In-Medium SRG Approaches for Open-Shell Nuclei

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Outline

- The Similarity Renormalization Group
- In-Medium SRG
- Ground States of Closed- and Open-Shell Nuclei
- IM-SRG Interactions for the Shell Model
- Next Steps
- Conclusions

Prelude:

Similarity Renormalization Group

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

R. Roth, S. Reinhardt, and H. H., Phys. Rev. **C77** (2008), 064003

H. H. and R. Roth, Phys. Rev. **C75** (2007), 051001

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.,

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

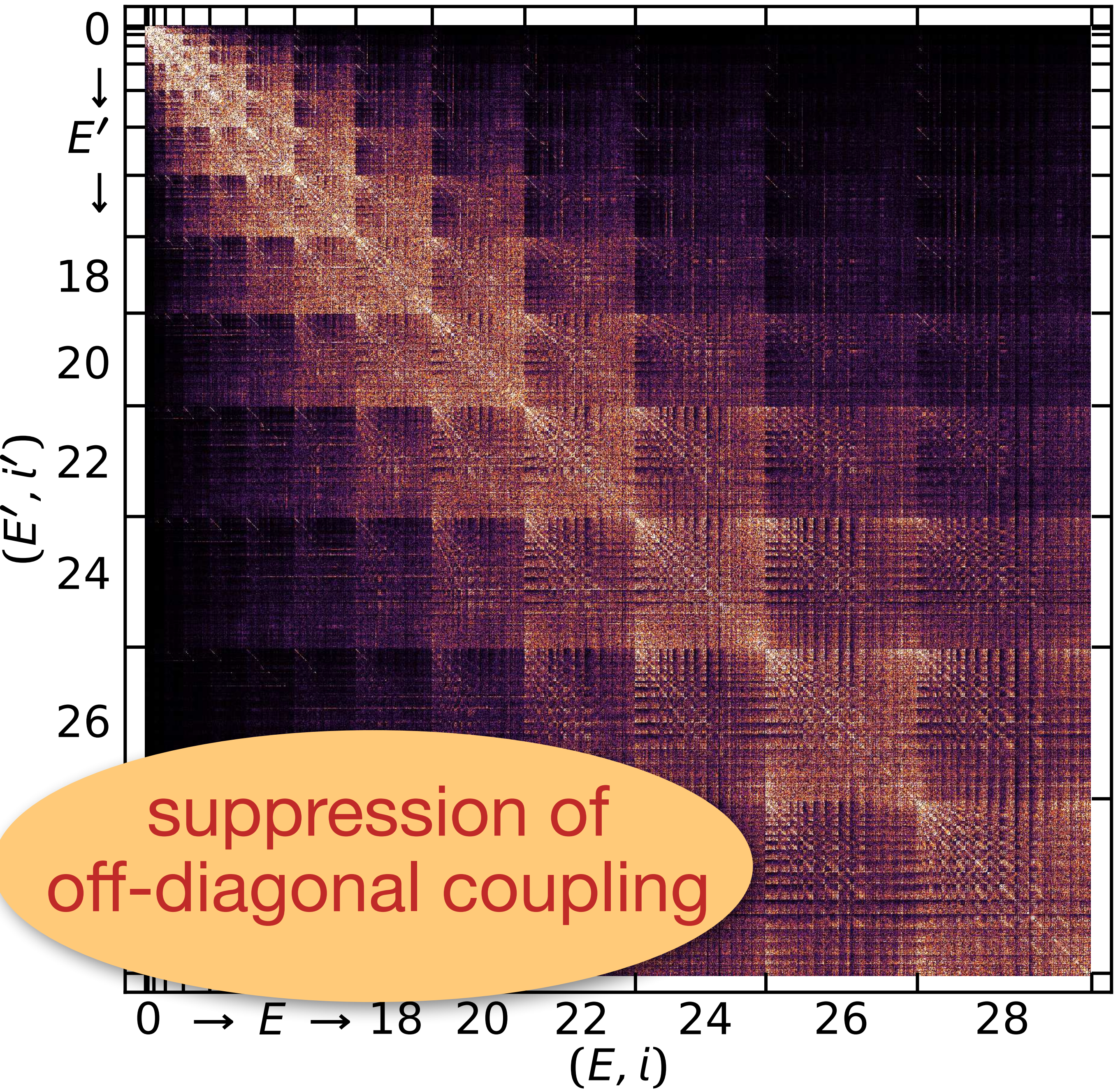
to suppress (suitably defined) off-diagonal Hamiltonian

- consistent evolution for all observables of interest

SRG in Three-Body Space

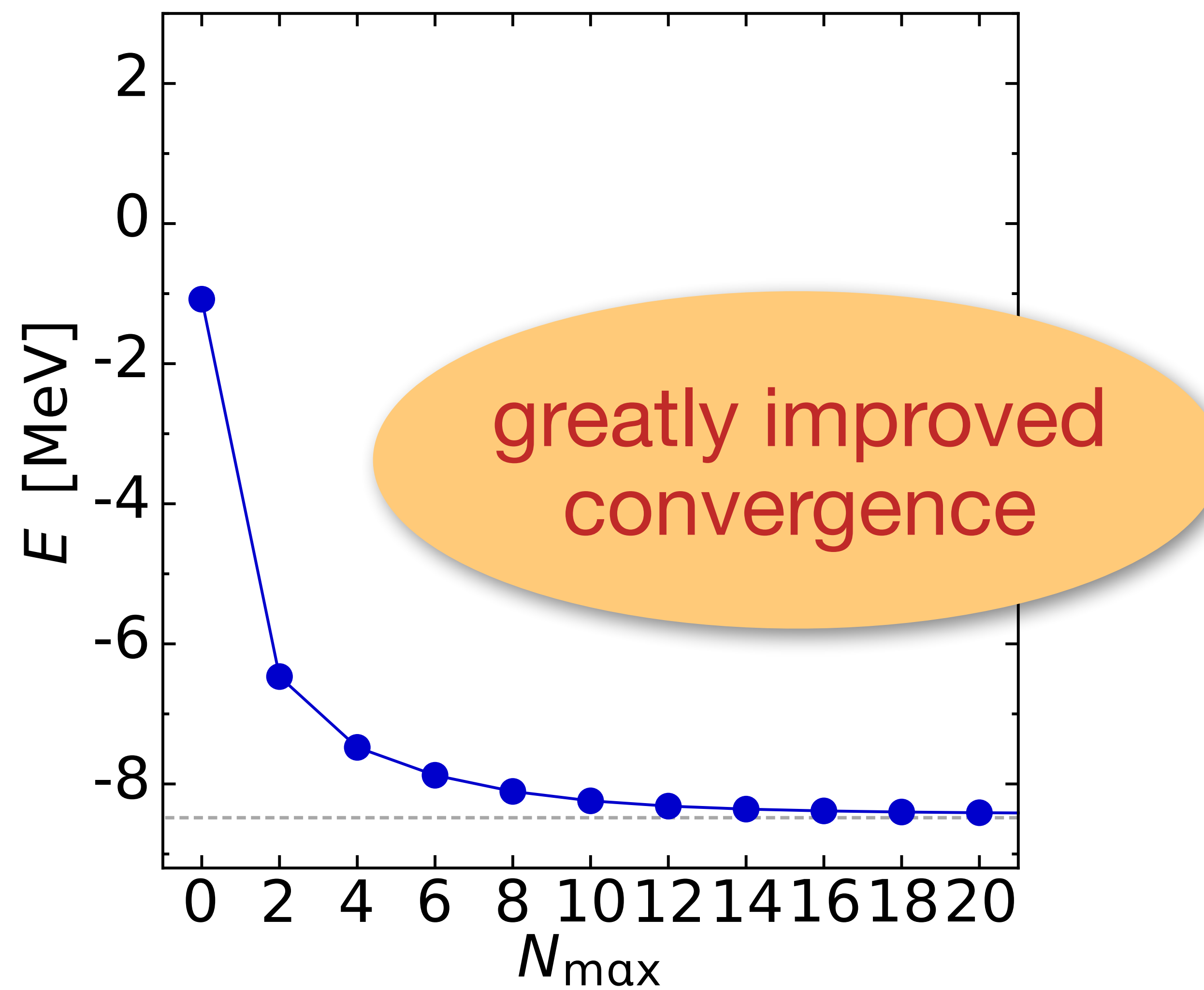
3B Jacobi-HO Matrix Elements

$J^\pi = \frac{1}{2}^+, T = \frac{1}{2}, \hbar\Omega = 28$ MeV



λ = 1.33 fm^{-1}

^{3}H ground-state (NCSM)



[figures by R. Roth, A. Calci, J. Langhammer]

In-Medium SRG

S. K. Bogner, H. H., T. Morris, A. Schwenk, and K. Tuskiyama, to appear in Phys. Rept.

H. H., 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)

Solving the Flow Equation

operator flow equation

$$\frac{d}{ds}H(s) = \left[\eta(s), H(s)\right]$$

encodes information for all systems described by H …

… but solving multiple systems at once requires an increasingly complicated unitary transformation

Solving the Flow Equation

manage complexity by defining / choosing

- truncation / organization scheme,
- basis (for operator algebra and/or Hilbert space), …

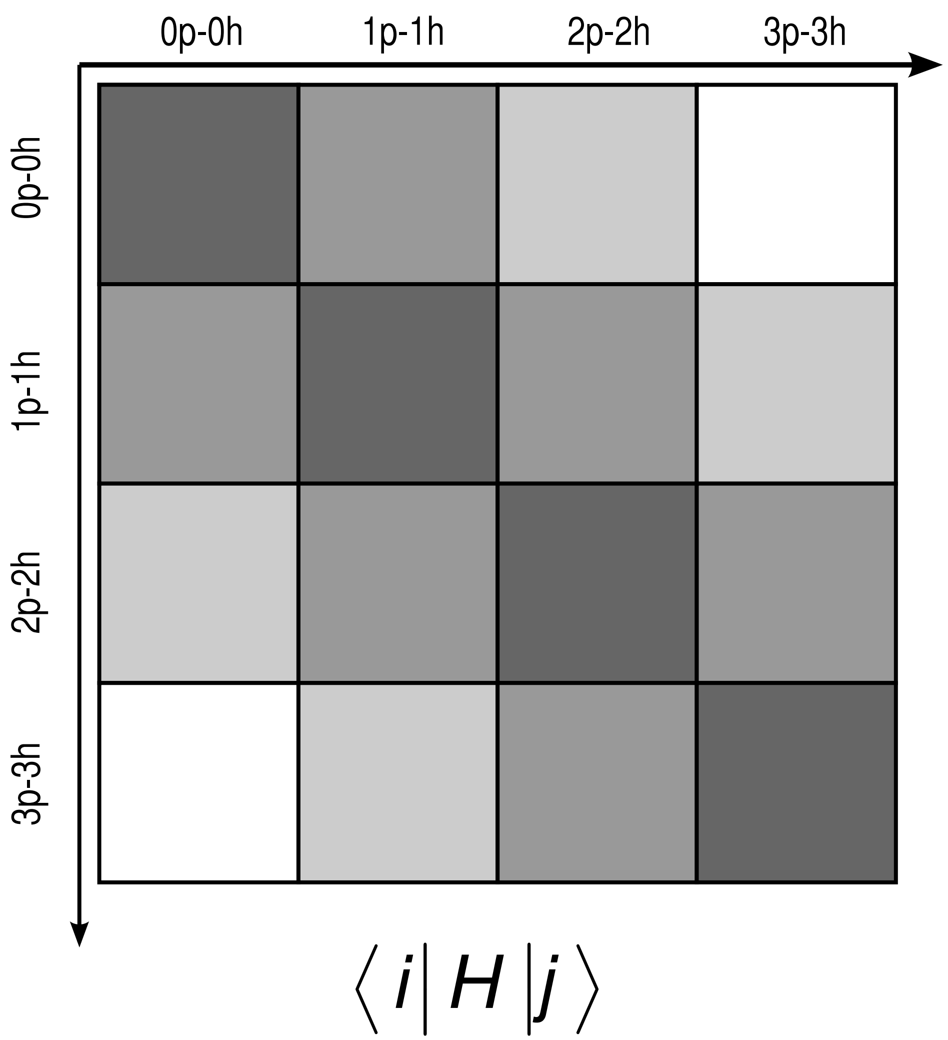
… but this introduces restrictions (e.g., to systems with fixed particle number), uncertainties

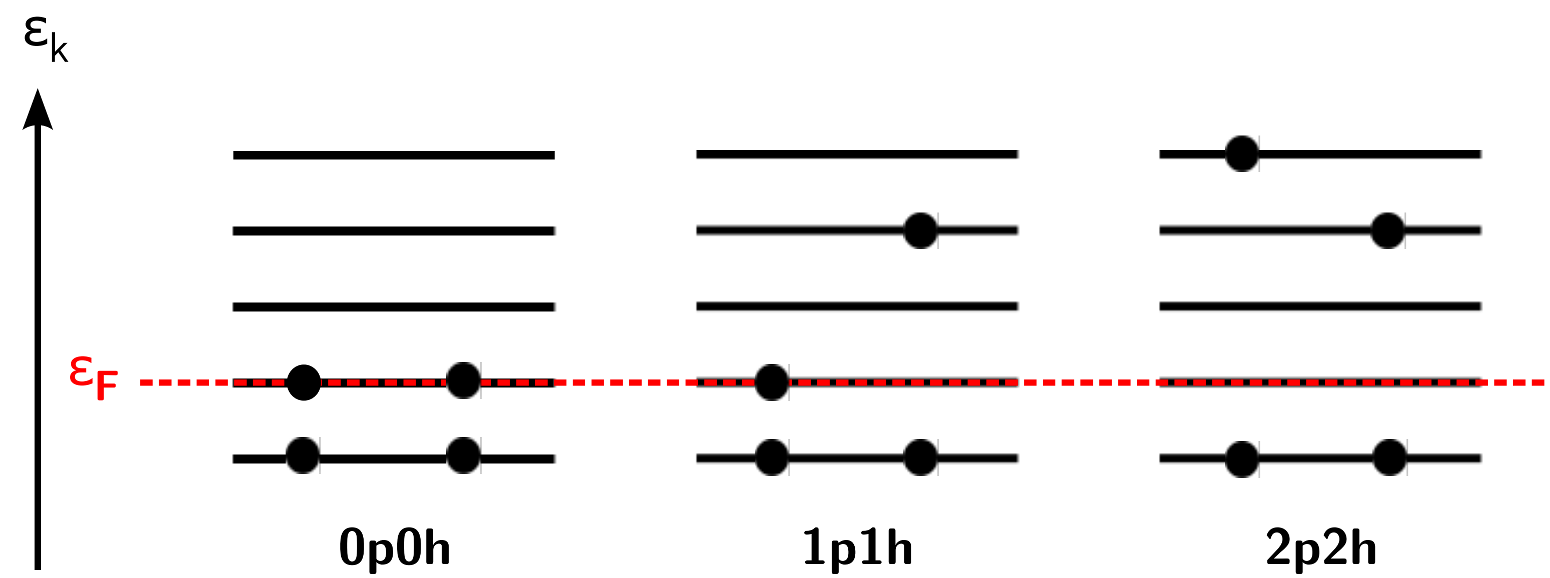
Solving the Flow Equation

- define decoupling condition(s)
- choose a generator

use flexibility to introduce information from target system (e.g. reference state), optimize transformation, reduce uncertainties

Decoupling in A-Body Space





excitations relative to reference state:
→ 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:

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

- 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

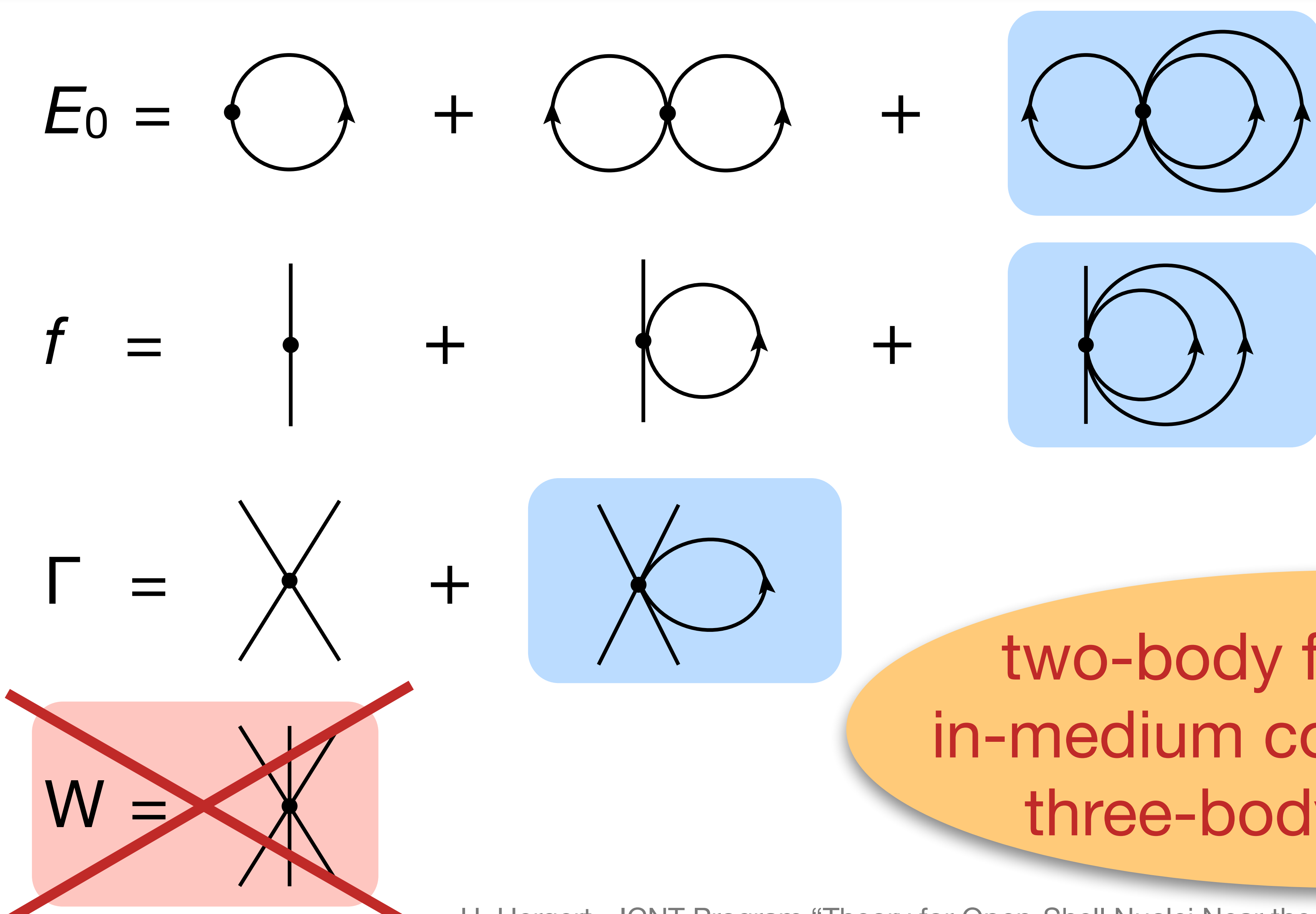
$$\left\langle\Phi\right| :A^{k_1\dots k_N}_{l_1\dots l_N}: \left|\Phi\right\rangle = 0$$

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

Normal-Ordered Hamiltonian

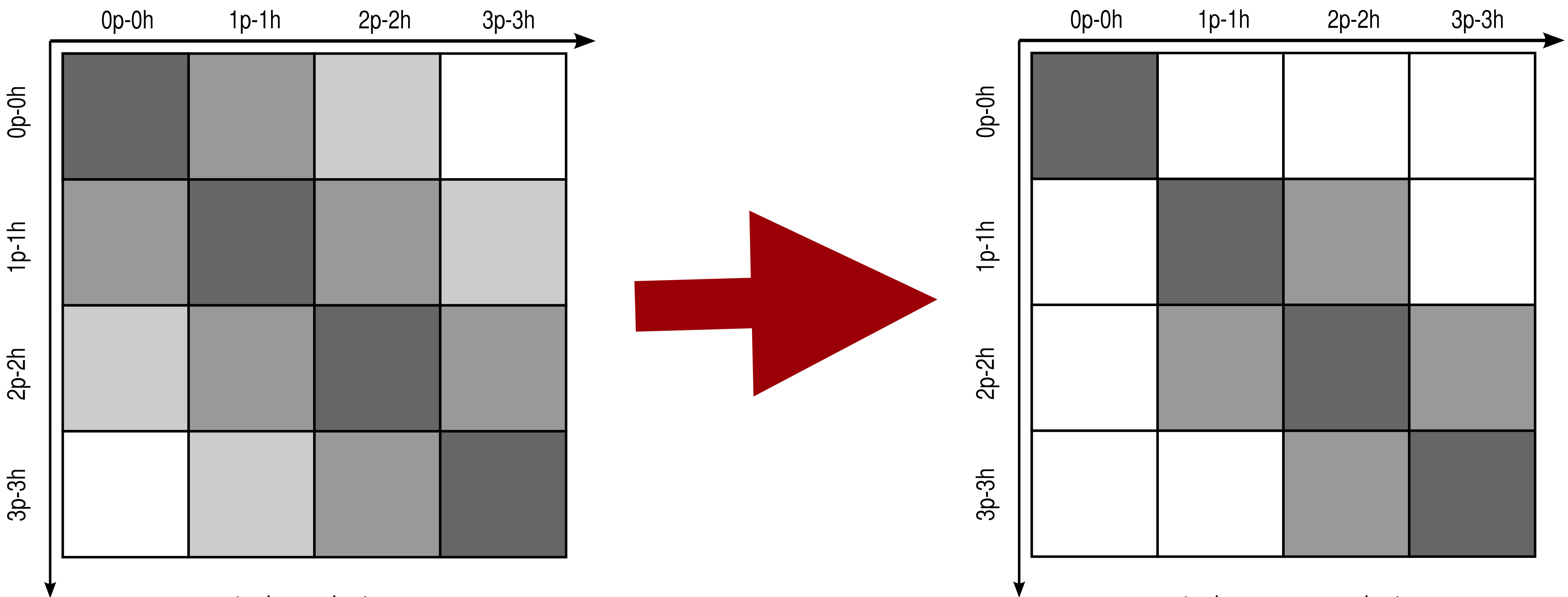
Normal-Ordered Hamiltonian

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



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

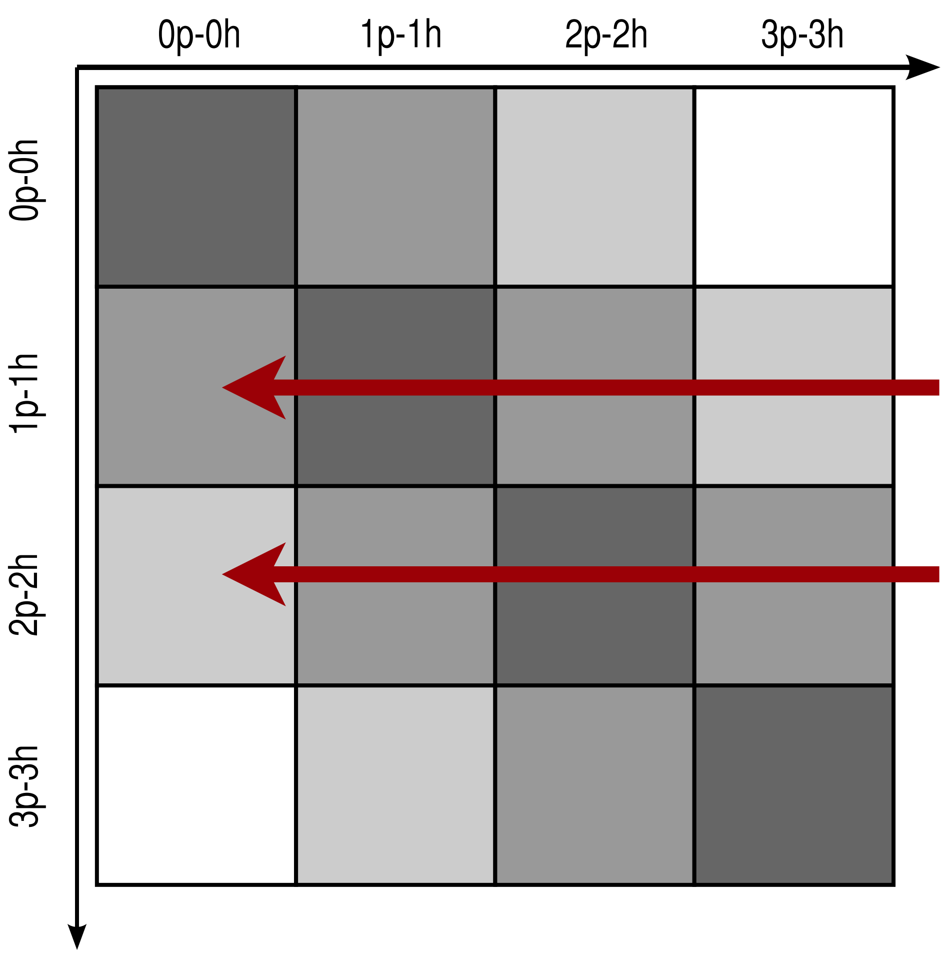
Decoupling in A-Body Space



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

aim: decouple reference state $|\Phi\rangle$ (0p-0h) from excitations

Decoupling in A-Body Space



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

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

- 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: $$\eta^{I} = [H_d, H_{od}]$$
- 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)

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

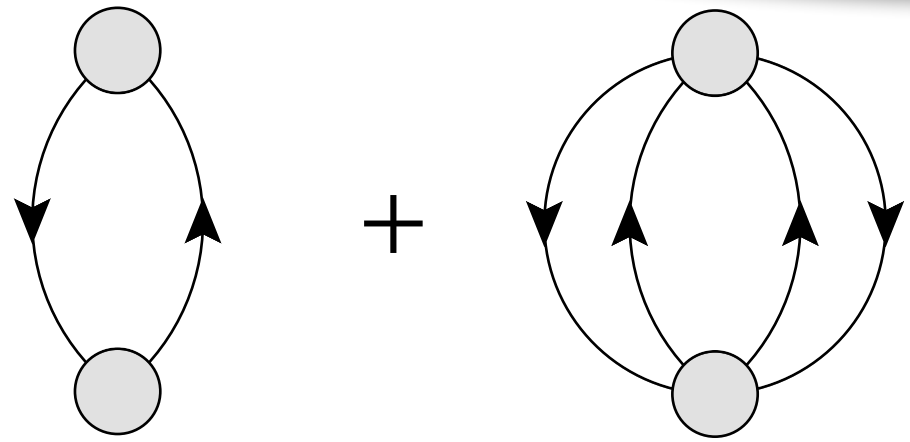
- off-diagonal matrix elements are suppressed like $e^{-\Delta^2 s}$ (Wegner), e^{-s} (White), and $e^{-|\Delta| s}$ (imaginary time)
- g.s. energies ($s \to \infty$) differ by $\ll 1\%$

IM-SRG(2) Flow Equations

0-body Flow

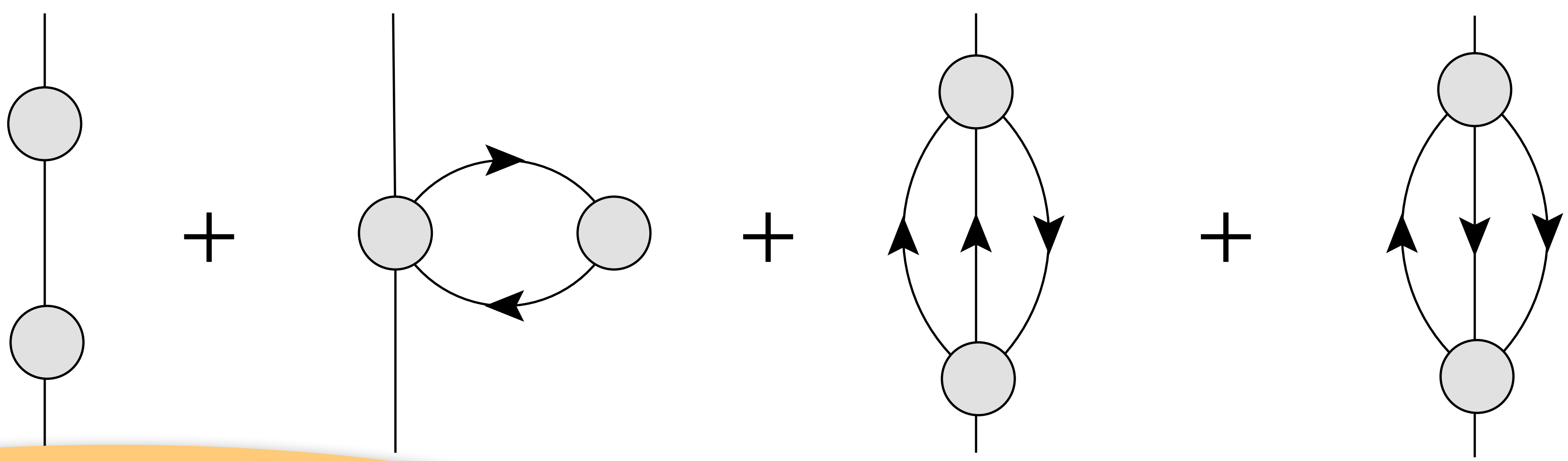
~ 2nd order MBPT for *H(s)*

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



1-body Flow

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



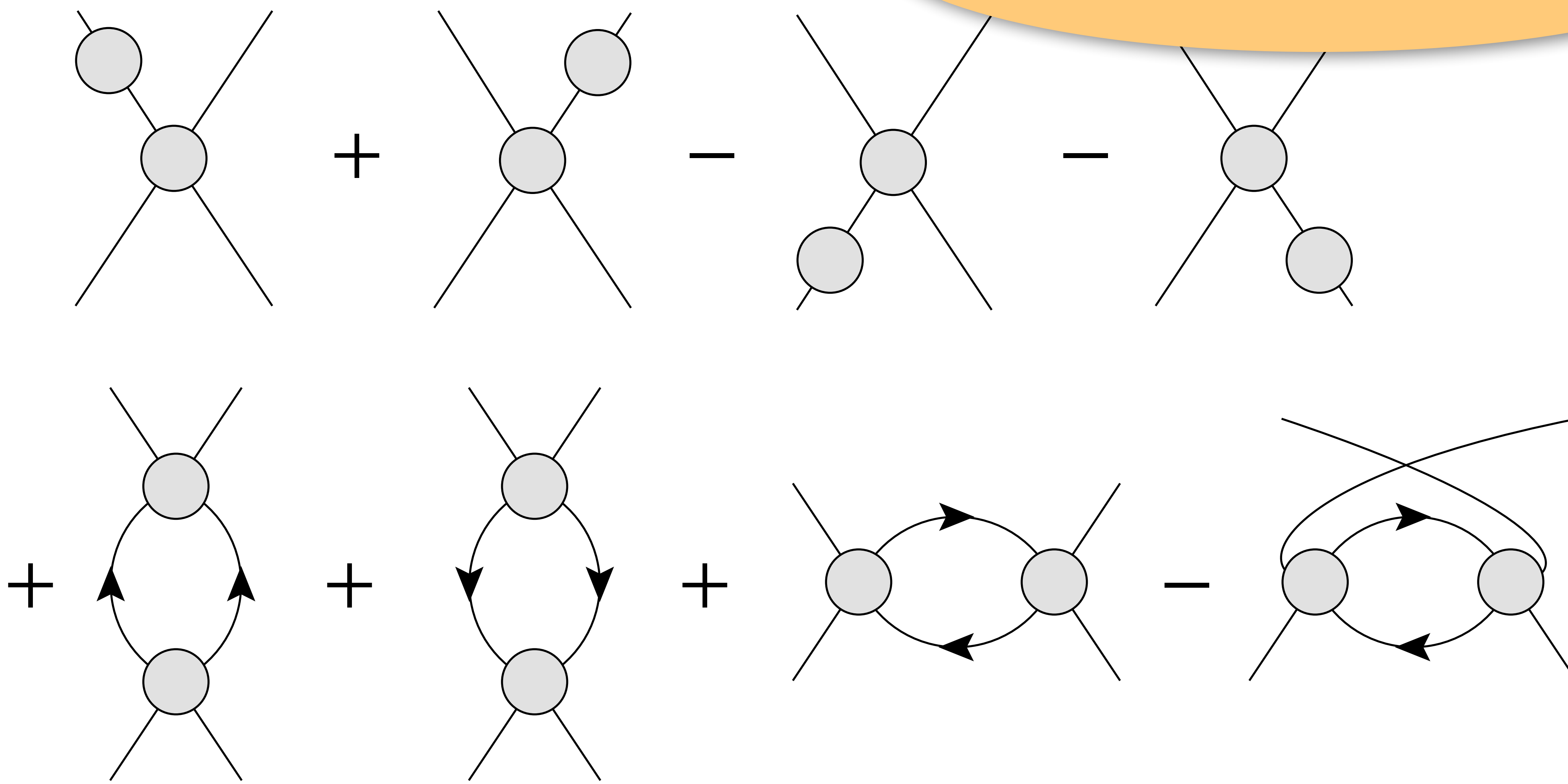
IM-SRG(2): truncate ops. at two-body level

IM-SRG(2) Flow Equations

2-body Flow

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

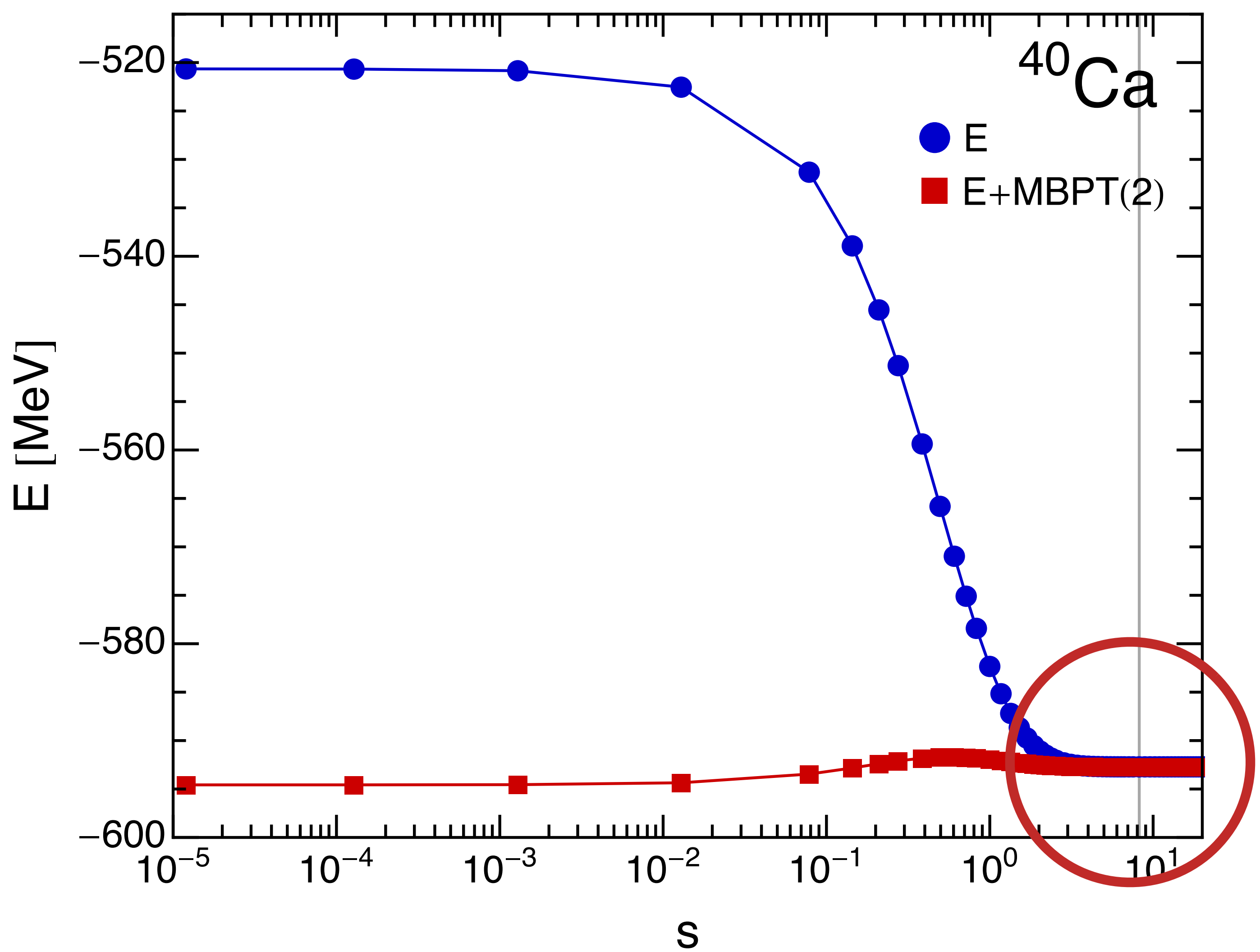
$$\frac{d\Gamma}{ds} =$$

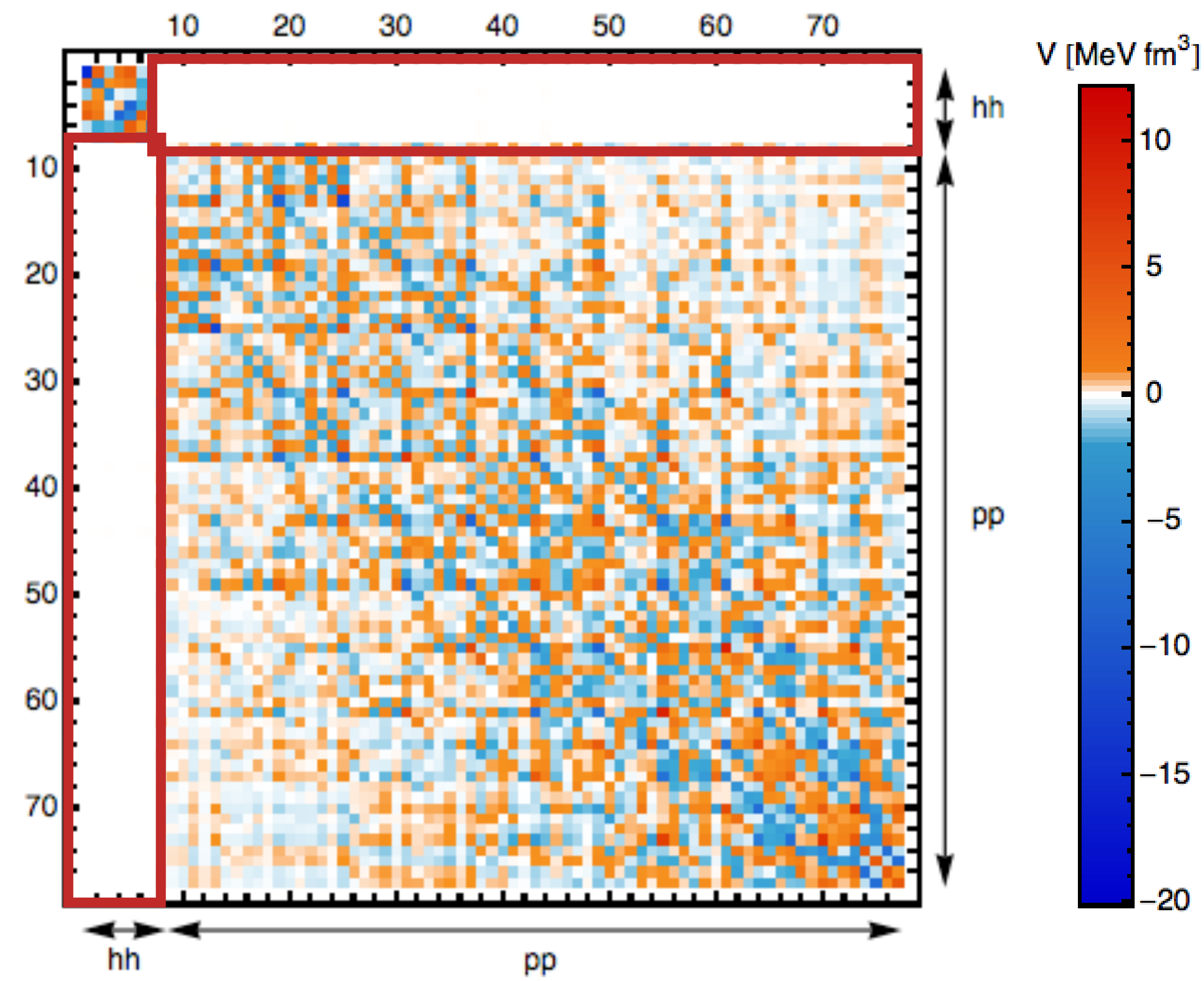


s channel — ladders

t channel, *u* channel — rings

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

Ground States of Closed and Open-Shell Nuclei

H. H., in preparation

H. H., S. Bogner, T. Morris, S. Binder, A. Calci, J. Langhammer, R. Roth, Phys. Rev. C **90**, 041302 (2014)

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

H. H., S. K. Bogner, S. Binder, A. Calci, J. Langhammer, R. Roth, and A. Schwenk, Phys. Rev. C **87**, 034307 (2013)

Hamiltonians

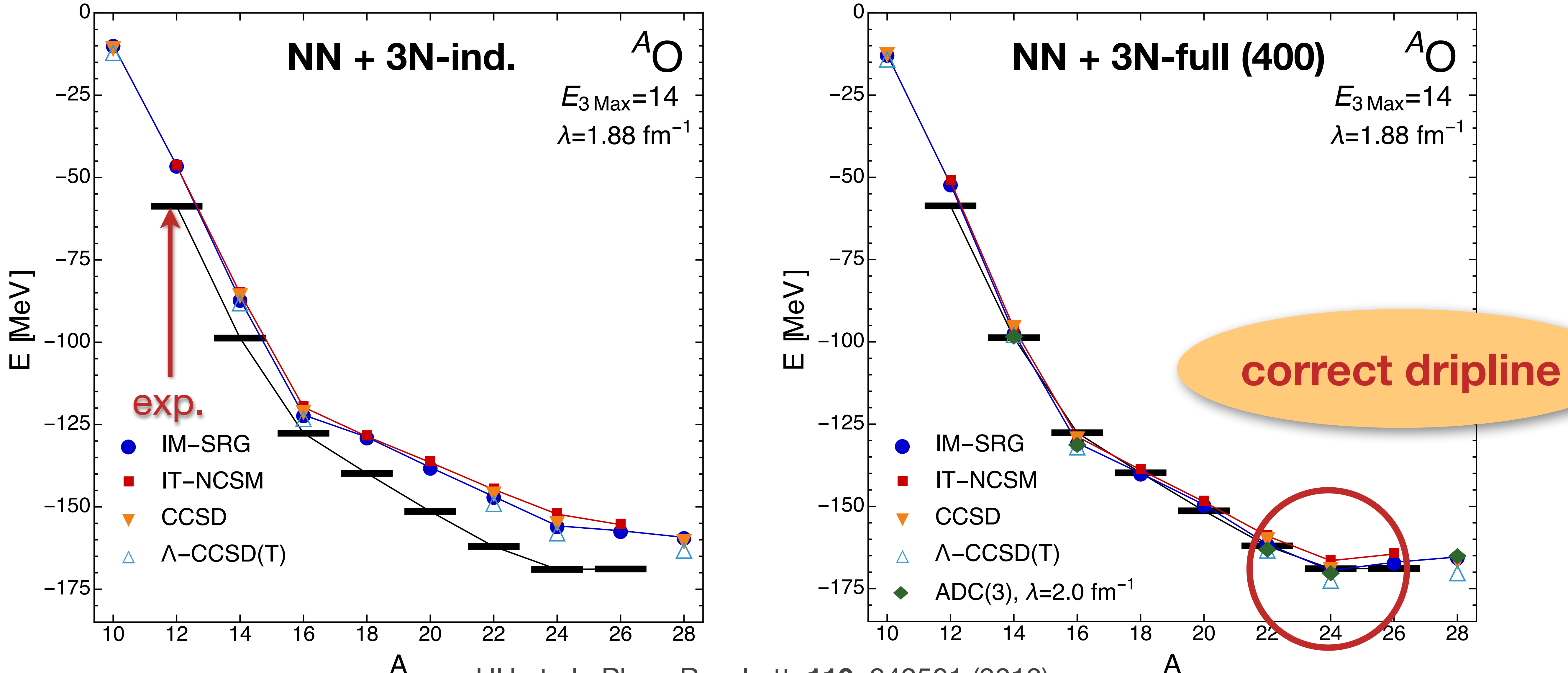
Initial Hamiltonian

- NN: chiral interaction at N^3LO (Entem & Machleidt)
- 3N: chiral interaction at N^2LO (c_D, c_E fit to ^3H, ^4He energies, β decay)

SRG-Evolved Hamiltonians

- **NN + 3N-induced:** start with initial NN Hamiltonian, keep two- and three-body terms
- **NN + 3N-full:** start with initial NN + 3N Hamiltonian, keep two- and three-body terms

Results: Oxygen Chain



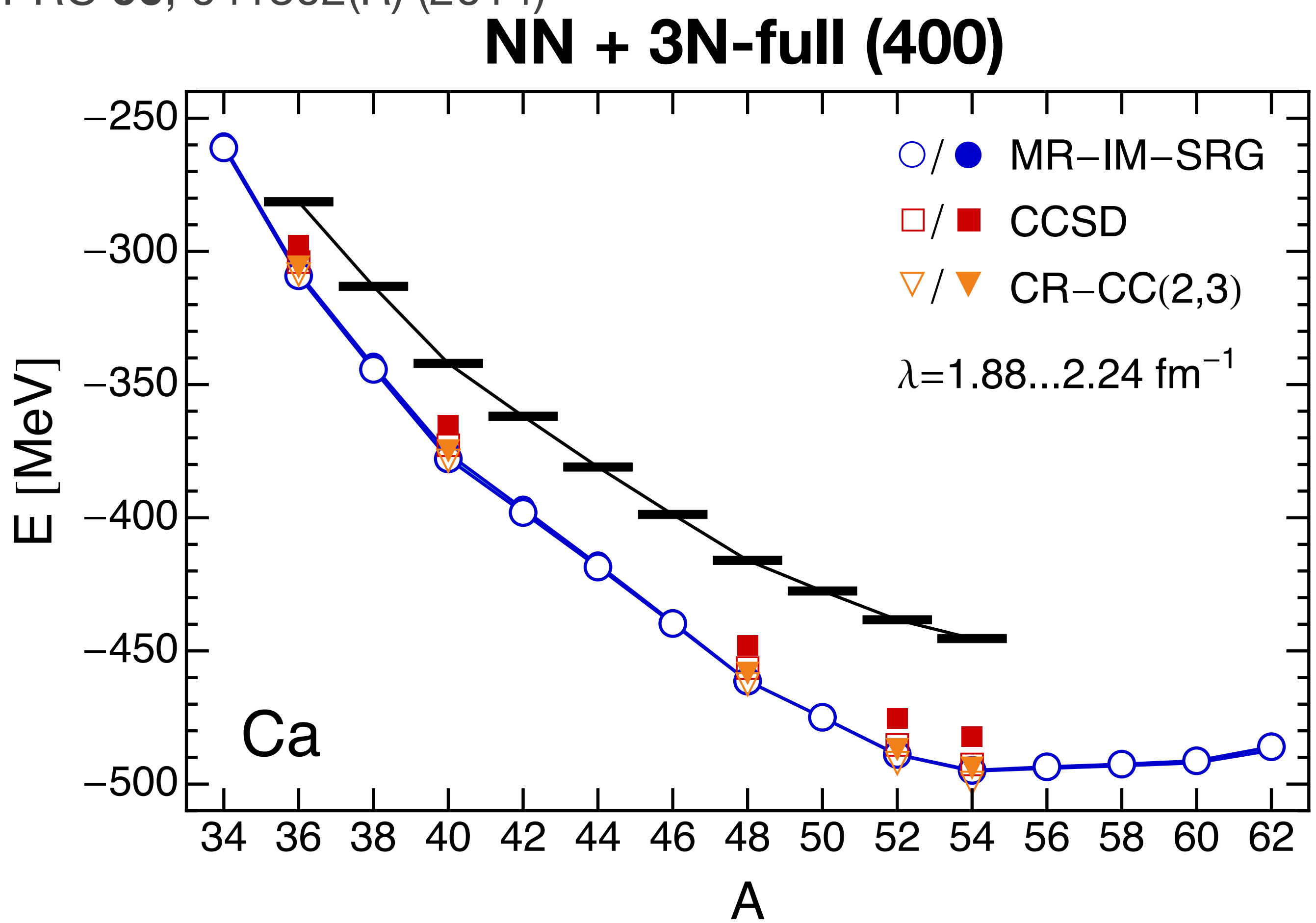
HH et al., Phys. Rev. Lett. **110**, 242501 (2013)

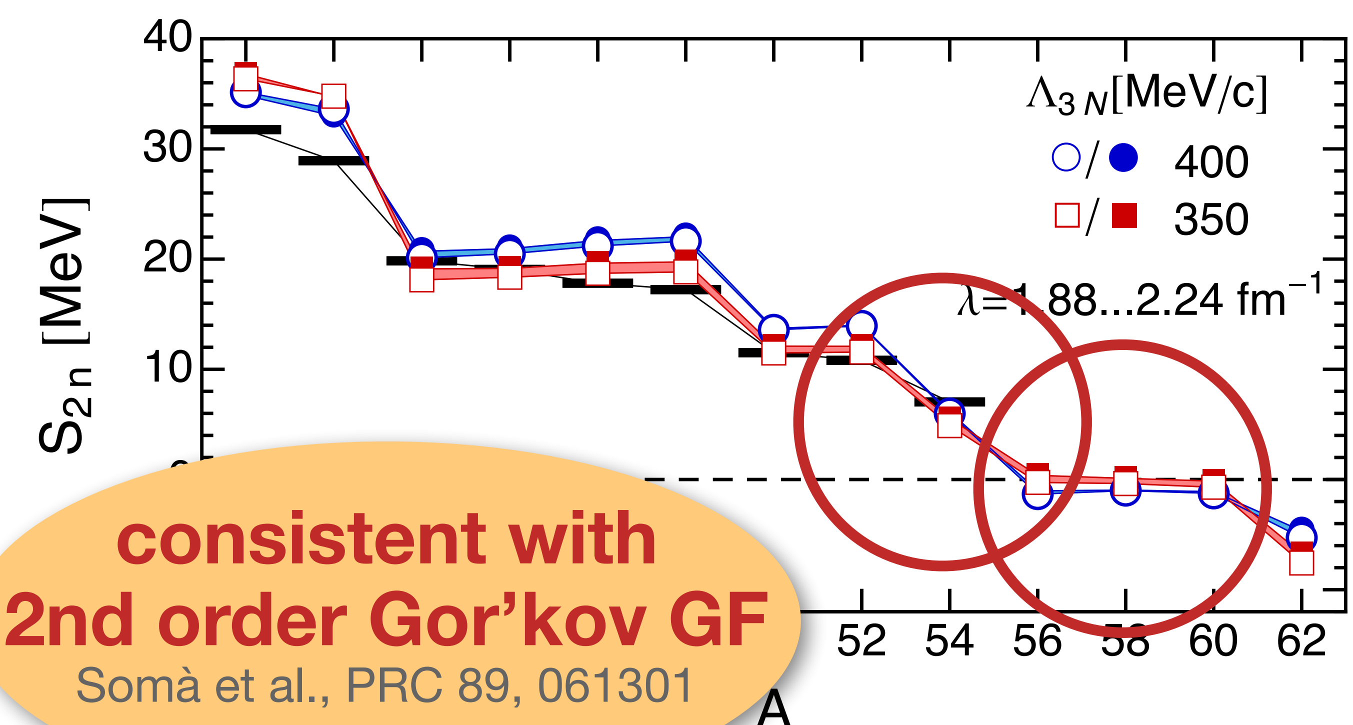
ADC(3): A. Cipollone et al., Phys. Rev. Lett. **111**, 242501 (2013)

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

Two-Neutron Separation Energies

PRC **90**, 041302(R) (2014)





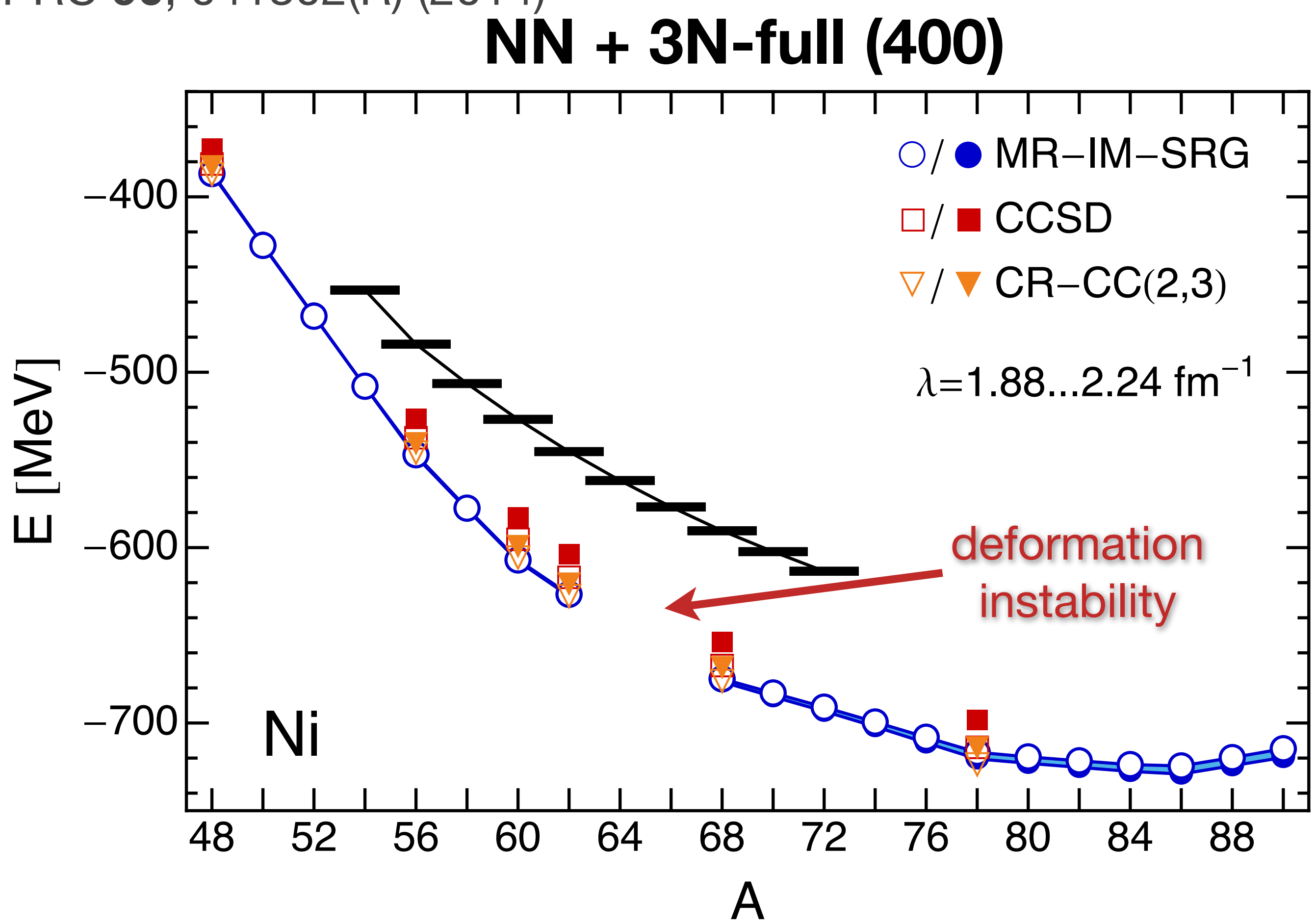
consistent with 2nd order Gor'kov GF

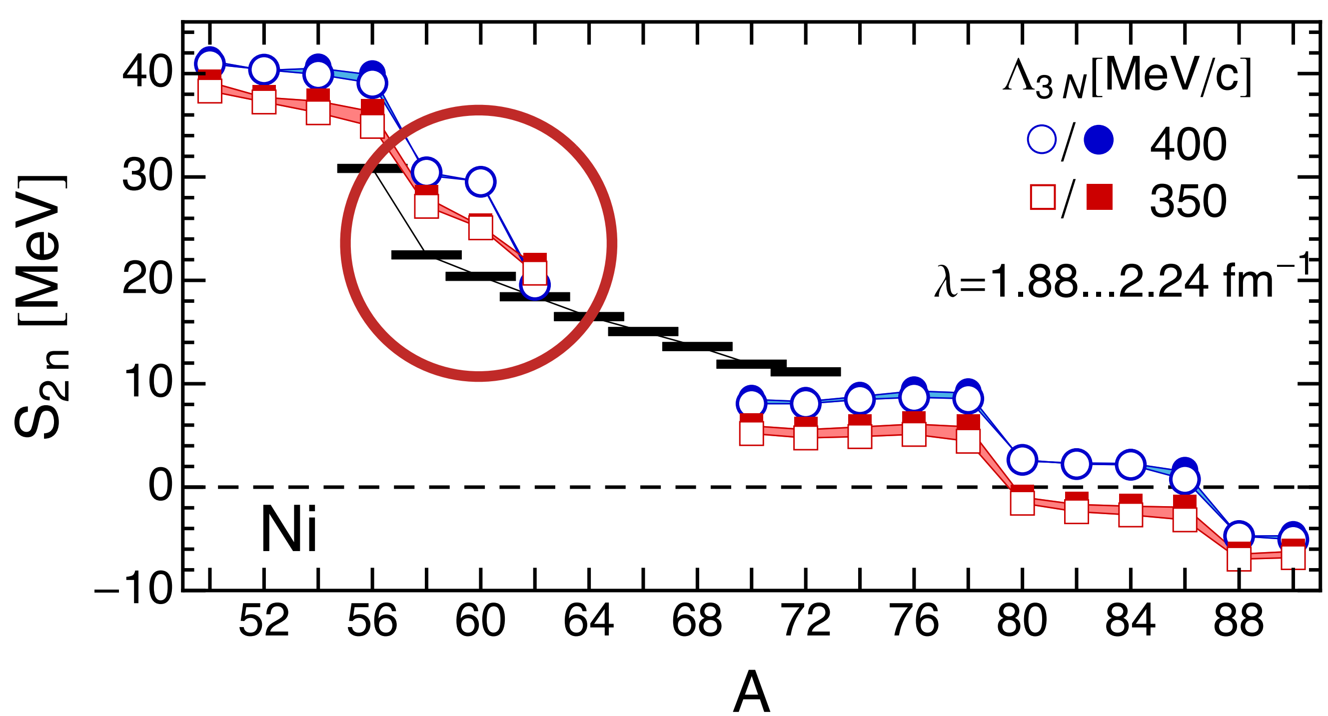
Somà et al., PRC 89, 061301

- 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

Two-Neutron Separation Energies

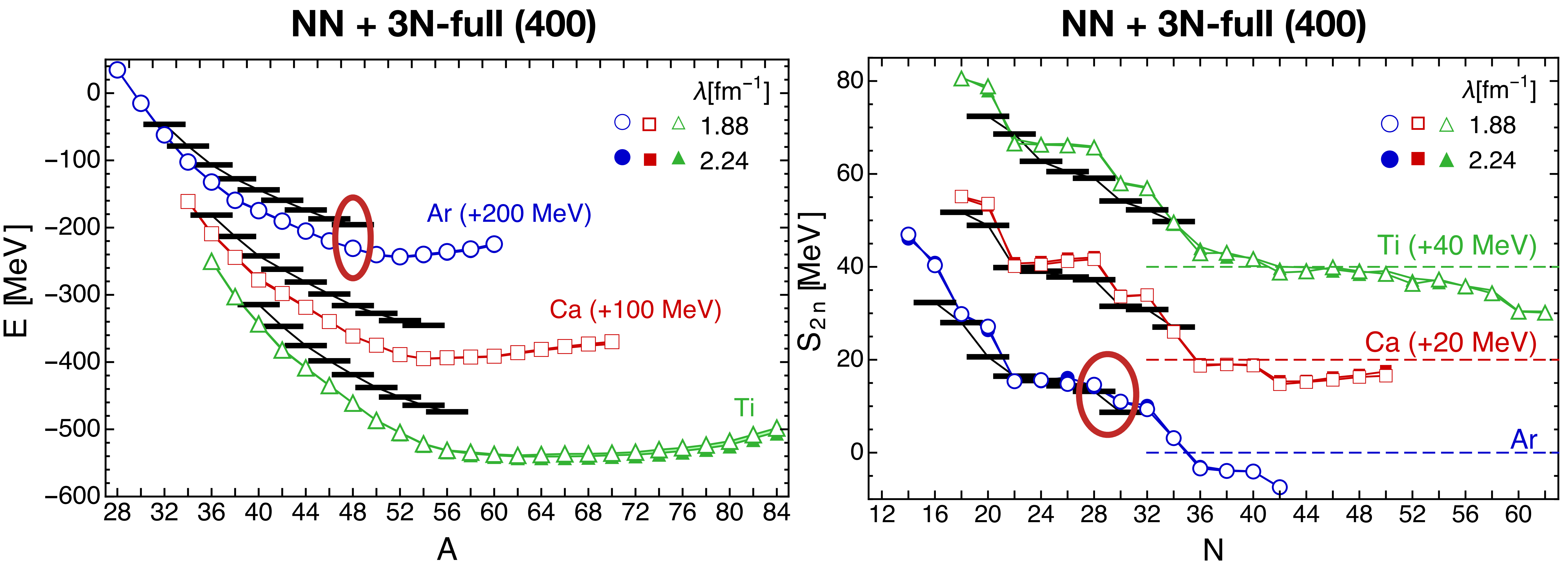
PRC **90**, 041302(R) (2014)





- flat trends for g. s. energies and S_{2n} (similar to Ca)
- deformation instability in ^{64,66}Ni calculations - issue with "shell" structure
- further evidence from 3N cutoff variation
- no continuum coupling yet, other S_{2n} uncertainties < 1MeV

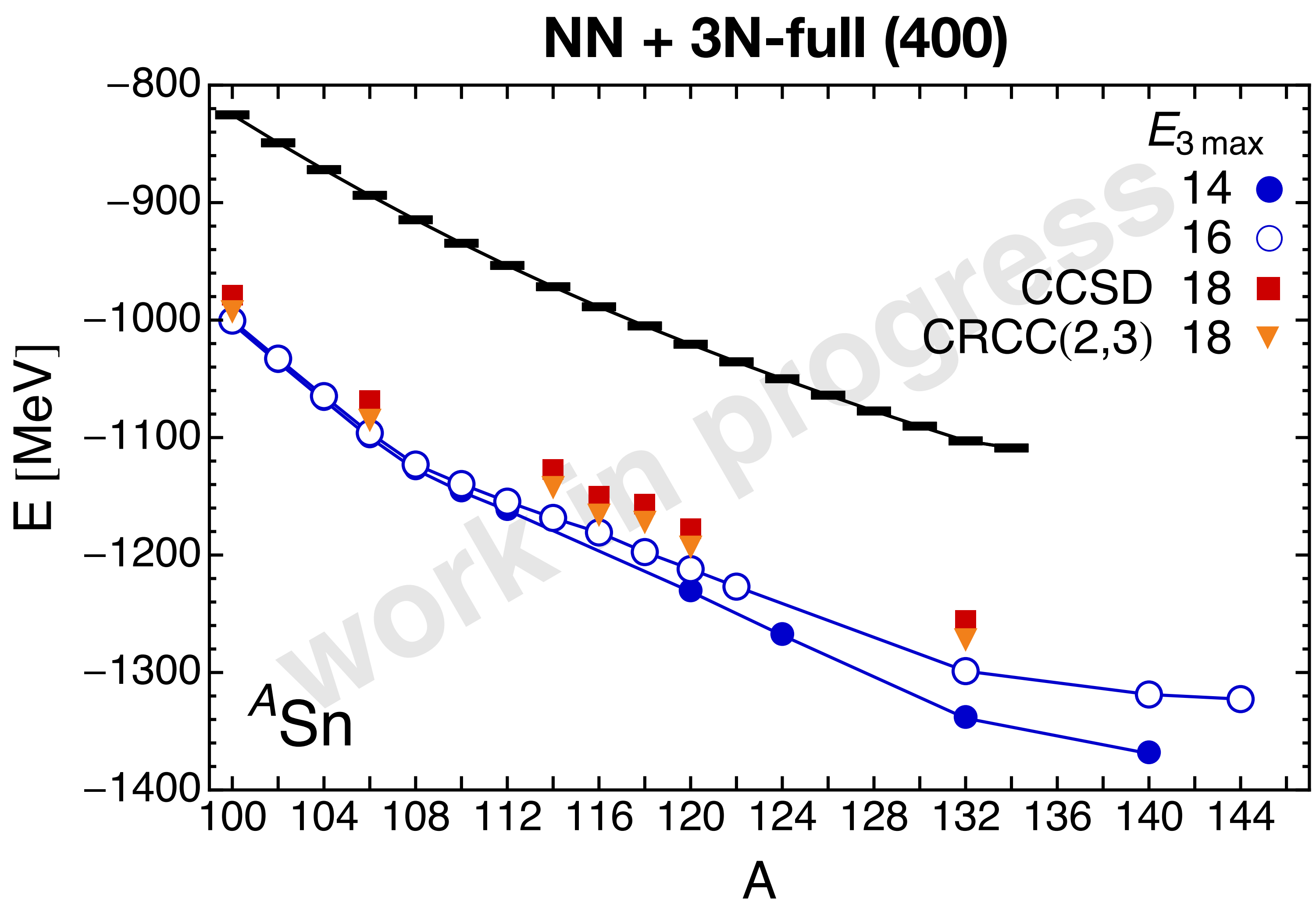
Isotopic Chains Around Ca



- 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 *Ab Initio* Mass Frontier: Tin



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

- systematics of overbinding similar to Ca/Ni
- 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

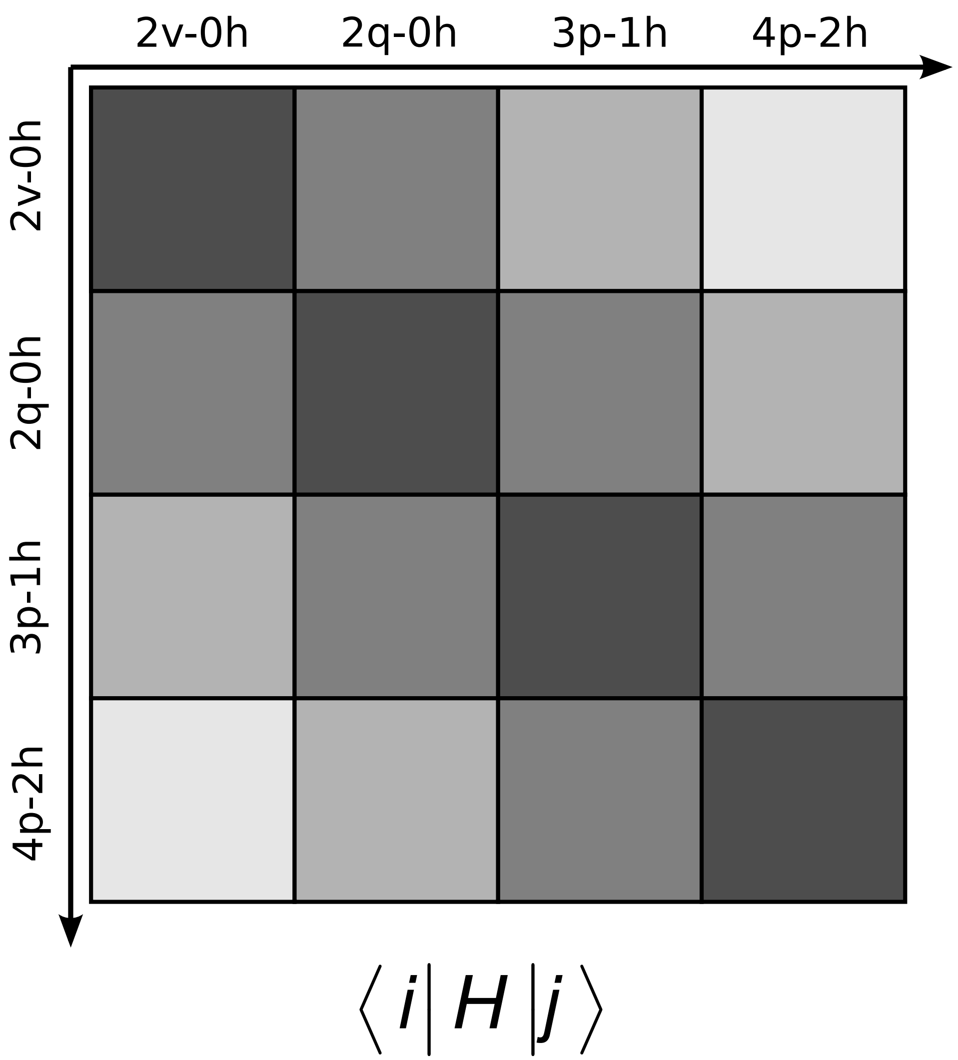
IM-SRG Interactions for the Shell Model

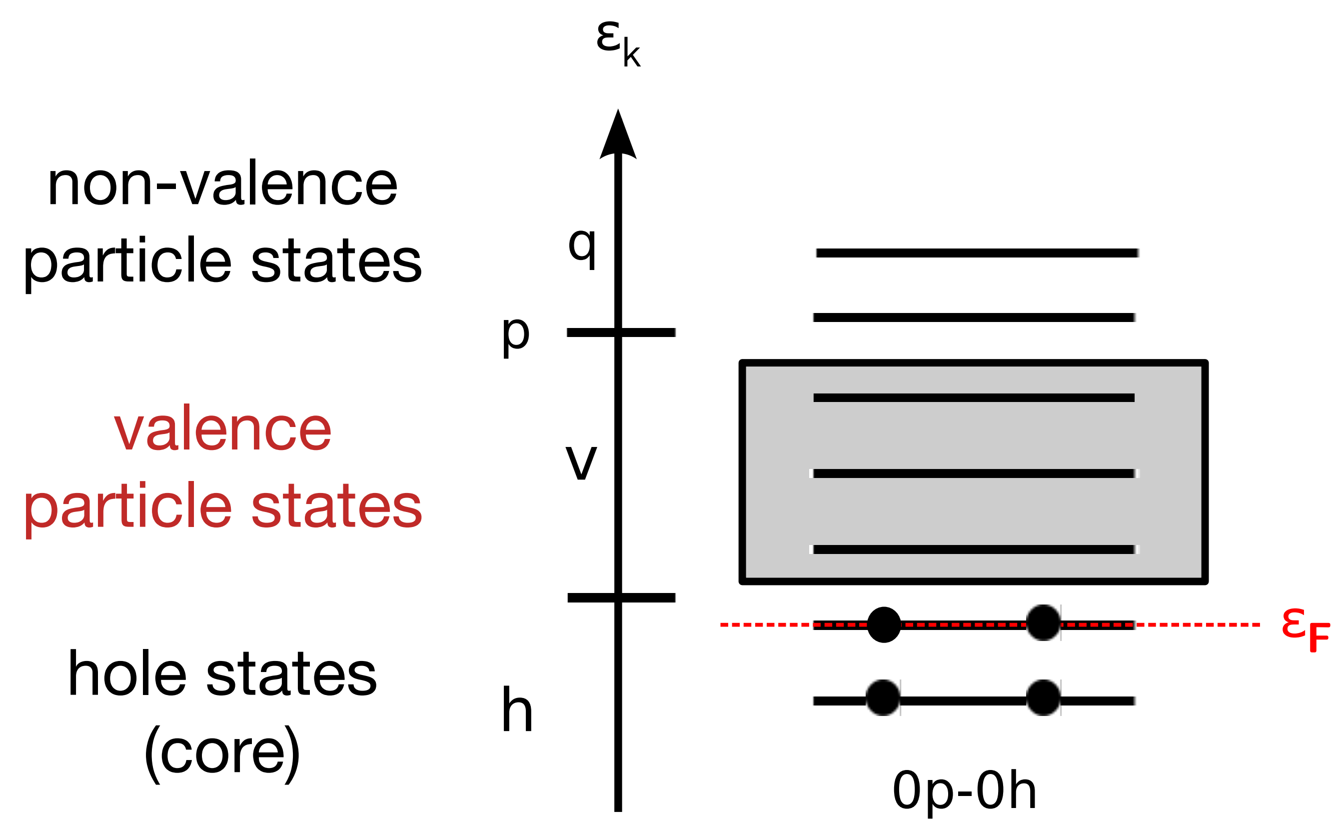
S. K. Bogner, H. H., J. D. Holt, A. Schwenk, in preparation

S. K. Bogner, H. H., J. D. Holt, A. Schwenk, S. Binder, A. Calci, J. Langhammer, R. Roth, Phys. Rev. Lett. 113, 142501 (2014)

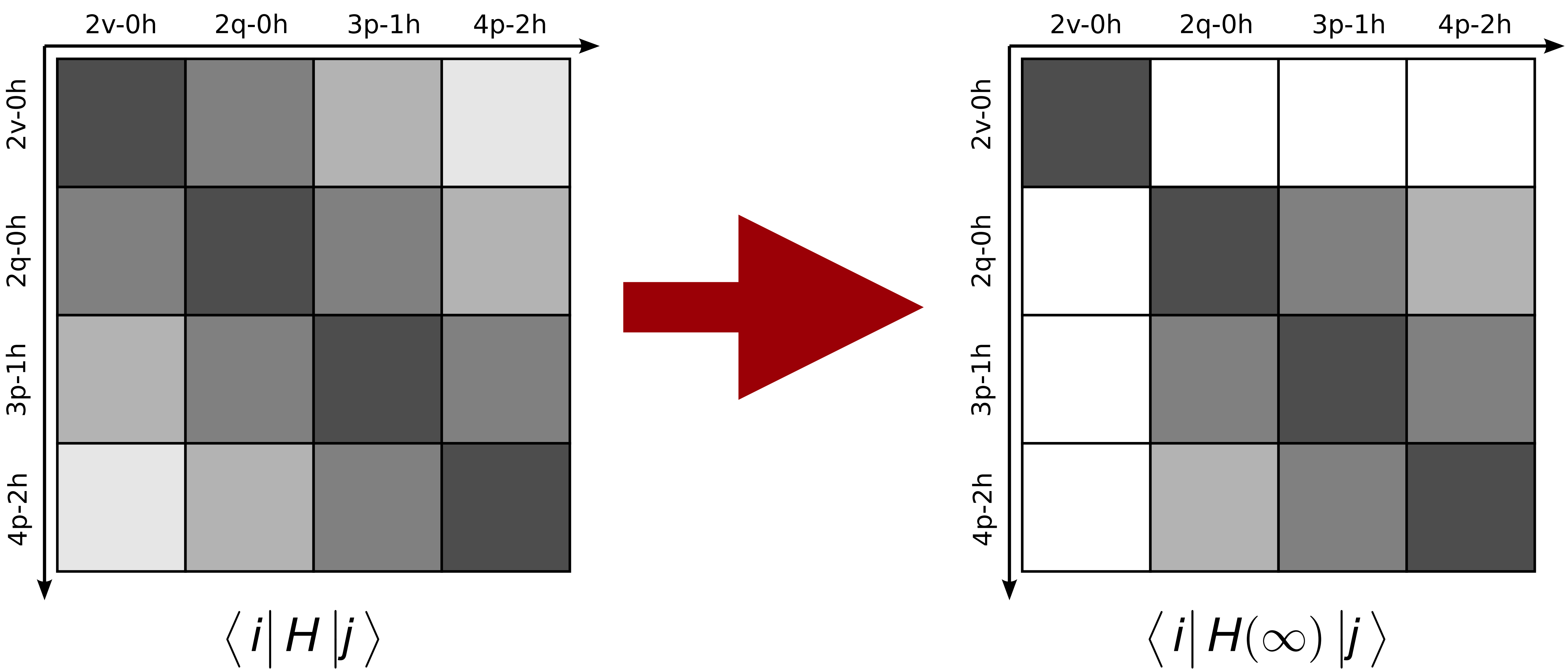
K. Tsukiyama, S. K. Bogner, and A. Schwenk, Phys. Rev. C **85**, 061304(R) (2012)

Valence Space Decoupling





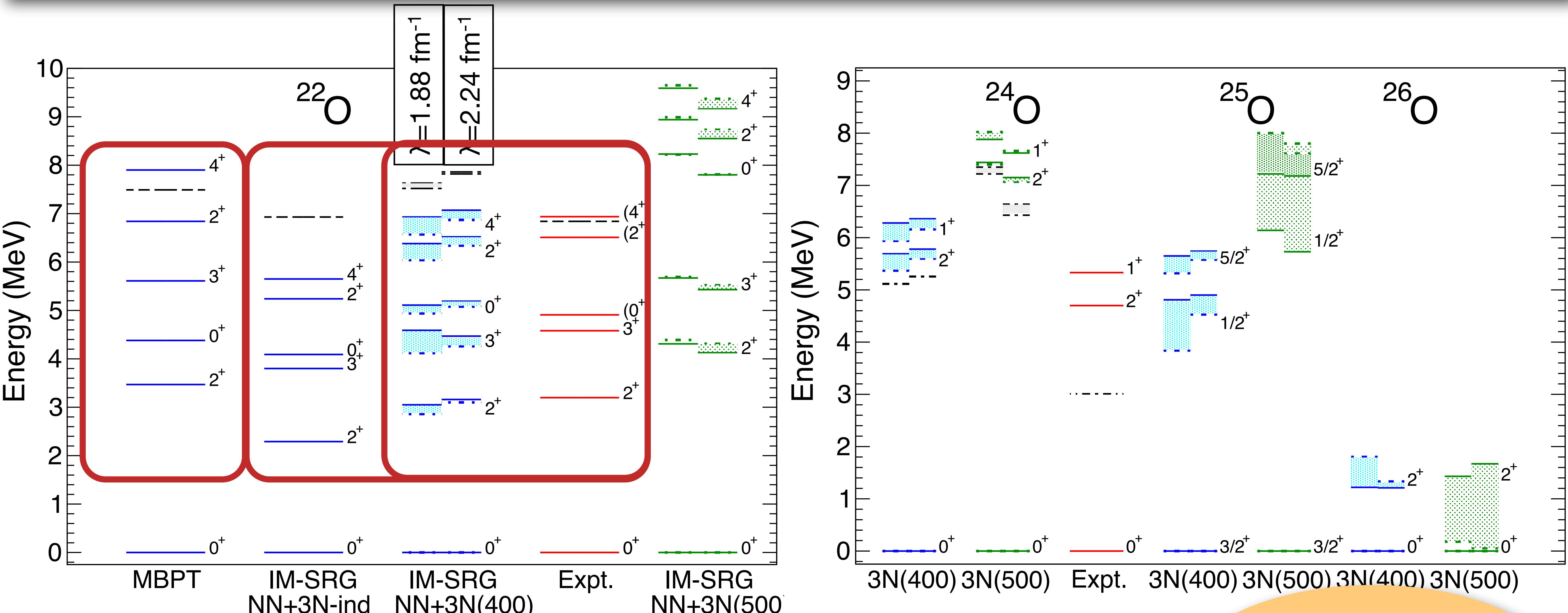
Valence Space Decoupling

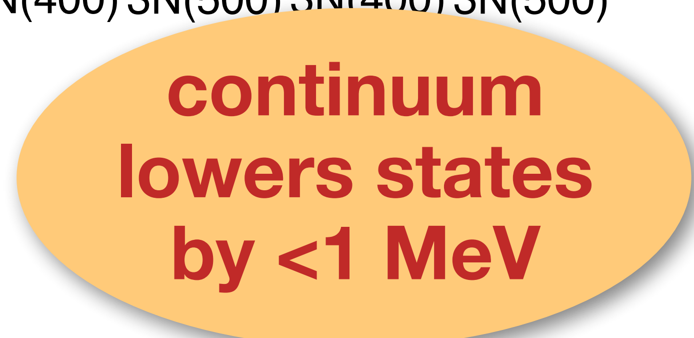


- construct generator from off-diagonal Hamiltonian

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

From Oxygen...



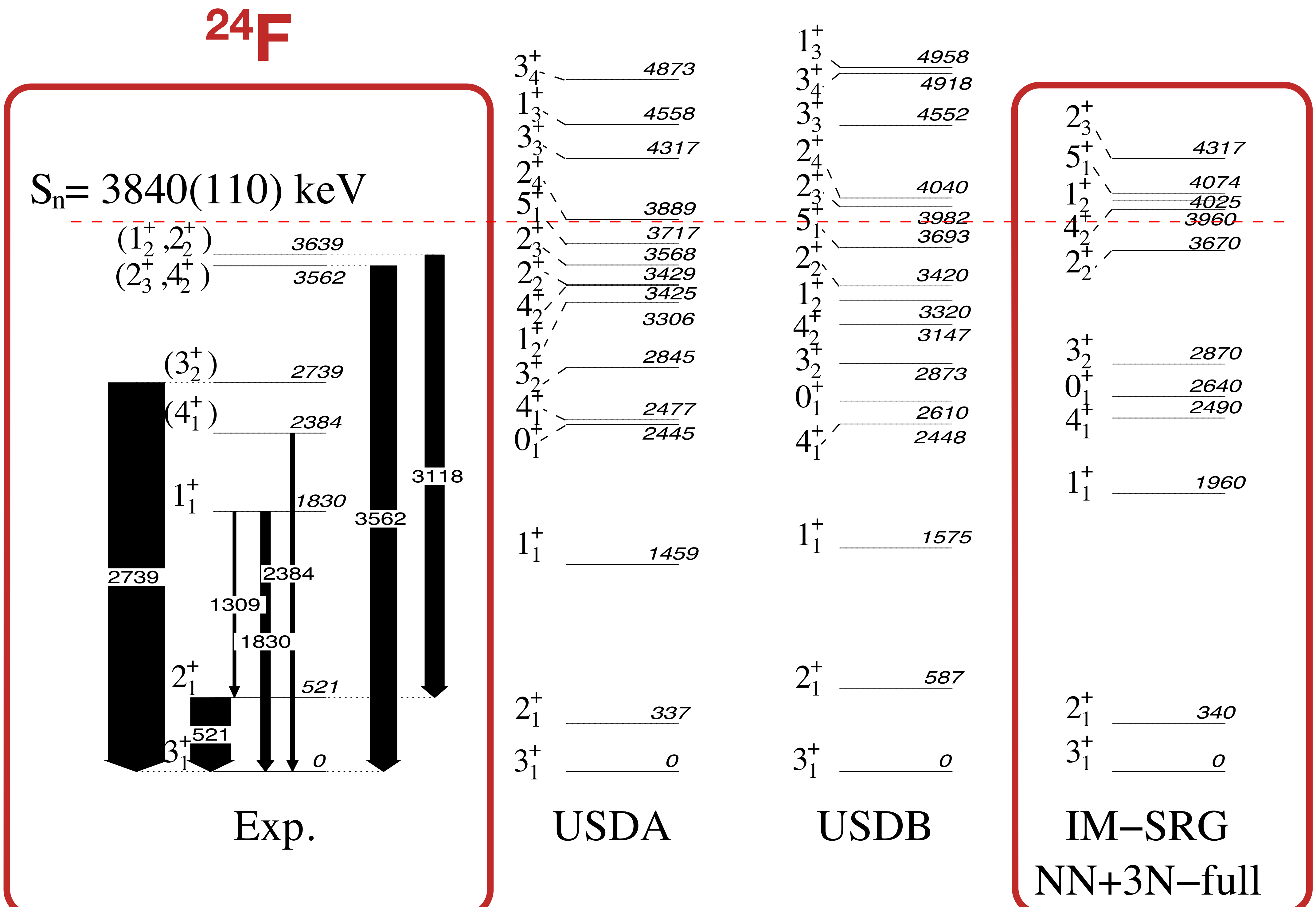


shading: $\hbar\Omega$ variation

Phys. Rev. Lett. **113**, 142501 (2014)

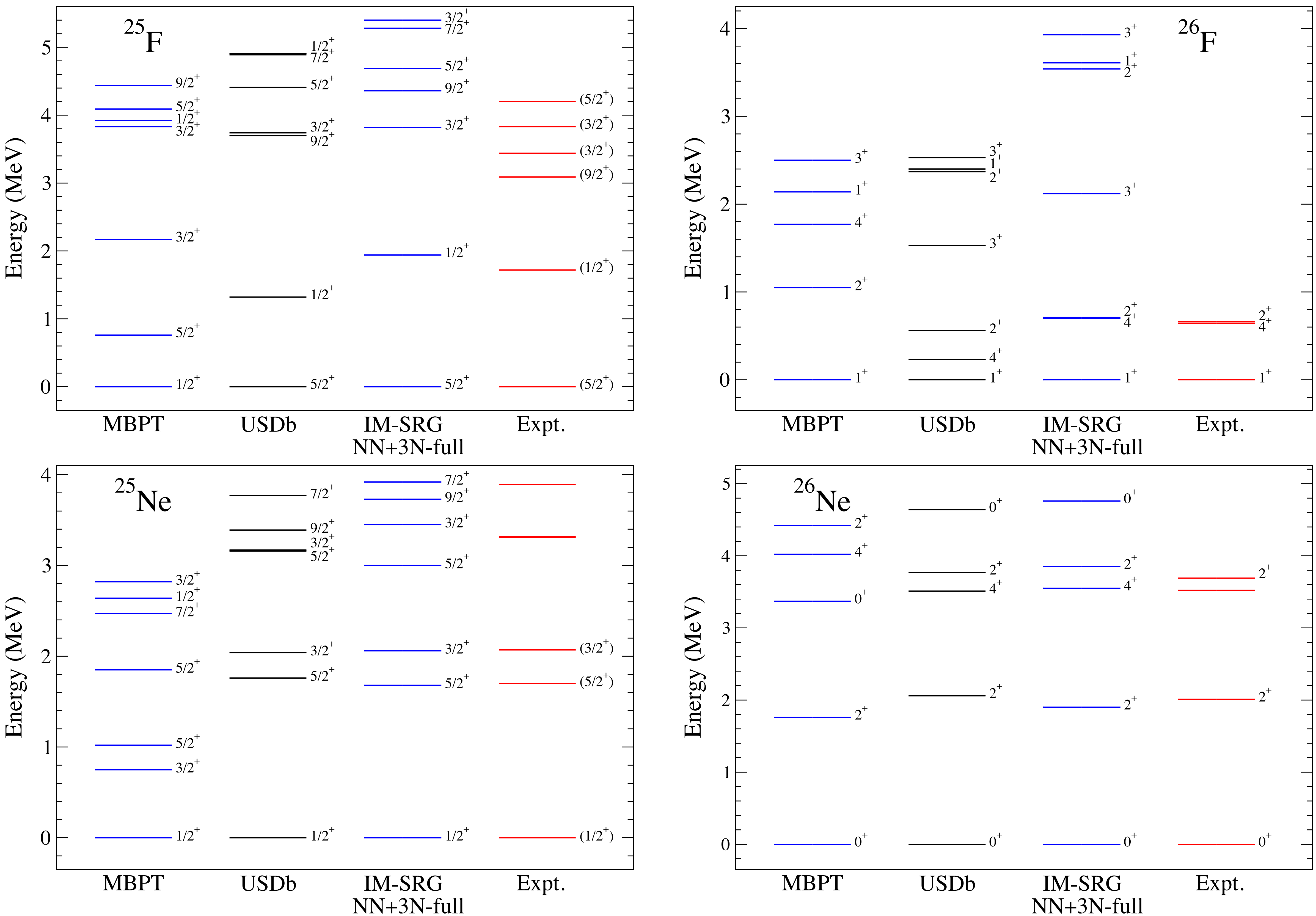
- **3N forces crucial**
- IM-SRG improves on finite-order MBPT effective interaction
- competitive with phenomenological calculations

... Into the *sd*-Shell...

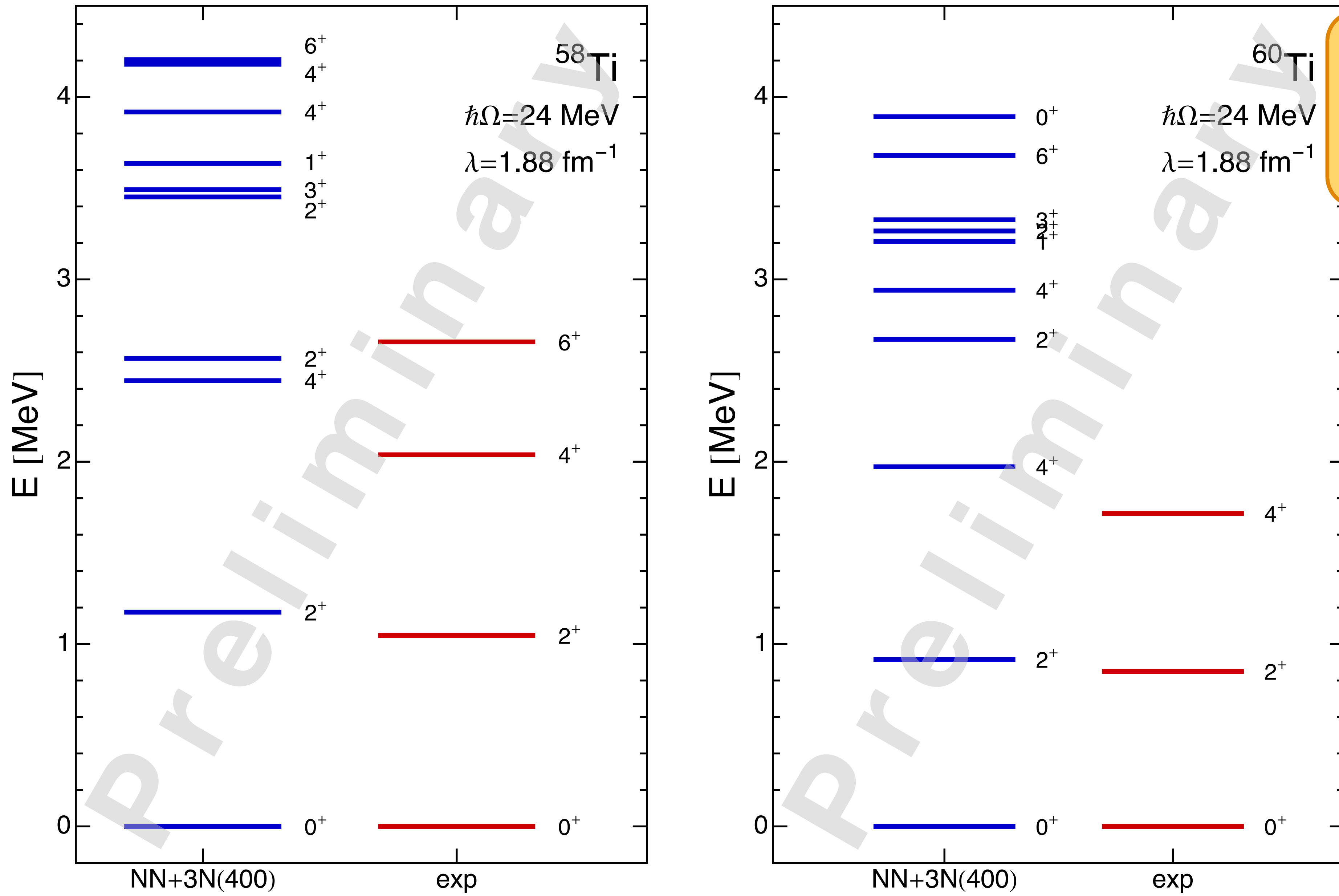


L. Carceres et al., arXiv:1501.01166 [nucl-th]

... Into the *sd*-Shell...



... And Beyond



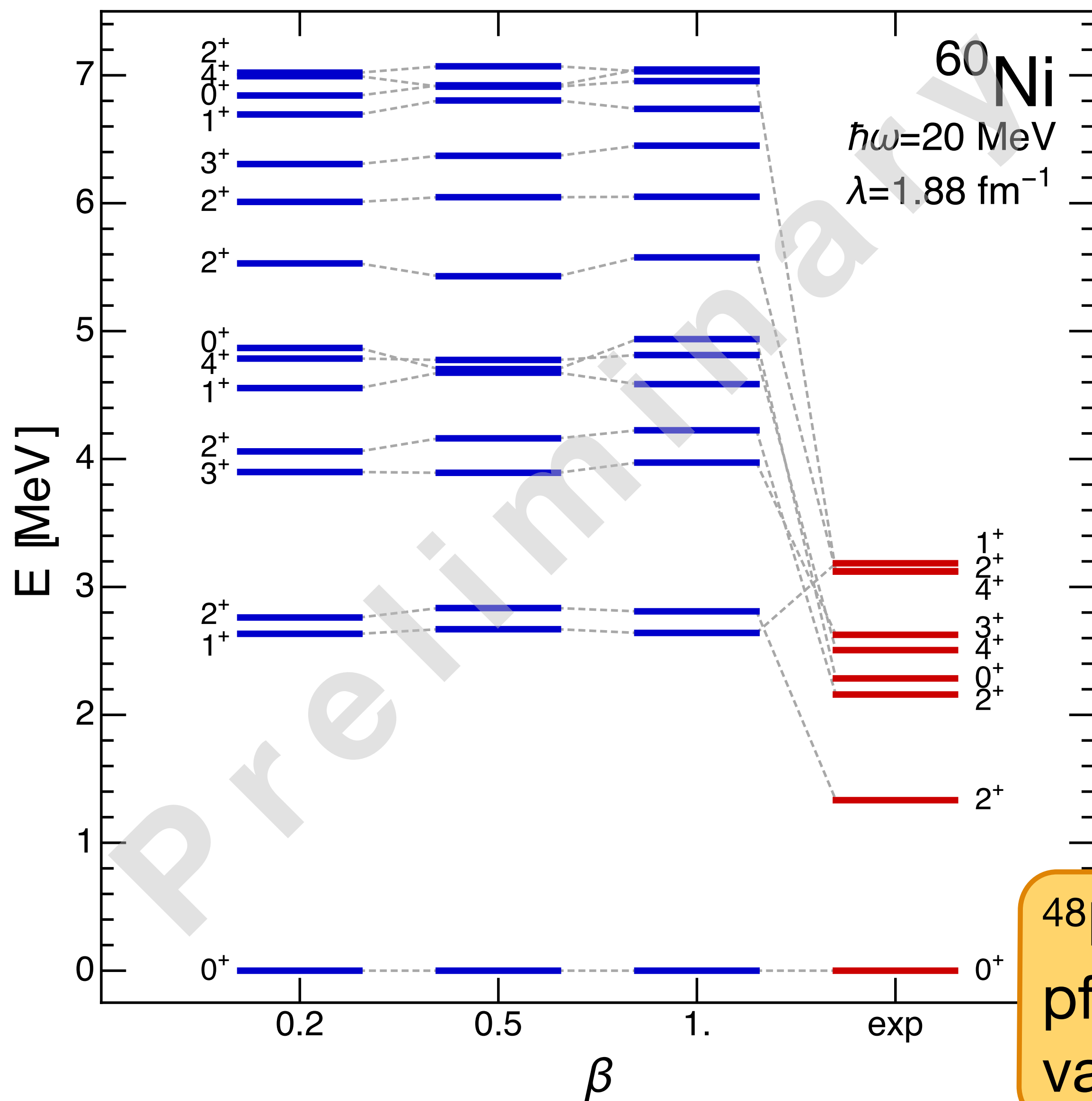
^{48}Ca core, $\nu pf_{5/2}$, πpf valence space

experimental data: A. Gade et al., Phys. Rev. Lett. **112**, 112503 (2014) and NNDC

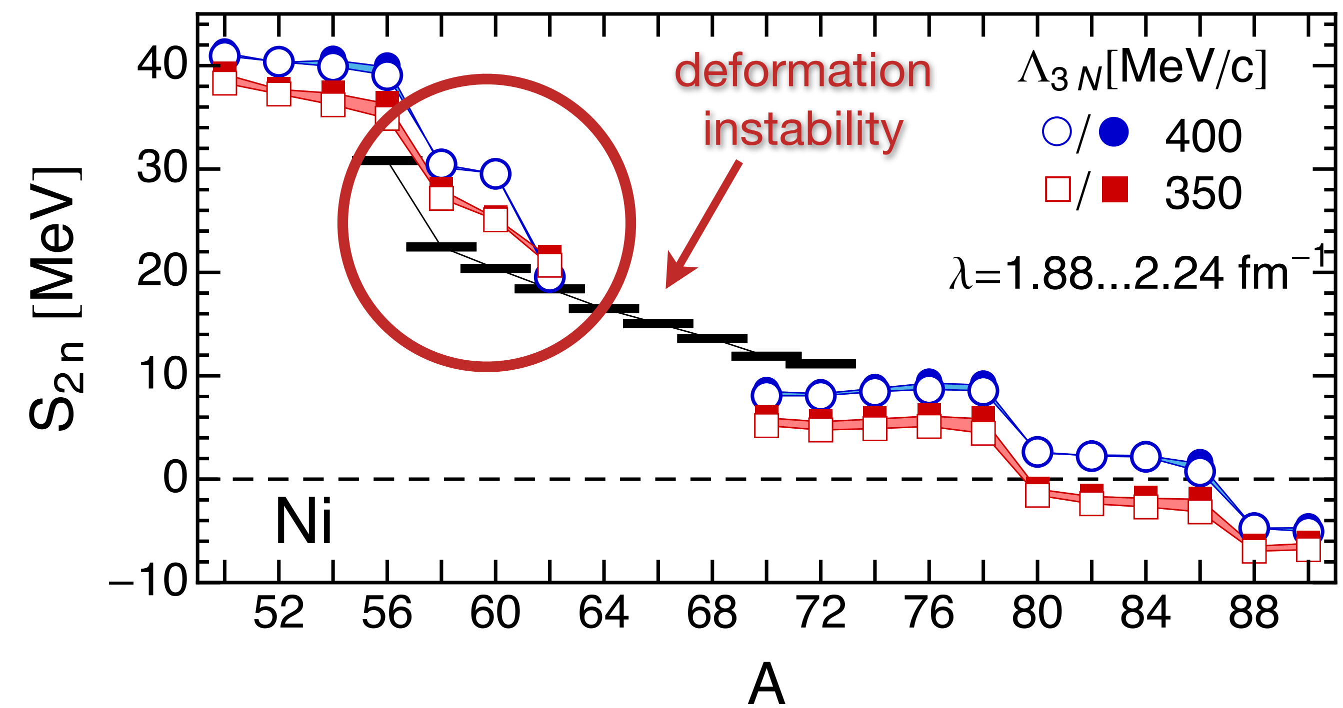
➡ theoretical level scheme similar to empirical interactions (LNPS, GXPF1A)

Multi-Shell Interactions

NN + 3N-full(400)



MR-IM-SRG, NN+3N-full

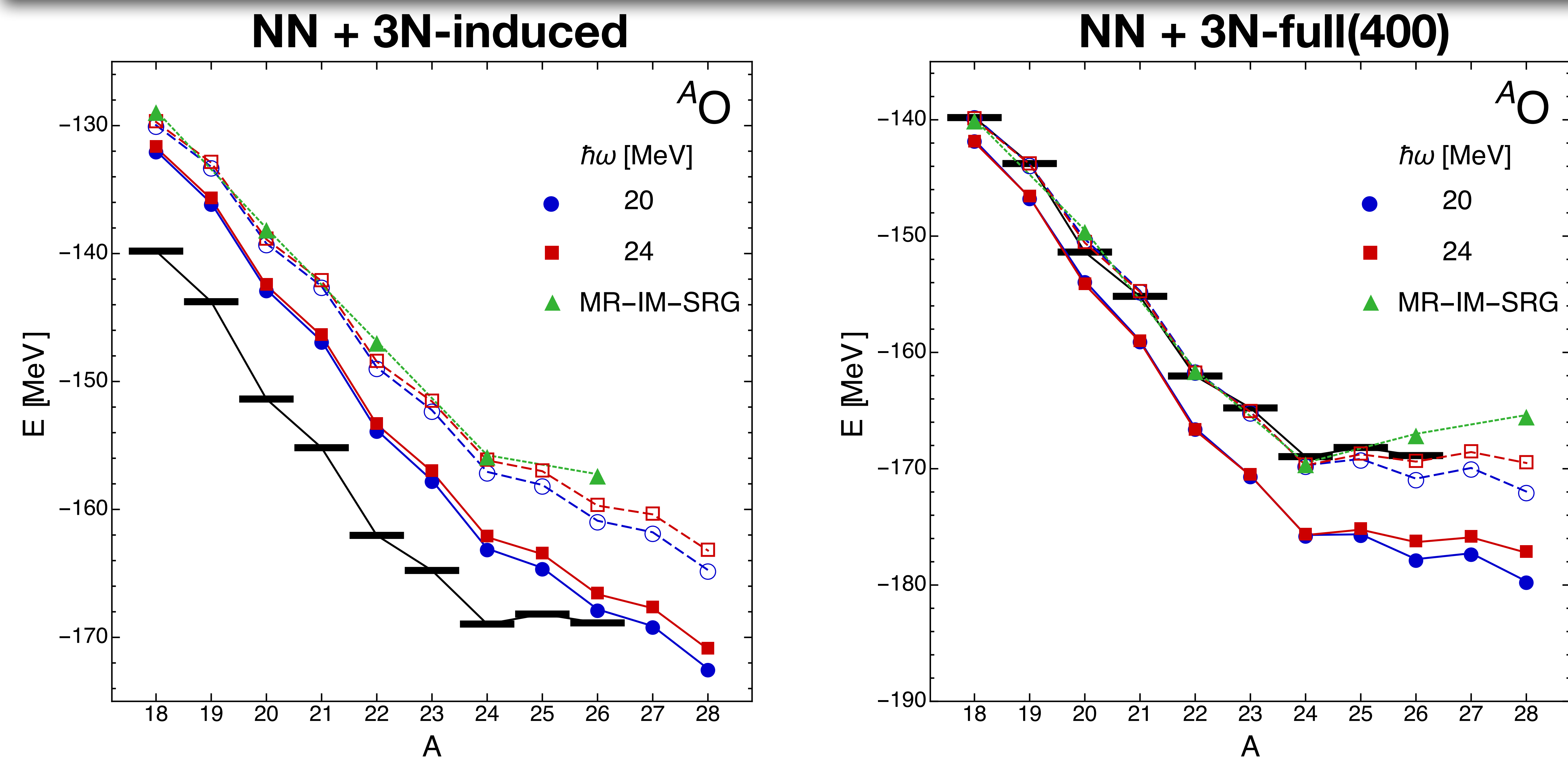


PRC **90**, 041302(R) (2014)

^{48}Ni core,
pfg$_{9/2}$
valence space

➡ elevated 2^+ energy consistent with S_{2n} from MR-IM-SRG g.s. calculations with same Hamiltonian

Open Issue



- looks like simple shift: $\Delta E \approx \frac{A_v}{A} \cdot \text{const.}$ …
- … but it's more complicated; take more information on target into account (occupation of states, etc.) ?

Next Steps

Magnus Series Formulation

talk by T. Morris, week 2

- construct unitary transformation explicitly:

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

- flow equation for Magnus operator :

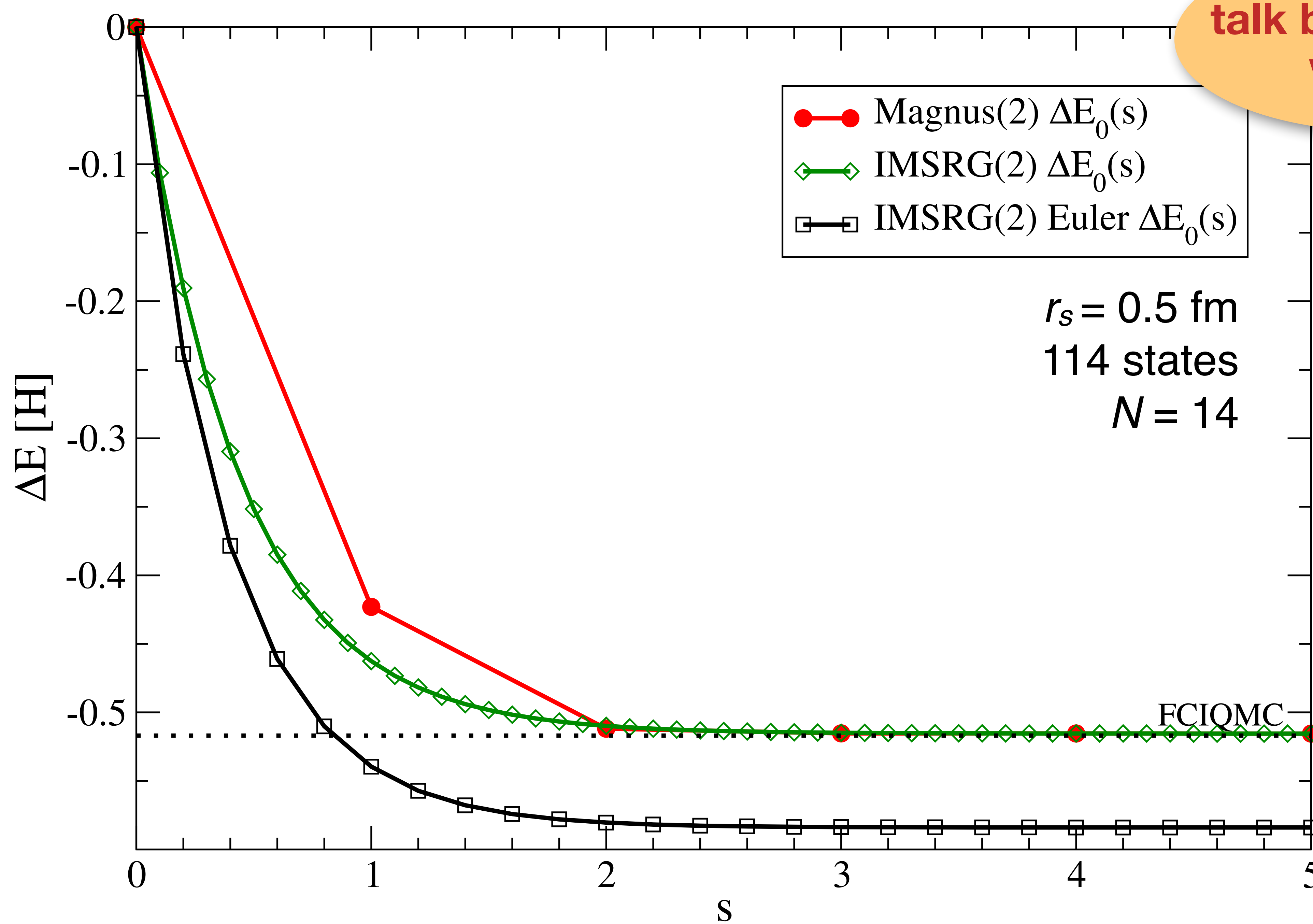
$$\frac{d}{ds}\Omega = \sum_{k=0}^{\infty} \frac{B_k}{k!} \mathrm{ad}_{\Omega}^{k}(\eta) \,, \quad \mathrm{ad}_{\Omega}(O) = [\Omega, O]$$

(B_k: Bernoulli numbers)

- construct $O(s) = U(s) O_0 U^{\dagger}(s)$ using Baker-Campbell-Hausdorff expansion (Hamiltonian + effective operators)
- generate systematic approximations to (MR-)IM-SRG(3)
- simple integrator sufficient (Euler!) - **unitarity built in**

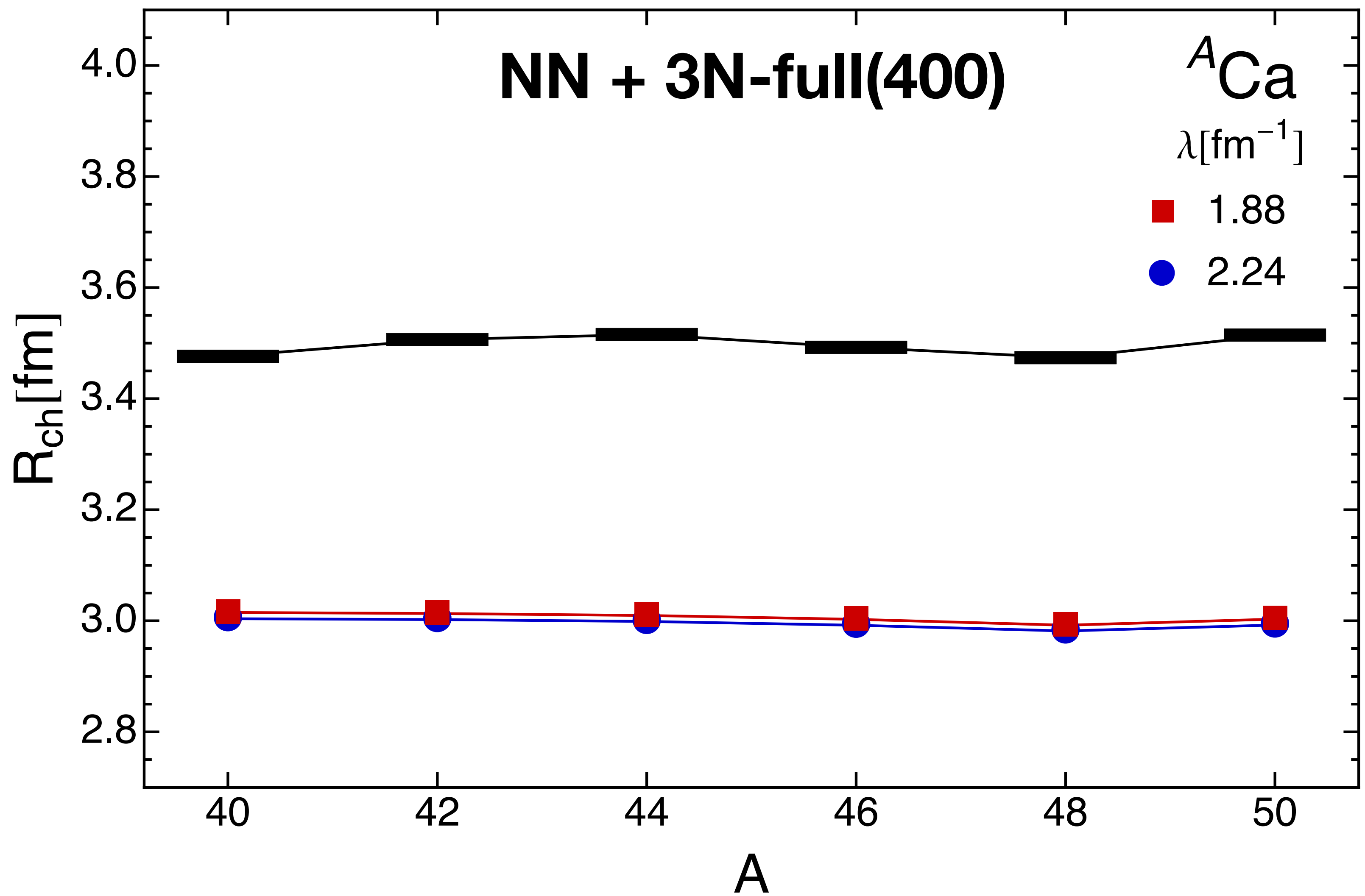
Example: Homogenous Electron Gas

talk by T. Morris, week 2



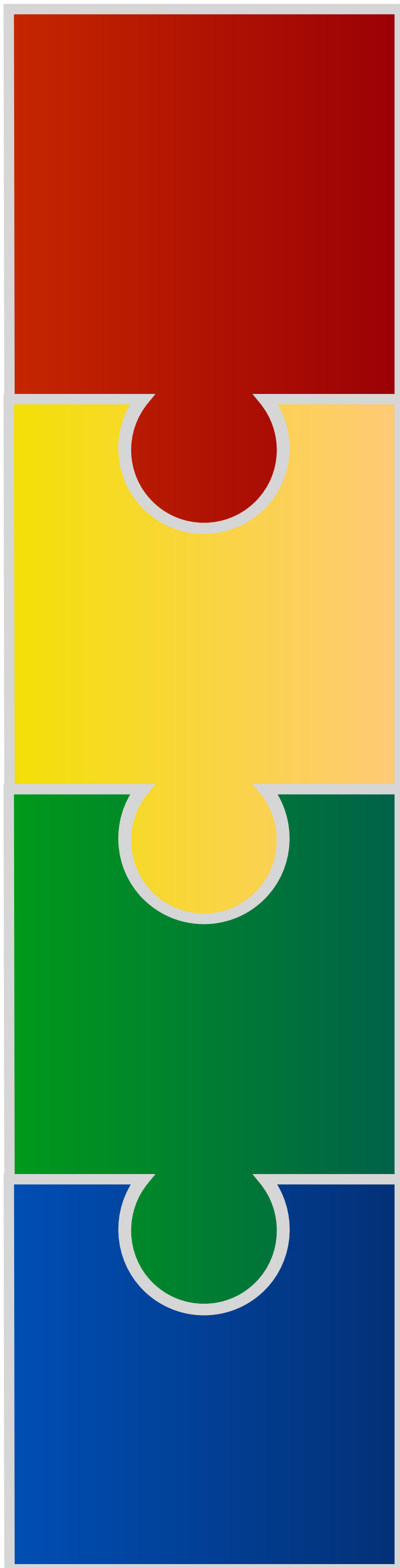
T. D. Morris, N. Parzuchowski, S. K. Bogner, in preparation

Effective Operators



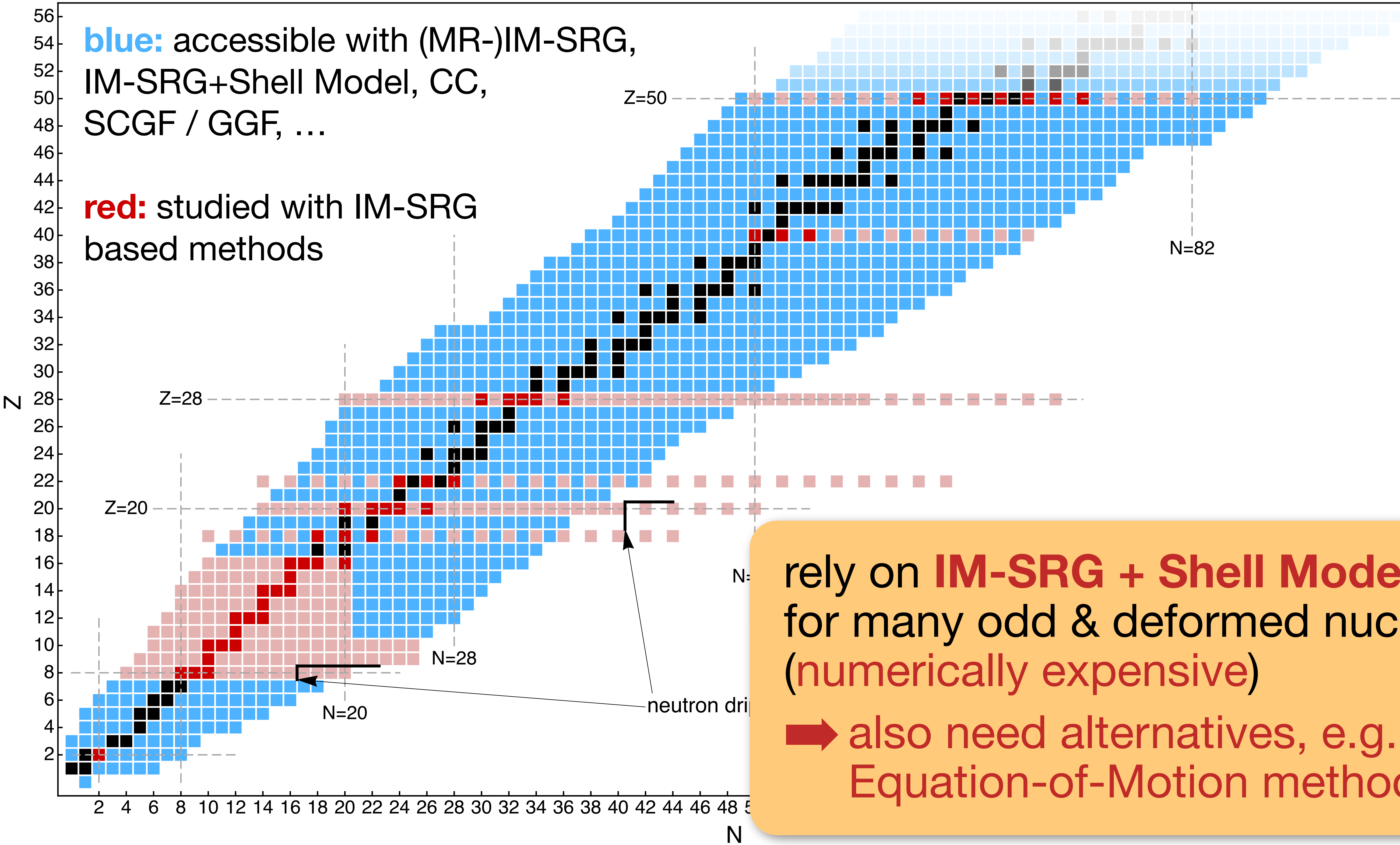
- small radii: interaction issue (power counting, regulators, LECs, …), also consider currents?
- scalar operators (radii, electromagnetic monopole, …) can be evaluated with existing code
- implementation of tensor operators in progress

Effective Operators



- (transition) operators from chiral EFT, including currents
  ➡ LECs consistent with nuclear interaction
- (S)RG evolution to resolution scale of the Hamiltonian / Hilbert space
- IM-SRG evolution consistent with Hamiltonian
- evaluation of 1B, 2B, (3B,…) transition operator, e.g., in Shell Model code
  ➡ transition densities in pn formalism (Coulomb, isospin breaking in nuclear interaction)

Reach of Ab Initio Methods



rely on **IM-SRG + Shell Model** for many odd & deformed nuclei (numerically expensive)

➡ also need alternatives, e.g., Equation-of-Motion methods

Conclusions

Status

- **IM-SRG Shell Model interactions**
  - nn, pn, pp matrix elements obtained simultaneously
  - single major-shell interactions available (p, sd, pf)
  - first tests of multi-shell interactions
  - first applications in Gamow Shell Model
    (talk by G. Papadimitriou, week 2)
- **effective operators**
  - electric monopole transitions accessible with existing technology
    (talk by R. Stroberg, week 2)
  - flow equations for non-scalar operators (1B, 2B) derived, implementation in progress

Status

- **(MR-)IM-SRG**
    - Magnus method for improved computational efficiency
    - new generators for ground- and excited-state decoupling
    - new types of reference states (NCSM, active-space CI, …)
    - approximations for (MR-)IM-SRG(3) derived, implementation in progress

Outlook

- exploration of available chiral NN + 3N Hamiltonians
- construction and validation of multi-shell interactions
- inclusion of continuum effects
- Equation-of-Motion methods as an alternative to Shell Model
- **consistent free-space SRG evolution of effective operators (and currents)**
- computational improvements & code optimization (w/ computer scientists)

Acknowledgments

S. Bogner, T. Morris,
N. Parzuchowski, F. Yuan
NSCL, Michigan State University

E. Gebrerufael, K. Hebeler,
R. Roth, A. Schwenk, J. Simonis,
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Supplement:

Multi-Reference IM-SRG

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H. H., S. Bogner, T. Morris, S. Binder, A. Calci, J. Langhammer, R. Roth, Phys. Rev. C **90**, 041302 (2014)

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

Multi-Reference IM-SRG

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

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

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

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

$$\ldots$$

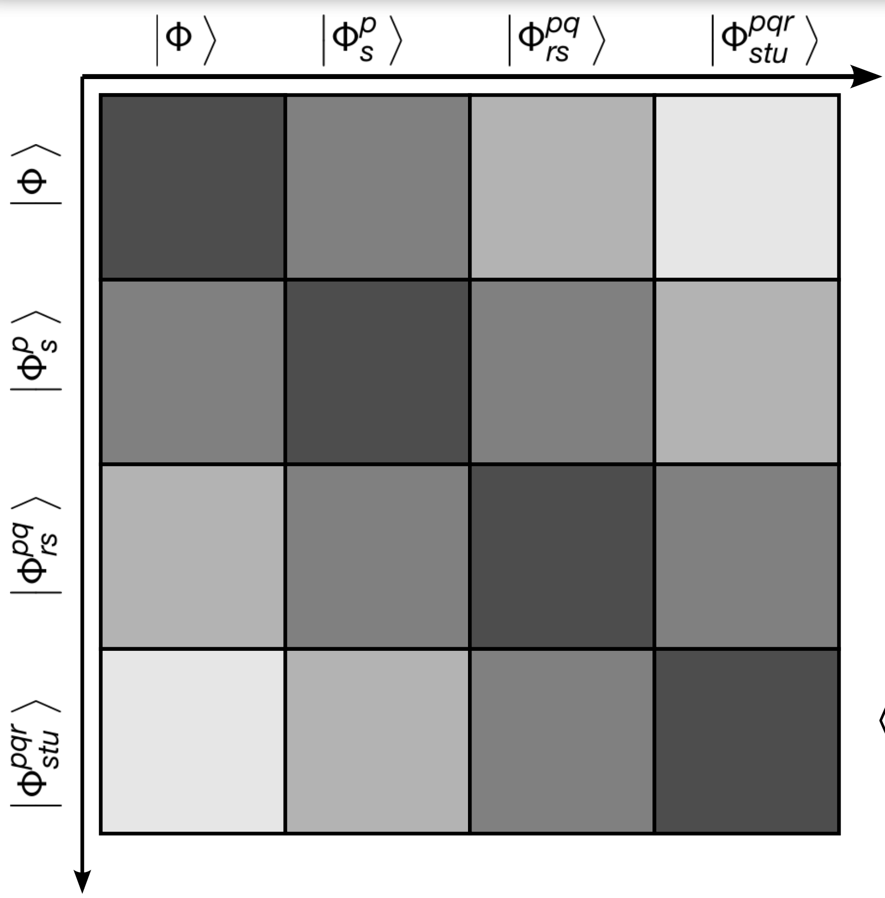
- irreducible densities give rise to additional contractions:

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

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

$$\ldots$$

Decoupling Revisited



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

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

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

- 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

Generators

$$\eta^{I} = [H_d, \boxed{H_{od}}]$$

$$\eta^{II} = \sum_{pr} \frac{\boxed{\bar{n}_p n_r f^p_r + \dots}}{\boxed{\Delta^p_r}} : A^p_r : + \frac{1}{4} \sum_{pqrs} \frac{\boxed{\bar{n}_p \bar{n}_q n_r n_s \Gamma^{pq}_{rs} + \dots}}{\boxed{\Delta^{pq}_{rs}}} : A^{pq}_{rs} : - \text{H.c.}$$

$$\eta^{III} = \sum_{pr} \boxed{\text{sgn}(\Delta^p_r)} (\boxed{\bar{n}_p n_r f^p_r + \dots}) : A^p_r : + \frac{1}{4} \sum_{pqrs} \boxed{\text{sgn}(\Delta^{pq}_{rs})} (\boxed{\bar{n}_p \bar{n}_q n_r n_s \Gamma^{pq}_{rs} + \dots}) : A^{pq}_{rs} : - \text{H.c.}$$

- White generator: small energy denominators due to near-degeneracies
- imaginary time generator: sign choice depends on approximate energies
- definition of H^{od} subject to density truncations

Brillouin Generator

- consider unitary variations of the energy functional

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

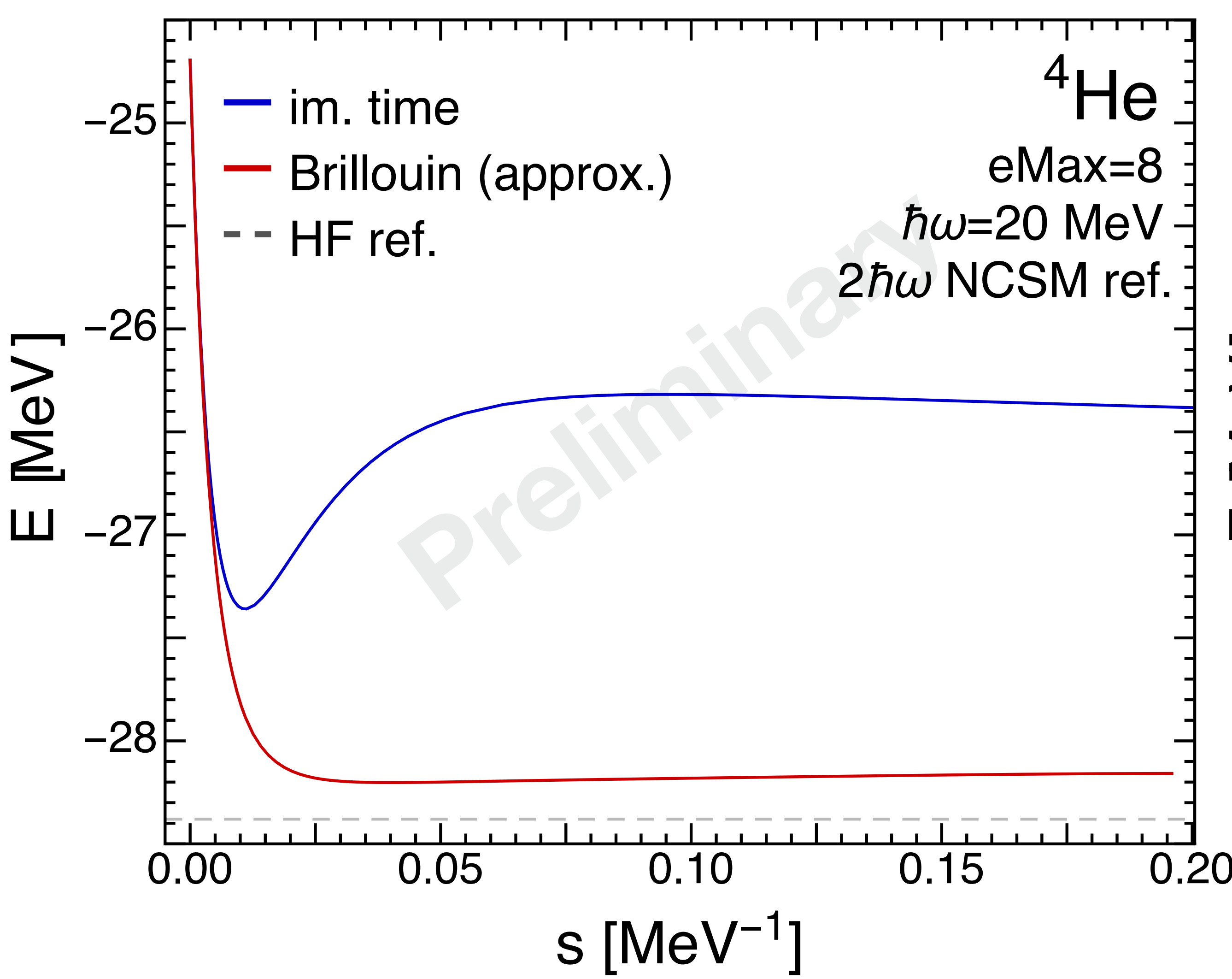
- define generator as the residual of the irreducible Brillouin condition (= gradient of E)

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

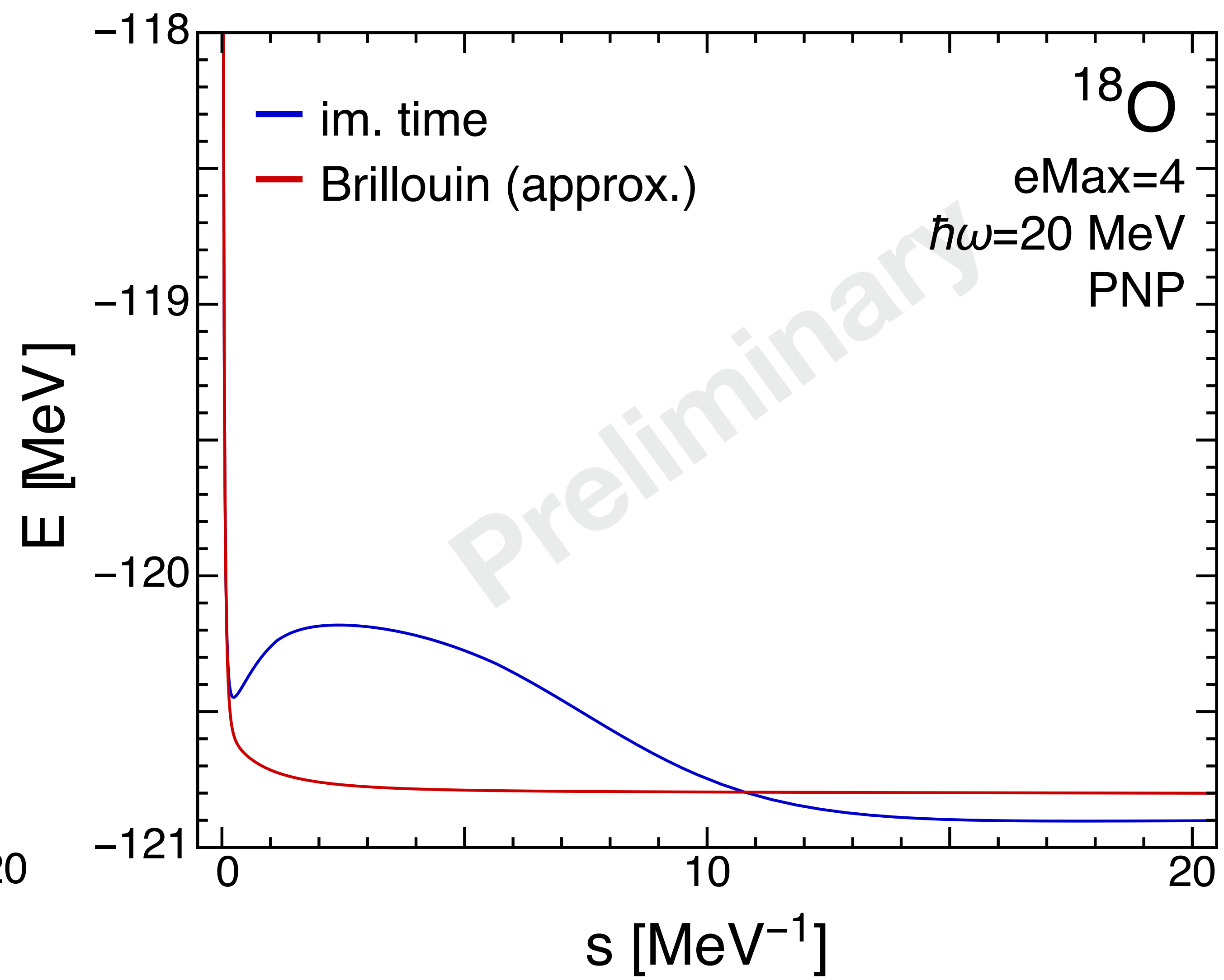
- fixed point ($\eta = 0$) is reached when IBC is satisfied, energy stationary (cf. ACSE approach in Quantum Chemistry)
- Brillouin generator depends linearly on $\lambda^p_s, \lambda^{pq}_{st}, \lambda^{pqr}_{stu}$, higher irreducible density matrices are not required

Brillouin Generator

NN-only, λ=1.88 fm^{-1}



NN+3N-ind., λ=2.0 fm^{-1}



- norm of Brillouin generator decays monotonically
  (approximation: 2B “particle-hole”-like term switched off, 3B density not yet implemented)

➡ use in Magnus formulation of MR-IM-SRG

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

2-body flow:

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

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

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

two-body flow unchanged,
O(N^6) scaling preserved

Particle-Number Projected HFB State

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

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

- calculate irreducible densities (project only once), e.g.,

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

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

$$\lambda^k_l = n_k \delta^k_l \left(= v_k^2 \delta^k_l\right) , \quad 0 \leq n_k \leq 1$$

- in NO basis, $\lambda^{kl}_{mn}, \lambda^{klm}_{nop}$ require only $N^2/2$, $N^3/4$ storage