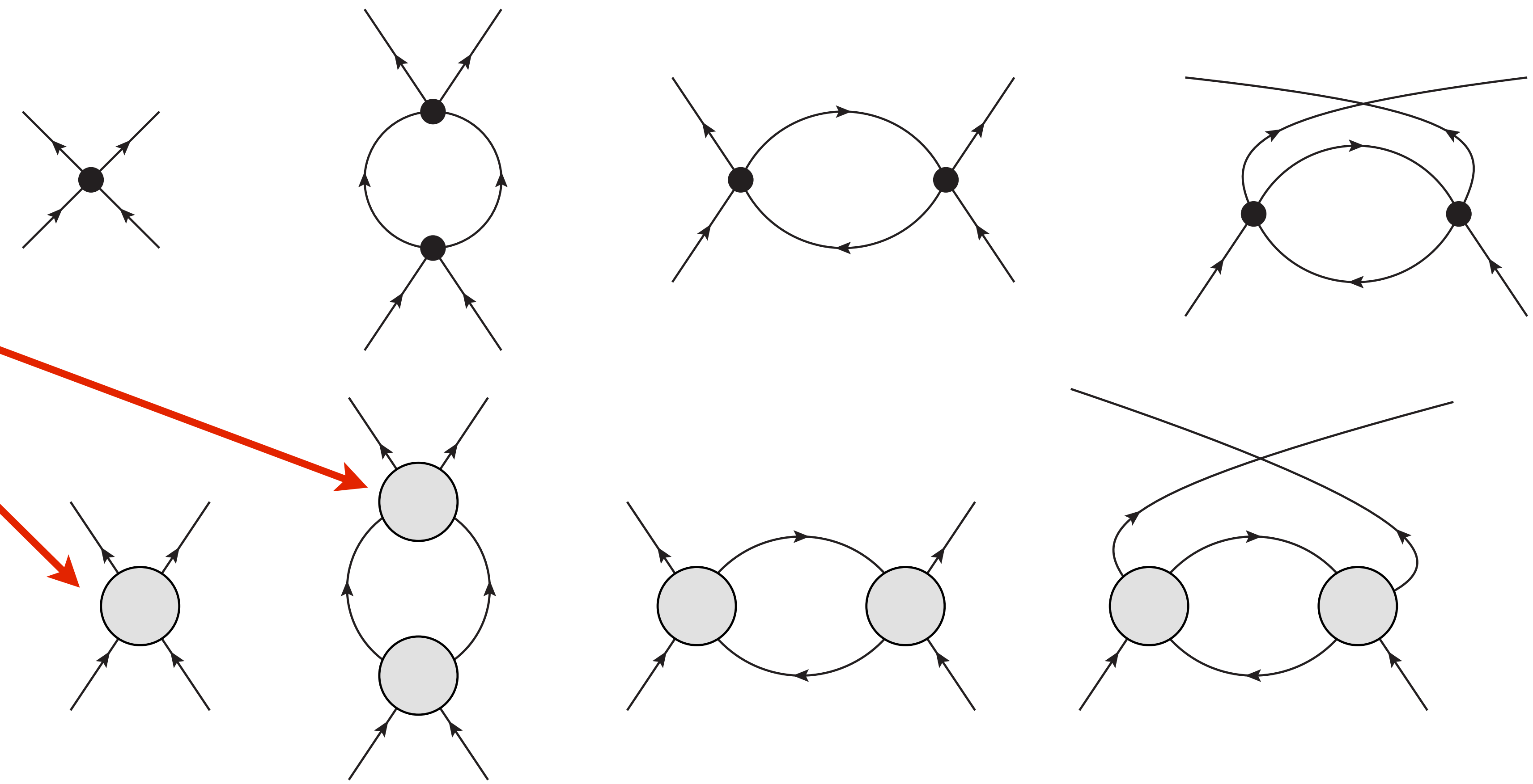
$$\Gamma(\delta s) \sim$$



Non-perturbative summation

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

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



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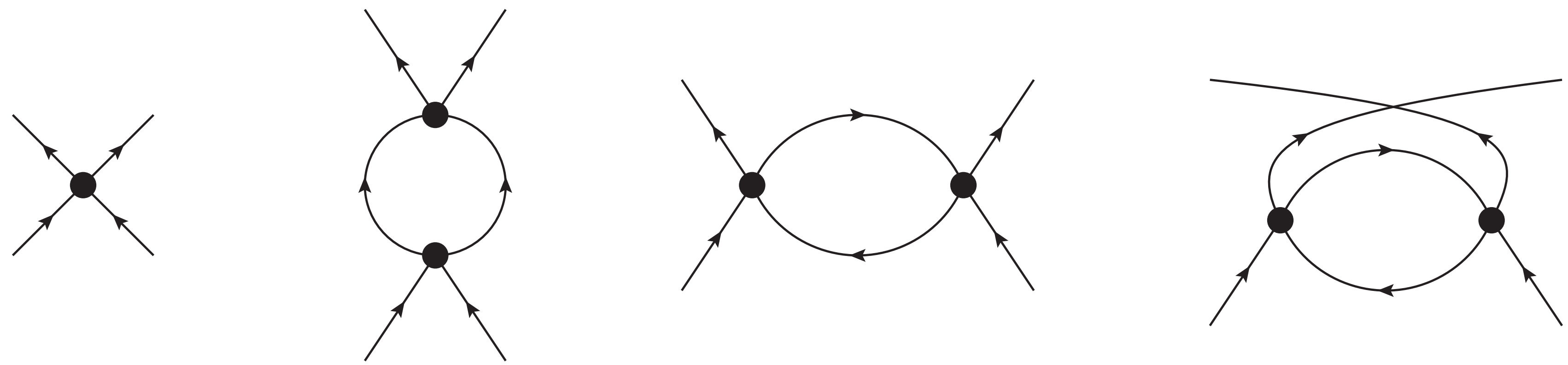
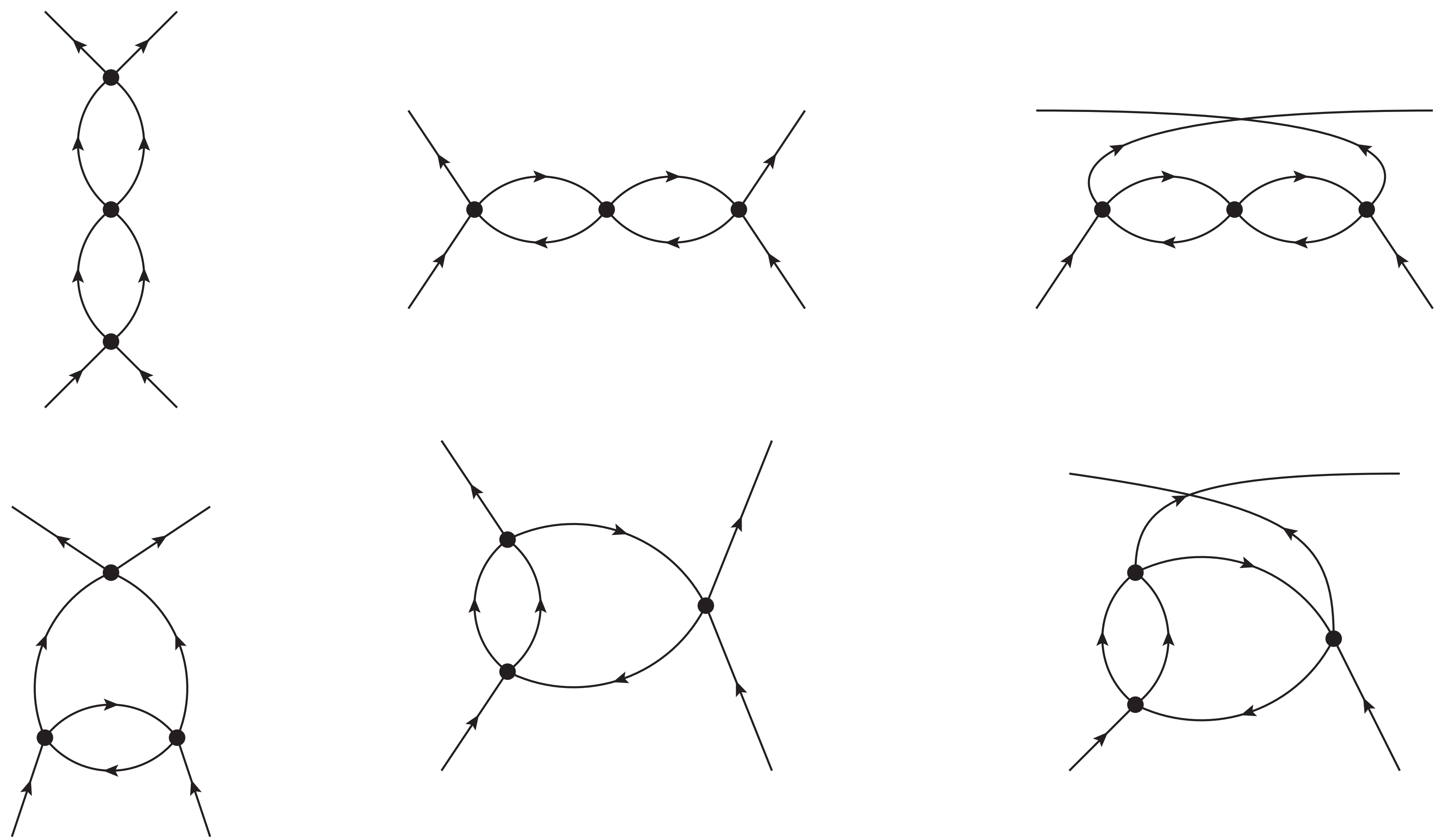


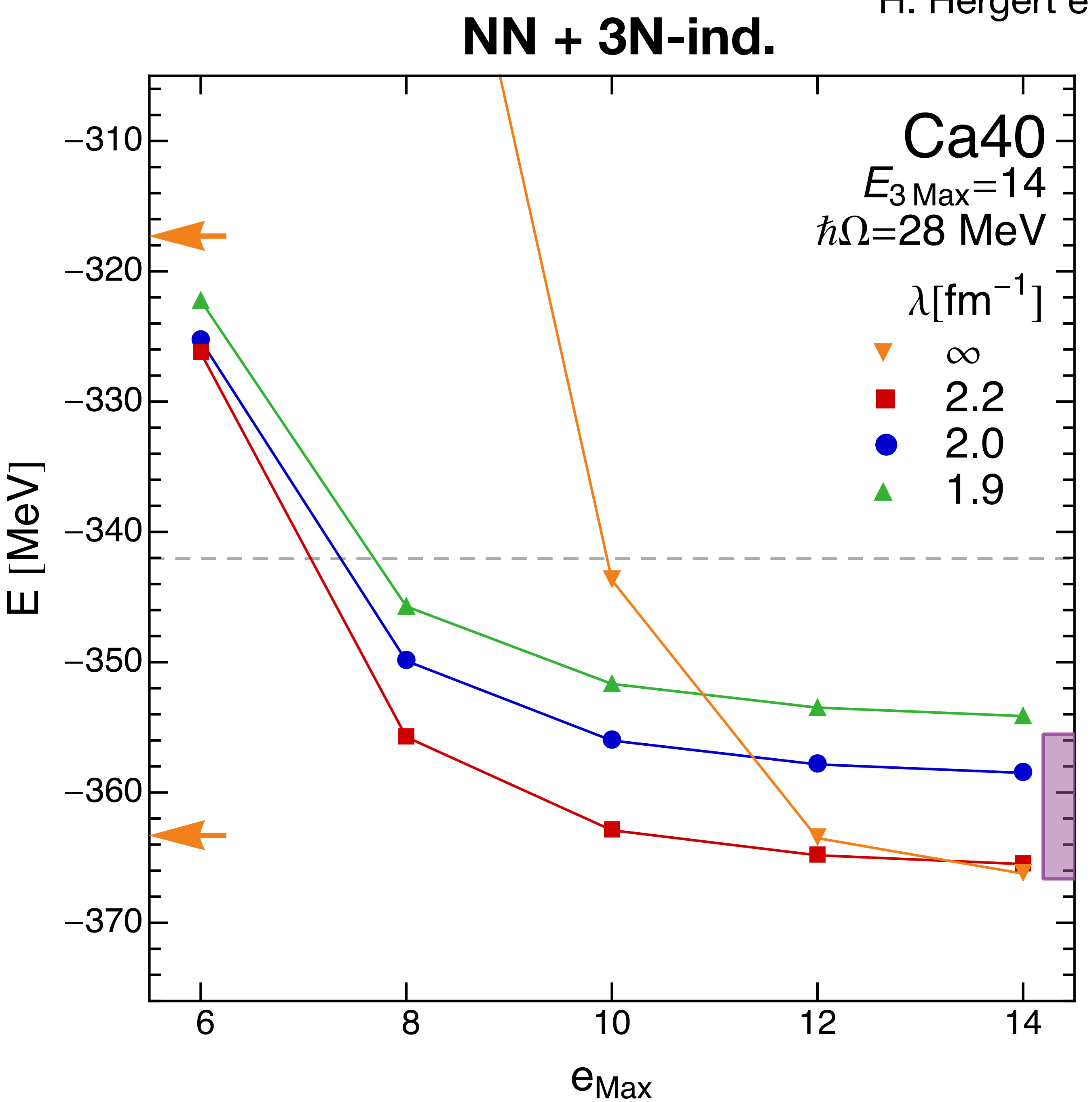
$\Gamma(2\delta s) \sim$



+ many more ...

Results: Closed-Shell Nuclei

H. Hergert et al., Phys. Rev. C **87**, 034307 (2013)



Bare N3LO(500) NN-only

Free-space SRG (NN + 3N-induced)

Normal-order in HF basis

IM-SRG(2) calculation

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)

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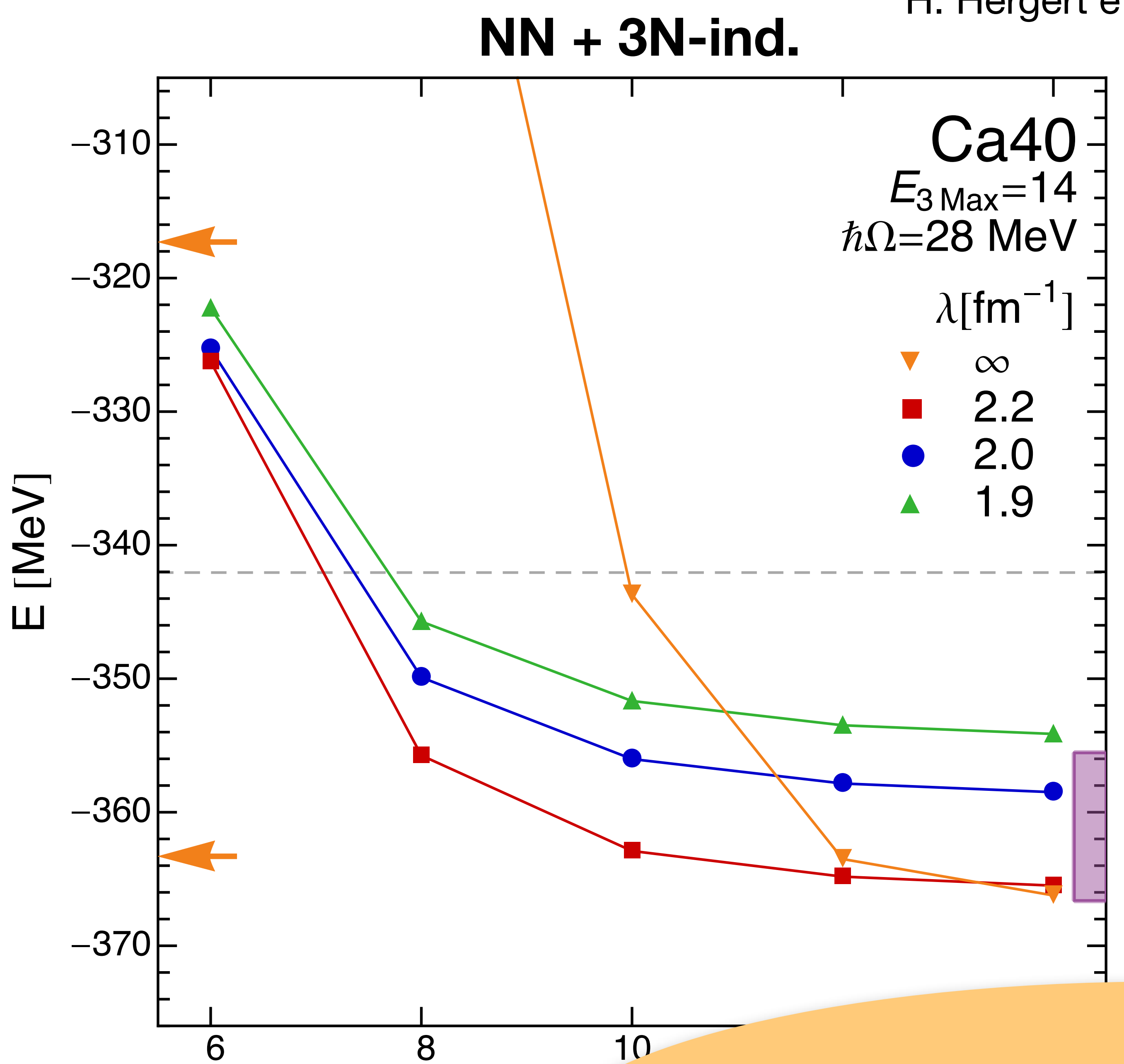

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Free-space SRG (NN + 3N-induced)

Normal-order in HF basis

...(2) calculation

IM-SRG(2) typically tracks Λ-CCSD(T) results

CCSD/Λ-CCSD(T), ...

Λ-CCSD(T), $\lambda = 1.9 - 2.2$ fm ... [nucl-th] & PRL 109, 052501 (2012)

Freedom of Choice for Generators

- Wegner

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

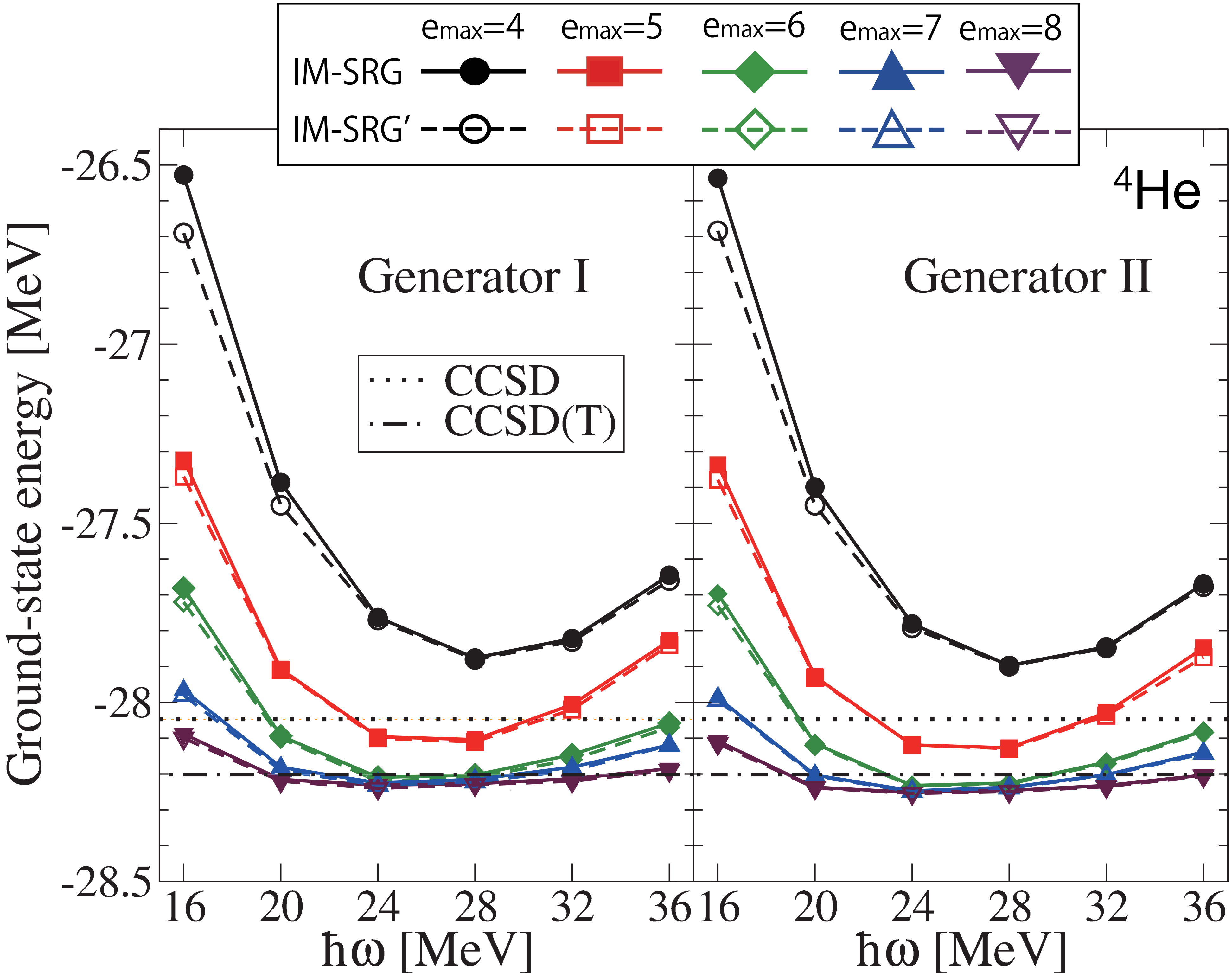
- White (J. Chem. Phys. 117, 7472)

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

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

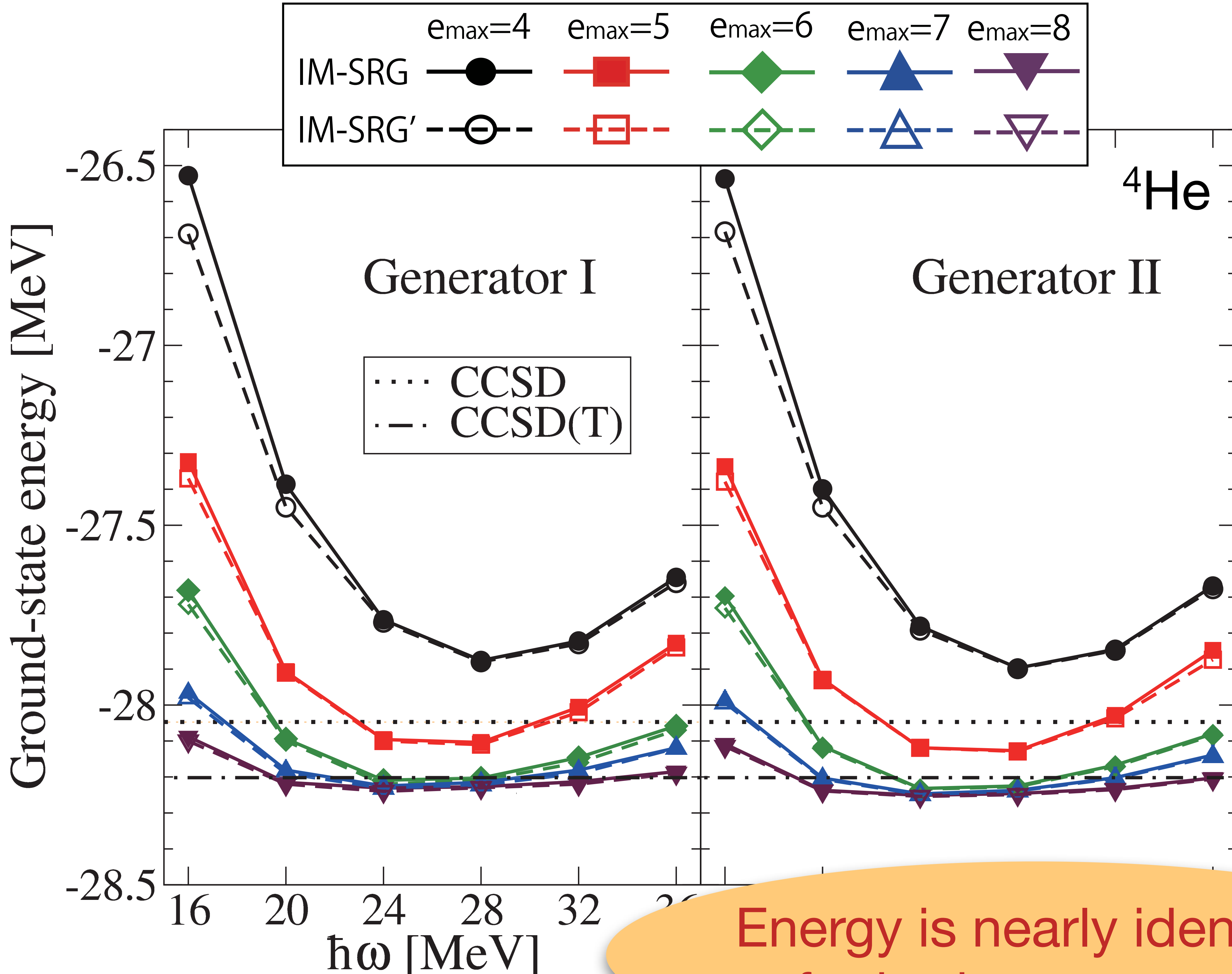
- g.s. energies ($s \to \infty$) for both generators agree within a few keV (measure of truncation error)

Generator Dependence



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

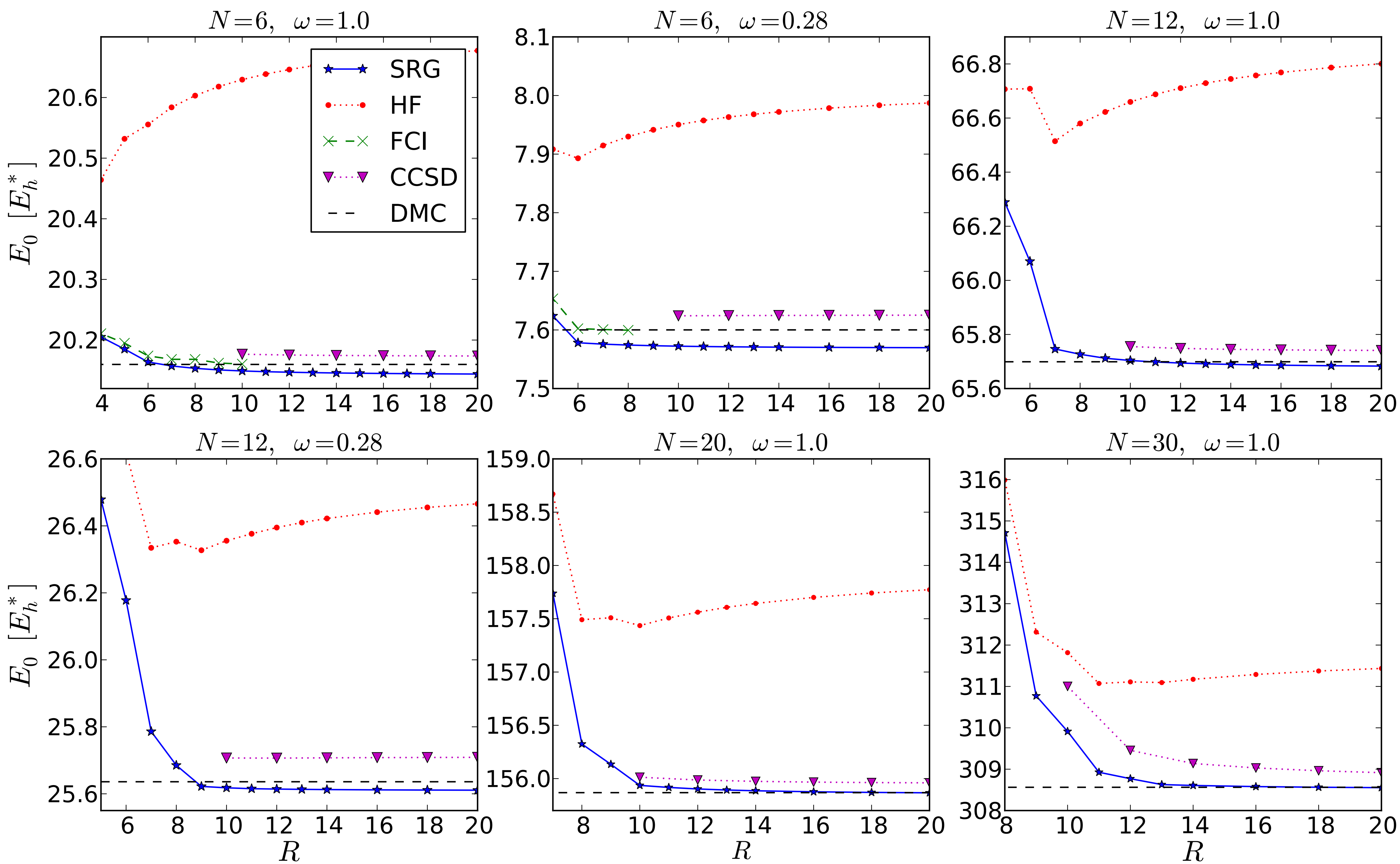
Generator Dependence



Energy is nearly identical for both generators!

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

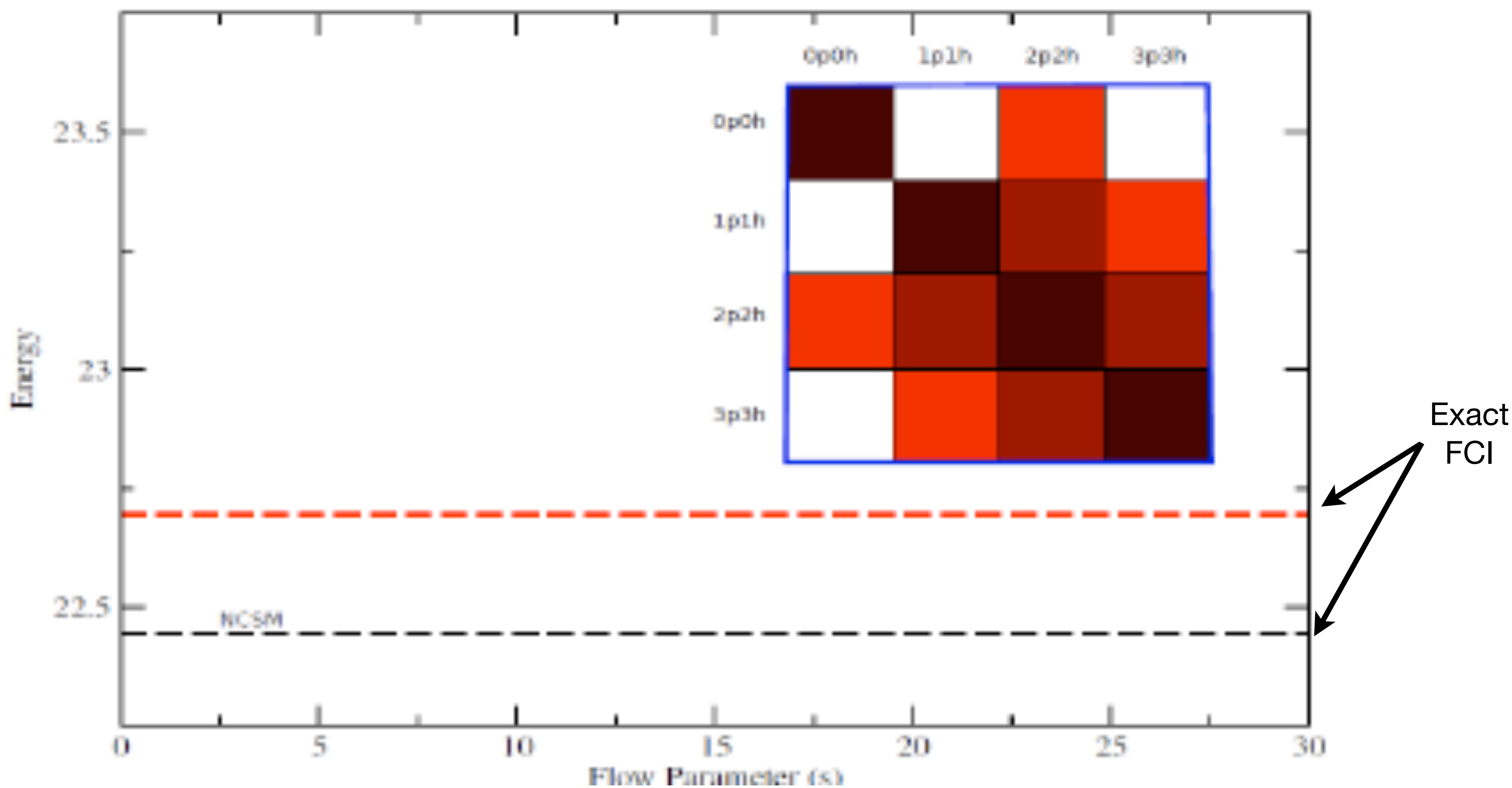
Non-nuclear application: Quantum Dots



Curiosity: higher accuracy than CCSD (both n^6 methods)

Extension to excited states

Ml=0 Ms=0 excited states in 2d Quantum Dots



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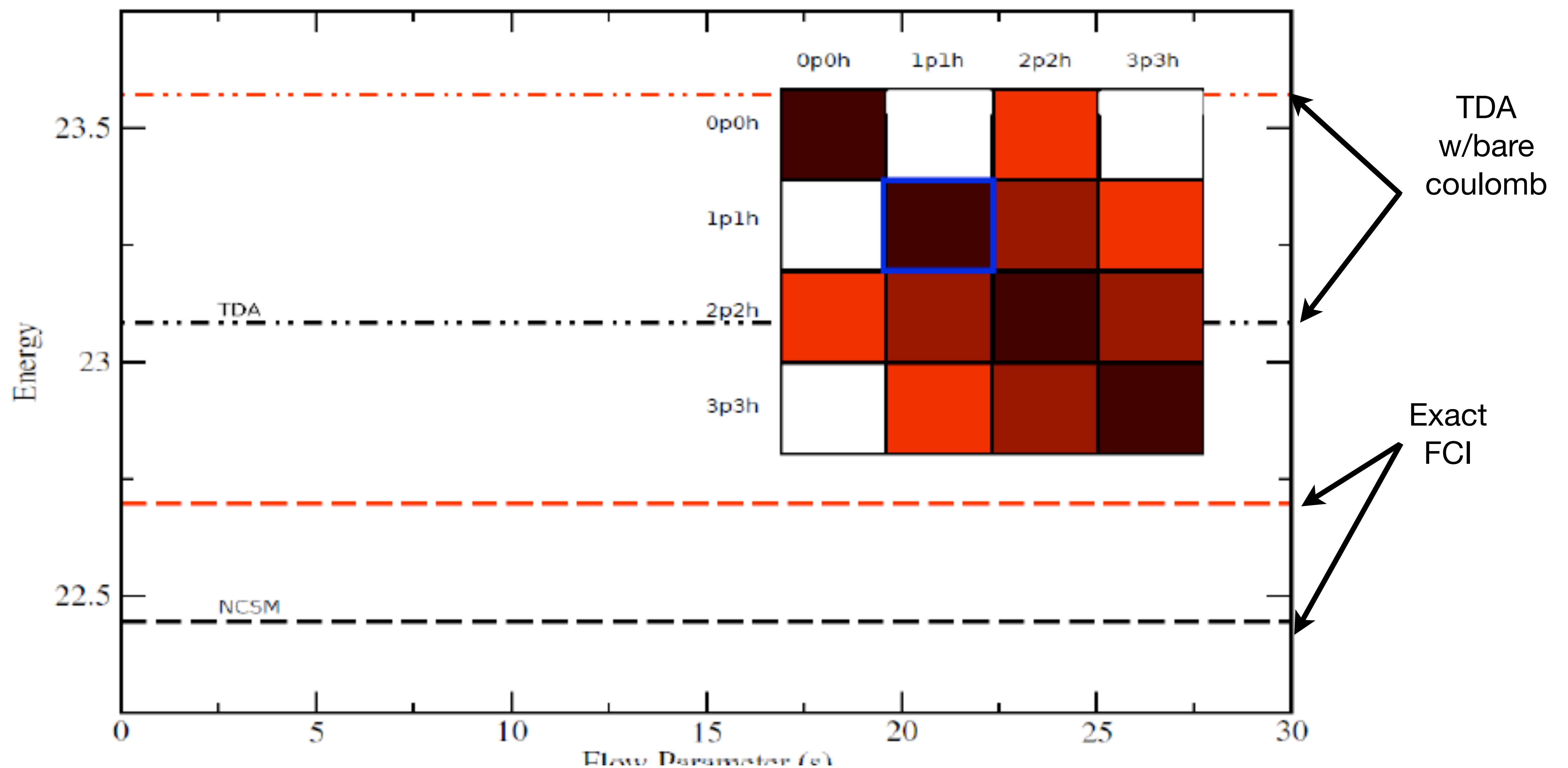
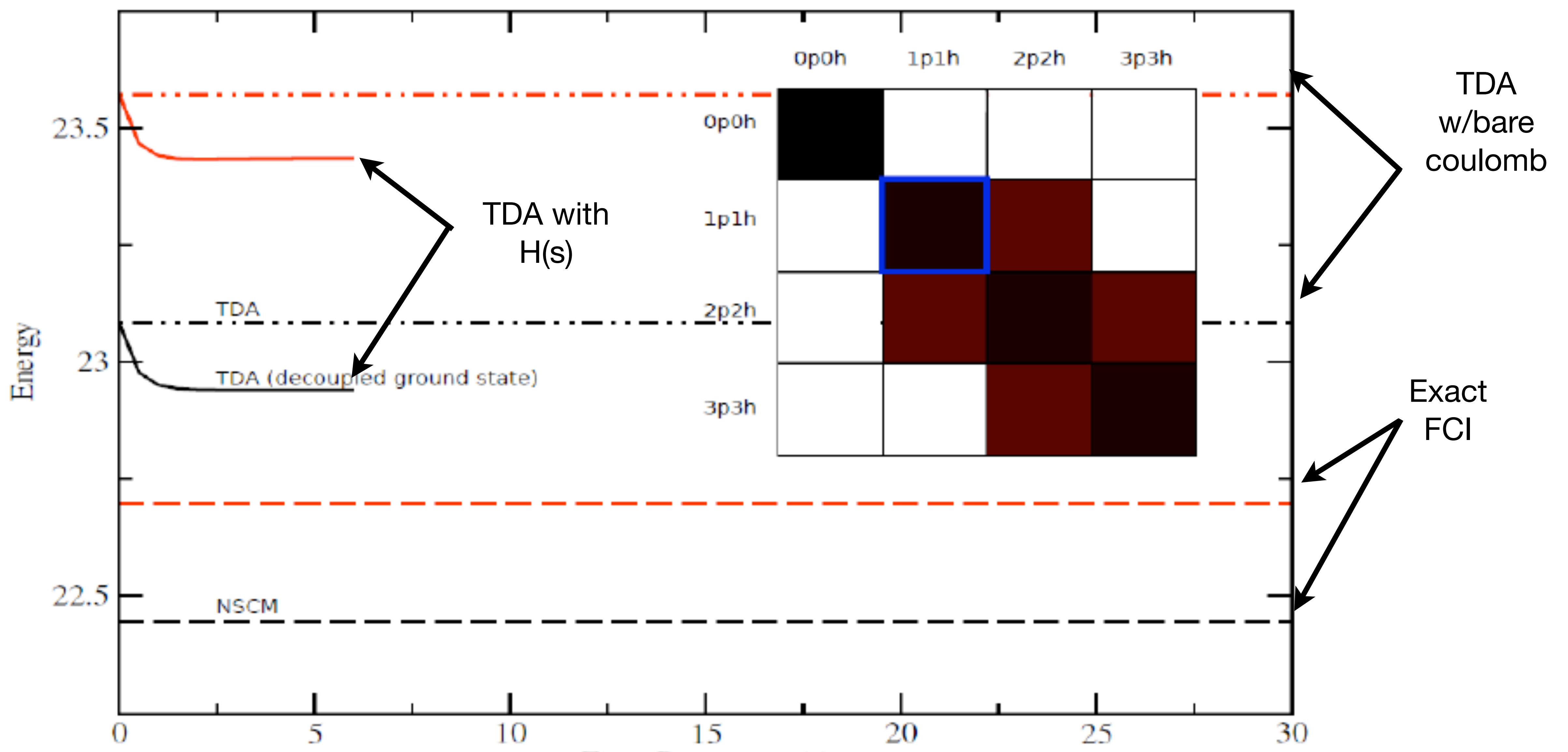


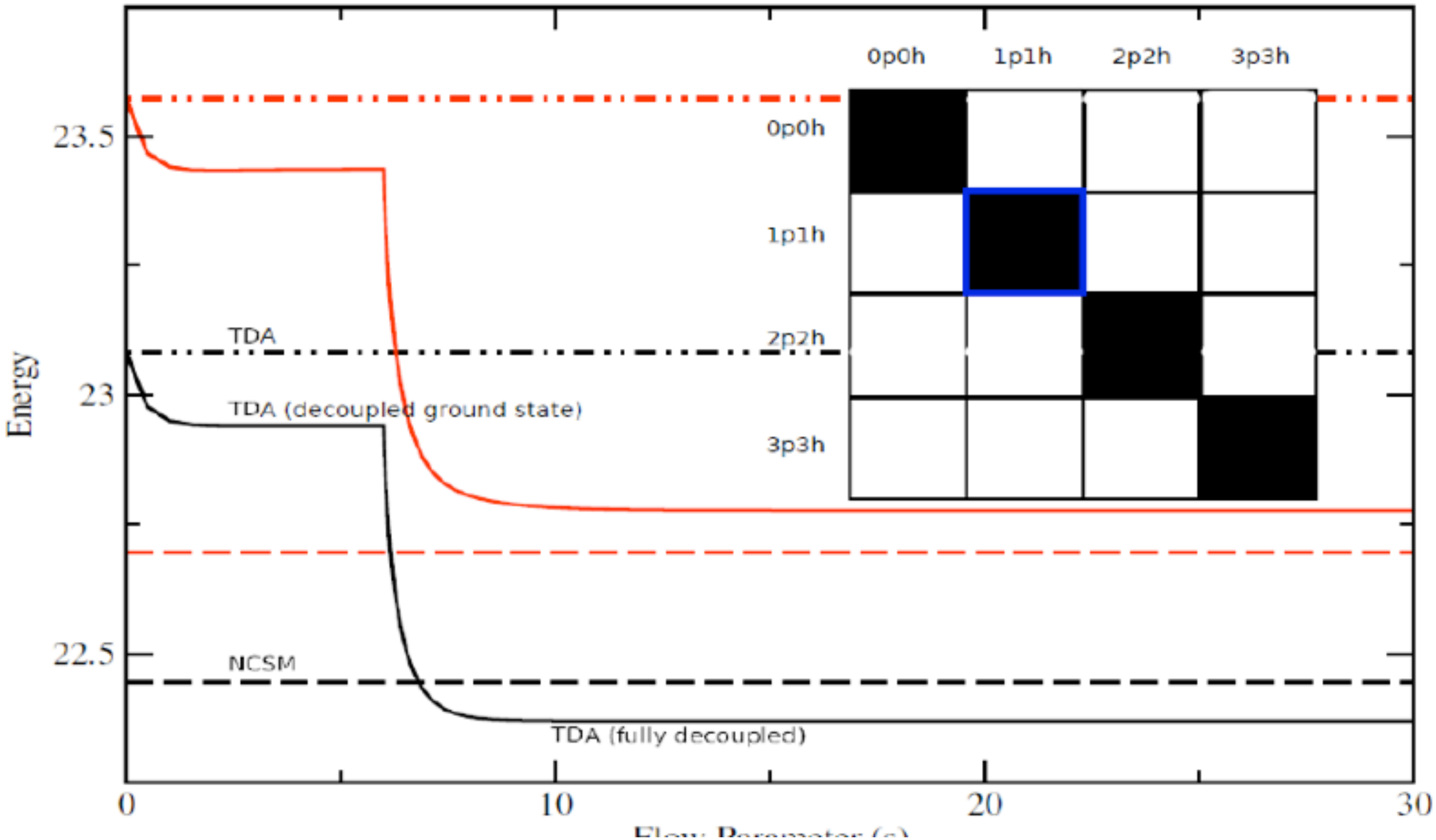
Extension to excited states

Ml=0 Ms=0 excited states in 2d Quantum Dots



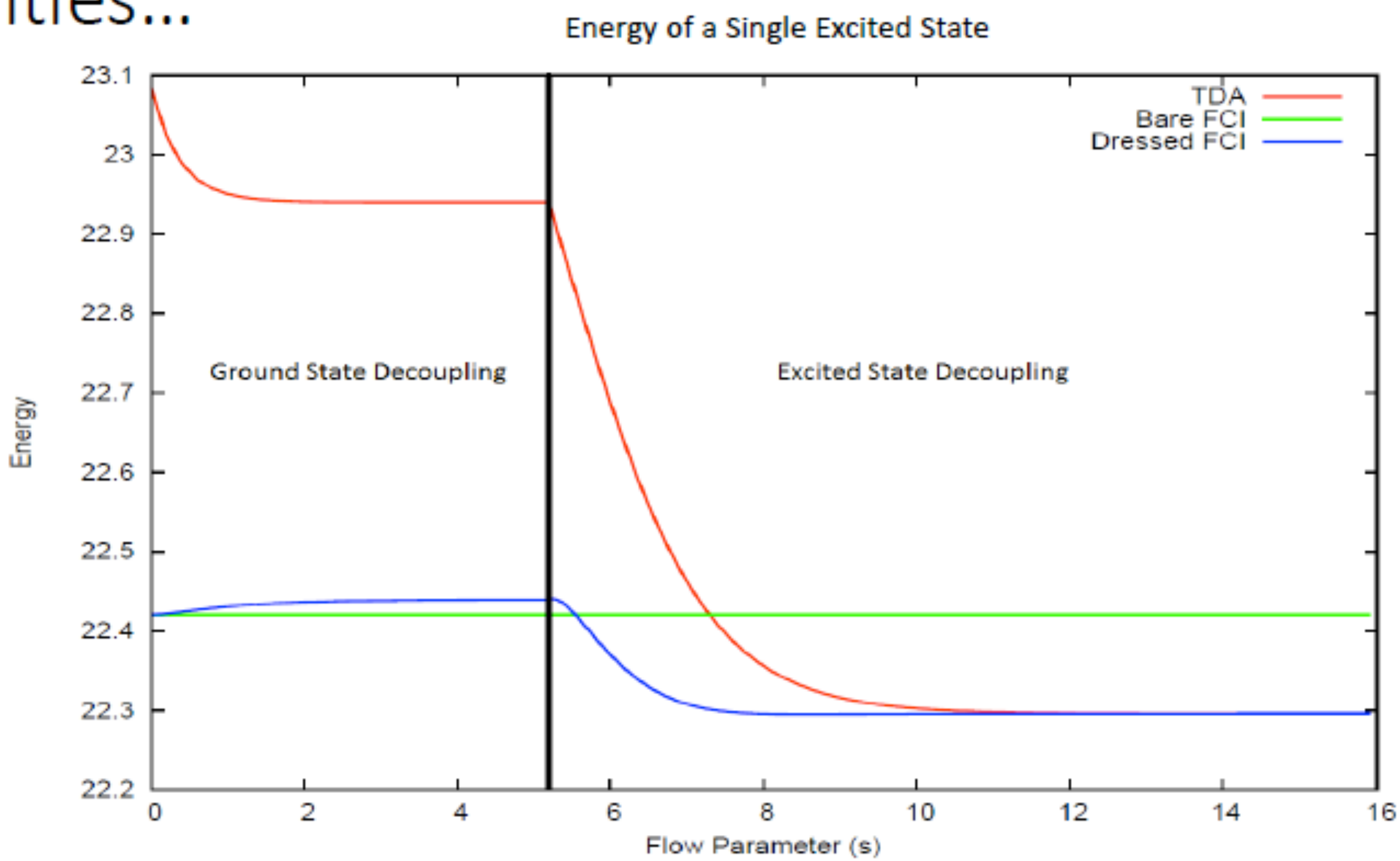
Extension to excited states

Ml=0 Ms=0 excited states in 2d Quantum Dots



Extension to excited states

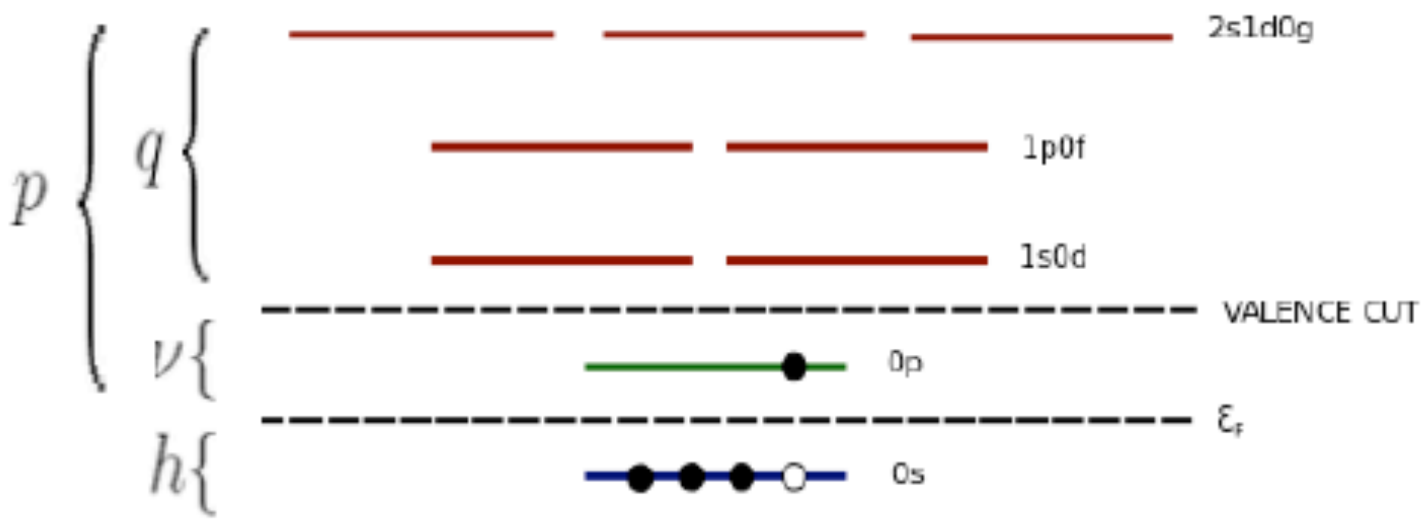
Difficulties...

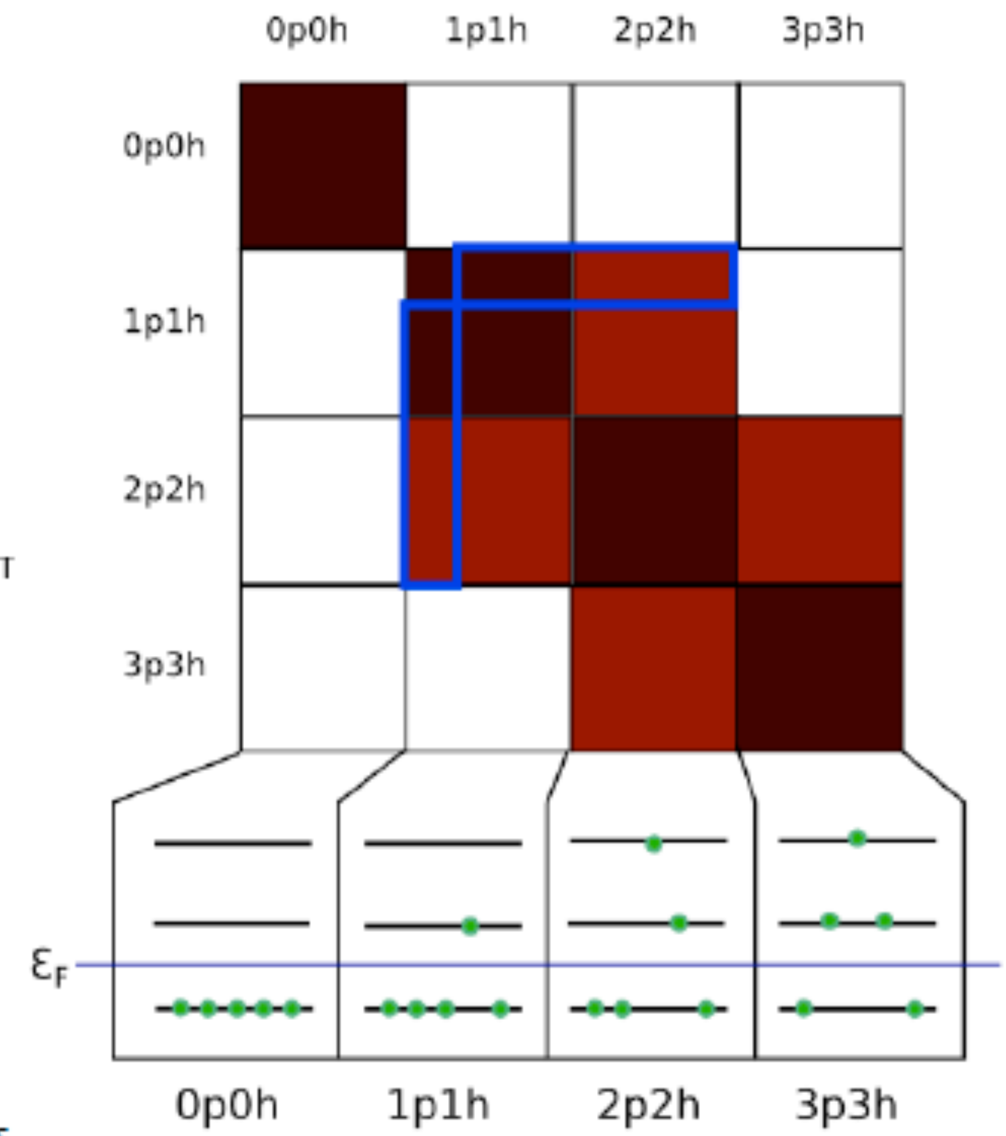


Over-rotation of H(s) in excited state decoupling?

Extension to excited states

Improved TDA calculation



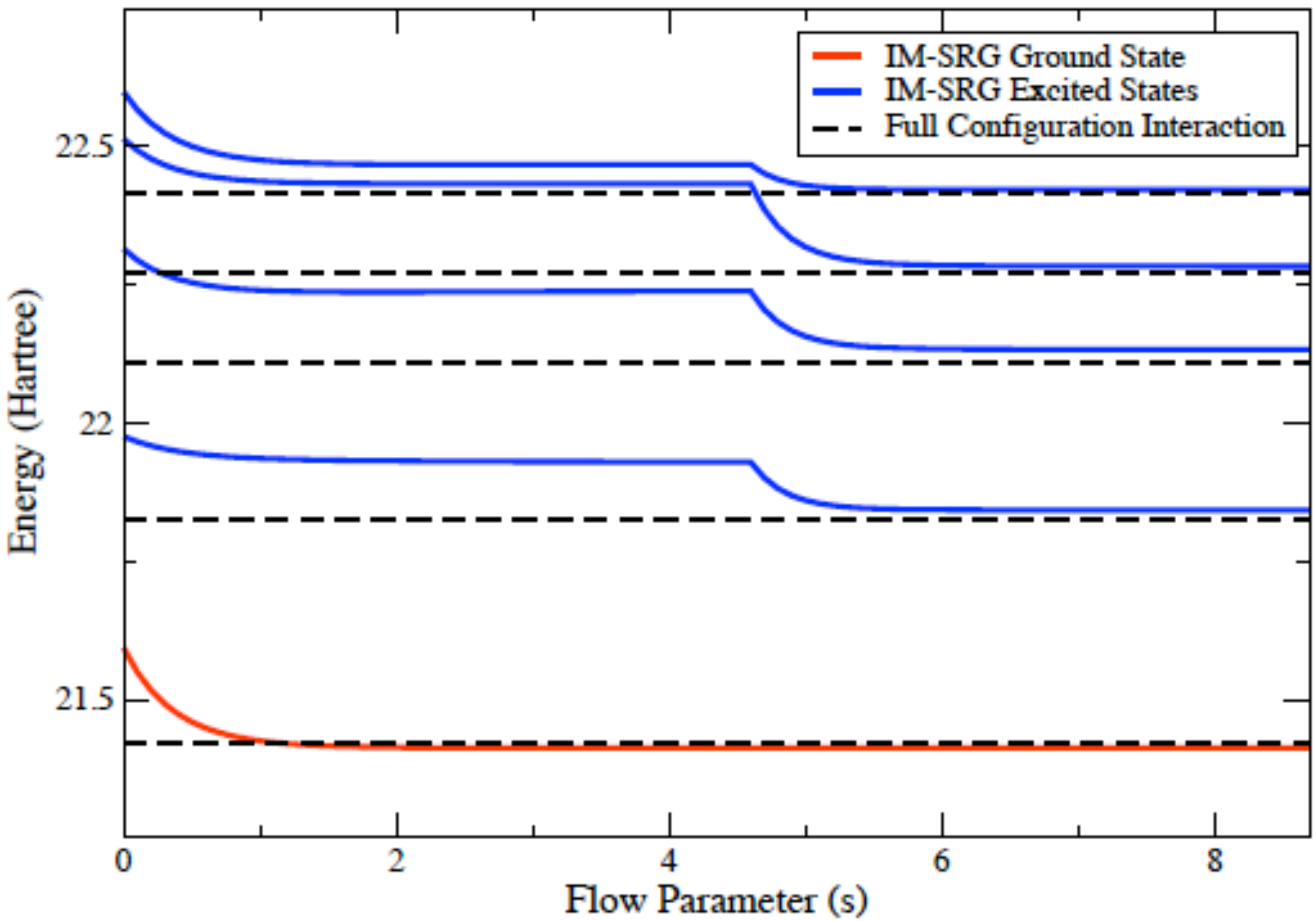


Smaller definition of off-diagonal leads to stable convergence

$$H^{od} : \{f_{q\nu}, \Gamma_{qh'\nu h}, \Gamma_{pp'\nu h}, \Gamma_{hph'h''}\}$$

A more minimal definition can be constructed using conserved quantities

Extension to excited states



IM-SRG for Open-Shell Systems

K. Tsukiyama, SKB and A. Schwenk, Phys. Rev. C **85**, 061304(R) (2012)
SKB, H. Hergert, J. D. Holt, A. Schwenk, S. Binder, A. Calci, J. Langhammer, and R. Roth, Phys. Rev. Lett. **113**, 142501 (2014)
H.Hergert, S. Binder, A. Calci, J. Langhammer, and R. Roth, Phys. Rev. Lett **110**, 242501 (2013)

IM-SRG for Open-Shell

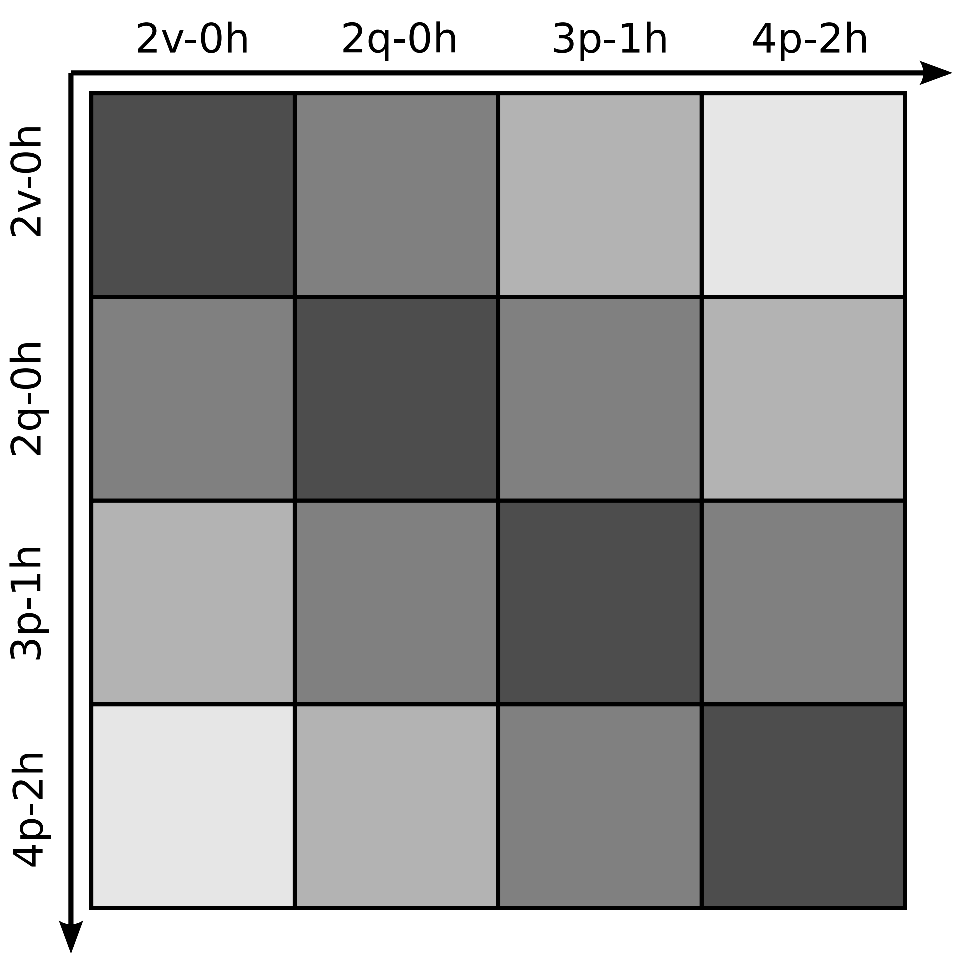
- Two possibilities

1. Use IM-SRG to derive effective hamiltonian/operators for valence shell model calculations [K. Tsukiyama, SKB, A. Schwenk PRC 85, 061304 (2012)]

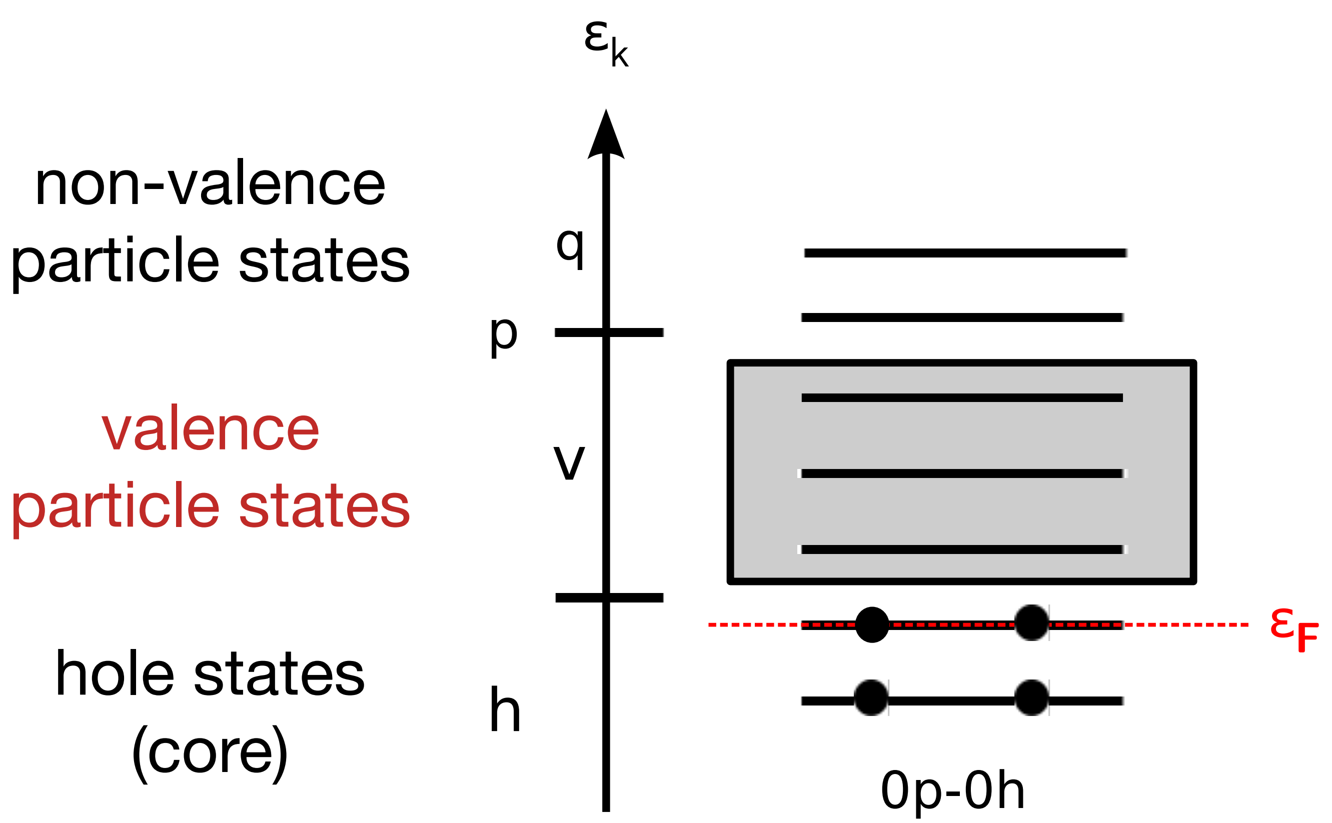
2. Solve open-shell directly with IM-SRG with suitable open-shell reference state (Multireference)
   - Number-projected HFB state

   H.Hergert, S. Binder, A. Calci, J. Langhammer, and R. Roth, Phys. Rev. Lett **110**, 242501 (2013)

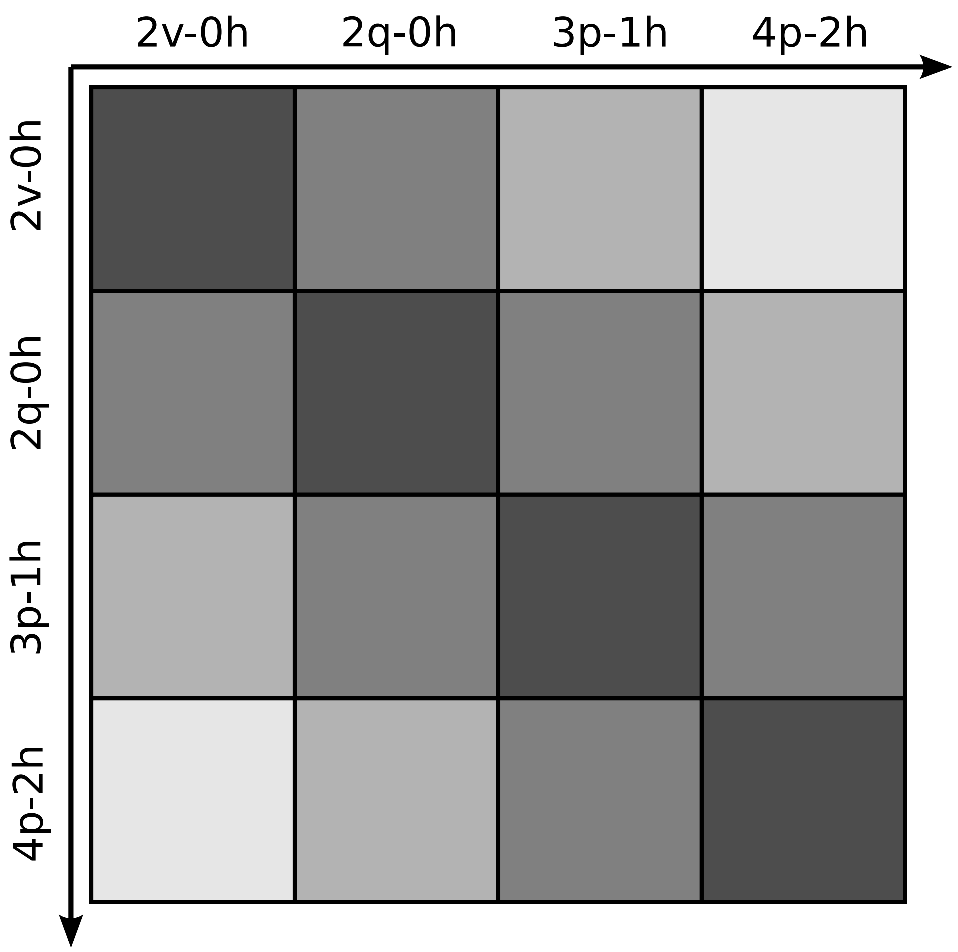
Valence Shell Model Decoupling



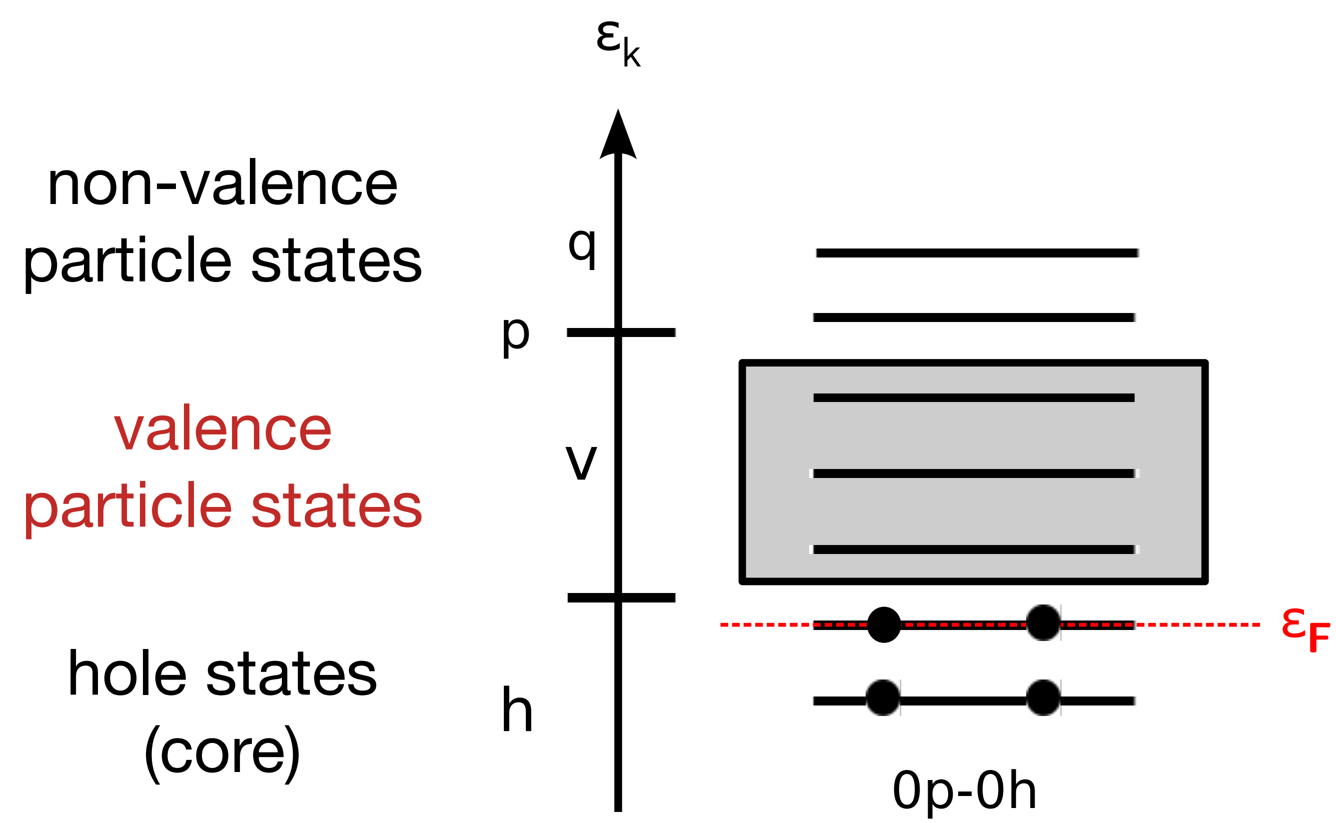
$\langle i | H | j \rangle$



Valence Shell Model Decoupling



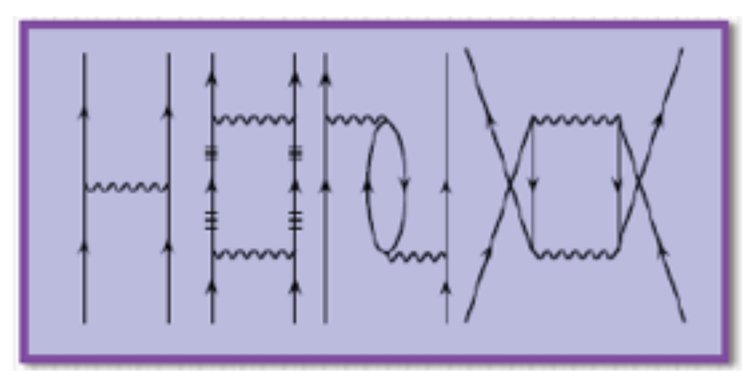
$$\langle i | H | j \rangle$$



Solve SM problem

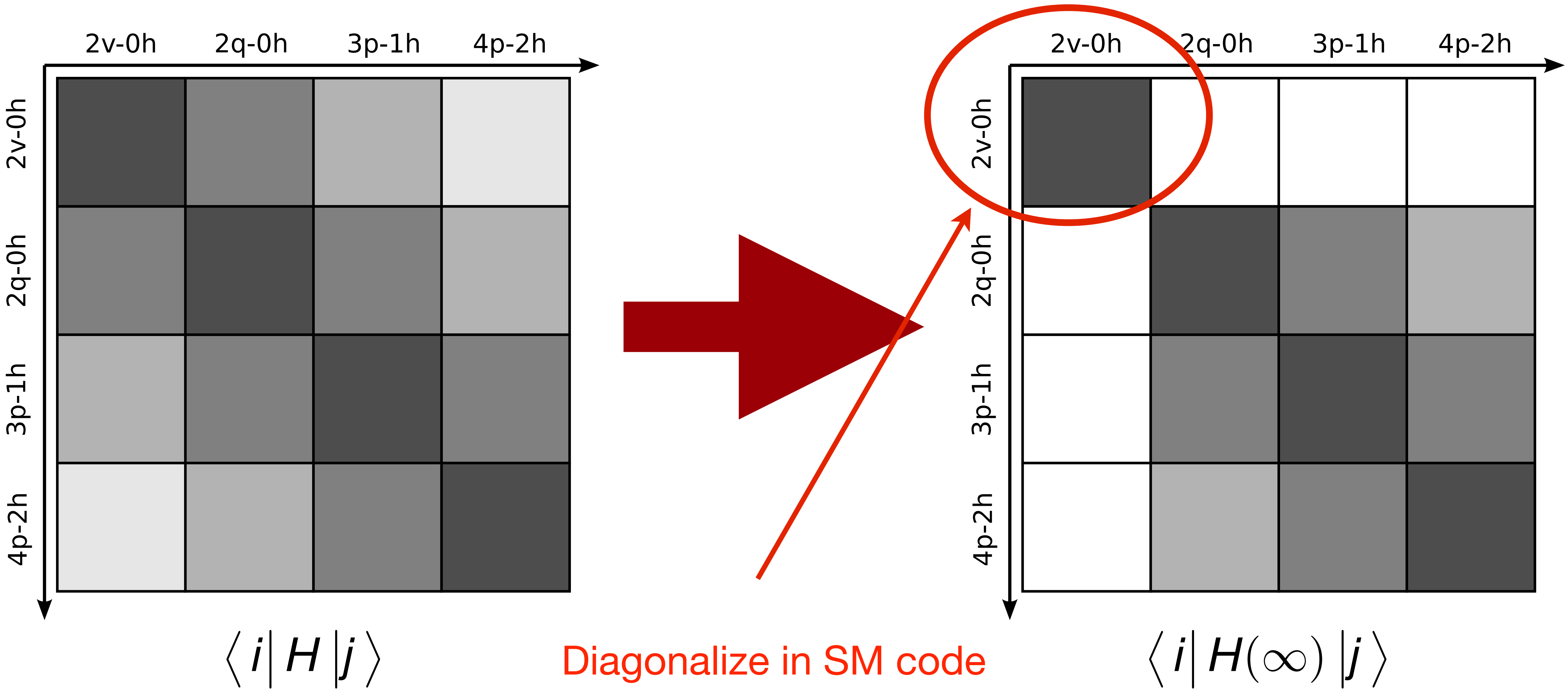
$$P H_{eff} P|\Psi\rangle = (E - E_c) P|\psi\rangle$$

Previously, H_{eff} from MBPT

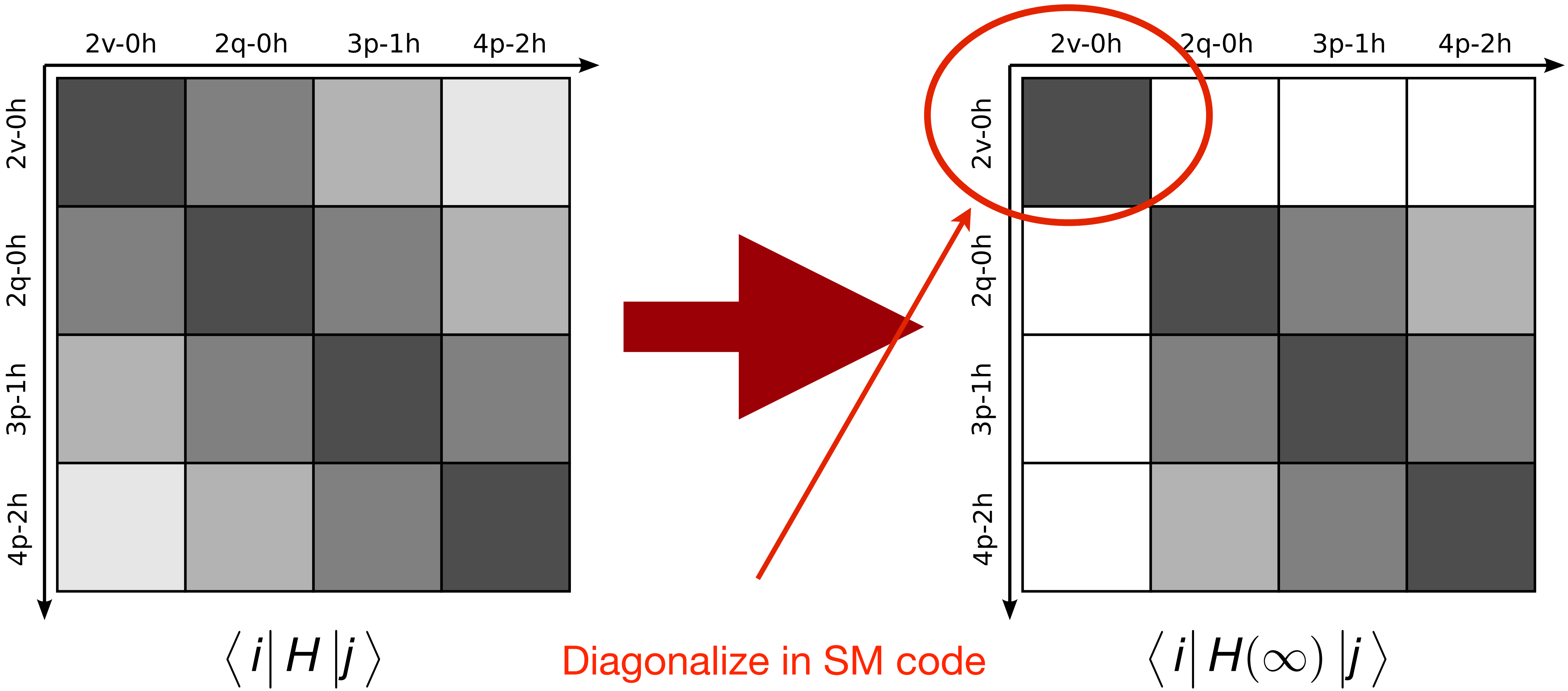


Can we use the IM-SRG to do this?

Valence Shell Model Decoupling



Valence Shell Model Decoupling

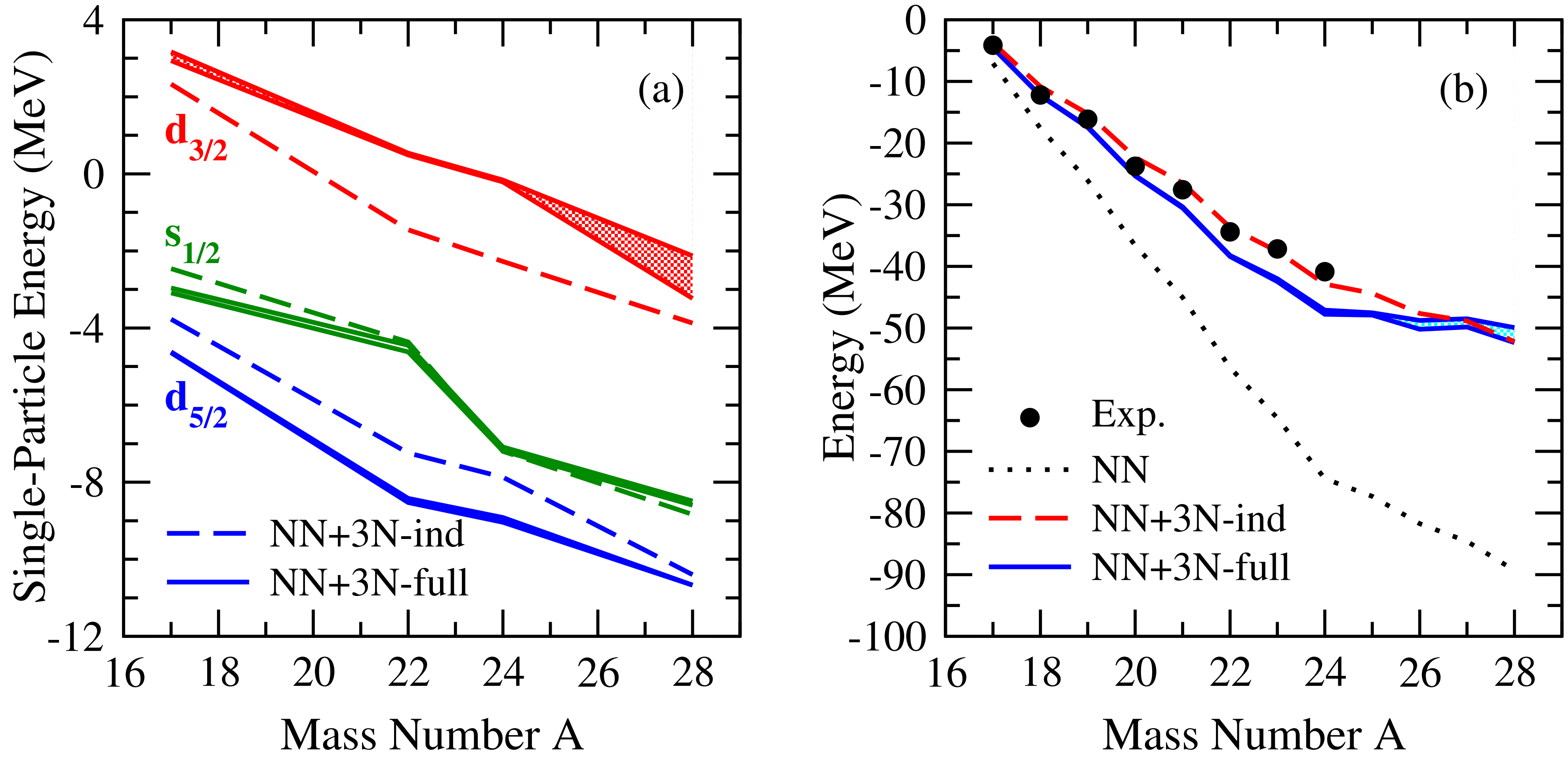


- use White-type generator with off-diagonal Hamiltonian

$$\left\{H^{od}\right\} = \{f_{h'}^{h}, f_{p'}^{p}, f_{h}^{p}, f_{v}^{q}, \Gamma_{hh'}^{pp'}, \Gamma_{hv}^{pp'}, \Gamma_{vv'}^{pq}\} \text{ \& H.c.}$$

Oxygen isotopes from NN + NNN

SKB et al., arXiv:1402.1407

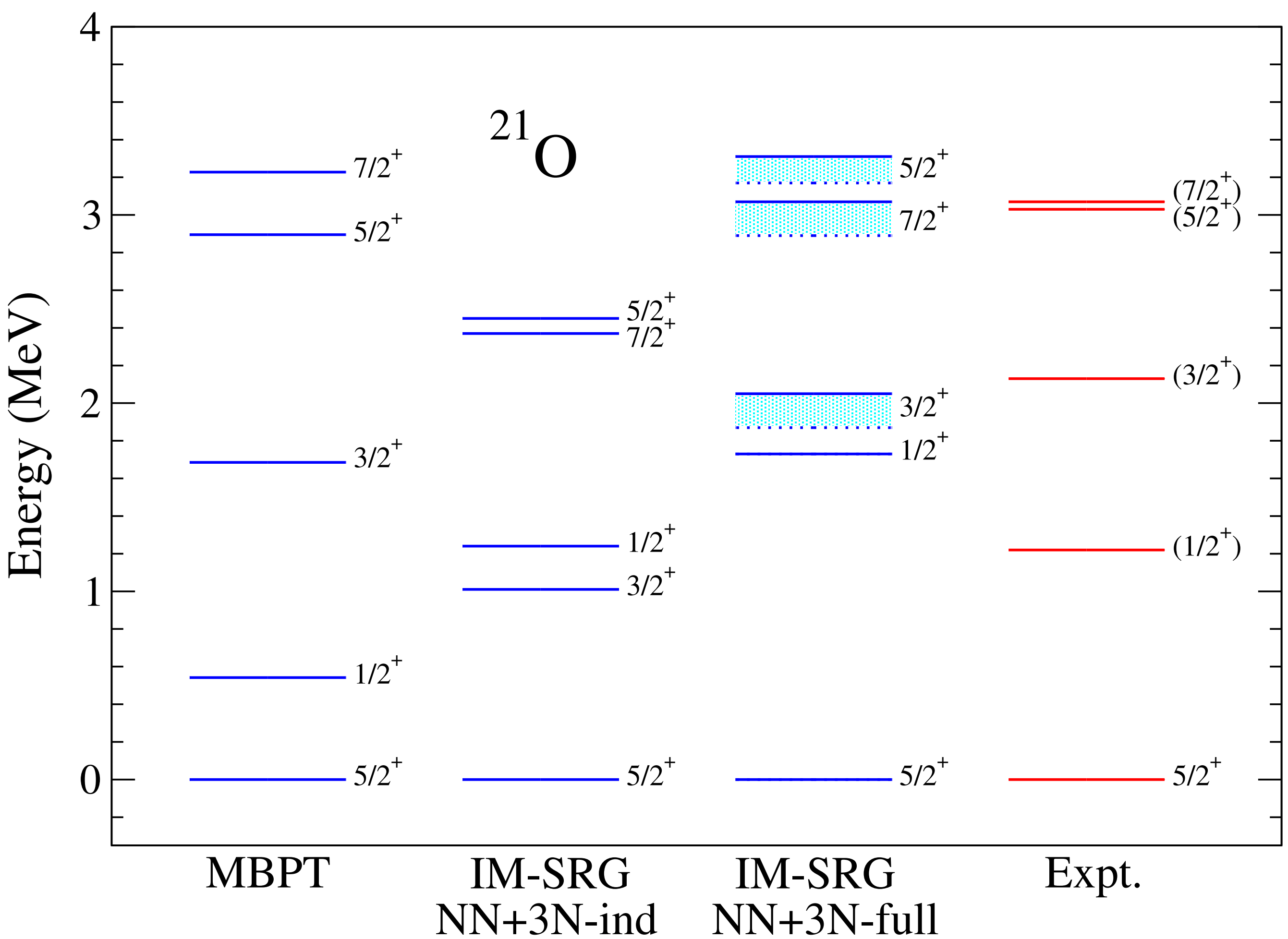


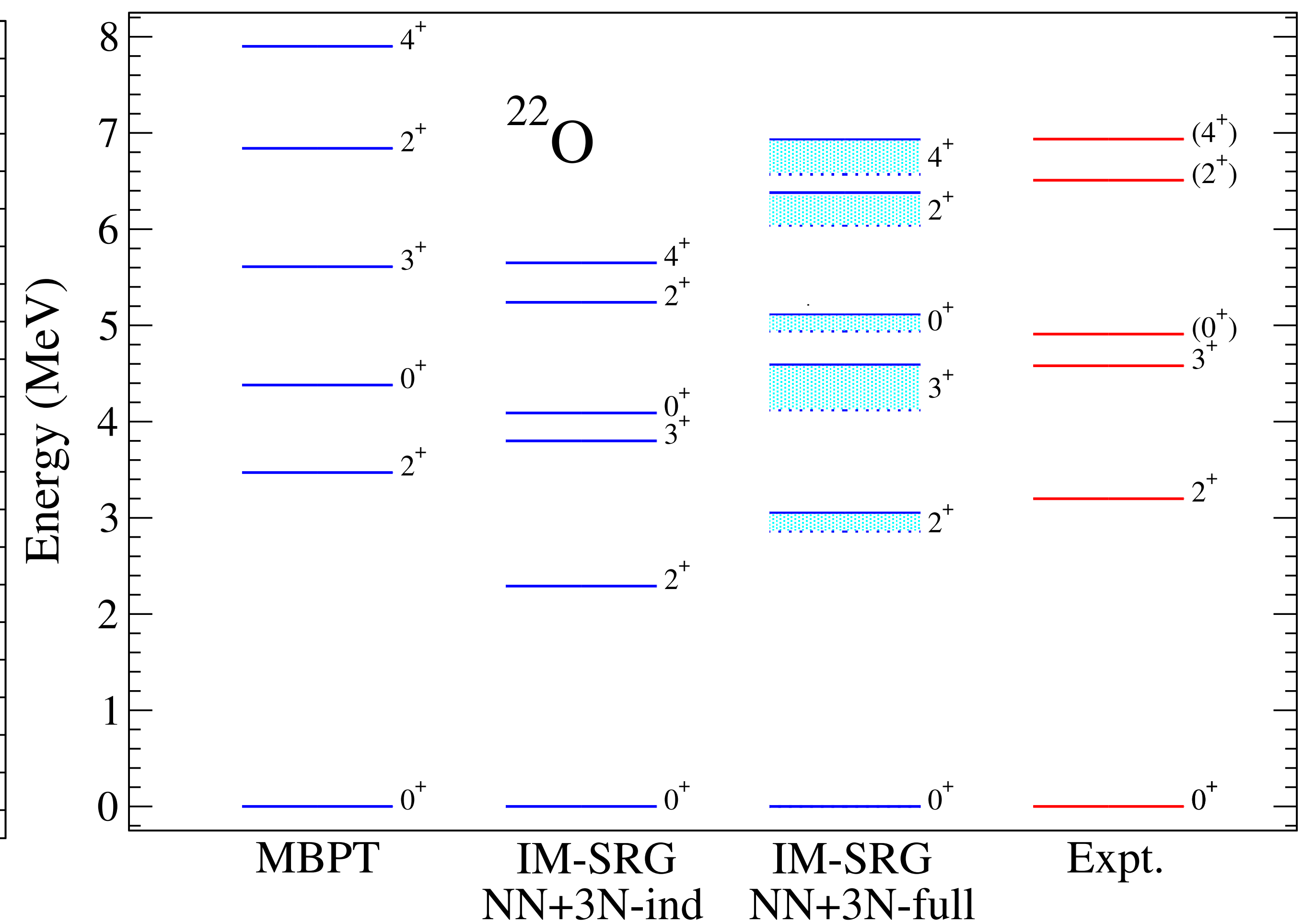
NN + 3N-ind = N3LO(500) NN, SRG-evolved to λ, omits induced 4N

NN + 3N-full = N3LO(500) NN + N2LO(400) 3N, SRG-evolved to λ, omits induced 4N

Oxygen Spectra

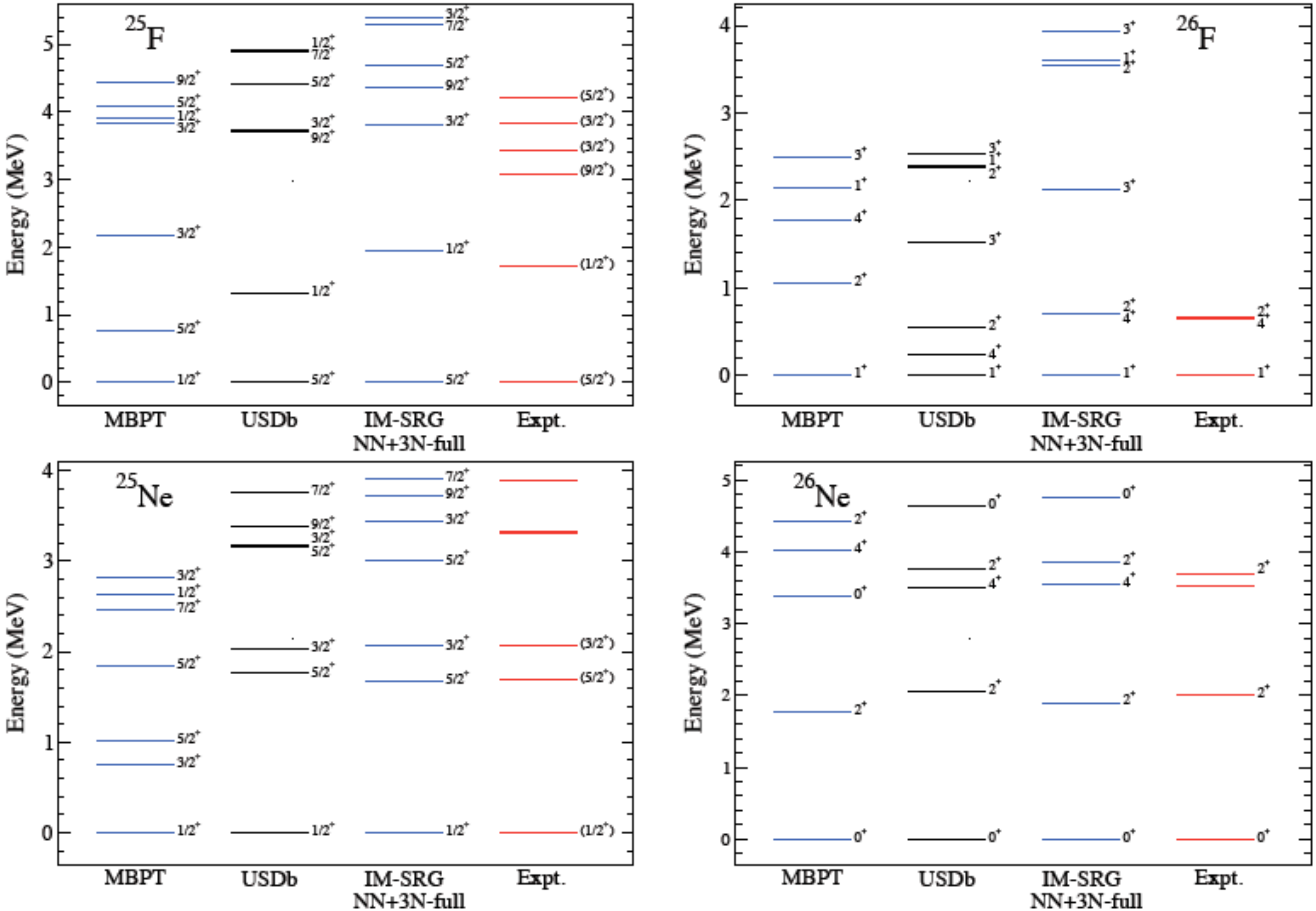
SKB et al., arXiv:1402.1407





- Importance of 3NF's
- No need for extended valence space (a-la MBPT)
- weak $\hbar\omega$ dependence (20-24 MeV)

Fluorine and Neon



Multi-reference IM-SRG (Heiko's talk)

- IM-SRG Shell model approach gives easy access to spectra, odd-nuclei, intrinsic deformation, etc., but limited by cost of diagonalization
- Is it possible to use IM-SRG directly to solve for open-shell systems?

Yes! Provided we use a reference state that's appropriate for an open-shell nucleus.

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

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

Multi-reference In-Medium SRG

- generalized normal ordering & Wick theorem for arbitrary reference state (Kutzelnigg & Mukherjee)
- ref. state correlations are encoded in irreducible n-body density matrices:

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

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

- additional terms in normal-ordered operators:

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

- additional contractions, e.g.,

$$:A^{ab}_{cd}::A^{kl}_{mn}: = \lambda^{ab}_{mn} :A^{kl}_{cd}:$$

$$:A^{abc}_{def}::A^{klm}_{nop}: = -\lambda^{abm}_{dop} :A^{ckl}_{efn}:$$

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

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:

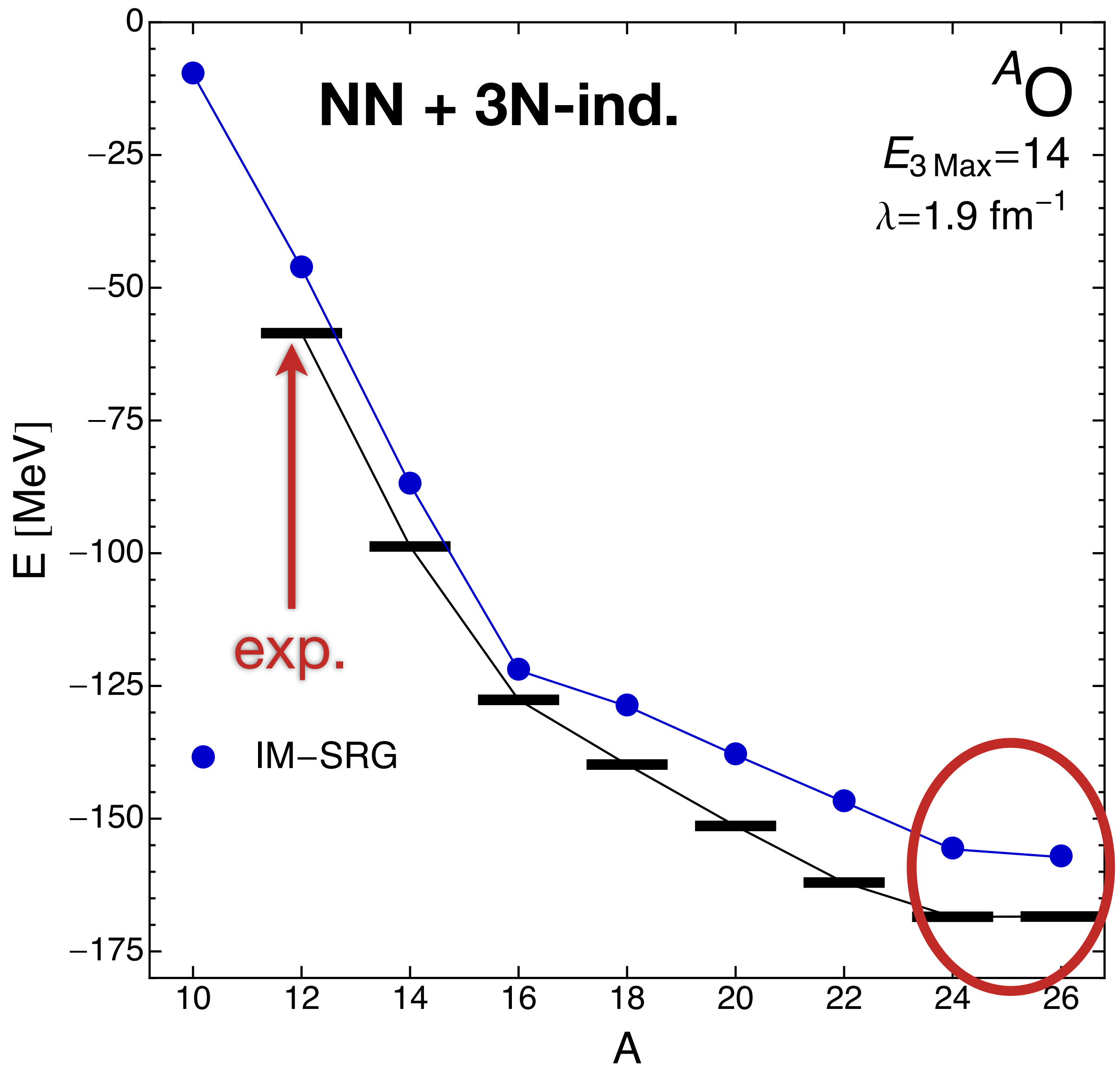
$$\frac{d}{ds}\Gamma^{12}_{34} = \sum_a \left(\eta^1_a \Gamma^{a2}_{34} + \eta^2_a \Gamma^{1a}_{34} - \eta^a_3 \Gamma^{12}_{a4} - \eta^a_4 \Gamma^{12}_{3a} - f^1_a \eta^{a2}_{34} - f^2_a \eta^{1a}_{34} + f^a_3 \eta^{12}_{a4} + f^a_4 \eta^{12}_{3a}\right)$$

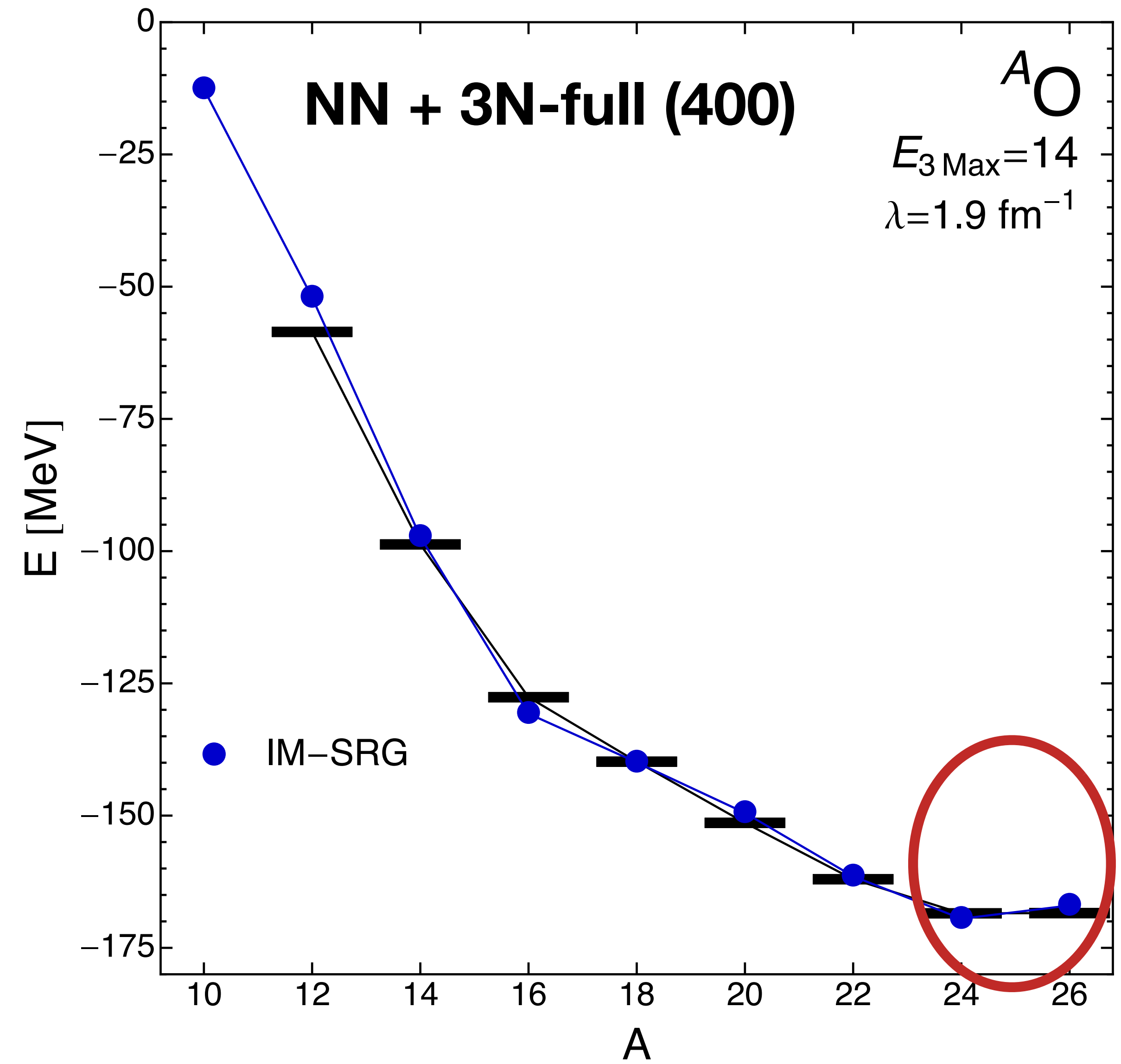
$$+ \frac{1}{2}\sum_{ab}\left(\eta^{12}_{ab}\Gamma^{ab}_{34} - \Gamma^{12}_{ab}\eta^{ab}_{34}\right)(1 - n_a - n_b)$$

$$+ \sum_{ab}(n_a - n_b)\left(\left(\eta^{1a}_{3b}\Gamma^{2b}_{4a} - \Gamma^{1a}_{3b}\eta^{2b}_{4a}\right) - \left(\eta^{2a}_{3b}\Gamma^{1b}_{4a} - \Gamma^{2a}_{3b}\eta^{1b}_{4a}\right)\right)$$

2-body flow unchanged

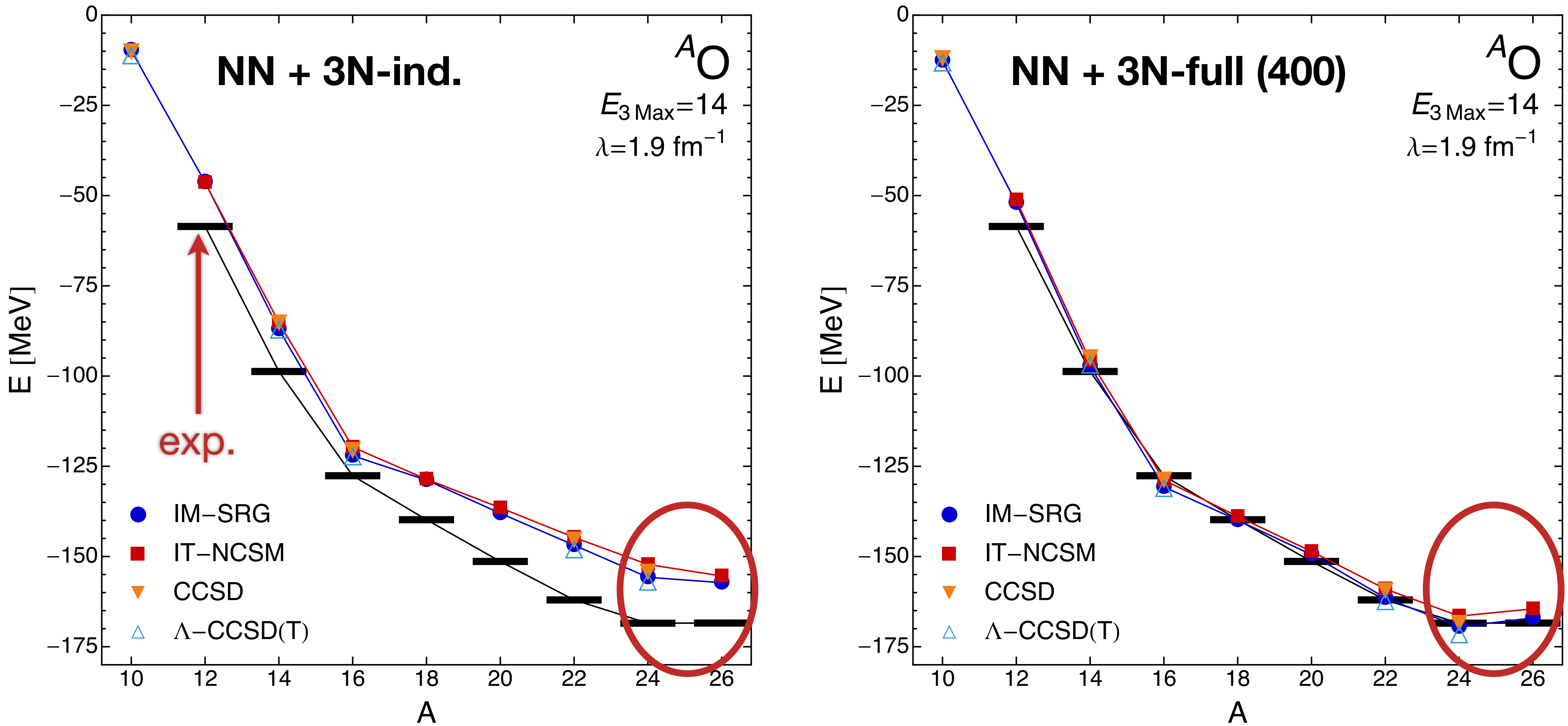
Results: Oxygen Chain





- ref. state: number-projected Hartree-Fock-Bogoliubov vacuum
- results (mostly) insensitive to choice of generator for same H^{od}

Results: Oxygen Chain



- ref. state: number-projected Hartree-Fock-Bogoliubov vacuum
- results (mostly) insensitive to choice of generator for same H^{od}
- **consistency between different many-body methods**

Solving the IM-SRG equations via the Magnus Expansion

Titus Morris, N. Parzuchowski and SKB, in preparation

Constructing the SRG unitary transformation directly?

$$\frac{dU_s}{ds} = \eta_s U_s \quad \Rightarrow \quad U_s = \mathcal{S}\exp\left(\int_0^s \eta_{s'} ds'\right)$$

$$= 1 + \int_0^s \eta_{s'} ds' + \int_0^s \eta_{s'} \int_0^{s'} \eta_{s''} \, ds' ds'' + \ldots$$

Constructing the SRG unitary transformation directly?

$$\frac{dU_s}{ds} = \eta_s U_s \quad \Rightarrow \quad U_s = \mathcal{S} \exp\left(\int_0^s \eta_{s'} ds'\right)$$

$$= 1 + \int_0^s \eta_{s'} ds' + \int_0^s \eta_{s'} \int_0^{s'} \eta_{s''} \, ds' ds'' + \ldots$$

Impractical due to S-ordered exponential

Would need to store η_s at all s values

How to apply it to transform H (and other operators)?

Constructing the SRG unitary transformation directly?

Magnus Expansion W. Magnus. *Comm. Pure and Appl. Math.*, VII:649–673, 1954.

$$U_s = \exp(\Omega_s)$$

$$\frac{d\Omega_s}{ds} = \eta_s + \frac{1}{2}[\Omega_s, \eta_s] + \frac{1}{12}[\Omega_s, [\Omega_s, \eta_s]] + \cdots \equiv \sum_{k=0}^{\infty} \frac{B_k}{k!} ad_{\Omega_s}^k(\eta_s)$$

$$ad_{\Omega}^k(\eta) = [\Omega, ad_{\Omega}^{k-1}(\eta)] \qquad B_k = \text{Bernoulli numbers}$$

Constructing the SRG unitary transformation directly?

Magnus Expansion W. Magnus. *Comm. Pure and Appl. Math.*, VII:649–673, 1954.

$$
\begin{aligned}
U_s &= \exp(\Omega_s) \\
\frac{d\Omega_s}{ds} &= \eta_s + \frac{1}{2}[\Omega_s, \eta_s] + \frac{1}{12}[\Omega_s, [\Omega_s, \eta_s]] + \cdots \equiv \sum_{k=0}^{\infty} \frac{B_k}{k!} ad^k_{\Omega_s}(\eta_s)
\end{aligned}
$$

$$
ad^k_{\Omega}(\eta) = [\Omega, ad^{k-1}_{\Omega}(\eta)] \qquad B_k = \text{Bernoulli numbers}
$$

$$
\begin{aligned}
H_s &= \exp(\Omega_s) H \exp(-\Omega_s) = H + [\Omega_s, H] + \frac{1}{2}[\Omega_s, [\Omega_s, H]] + \dots \\
O_s &= \exp(\Omega_s) O \exp(-\Omega_s) = O + [\Omega_s, O] + \frac{1}{2}[\Omega_s, [\Omega_s, O]] + \dots
\end{aligned}
$$

Magnus expansion implementation of IM-SRG(2)

$H_s\ , \eta_s\ , \Omega_s$ truncated to N-ordered 2-body terms

$$\frac{d\Omega_s}{ds} = \eta_s + \frac{1}{2}[\Omega_s, \eta_s]_{2B} + \frac{1}{12}\left[\Omega_s, [\Omega_s, \eta_s]_{2B}\right]_{2B} + \cdots$$

$$H_s = H + [\Omega_s, H]_{2B} + \frac{1}{2}\left[\Omega_s, [\Omega_s, H]_{2B}\right]_{2B} + \cdots$$

Truncate infinite Magnus and BCH commutator series numerically

Magnus expansion implementation of IM-SRG(2)

$H_s\,, \eta_s\,, \Omega_s$ truncated to N-ordered 2-body terms

$$\frac{d\Omega_s}{ds} = \eta_s + \frac{1}{2}[\Omega_s, \eta_s]_{2B} + \frac{1}{12}\left[\Omega_s, [\Omega_s, \eta_s]_{2B}\right]_{2B} + \cdots$$

$$H_s = H + [\Omega_s, H]_{2B} + \frac{1}{2}\left[\Omega_s, [\Omega_s, H]_{2B}\right]_{2B} + \cdots$$

Magnus expansion implementation of IM-SRG(2)

H_s , η_s , Ω_s truncated to N-ordered 2-body terms

$$\frac{d\Omega_s}{ds} = \eta_s + \frac{1}{2}[\Omega_s, \eta_s]_{2B} + \frac{1}{12}\left[\Omega_s, [\Omega_s, \eta_s]_{2B}\right]_{2B} + \cdots$$

$$H_s = H + [\Omega_s, H]_{2B} + \frac{1}{2}\left[\Omega_s, [\Omega_s, H]_{2B}\right]_{2B} + \cdots$$

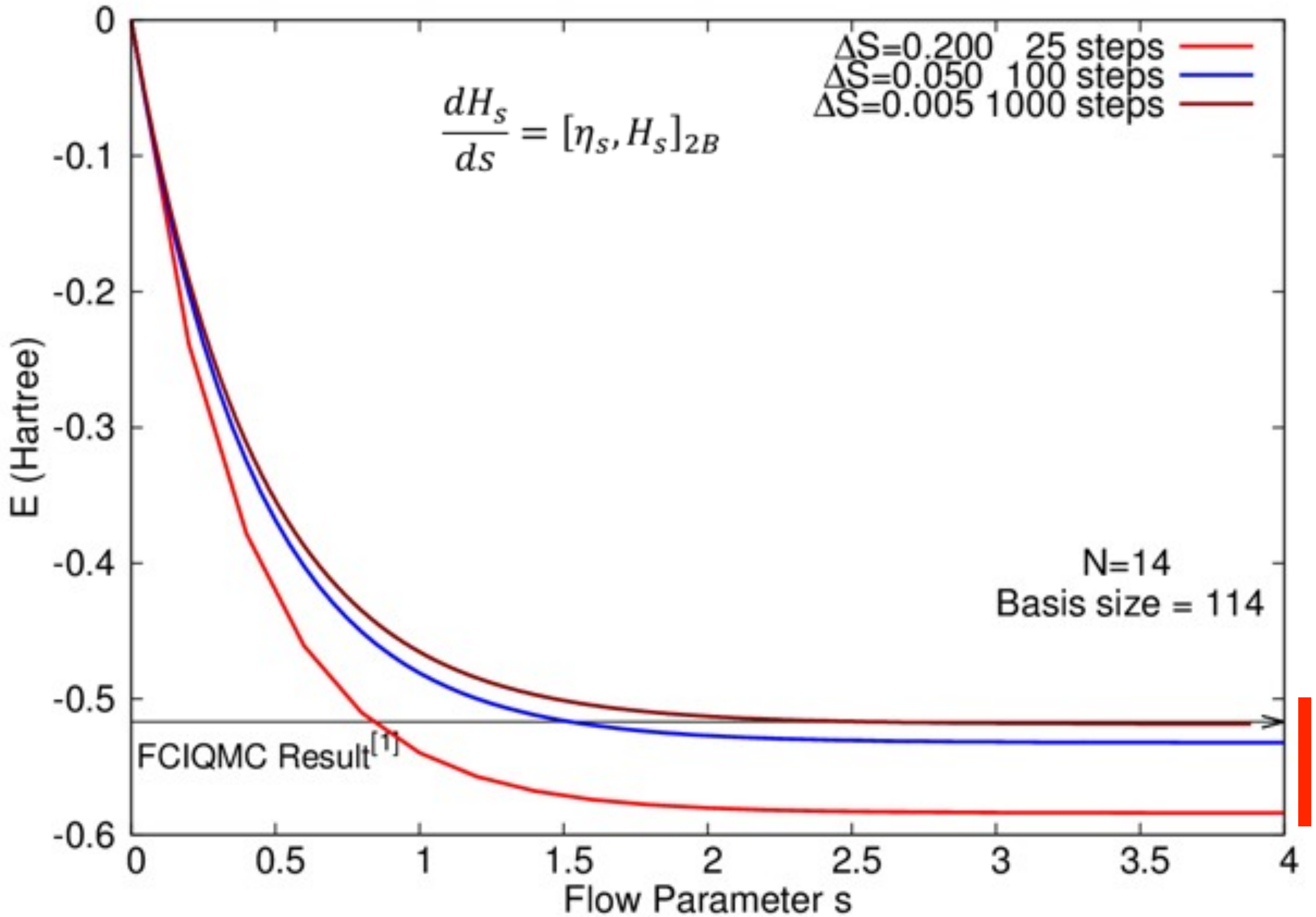
What makes this better than "usual" approach of solving dH/ds?

1) Reduced stiffness, decreased sensitivity to time-step error

2) Transformed observables at little extra cost (memory)

3) Computationally-feasible approximations to IM-SRG(3)

IM-SRG(2) evolution



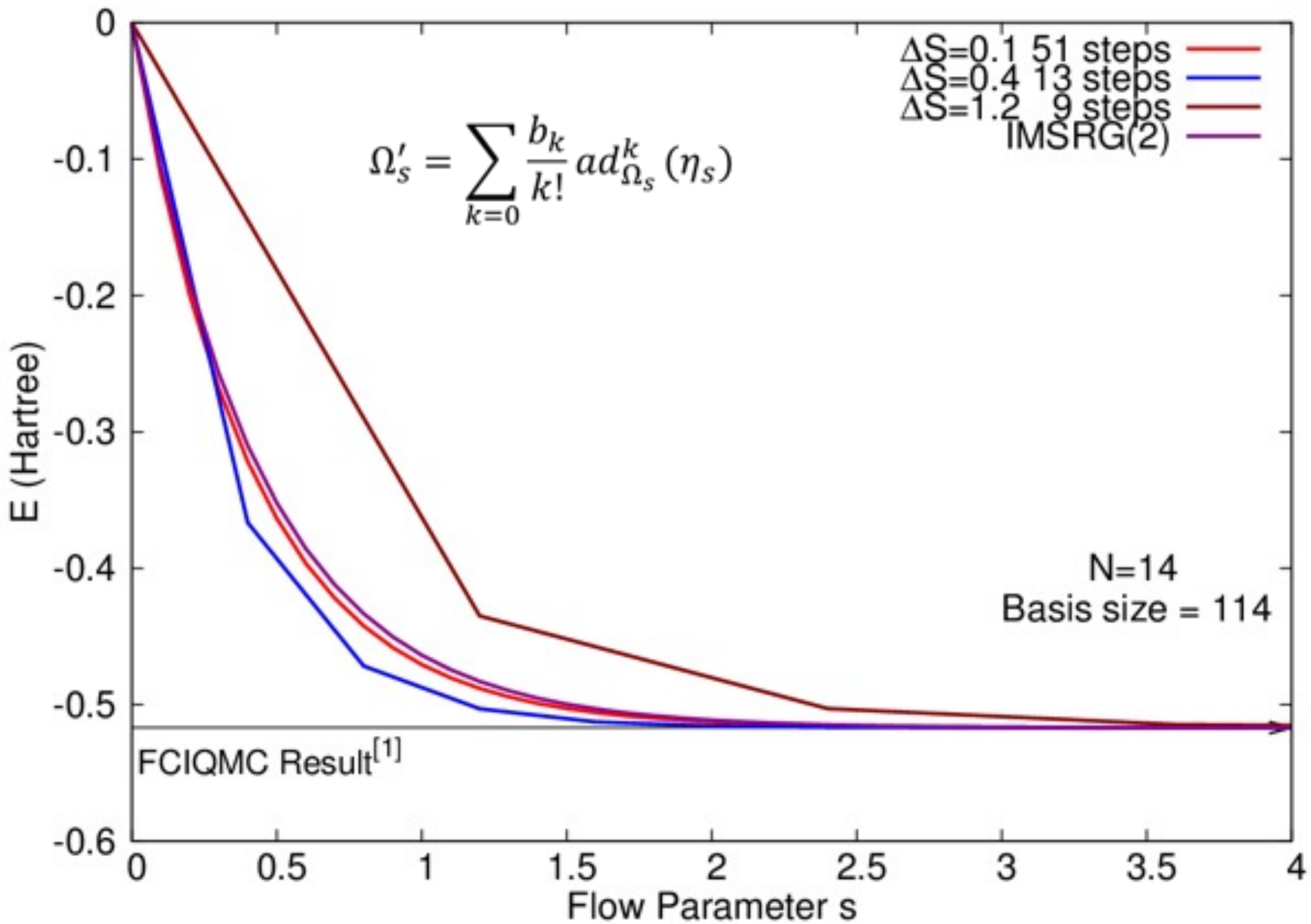
3d electron gas (box w/PBCs)

IM-SRG(2) equations solved by naive 1st-order Euler method

Need small step sizes to control error

In practice: higher-order adaptive ODE solver

Magnus IM-SRG(2) evolution



3d electron gas (box w/PBCs)

Magnus IM-SRG(2) equations solved by naive 1st-order Euler method

Independent of step size!

Converges in 9 steps (vs ~ 1000)

Why it works

It's ok to make a sloppy (e.g., 1st-order Euler) calculation of Ω_s

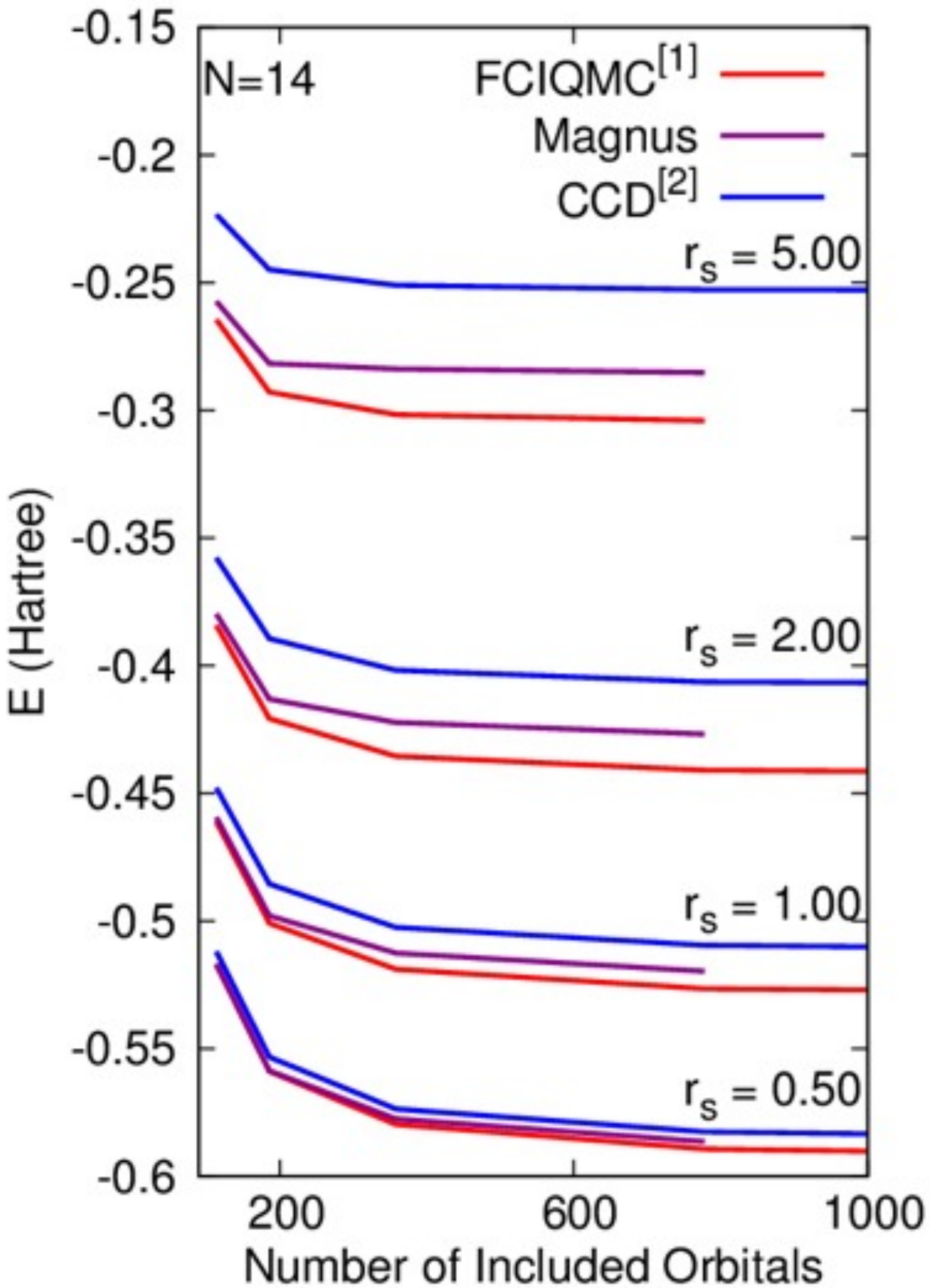
$$\Omega_s = \Omega_s^{true} + \Delta\Omega_s$$

$$H_s^{\text{Euler}} = \exp(\Omega_s) H \exp(-\Omega_s) \neq H_s^{true}$$

Nevertheless, H^{Euler} and H^{true} unitarily equivalent to each other (and to H)

Only requirement is that stepsize decreases strength of H^{OD}

Comparison to FCIQMC



Orbitals	IMSRG(2) CPUHR	Magnus(2) CPUHR
114	0.1	0.06
186	0.5	0.3
358	5.33	1.05
778	35.3	5.5

[1] Shepherd et al., J. Chem. Phys. 136, 244101 (2012)
[2] G. Baardsen, U. Oslo, Unpublished

Observables

Conclusions

- IM-SRG is an efficient new Ab-initio framework suitable for closed- and open-shell medium-mass nuclei
  - ✦ scales like CCSD, tracks more closely to CCSD(T) in wide range of systems
  - ✦ new method for deriving shell model interactions from "first principles"
    - ✦ easy access to spectra, odd-A, intrinsic deformation,..
    - ✦ competitive with usdb interactions in Oxygen, Fluorine, Neon
    - ✦ extendable to operators (e.g., neutrinoless ββ)
  - ✦ multi-reference IM-SRG using HFB reference state
    - ✦ cheaper alternative to SM for even-even groundstates
    - ✦ Oxygen, Calcium, Nickel chains using chiral NN + NNN
    - ✦ extension to excited states/odd-A on the horizon