# Recent Developments in the In-Medium SRG


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**Titus Morris**

# 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

## Basic Concept

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

- evolved Hamiltonian

- flow equation:

- choose to drive *H(s)* to desired form

# Similarity Renormalization Group

## Basic Concept

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

- evolved Hamiltonian

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

- flow equation:

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

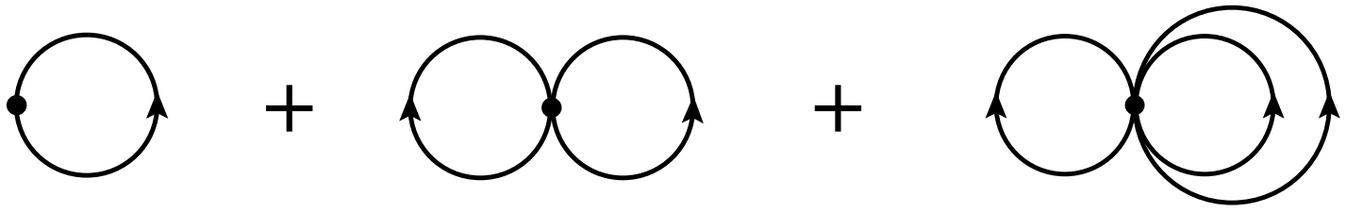
- choose $\eta(s)$ to drive *H(s)* to desired form

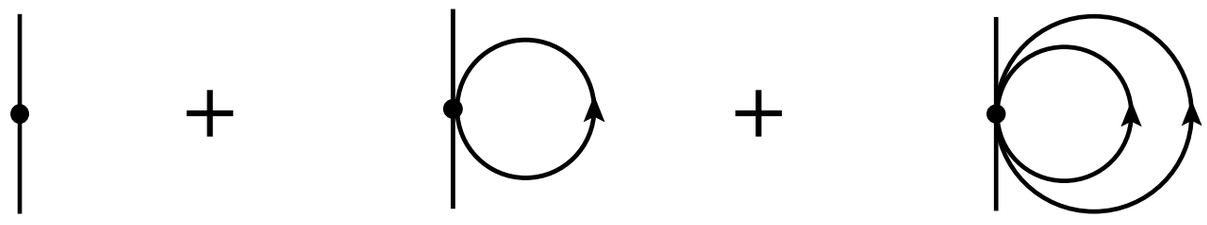
E.g. $$\eta(s) = [H_d(s), H_{od}(s)] \quad \Rightarrow \quad \lim_{s\to\infty} H_{od}(s) = 0$$

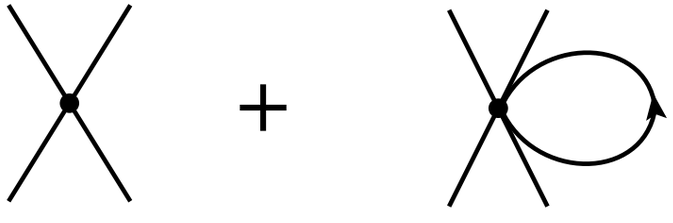
# Normal-Ordered Hamiltonian

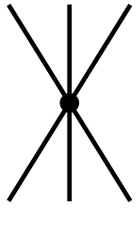
## Normal-Ordered Hamiltonian

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

$E_0 =$  $+$ $+$

$f =$  $+$ $+$

$\Gamma =$  $+$

$W =$ 

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

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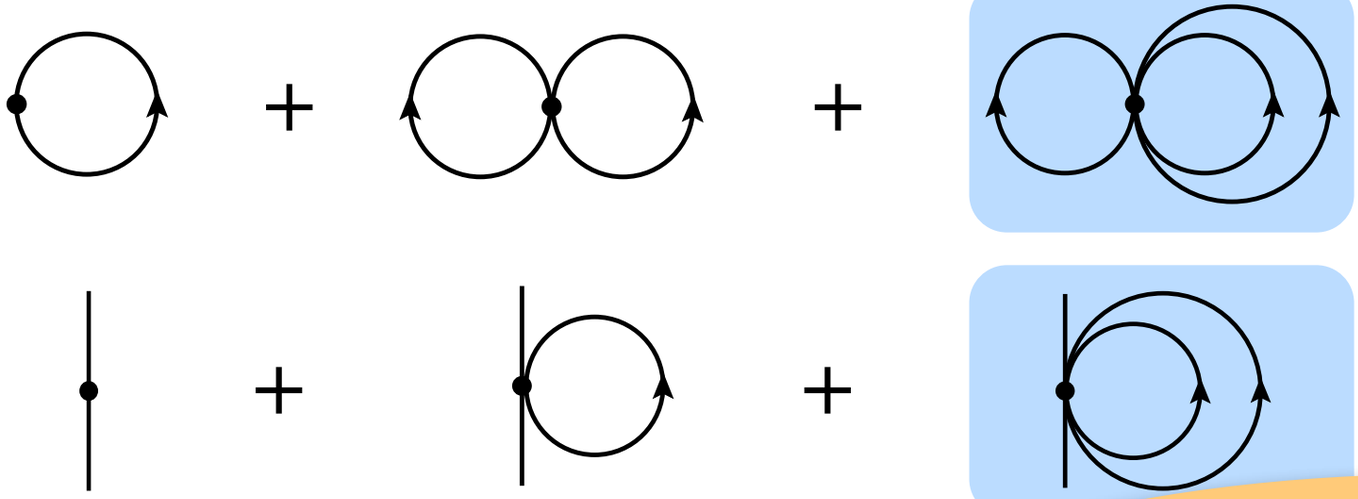
$E_0 =$ 

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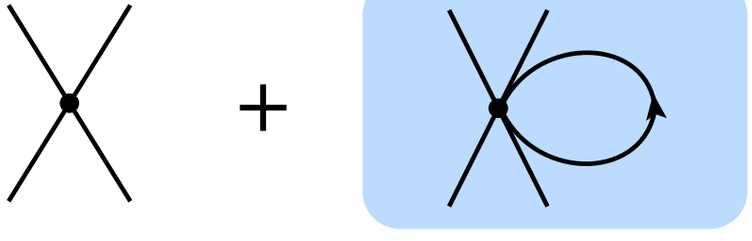
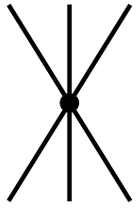
$\Gamma =$ 

$W =$ 

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

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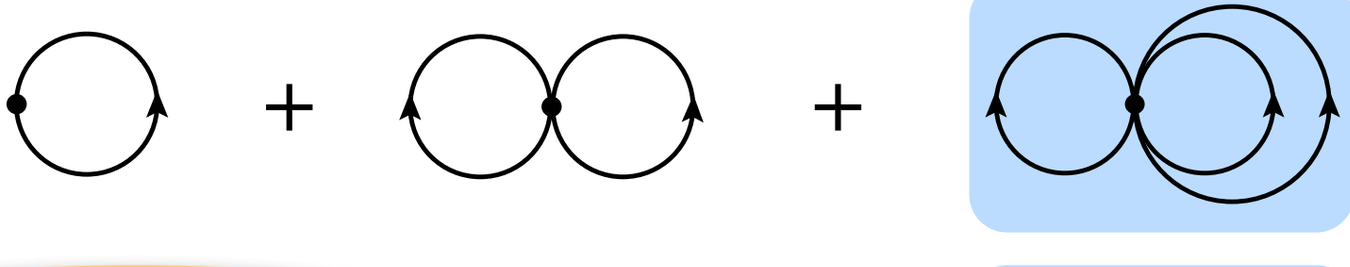
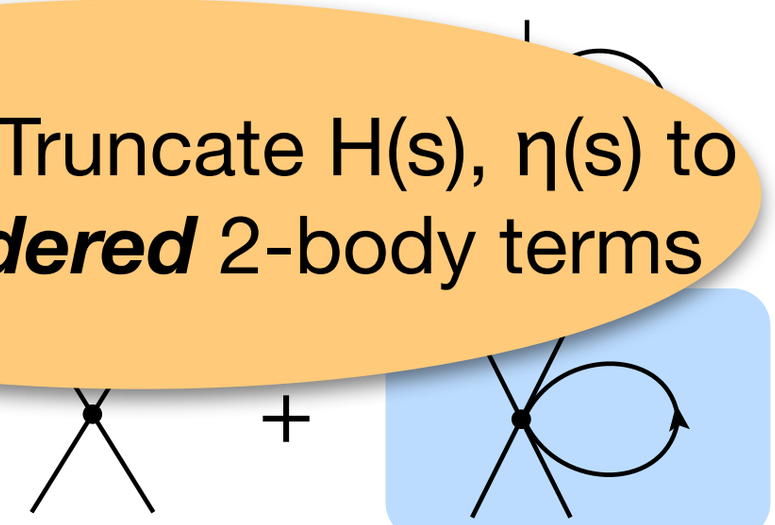
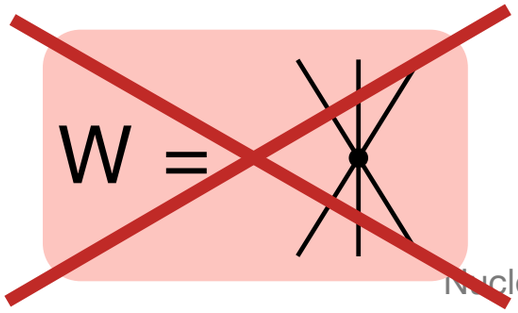
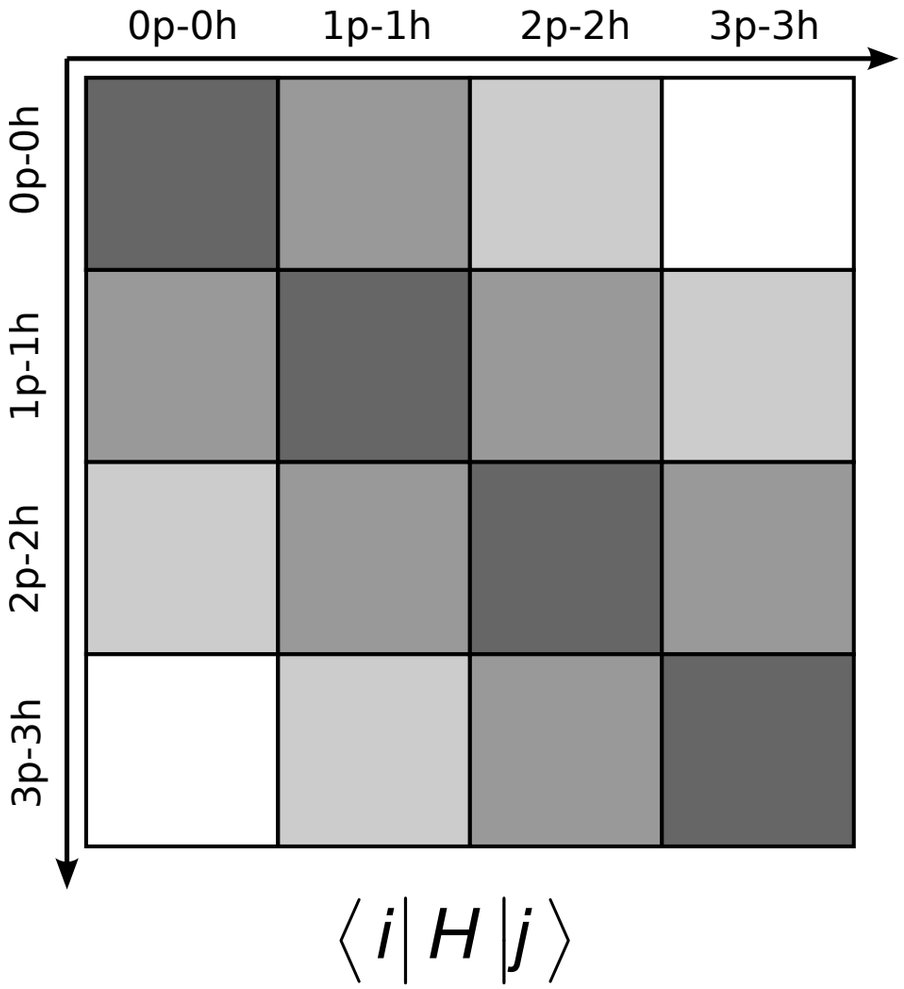
$E_0 =$  $+ \Gamma =$  $+ W =$ 

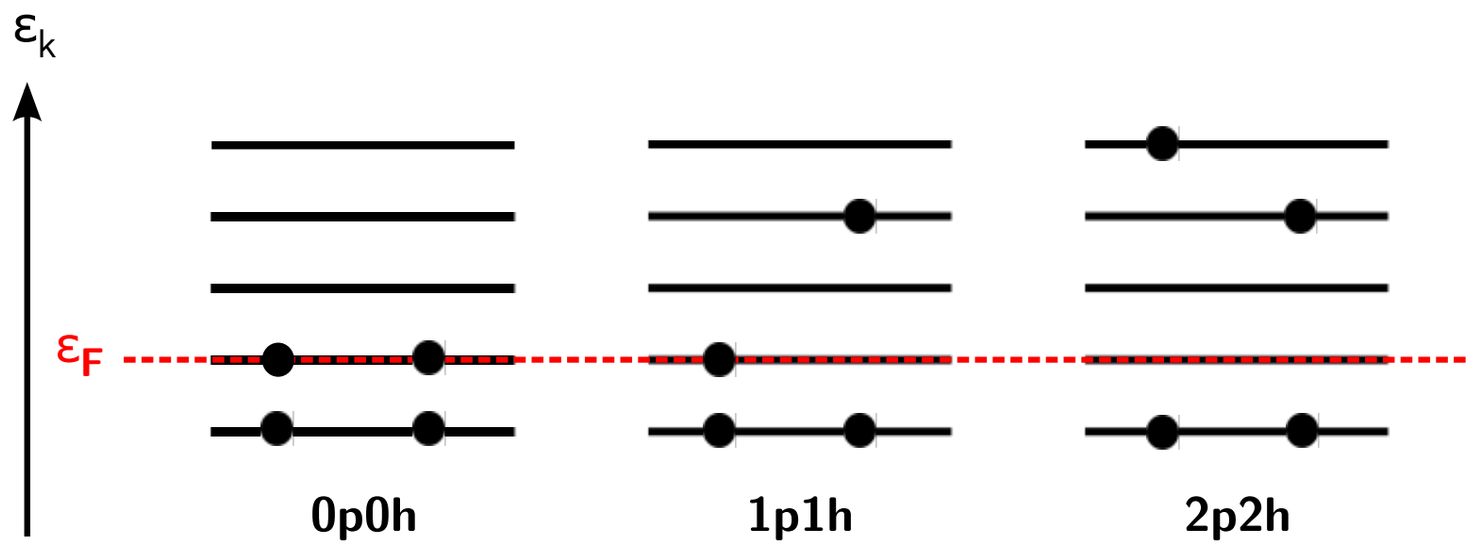
IM-SRG(2): Truncate H(s), η(s) to ***normal ordered*** 2-body terms

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



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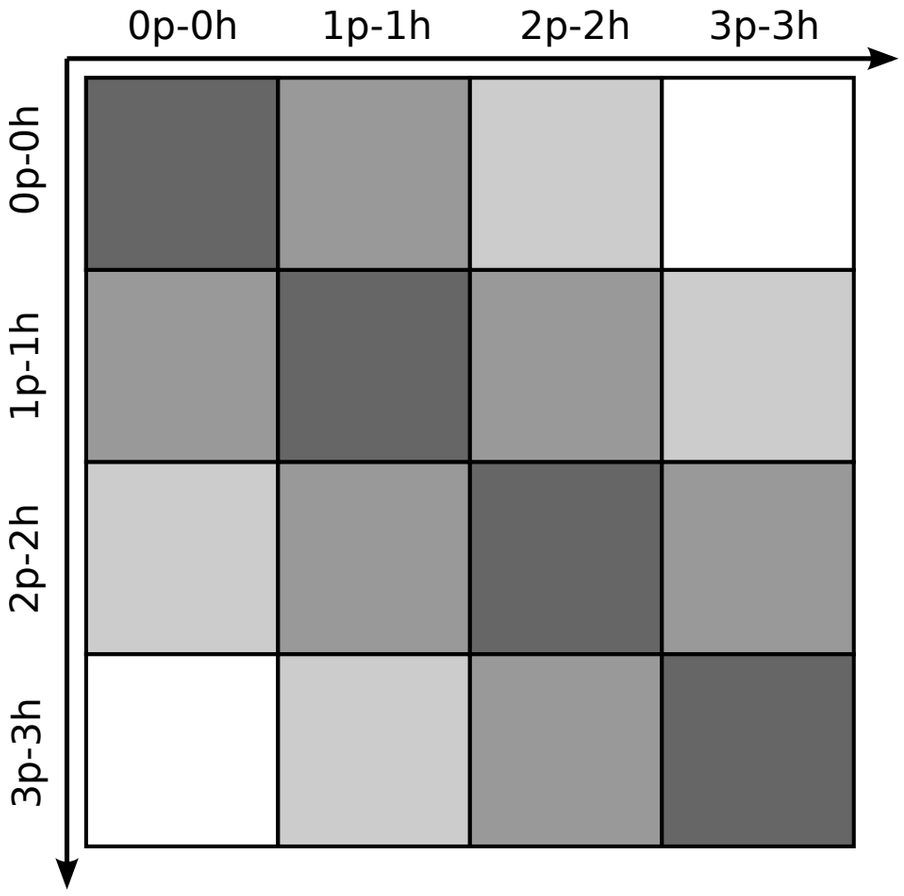
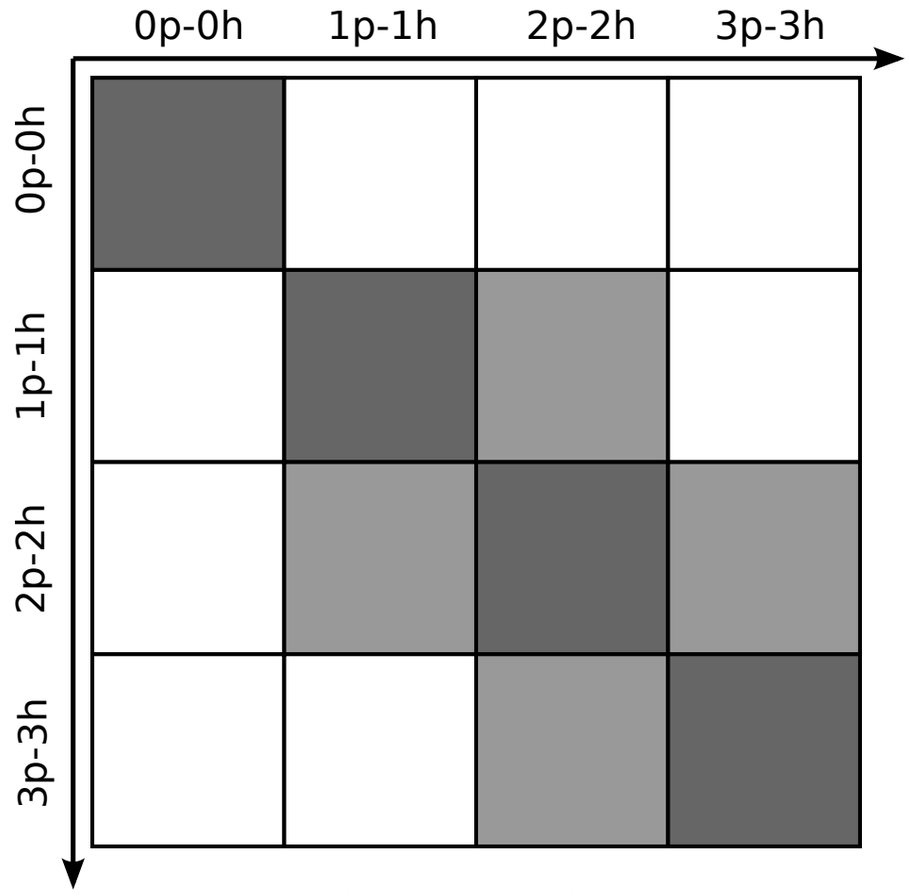



$\langle i | H | j \rangle$

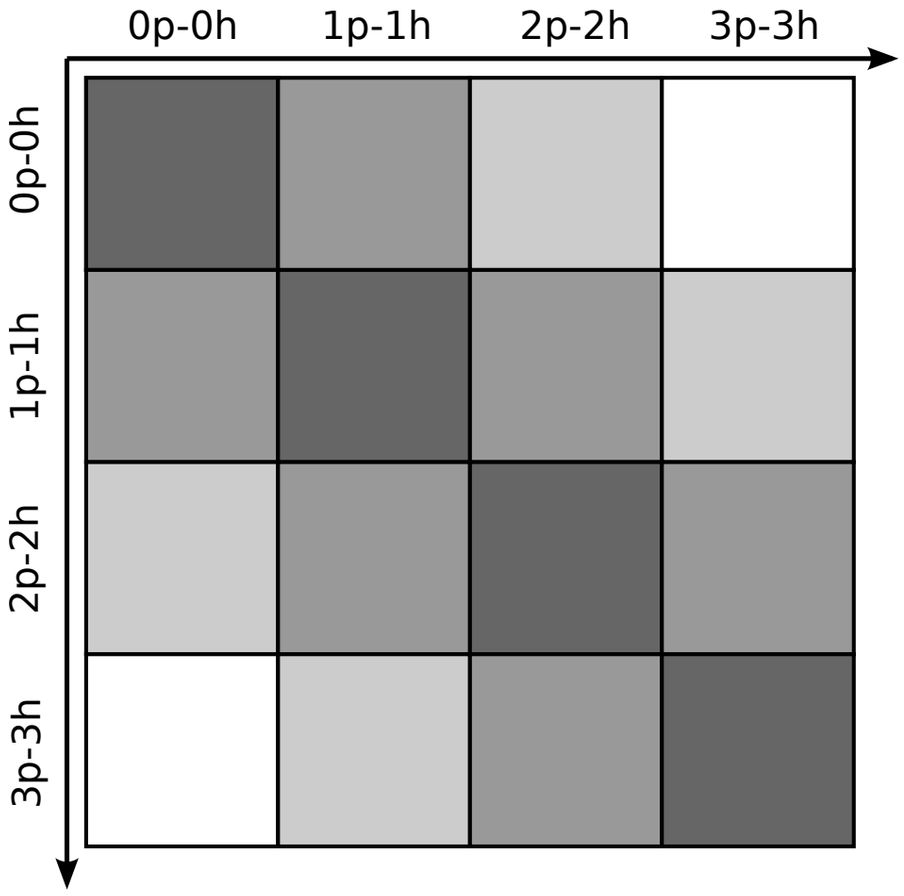



$\langle i | H(\infty) | j \rangle$

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

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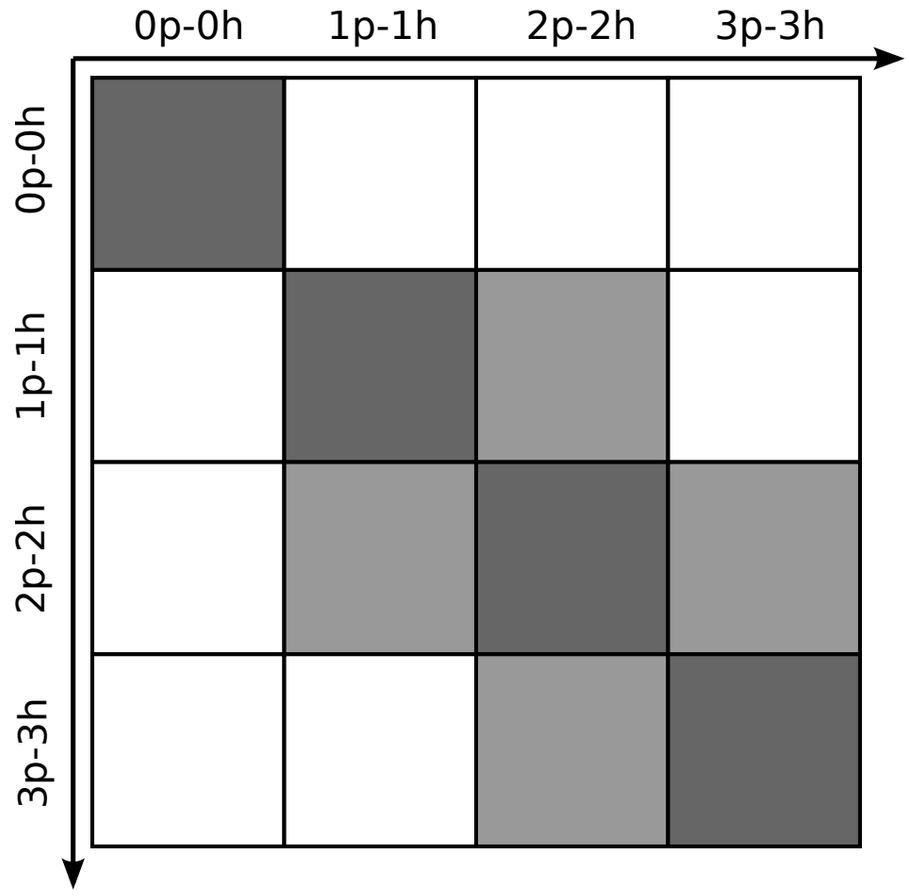



$\langle i | H(\infty) | j \rangle$

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

# Freedom of Choice for Generators

- Wegner

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

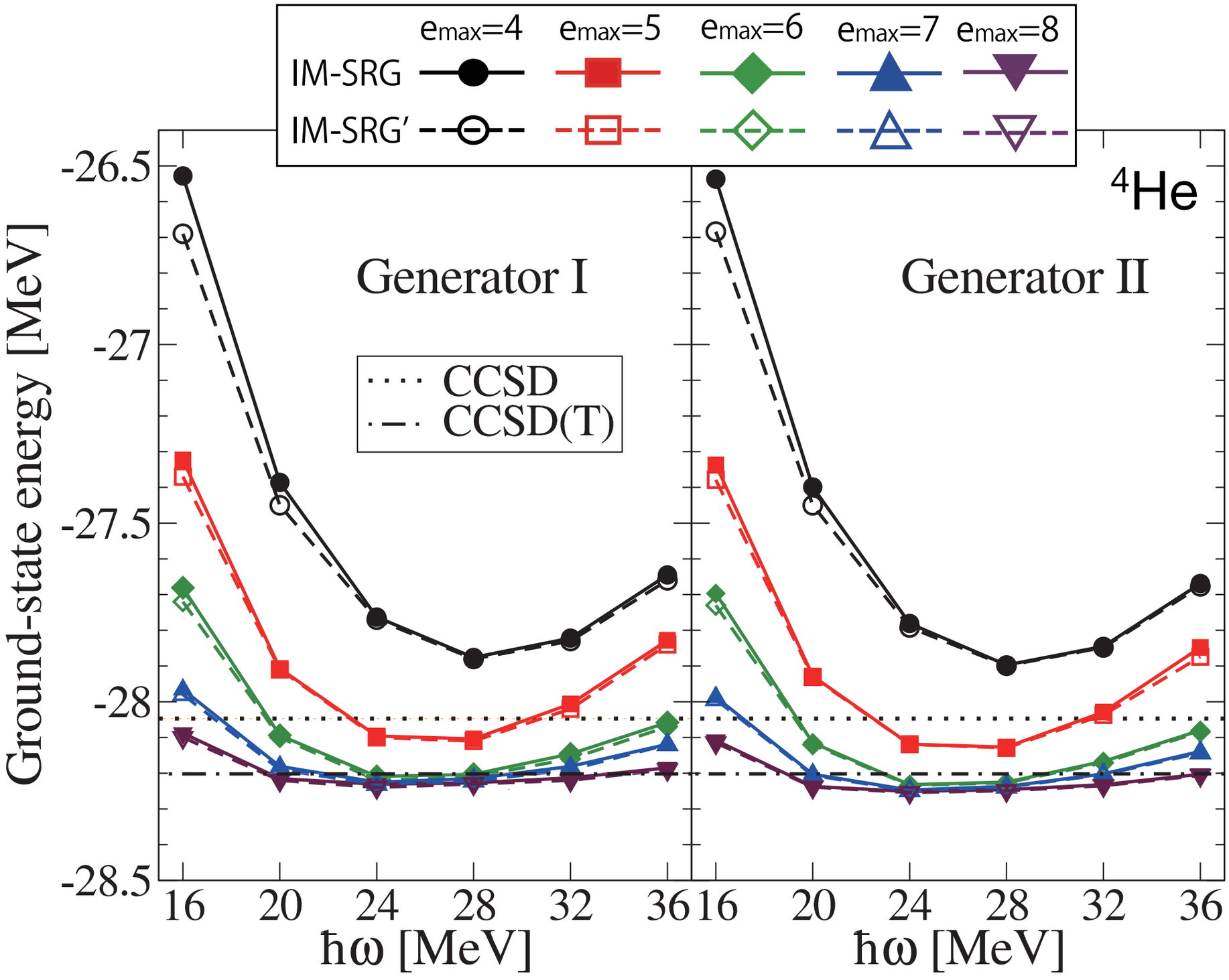
- White (J. Chem. Phys. 117, 7472)

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

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

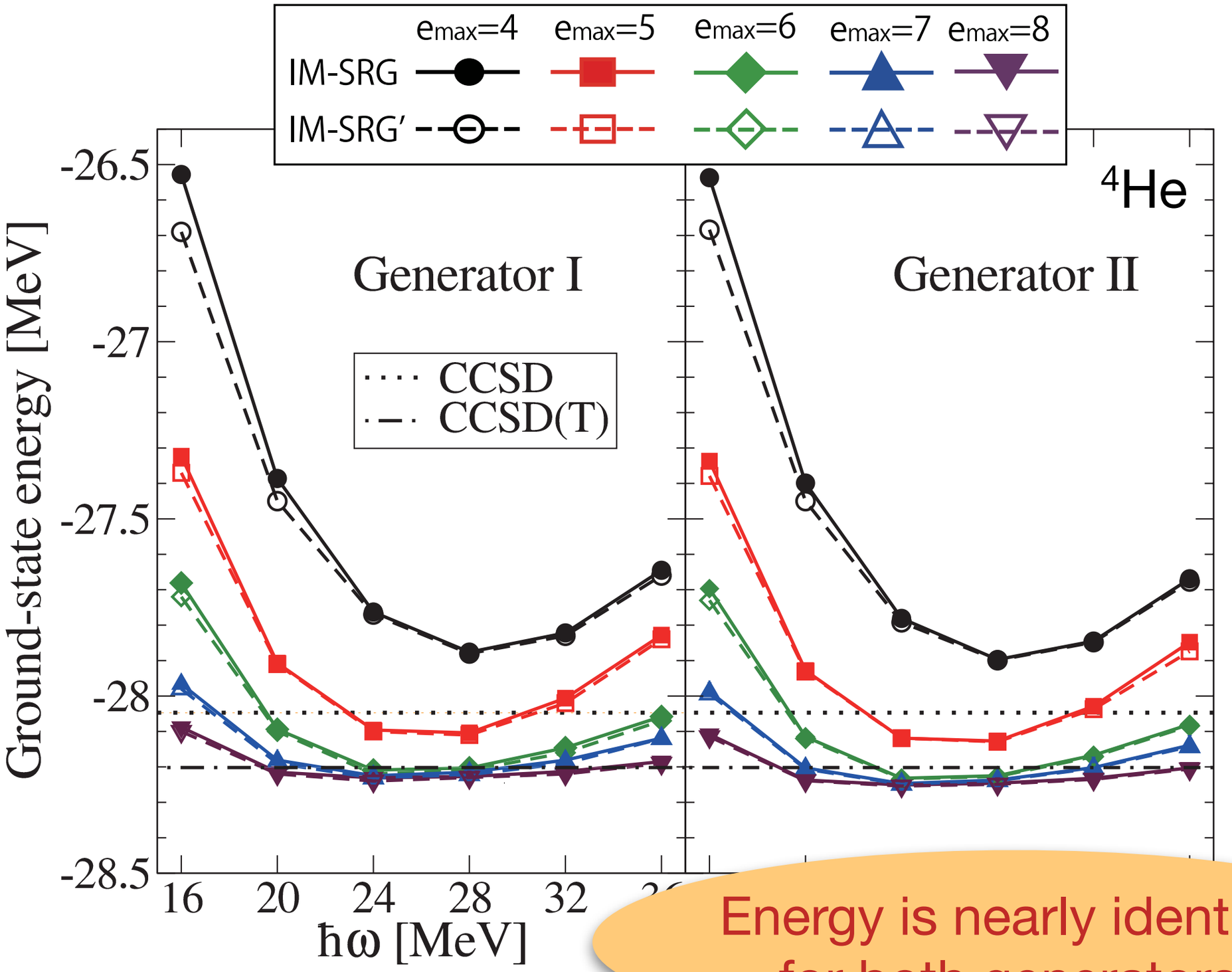
- g.s. energies ($s \to \infty$) for both generators agree within a few keV (measure of truncation error)

# Generator Dependence




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

# Generator Dependence

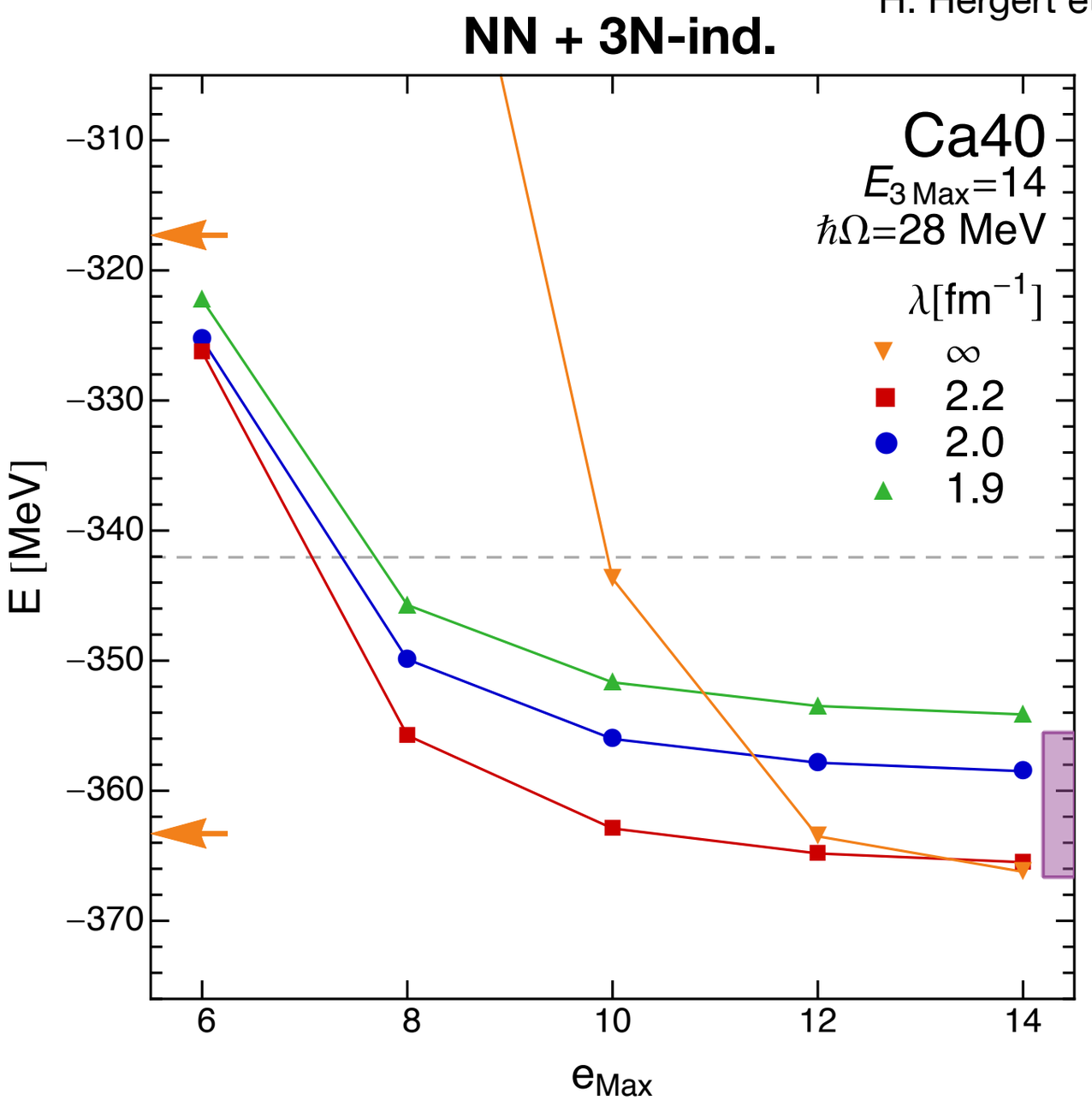



Energy is nearly identical for both generators!

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

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

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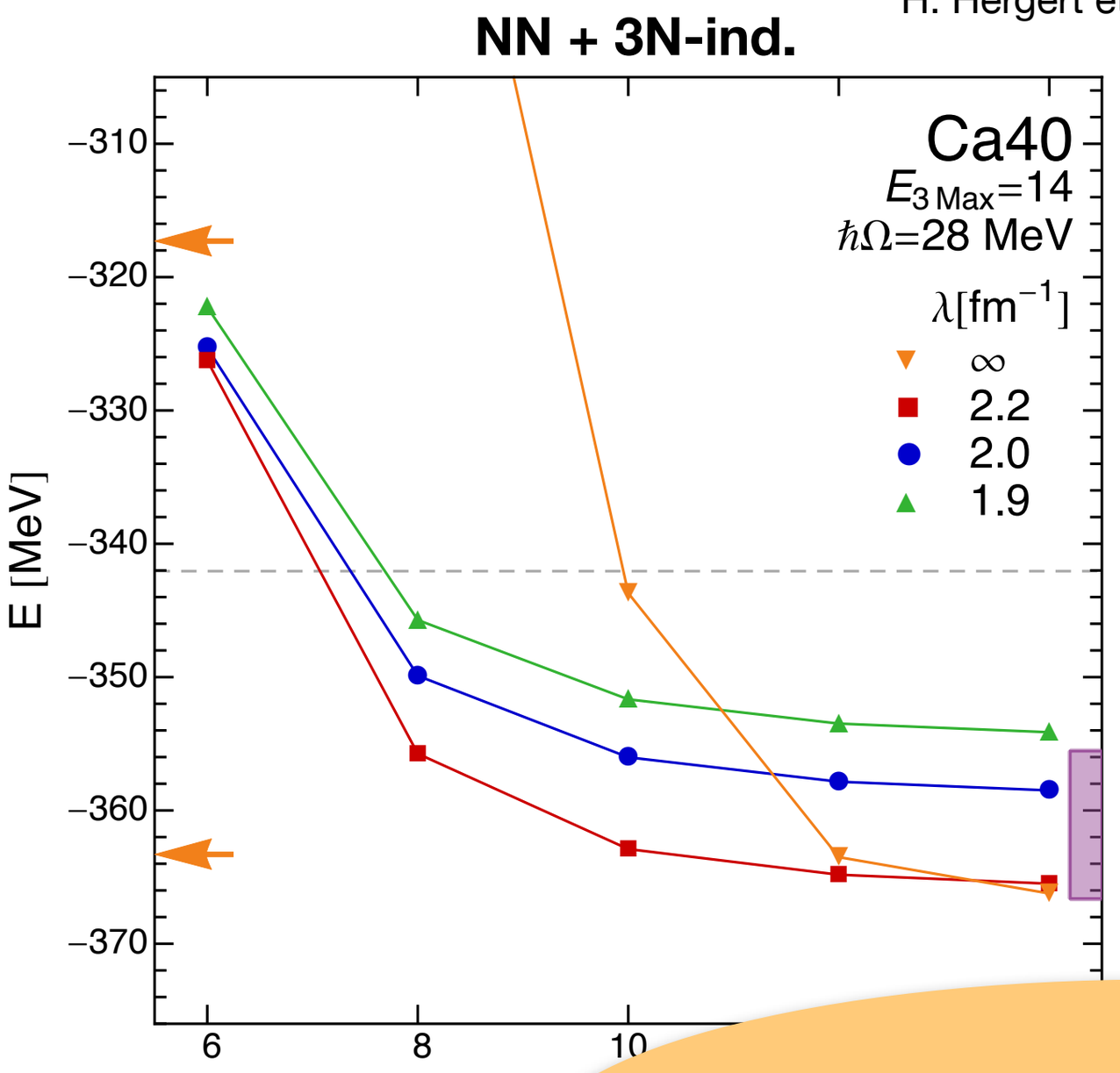


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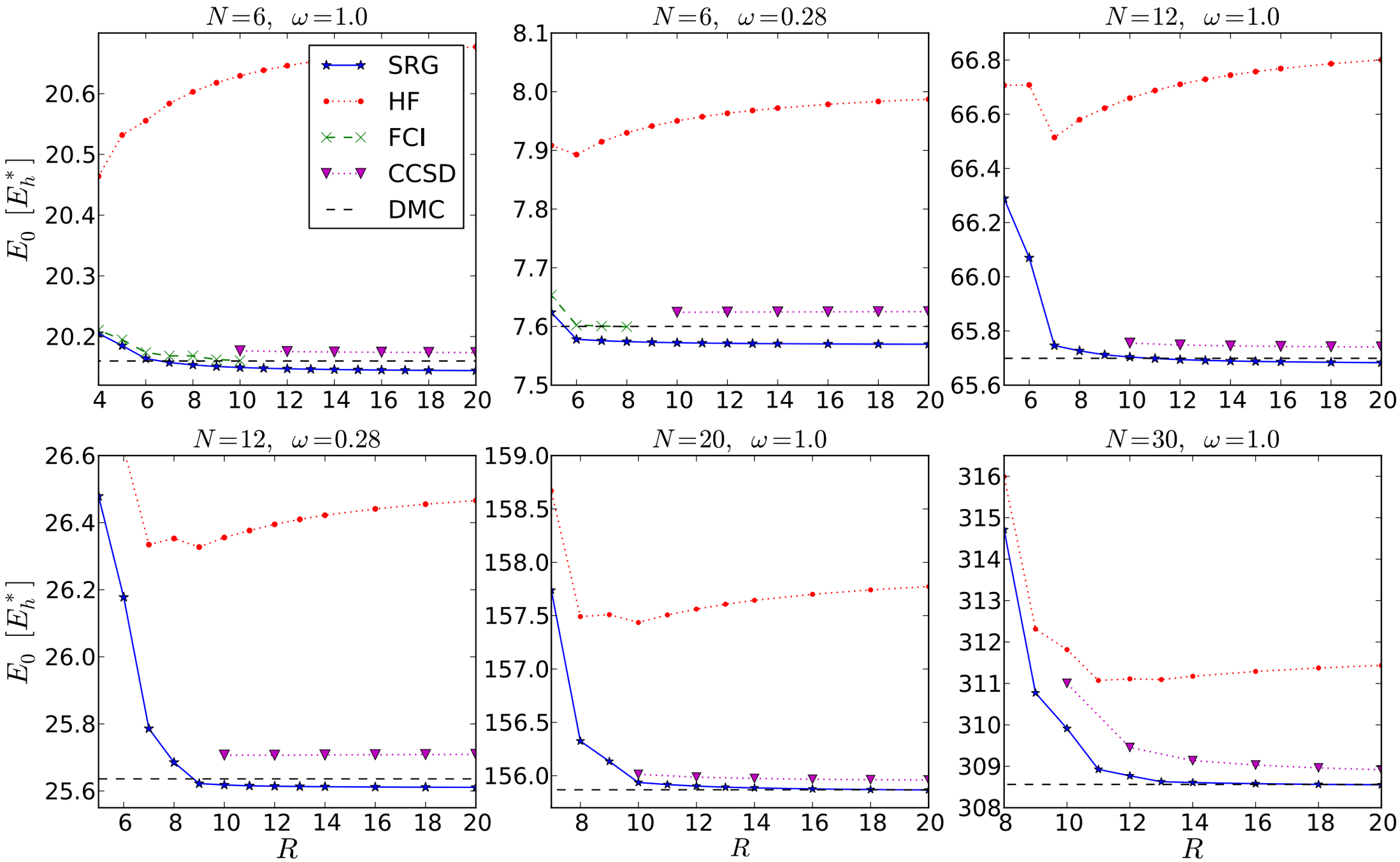
calculation

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

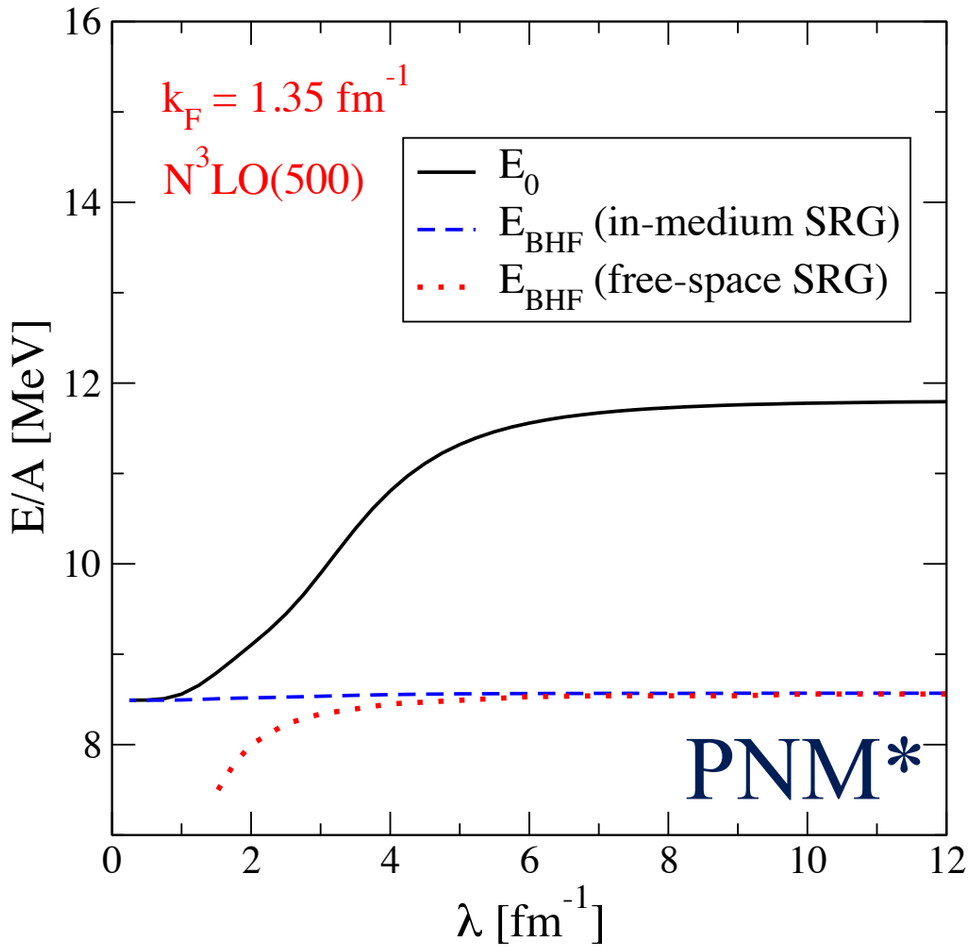
[nucl-th] & PRL 109, 052501 (2012)

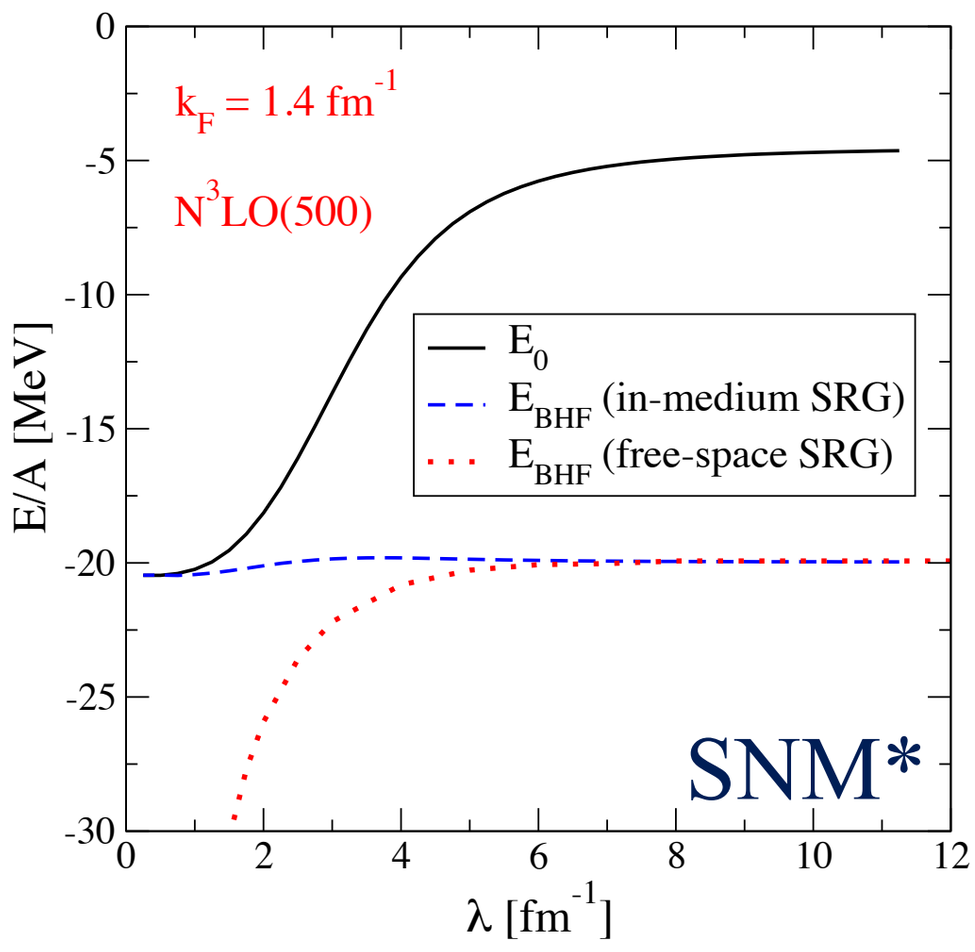
# Non-nuclear application: Quantum Dots




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

# Early Attempts at Infinite Matter




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

Weak λ-dependence => dominant 3,4,...-body terms evolved

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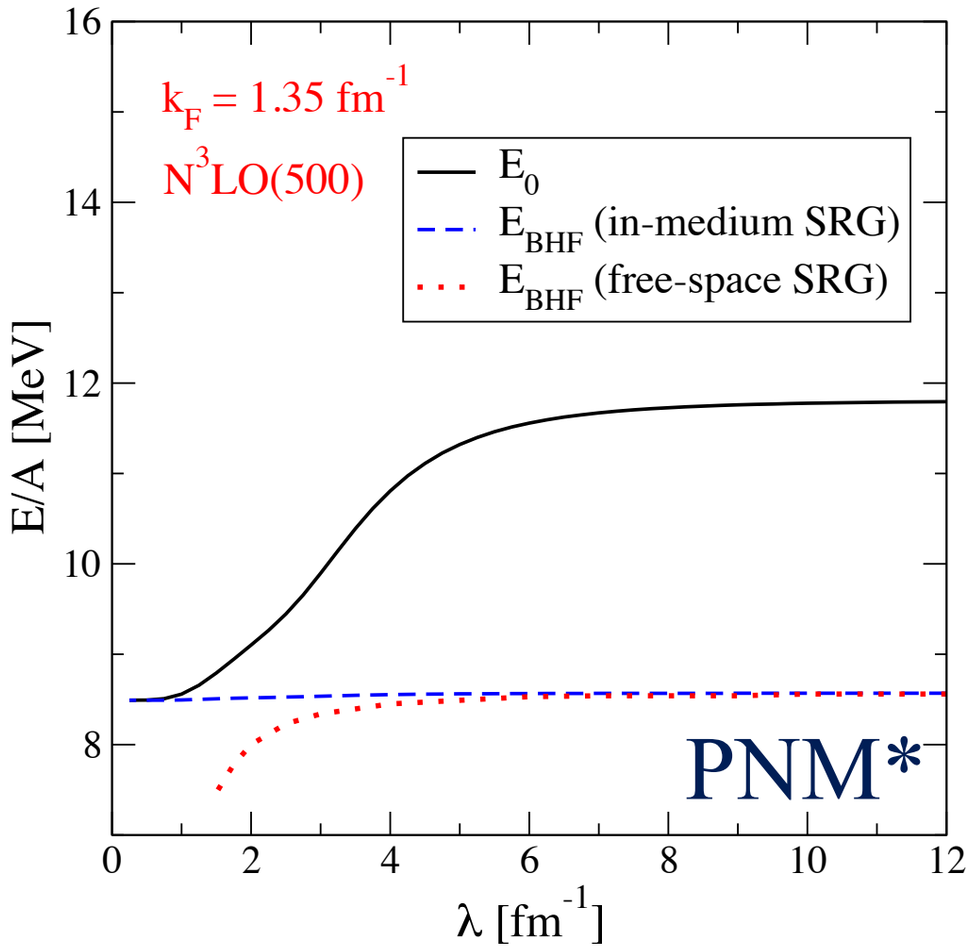


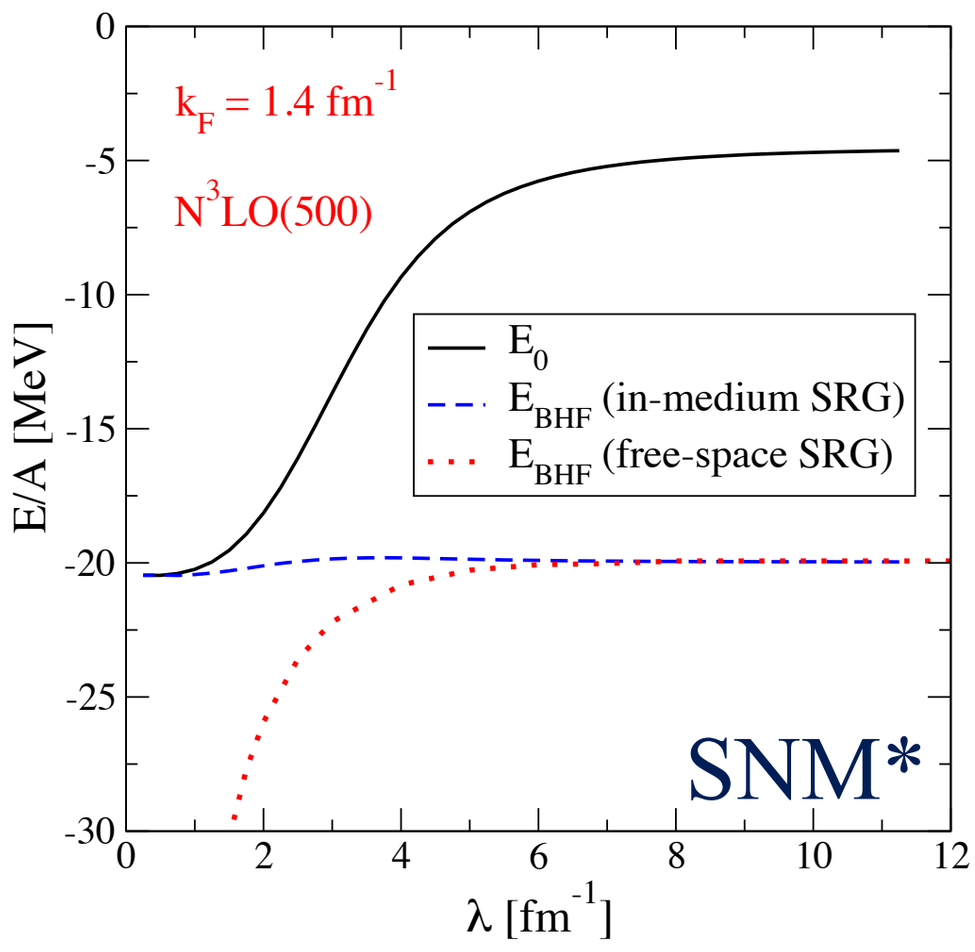


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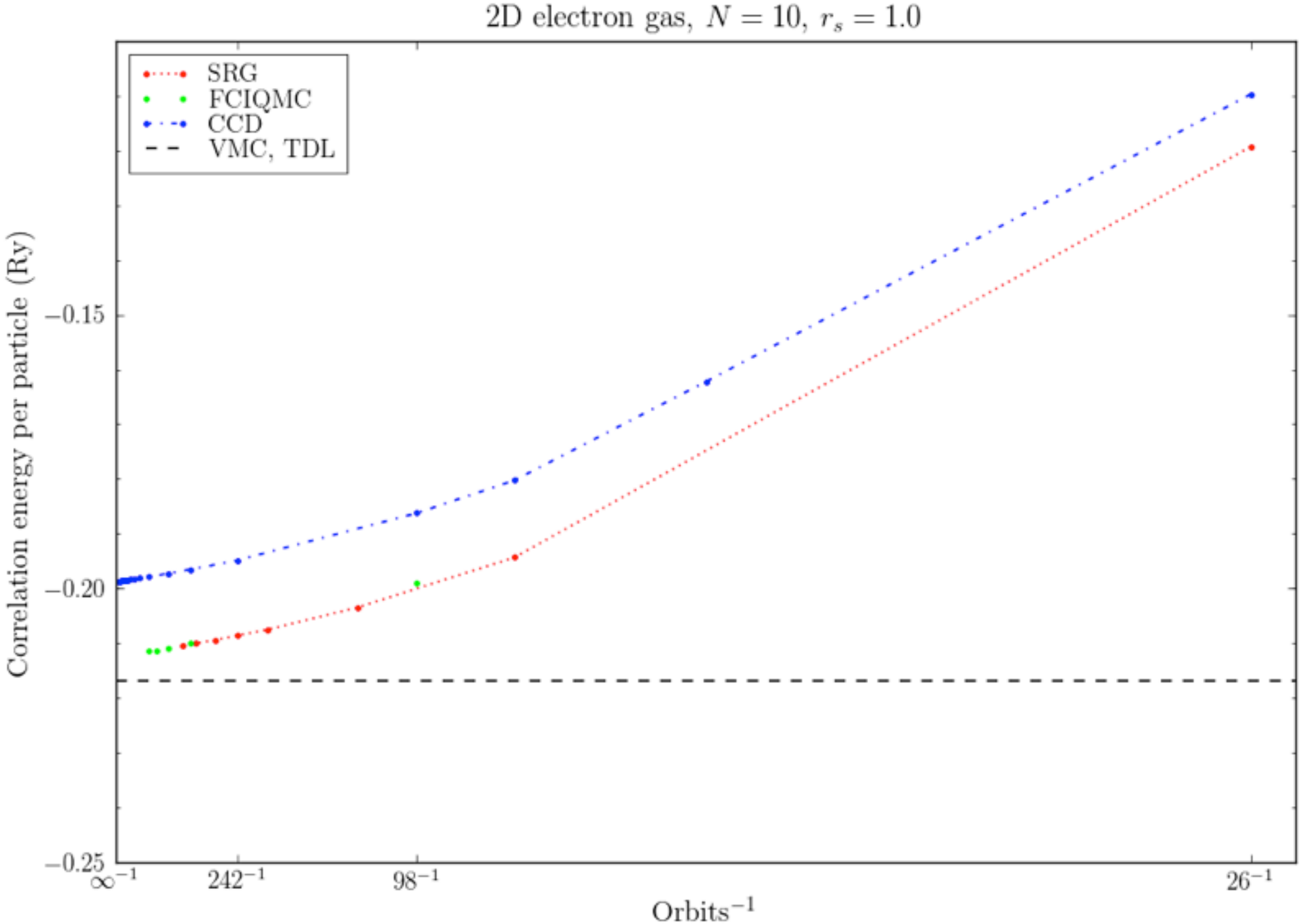
Weak λ-dependence => dominant 3,4,...-body terms evolved

BUT particle-hole channel neglected

Only becomes feasible in periodic box formulation

# Non-nuclear application: 2D $e^-$ gas




IM-SRG(2) tracks exact FCIQMC result

# Observations on IM-SRG(2)

★ Pros

- Intrinsically non-perturbative
- Commutators => linked diagrams/size extensive
- Scales as $N^6$ like CCSD but tracks CCSD(T) accuracy
- fits SM phenomenology (dominant mean-field + weak A-dependent NN interactions)

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★ Cons

- Observables possible but hard in practice
- $N^6$ scaling, but large prefactor (Stiff ODEs, need high-order solver,...)
- Lacking approximation schemes for IM-SRG(3)

# Solving the IM-SRG equations via the Magnus Expansion

**Titus Morris** and SKB, in preparation

# Constructing the SRG unitary transformation directly?

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

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

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Impractical due to S-ordered exponential

Would need to store $\eta_s$ 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.

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

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

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

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$$H_s = \exp(\Omega_s) H \exp(-\Omega_s) = H + [\Omega_s, H] + \frac{1}{2}\big[\Omega_s, [\Omega_s, H]\big] + \ldots$$

$$O_s = \exp(\Omega_s) O \exp(-\Omega_s) = O + [\Omega_s, O] + \frac{1}{2}\big[\Omega_s, [\Omega_s, O]\big] + \ldots$$

# Magnus expansion implementation of IM-SRG(2)

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

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

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

Truncate infinite Magnus and BCH commutator series numerically

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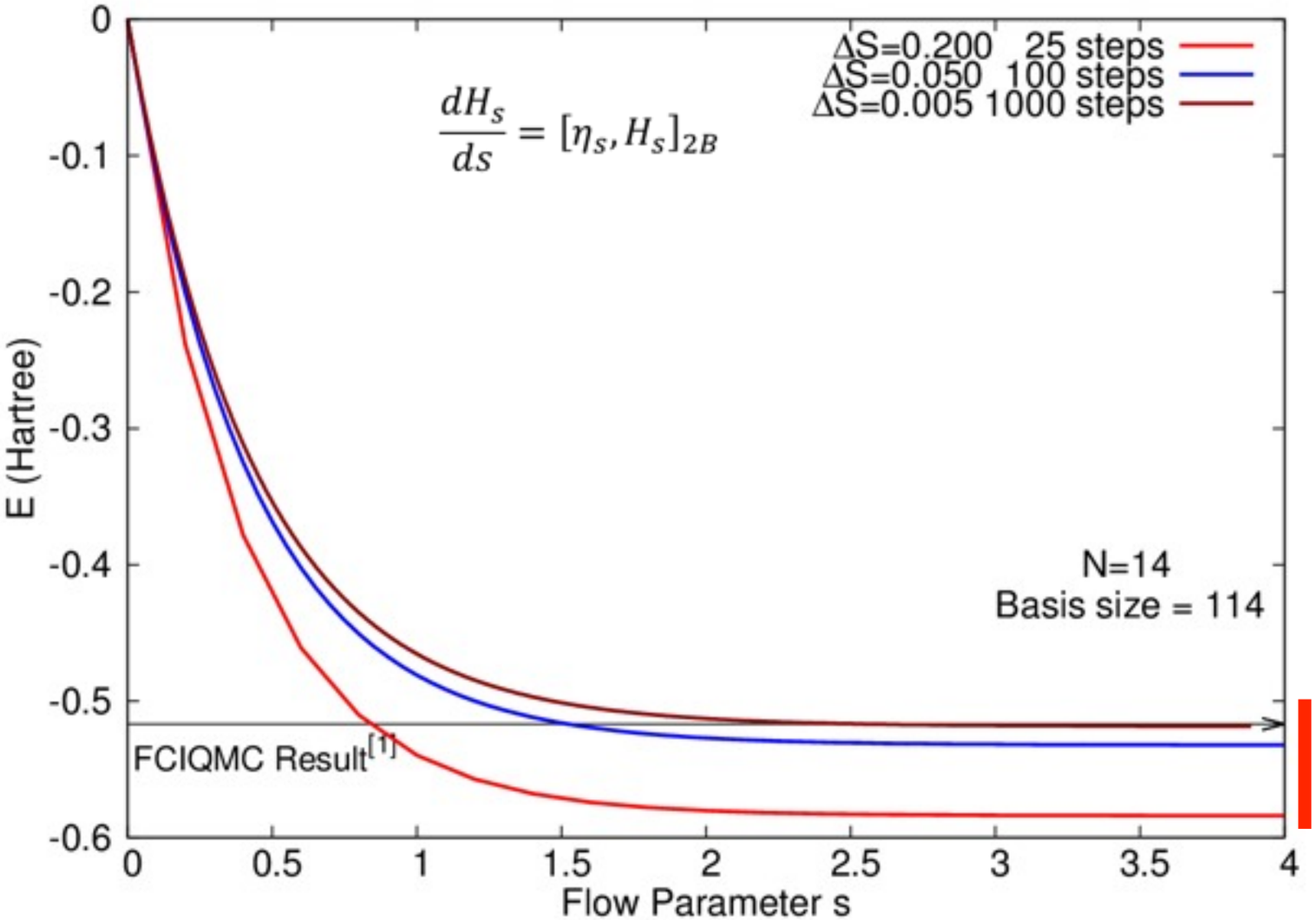
What makes this better/worse than “usual” approach of solving dH/ds?

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

2) Transformed observables at little extra cost

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

# IM-SRG(2) evolution



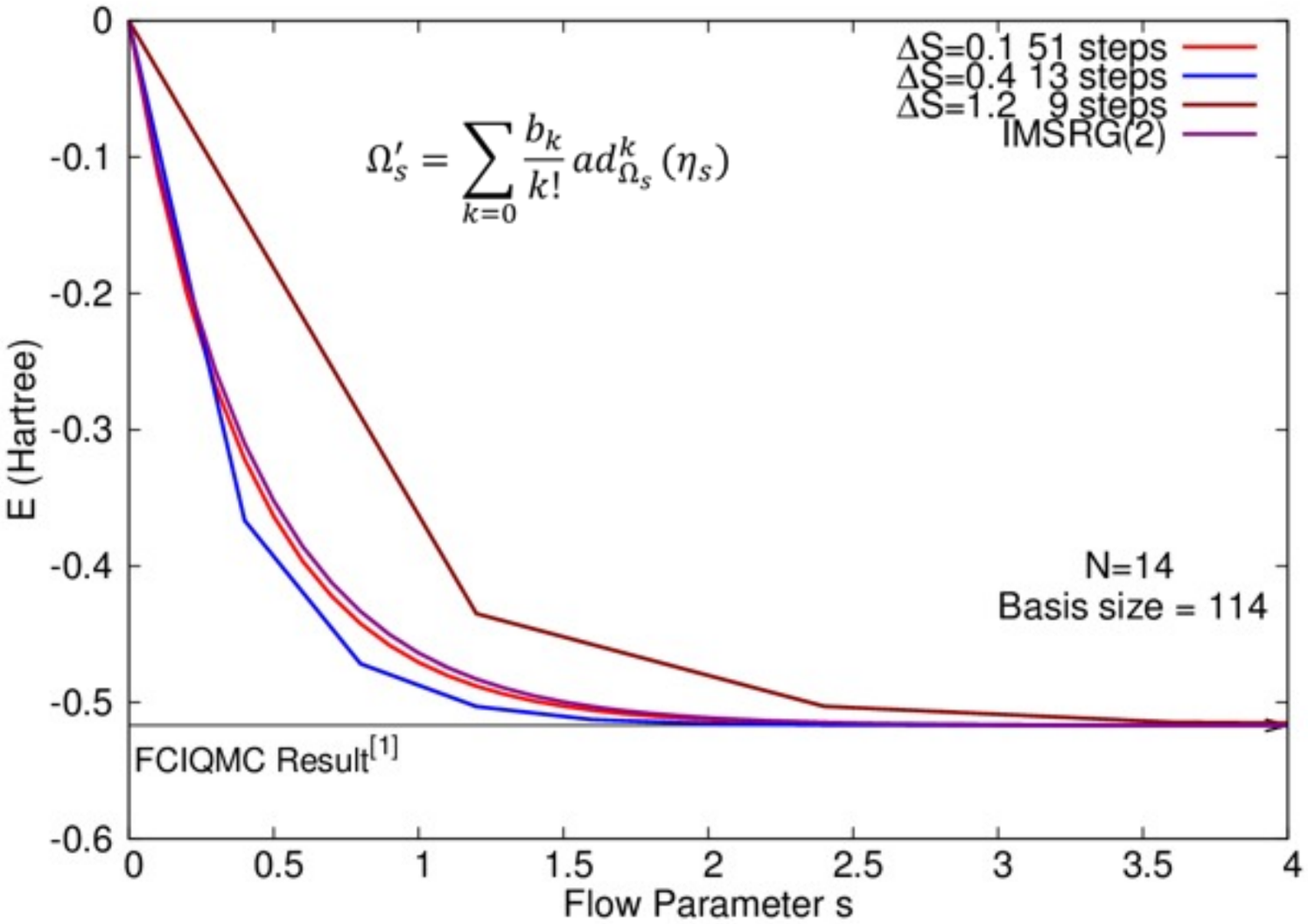

3d electron gas (box w/PBCs)

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 $\Omega_s$

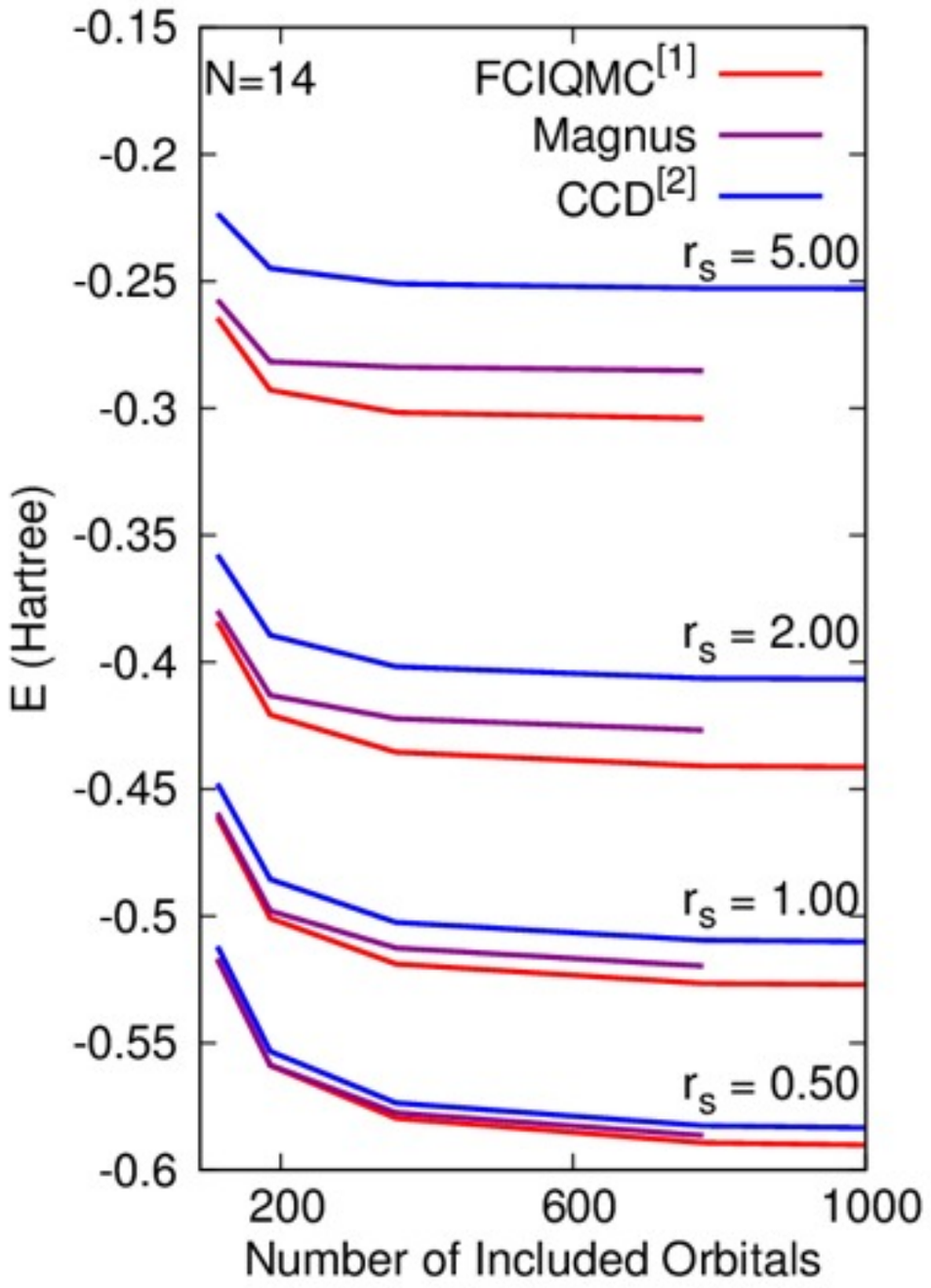
$$\Omega_s = \Omega_s^{true} + \Delta\Omega_s$$

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

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

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

# Comparison to FCIQMC

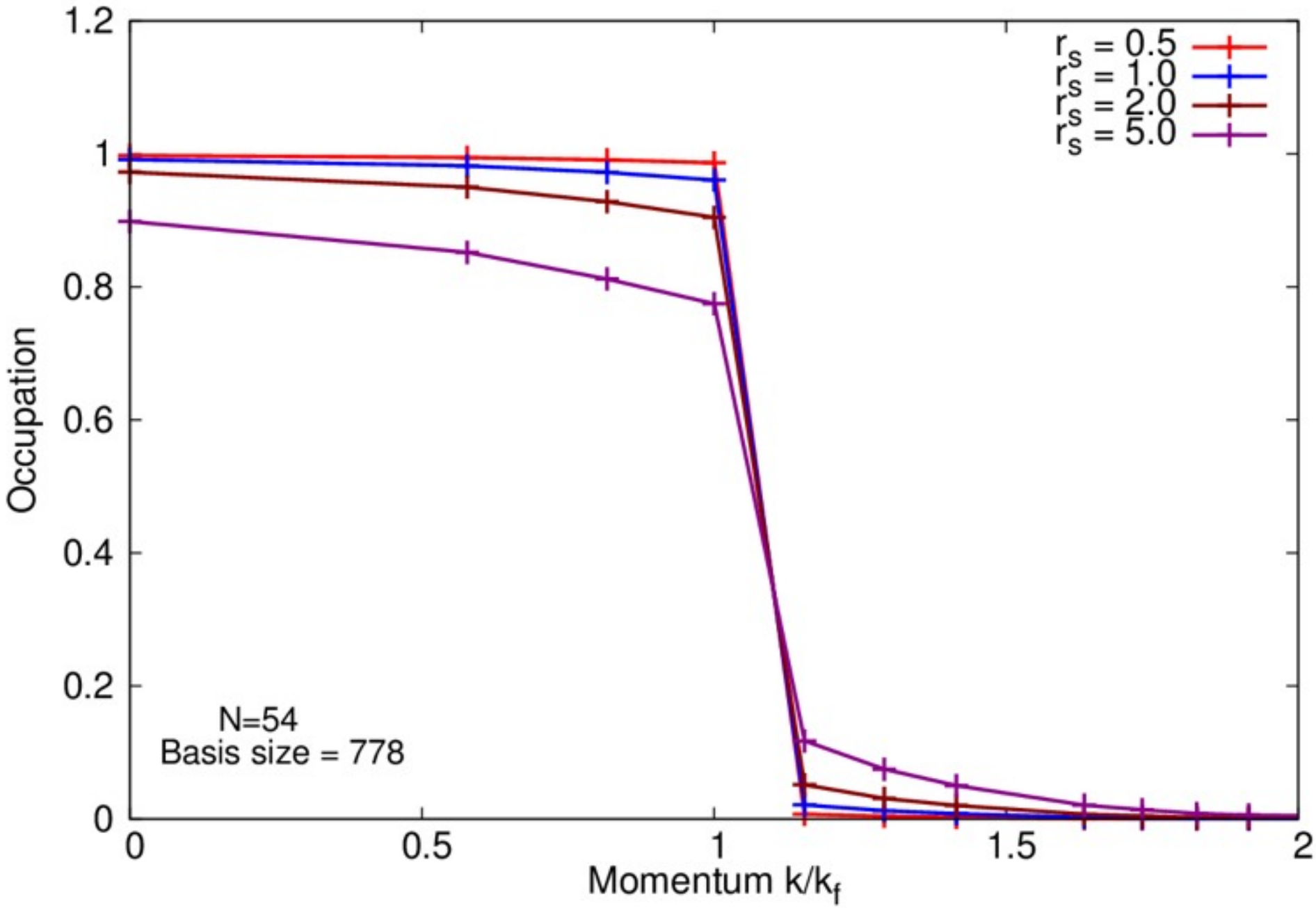



| Orbitals | IMSRG(2) CPUHR | Magnus(2) CPUHR |
|---|---|---|
| 114 | 0.1 | 0.06 |
| 186 | 0.5 | 0.3 |
| 358 | 5.33 | 1.05 |
| 778 | 35.3 | 5.5 |


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

# Observables

Ex: Momentum distributions in 3d electron gas



# 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, arXiv: 1402.1407
H.Hergert, S. Binder, A. Calci, J. Langhammer, and R. Roth, Phys. Rev. Lett **110**, 242501 (2013)

# IM-SRG for Open-Shell

- Two possibilities

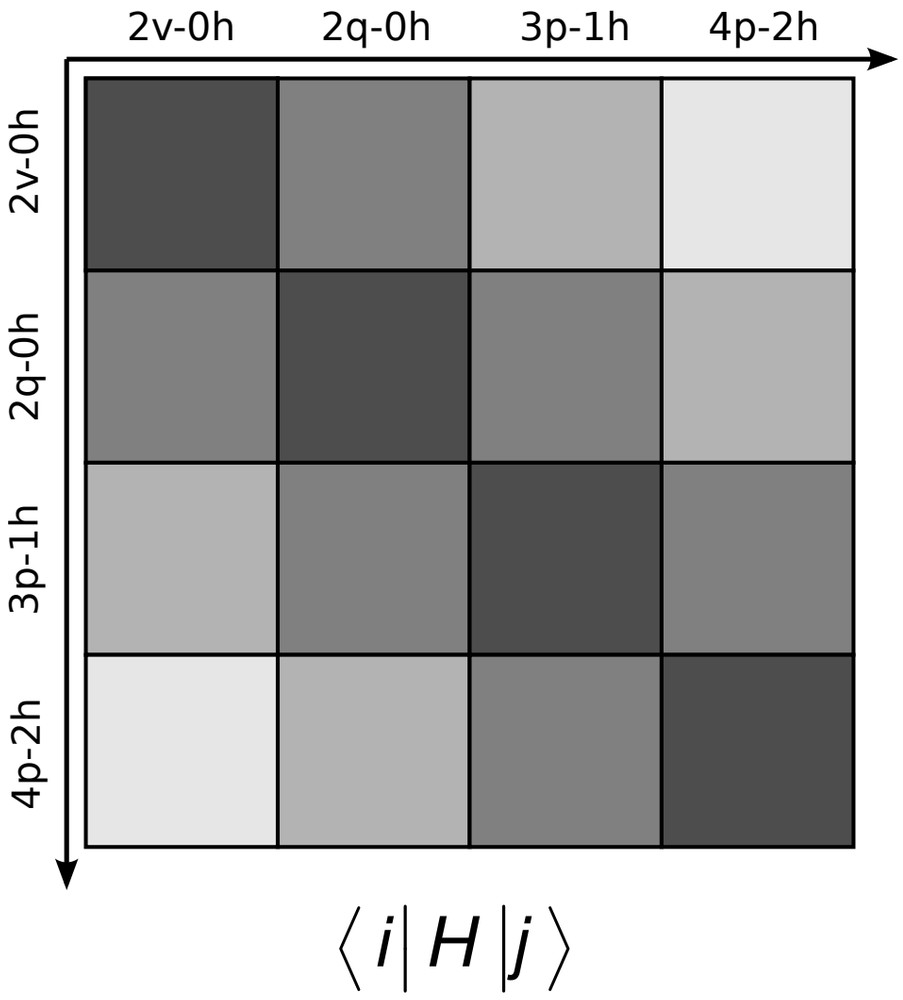
1. Use IM-SRG to derive effective hamiltonian/operators for valence shell model calculations [K. Tsukiyama, SKB, A. Schwenk PRC 85, 061304 (2012)]

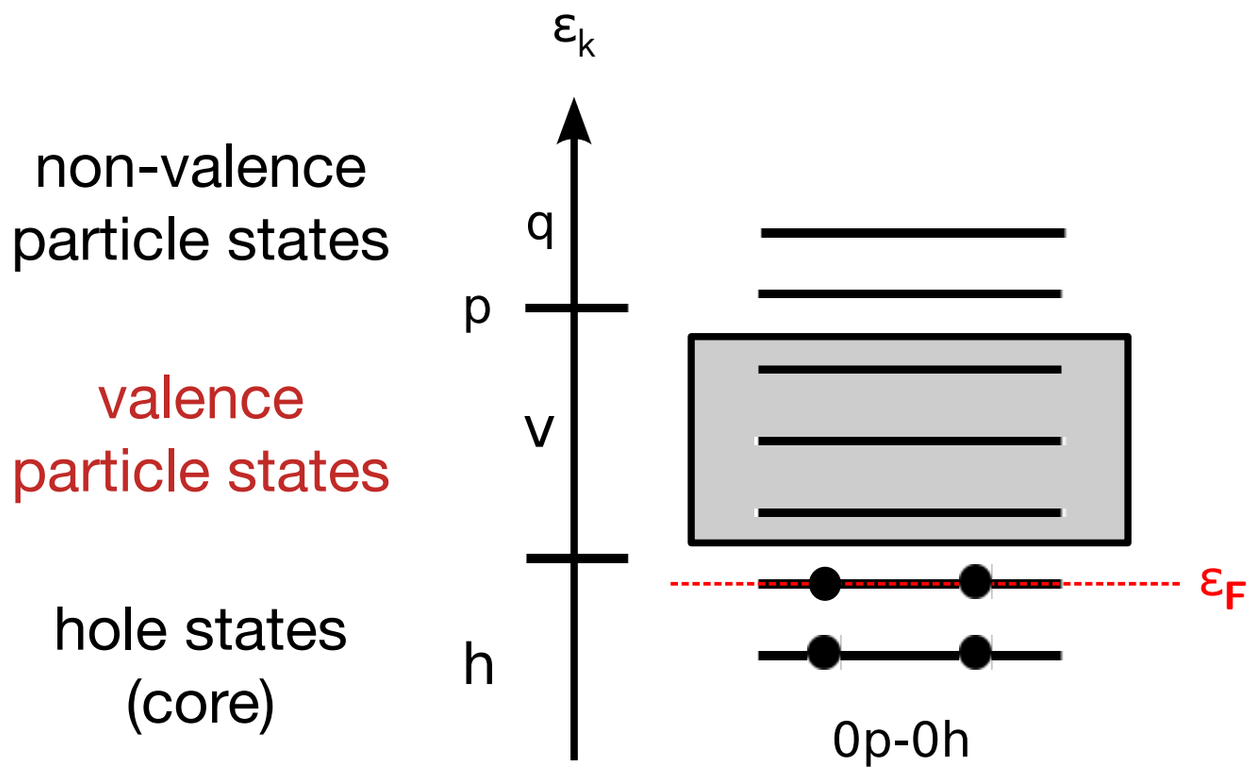
2. Solve open-shell directly with IM-SRG with suitable open-shell reference state (Multireference)

   - 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



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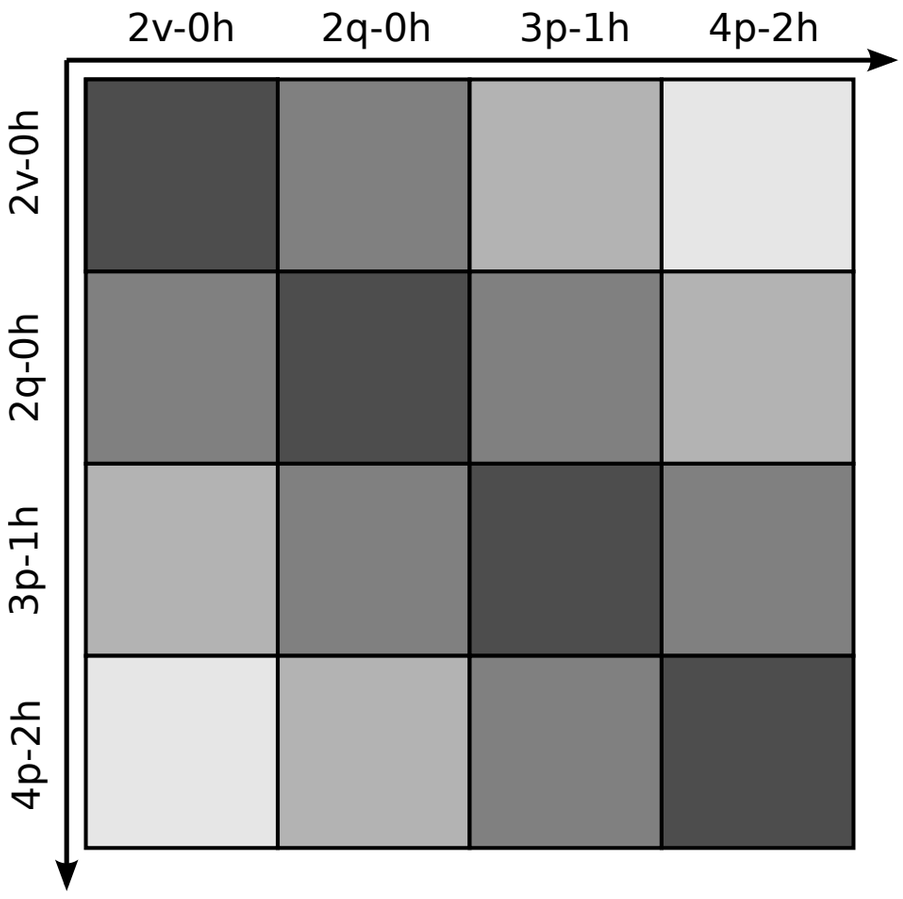


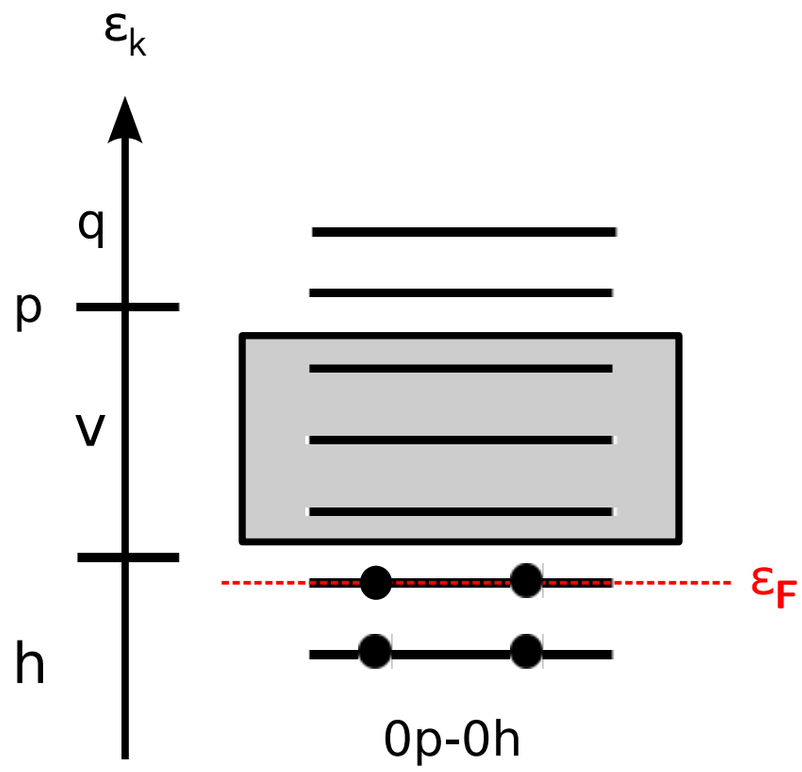

$$\langle i | H | j \rangle$$

Solve SM problem

non-valence particle states

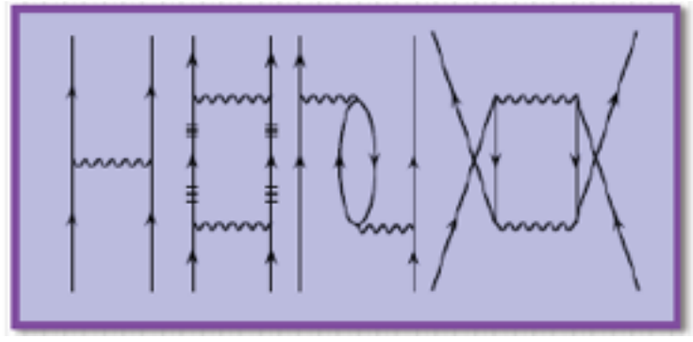
valence particle states

hole states (core)



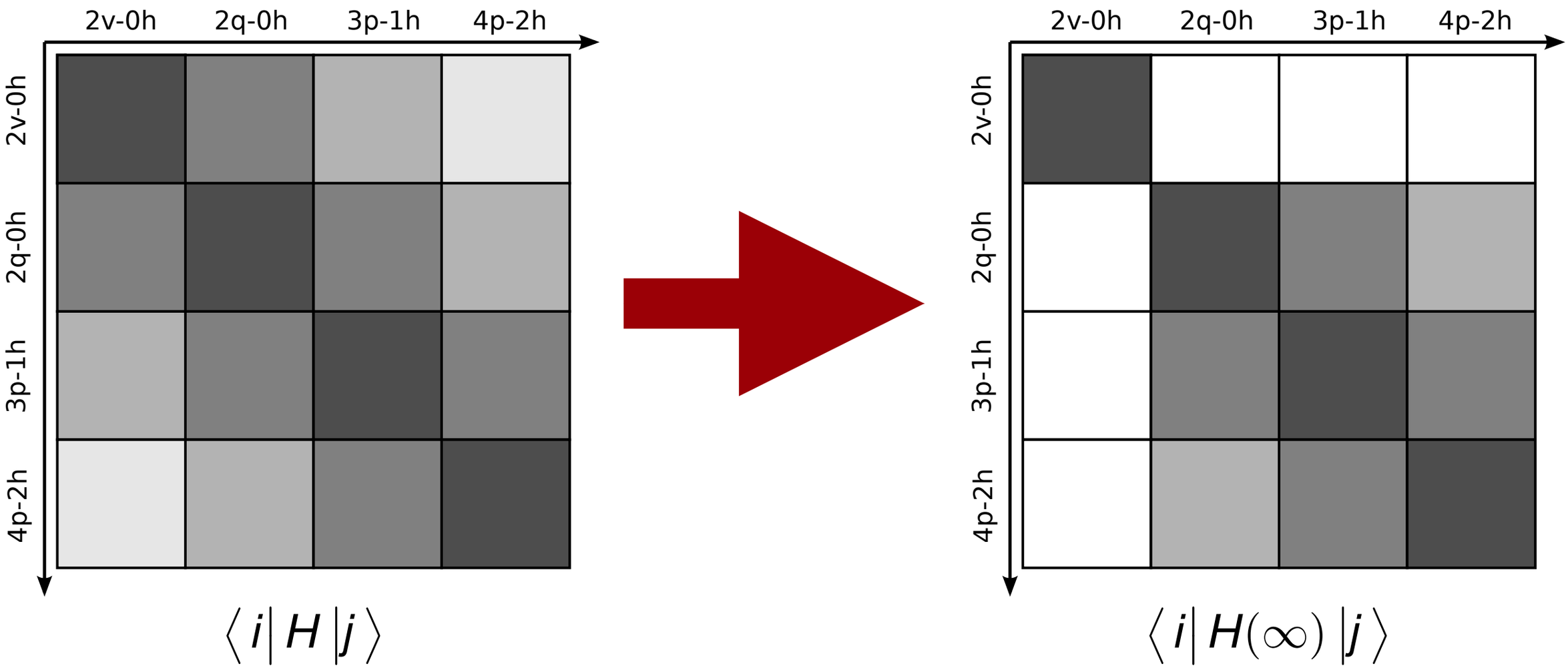

$$PH_{eff}P|\Psi\rangle = (E - E_c)P|\psi\rangle$$

Previously, $H_{eff}$ from MBPT



Can we use the IM-SRG to do this?

# Valence Shell Model Decoupling



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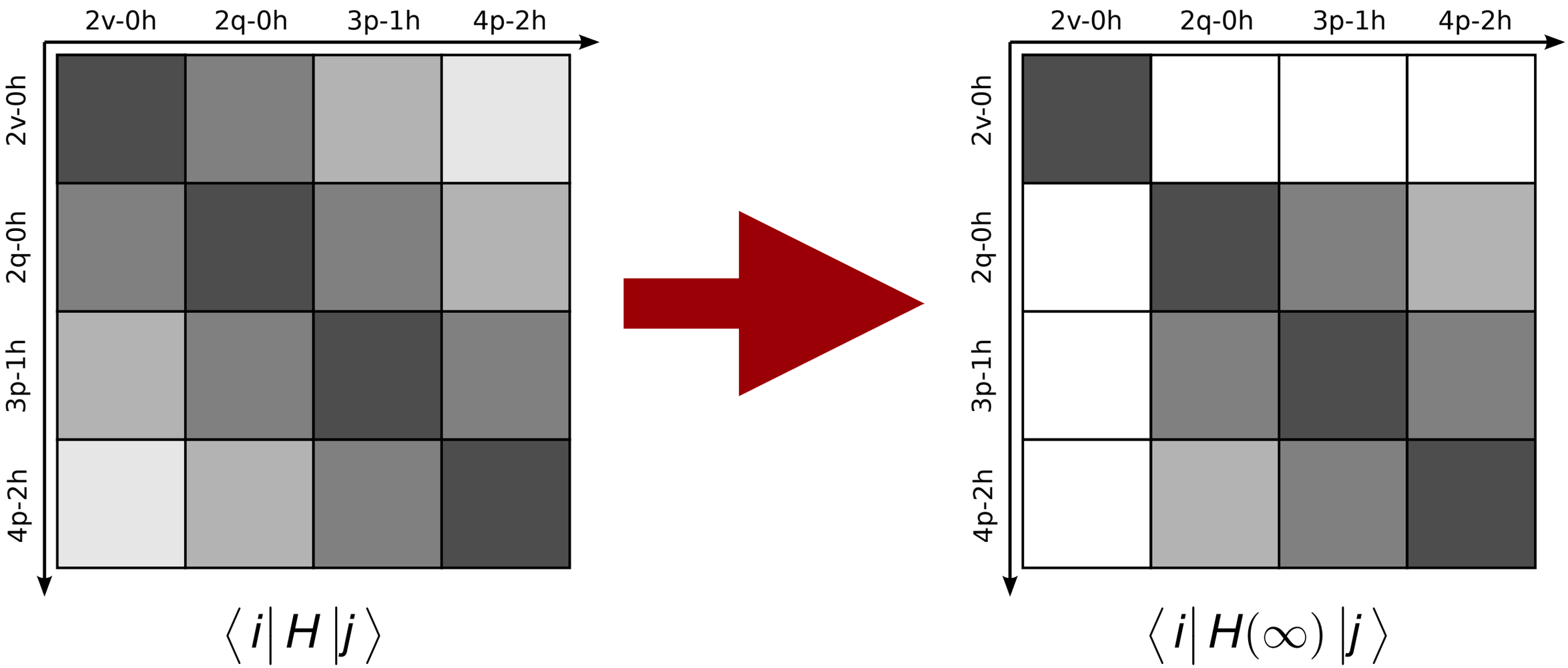


- use White-type generator with off-diagonal Hamiltonian

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

# IM-SRG(2) Shell Model Recipe

## 1) Generate HF basis w/full NN + NNN

$$H_A = \left(1 - \frac{1}{A}\right) \sum_i \frac{\mathbf{p}_i^2}{2m} + \sum_{i<j} \left( V_{ij} - \frac{\mathbf{p}_i \cdot \mathbf{p}_j}{Am} \right) + \sum_{i<j<k} V_{ijk}$$

A = target nucleus (NOT core)

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## 2) Normal order w.r.t. core HF gs and drop 3N (NO2B)

$$H_A = E_0 + \sum_{qr} f_r^q : A_r^q : + \frac{1}{4} \sum_{qrst} \Gamma_{st}^{qr} : A_{ts}^{qr} :$$

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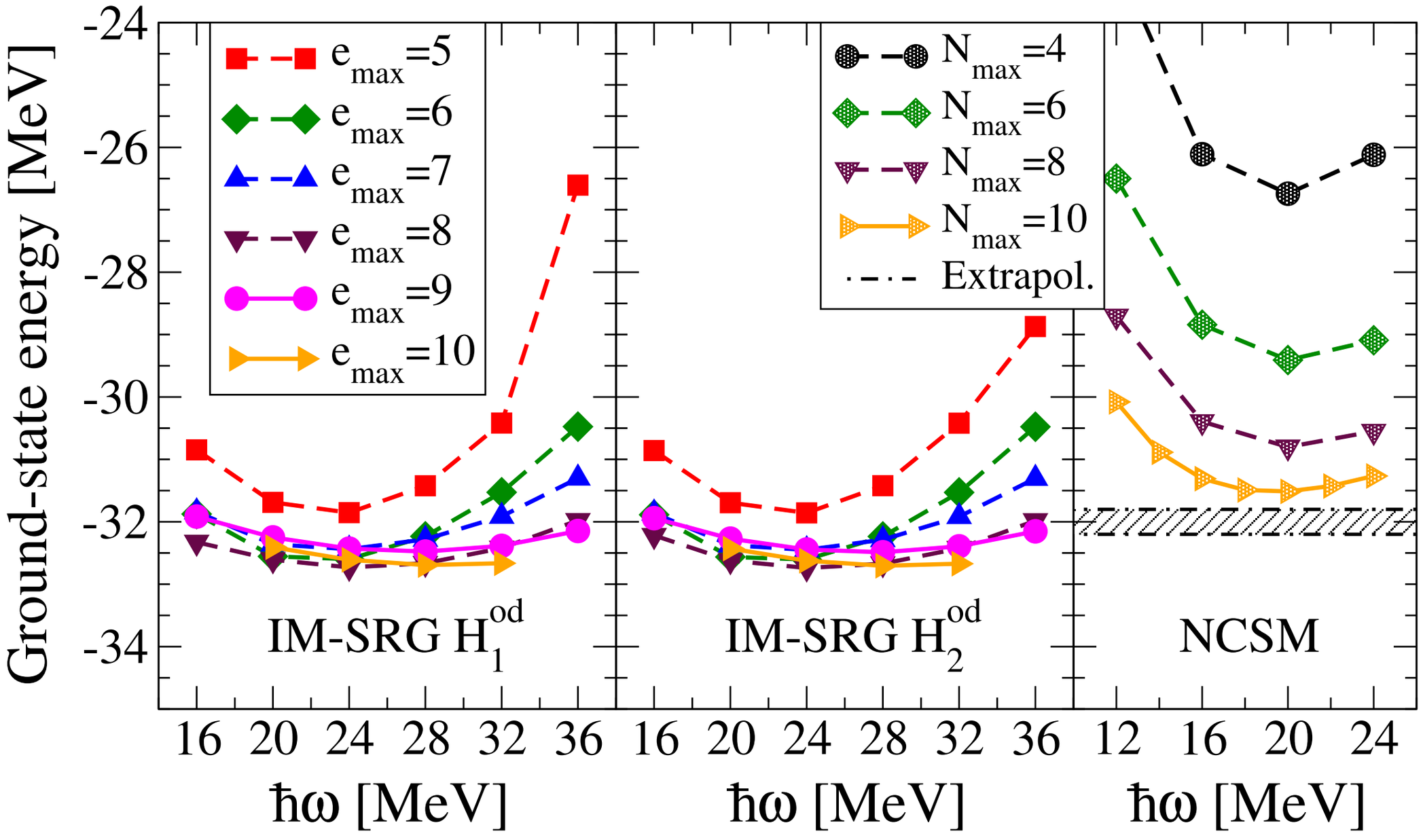
3) Solve IM-SRG(2) w/Valence decoupling

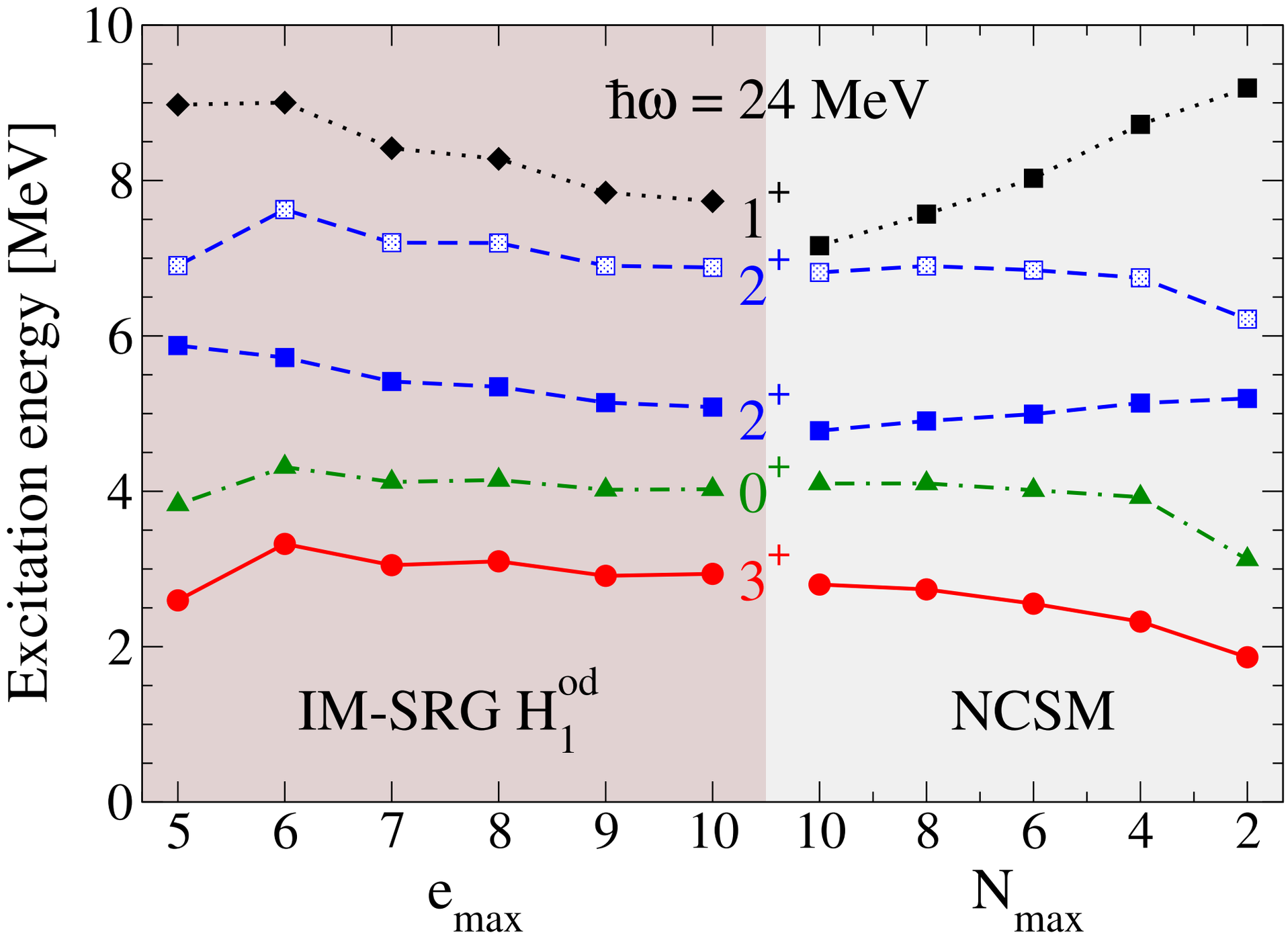
4) Diagonalize $H_A(\infty)$ in valence shell

# $^6$Li ground state: comparison to exact NCSM




K. Tsukiyama, SKB and A. Schwenk, Phys. Rev. C **85**, 061304(R) (2012)

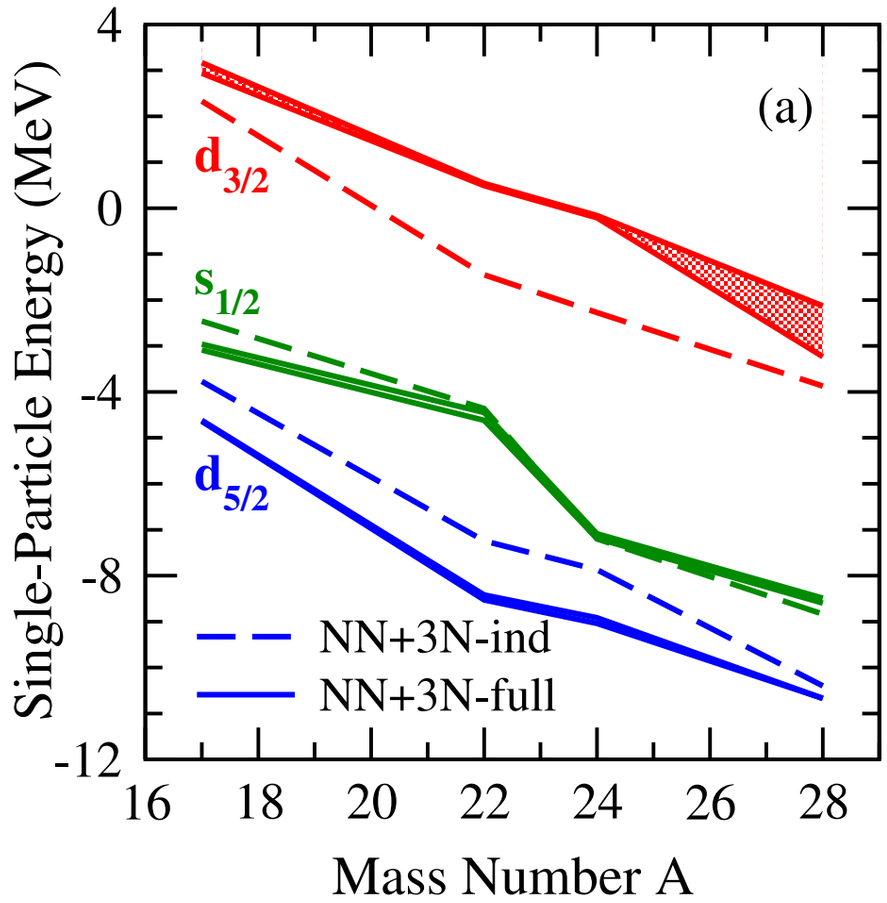
# $^6$Li spectra: comparison to NCSM

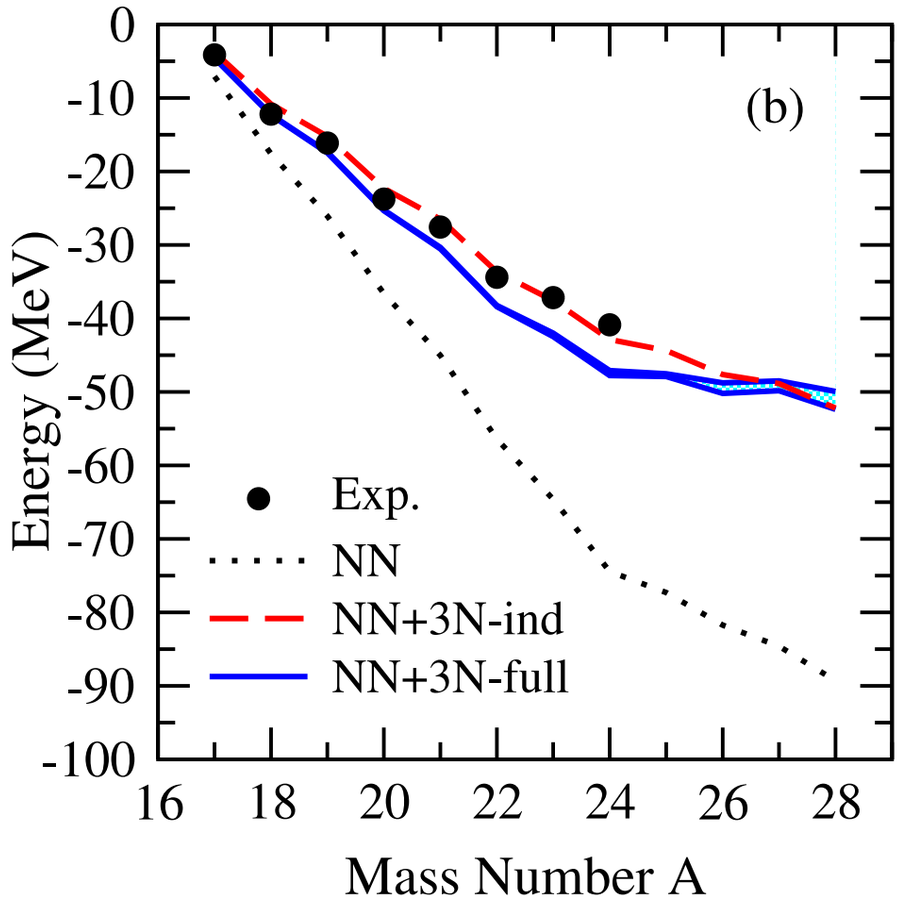



K. Tsukiyama, SKB and A. Schwenk, Phys. Rev. C **85**, 061304(R) (2012)

# Oxygen isotopes from NN + NNN

SKB et al., arXiv:1402.1407



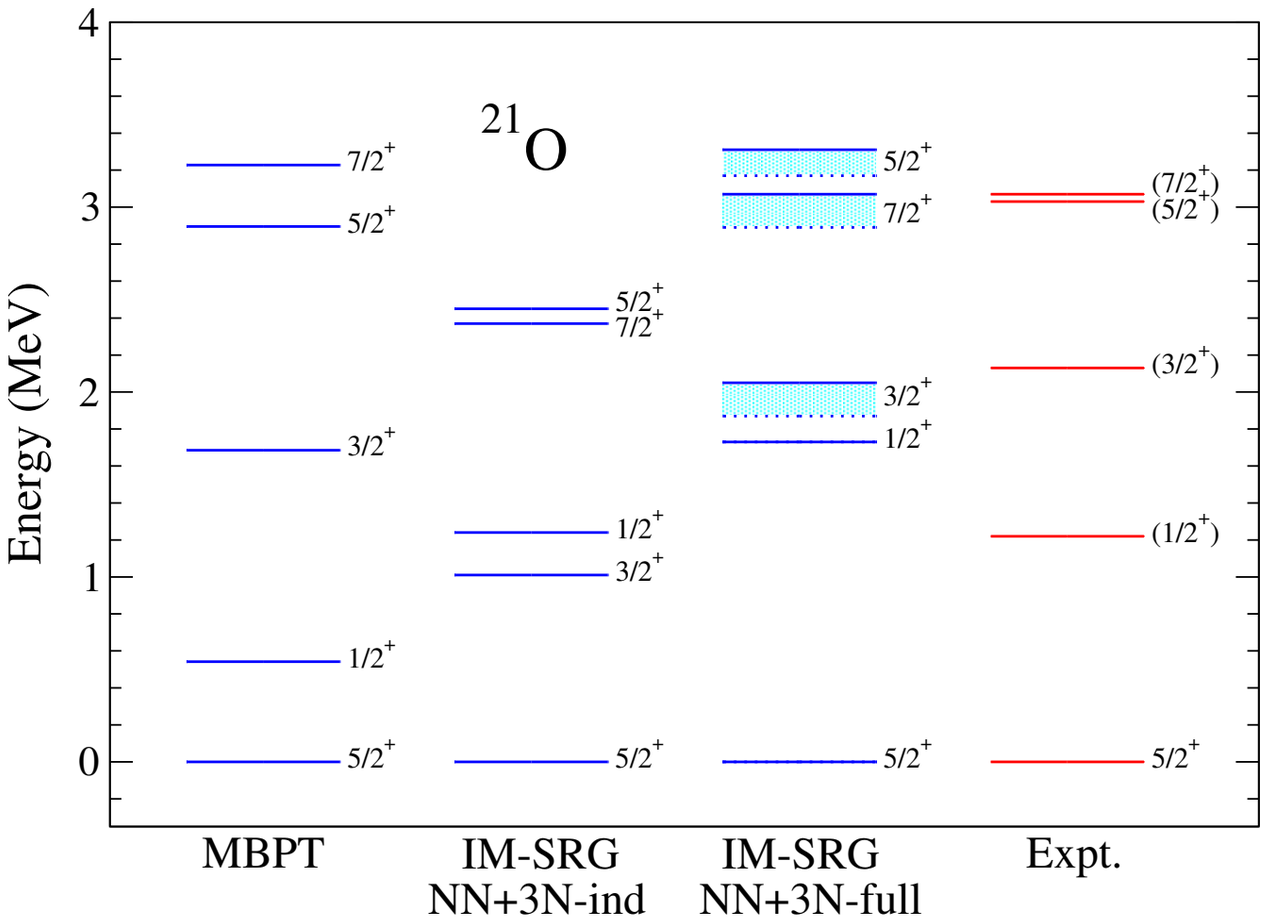



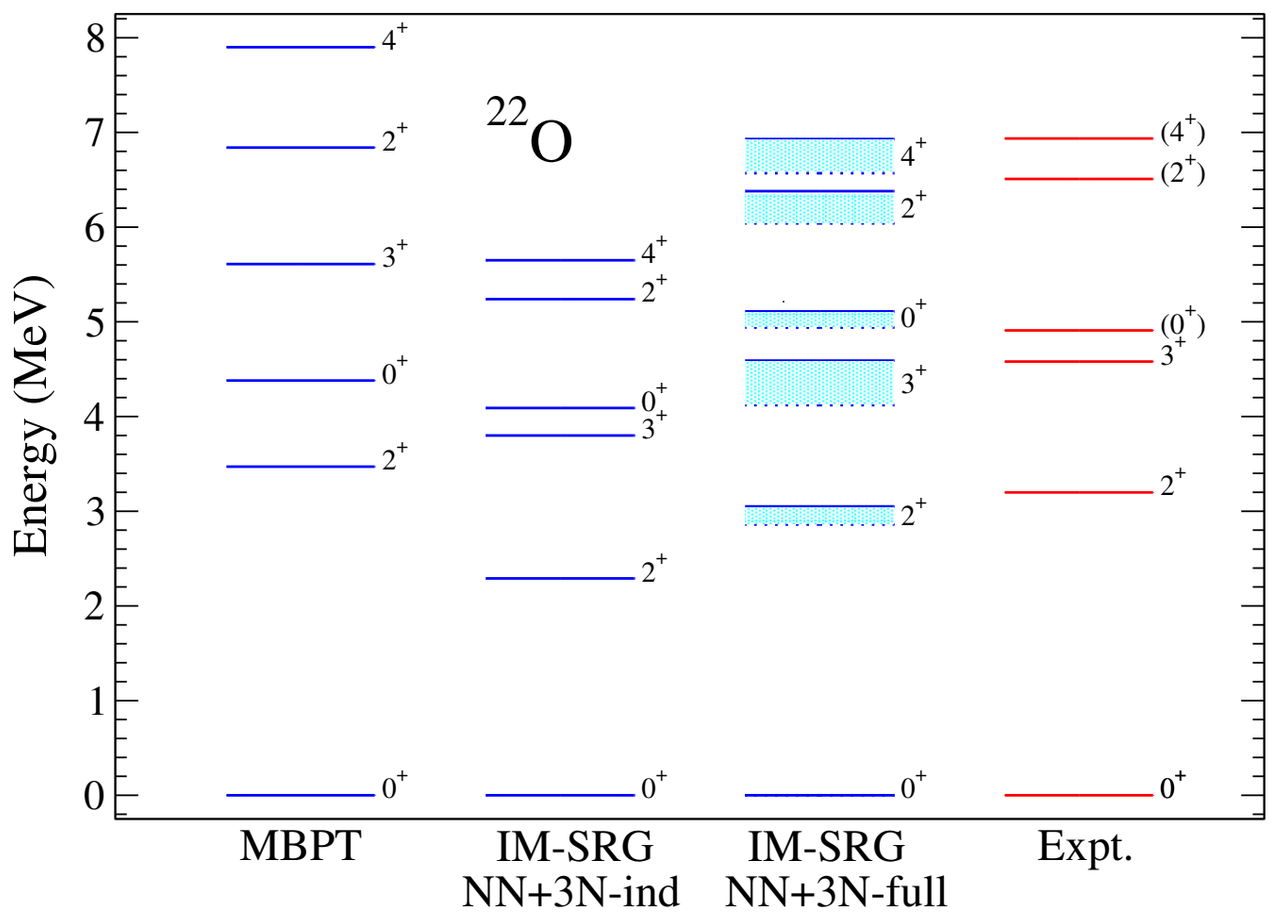

NN + 3N-ind = N3LO(500) NN, SRG-evolved to $\lambda$, omits induced 4N

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

# Oxygen Spectra

SKB et al., arXiv:1402.1407

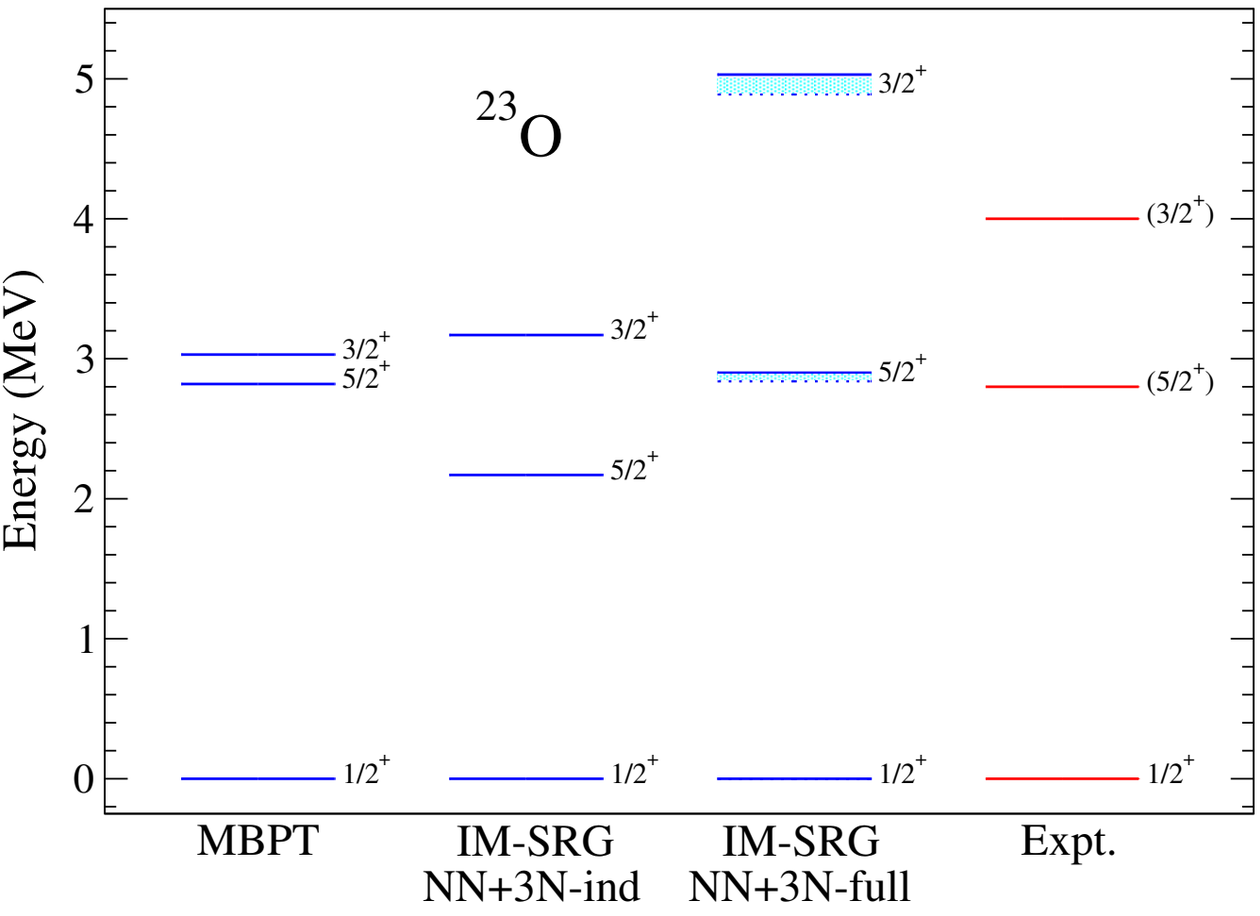


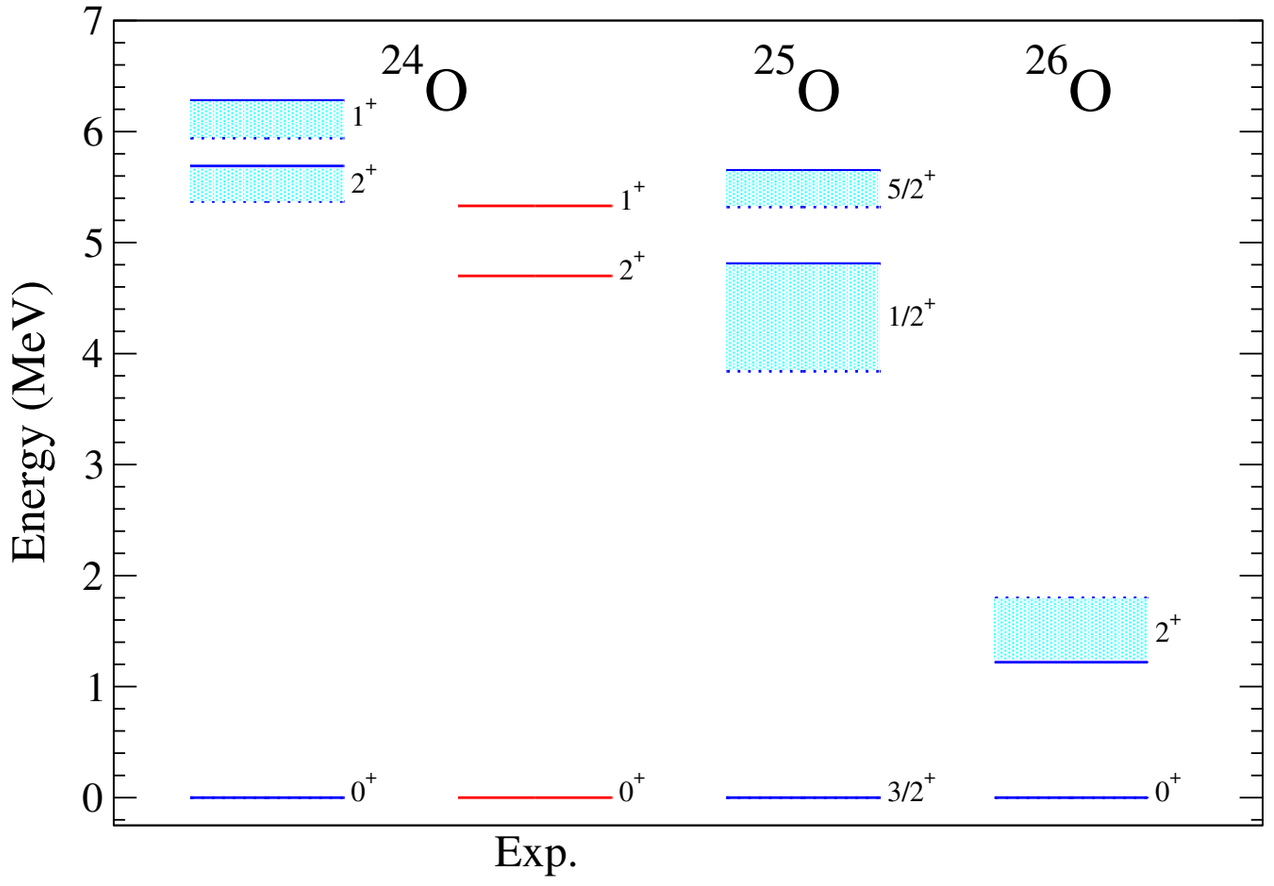




- Importance of 3NF's
- No need for extended valence space (a-la MBPT)
- weak $\hbar\omega$ dependence (20-24 MeV)

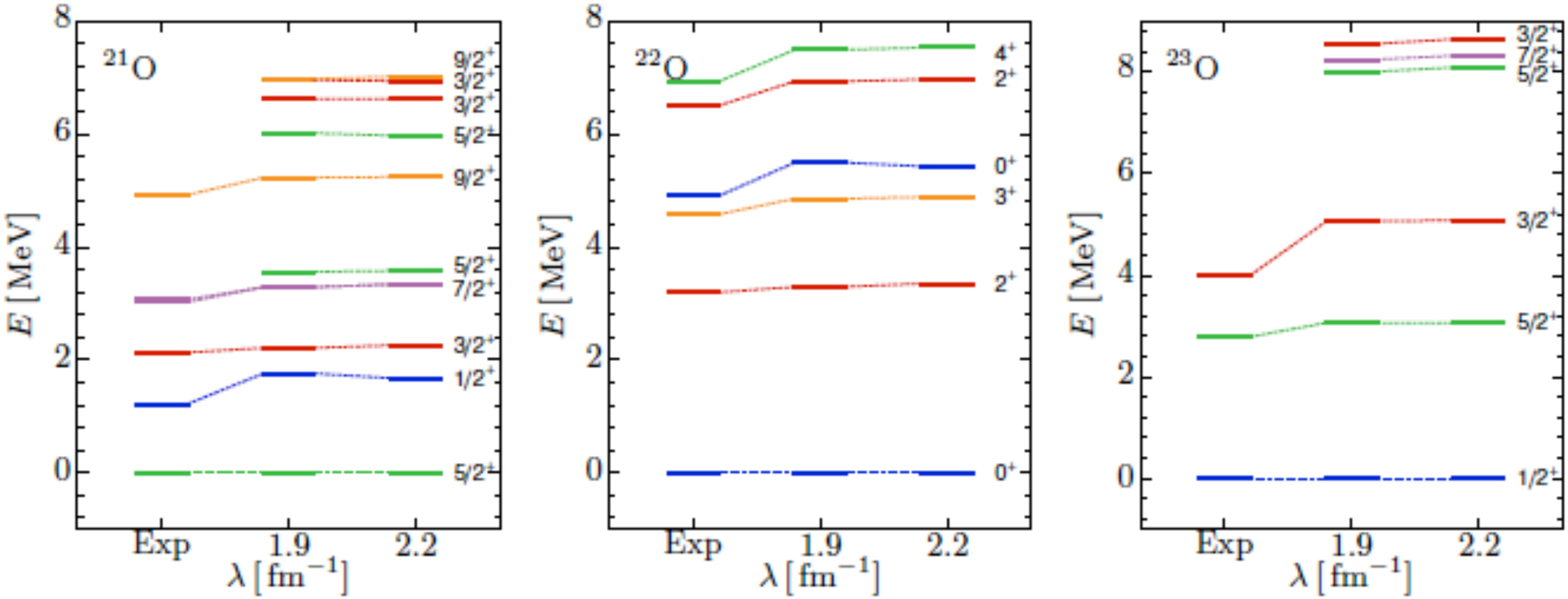
# Oxygen Spectra

SKB et al., arXiv:1402.1407



# Oxygen Spectra




Weak dependence on free-space SRG λ

# Conclusions

- closed shell nuclei thru $^{56}$Ni with initial 3NF in IM-SRG(2)
  - ✦ scales like CCSD, tracks more closely to CCSD(T)
  - ✦ same trend in various systems (nuclei, quantum dots, electron gas, neutron drops, molecules)
  - ✦ Magnus expansion => faster convergence, access to observables, approximations to IM-SRG(3)

- Ab-initio valence shell model
  - ✦ Ground states, spectra, odd-A “all in one”
  - ✦ Initial proof-of-principle in Oxygen w/initial 3NF; competitive with USDb
  - ✦ On the horizon: F, Ne, and Mg chains, extended model spaces, effective operators, comparisons to other methods (NSCMWC, CCEI, SCGF) etc...