In-Medium SRG for Closed and Open-Shell Nuclei

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Outline

- Introduction to the In-Medium SRG
- Multi-Reference IM-SRG
- Ground States of Closed- and Open-Shell Nuclei
- IM-SRG Interactions for the Shell Model
- Next Steps

Introduction to the In-Medium SRG

S. K. Bogner, H. H., T. D. 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)

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 $H(s) = U(s)HU^{\dagger}(s)$:

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

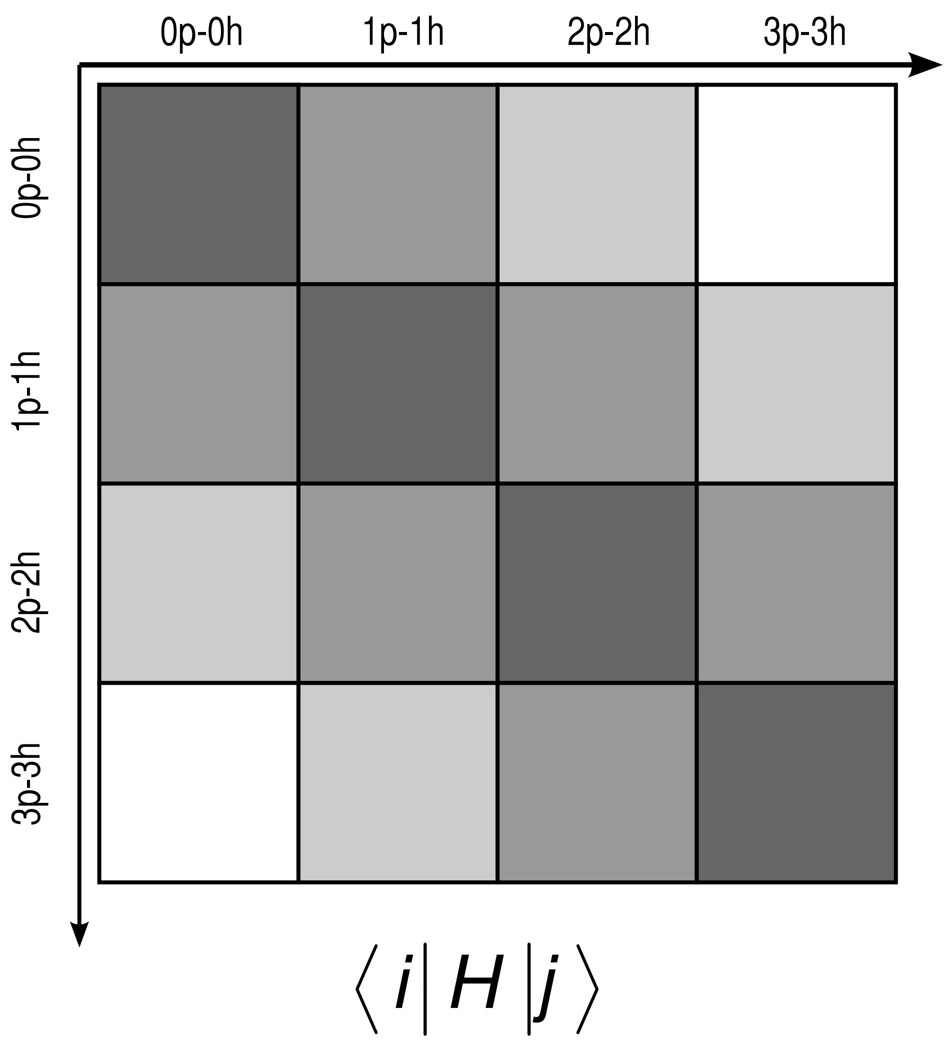
- choose $\eta(s)$ to achieve desired behavior, e.g.,

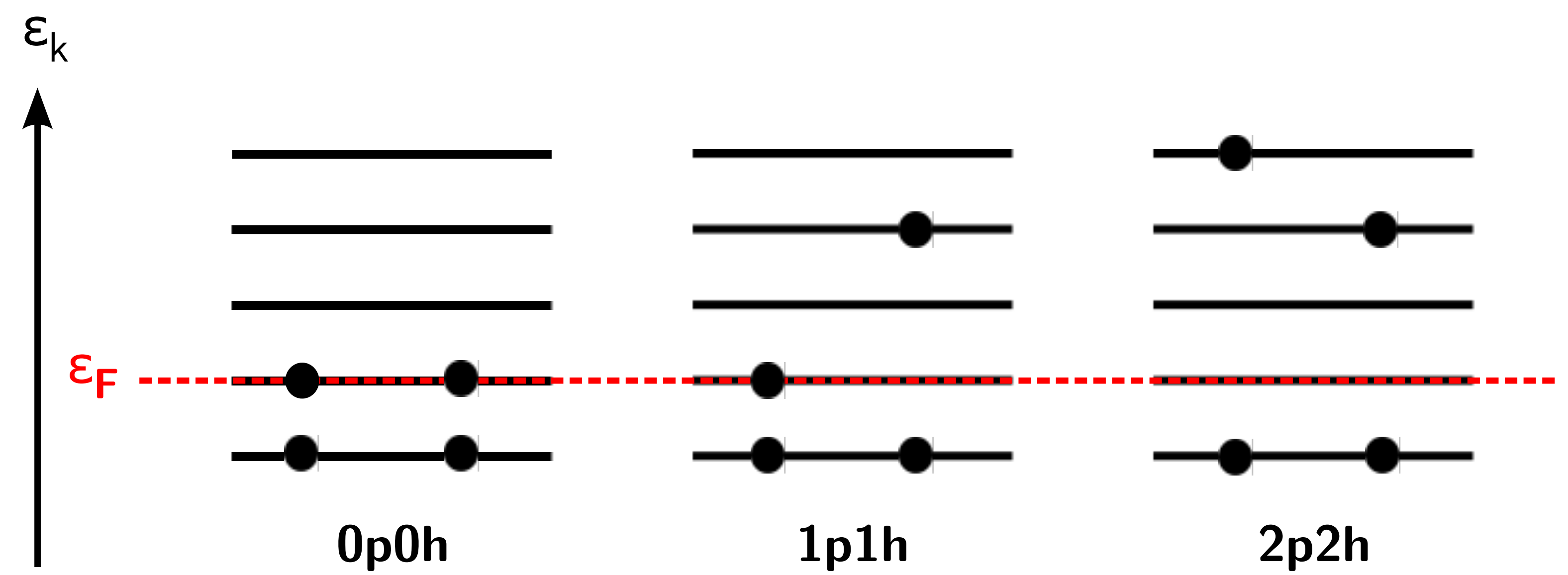
$$\eta(s) = \left[H_d(s), H_{od}(s)\right]$$

to suppress (suitably defined) off-diagonal Hamiltonian

- consistent evolution for all observables of interest

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:

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

- 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

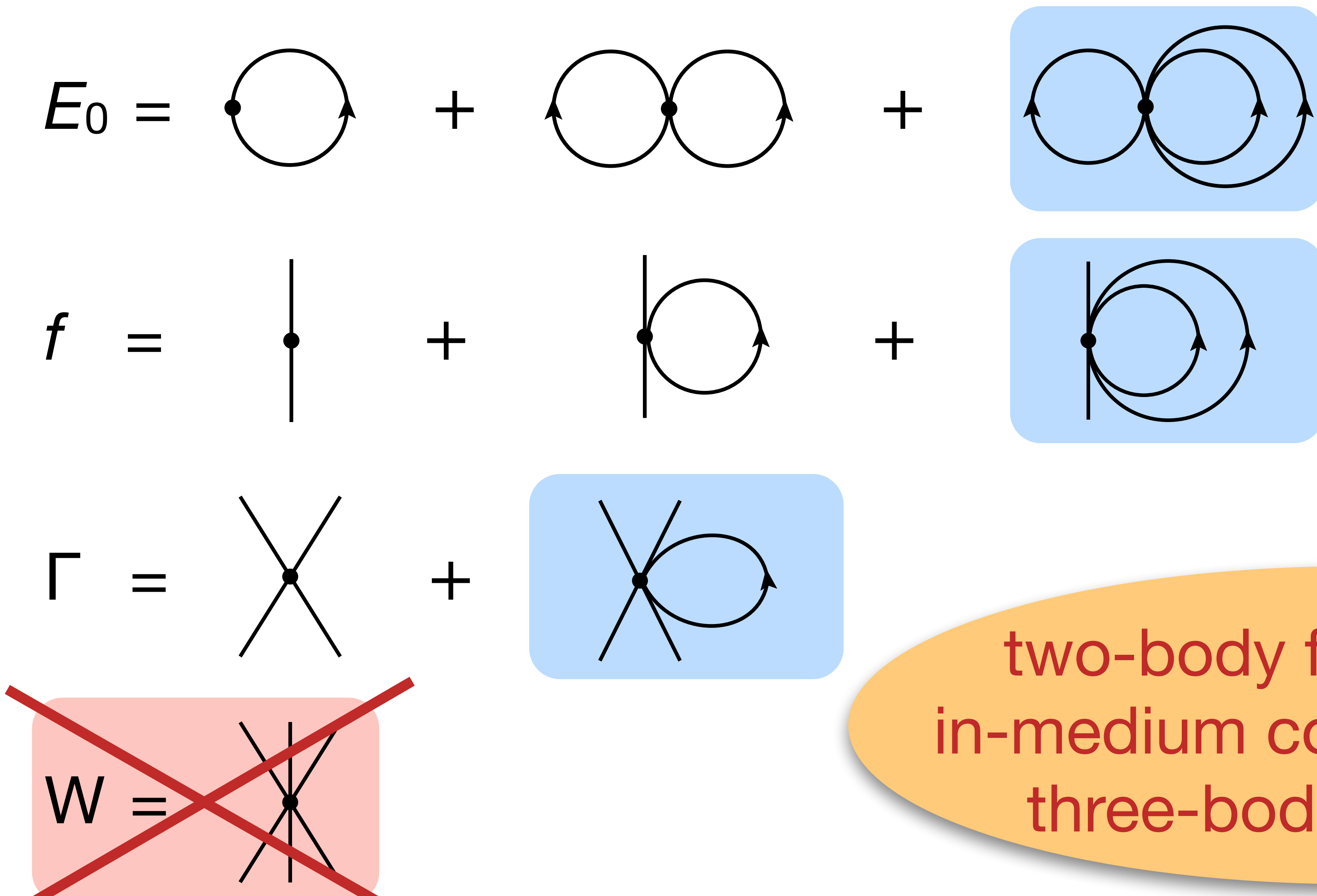
$$\langle \Phi | :A^{k_1 \dots k_N}_{l_1 \dots l_N}: | \Phi \rangle = 0$$

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

Normal-Ordered Hamiltonian

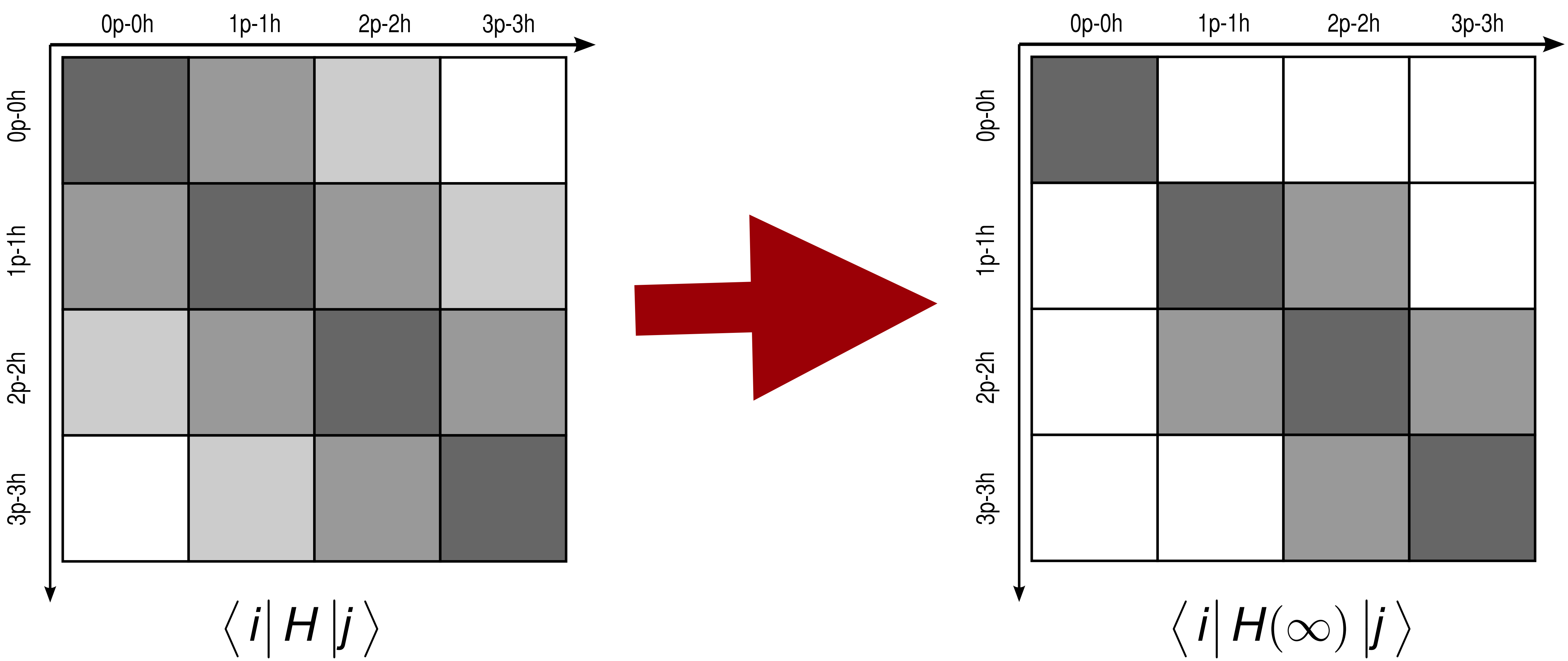
Normal-Ordered Hamiltonian

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



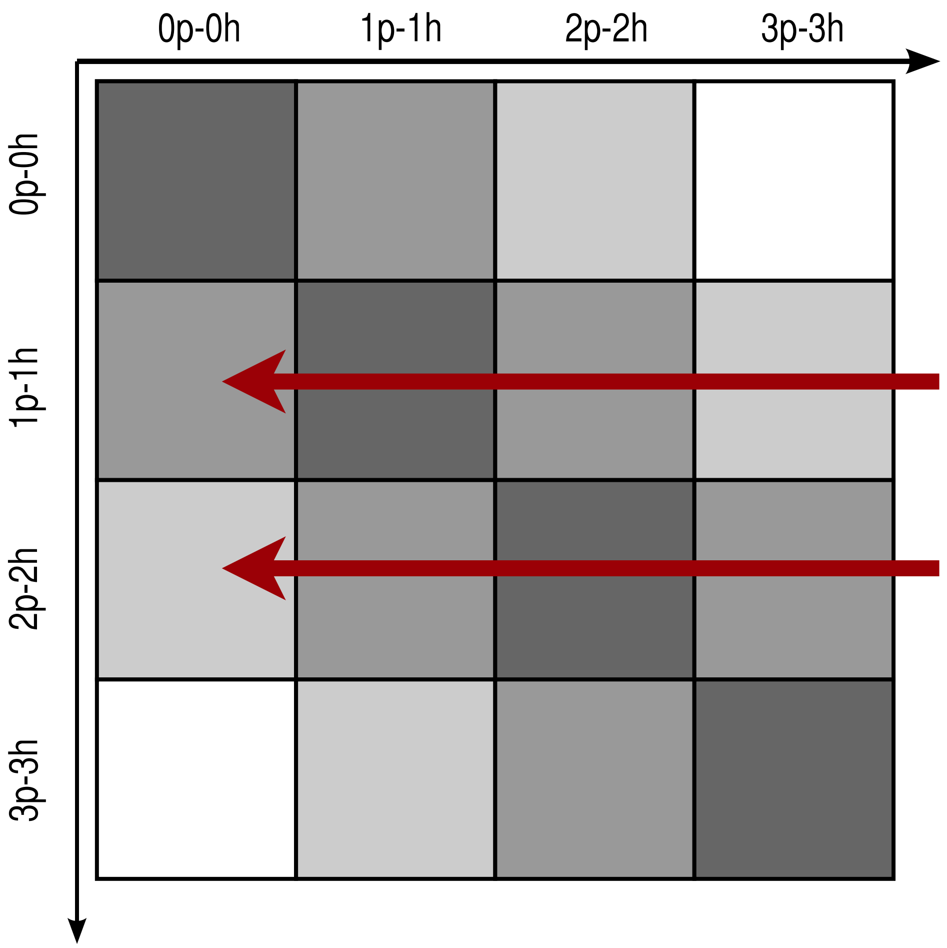
two-body formalism with in-medium contributions from three-body interactions

Decoupling in A-Body Space



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

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

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

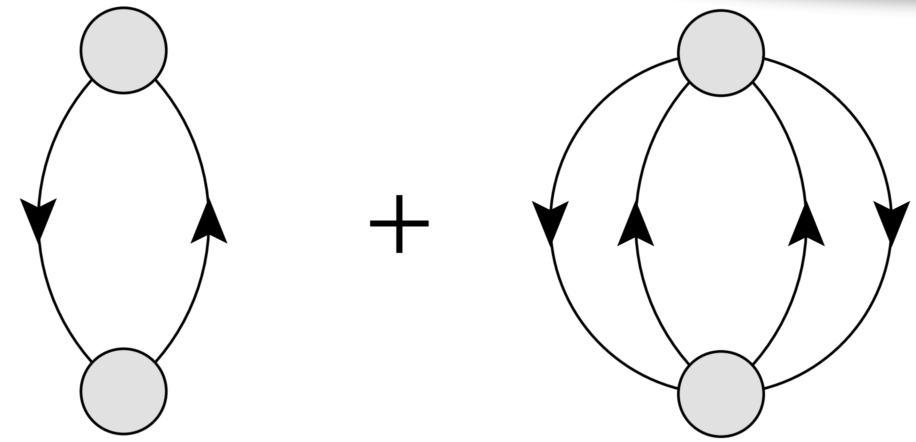
- off-diagonal matrix elements are suppressed like $e^{-\Delta^2 s}$ (Wegner), e^{-s} (White), and $e^{-|\Delta| s}$ (imaginary time)
- g.s. energies ($s \to \infty$) differ by $\ll 1\%$

IM-SRG(2) Flow Equations

0-body Flow

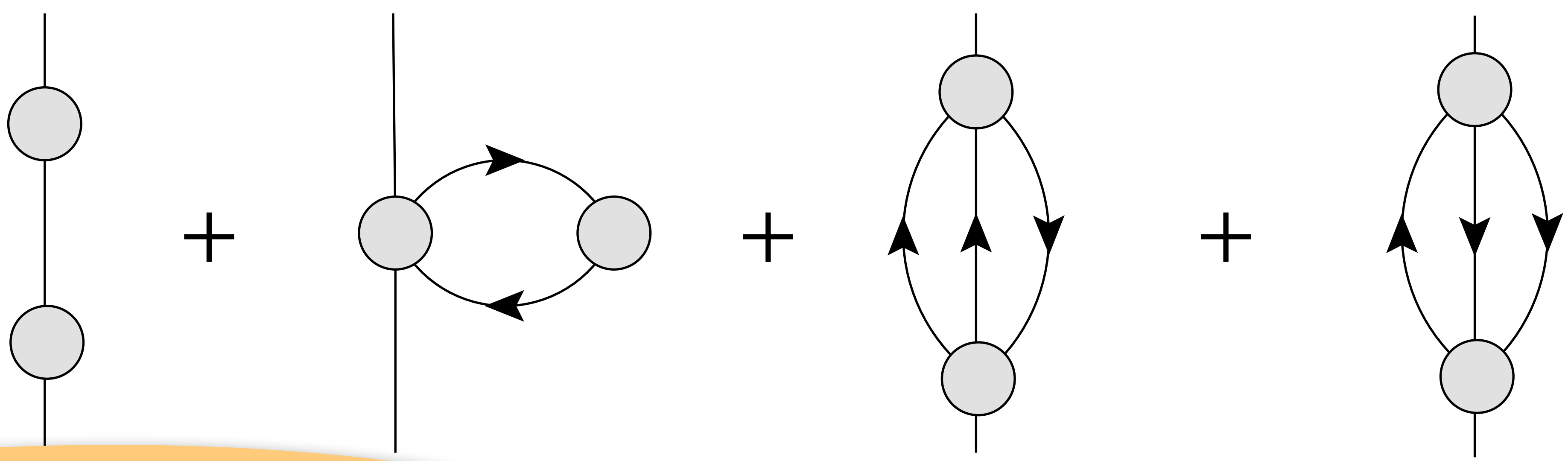
~ 2nd order MBPT for *H(s)*

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



1-body Flow

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



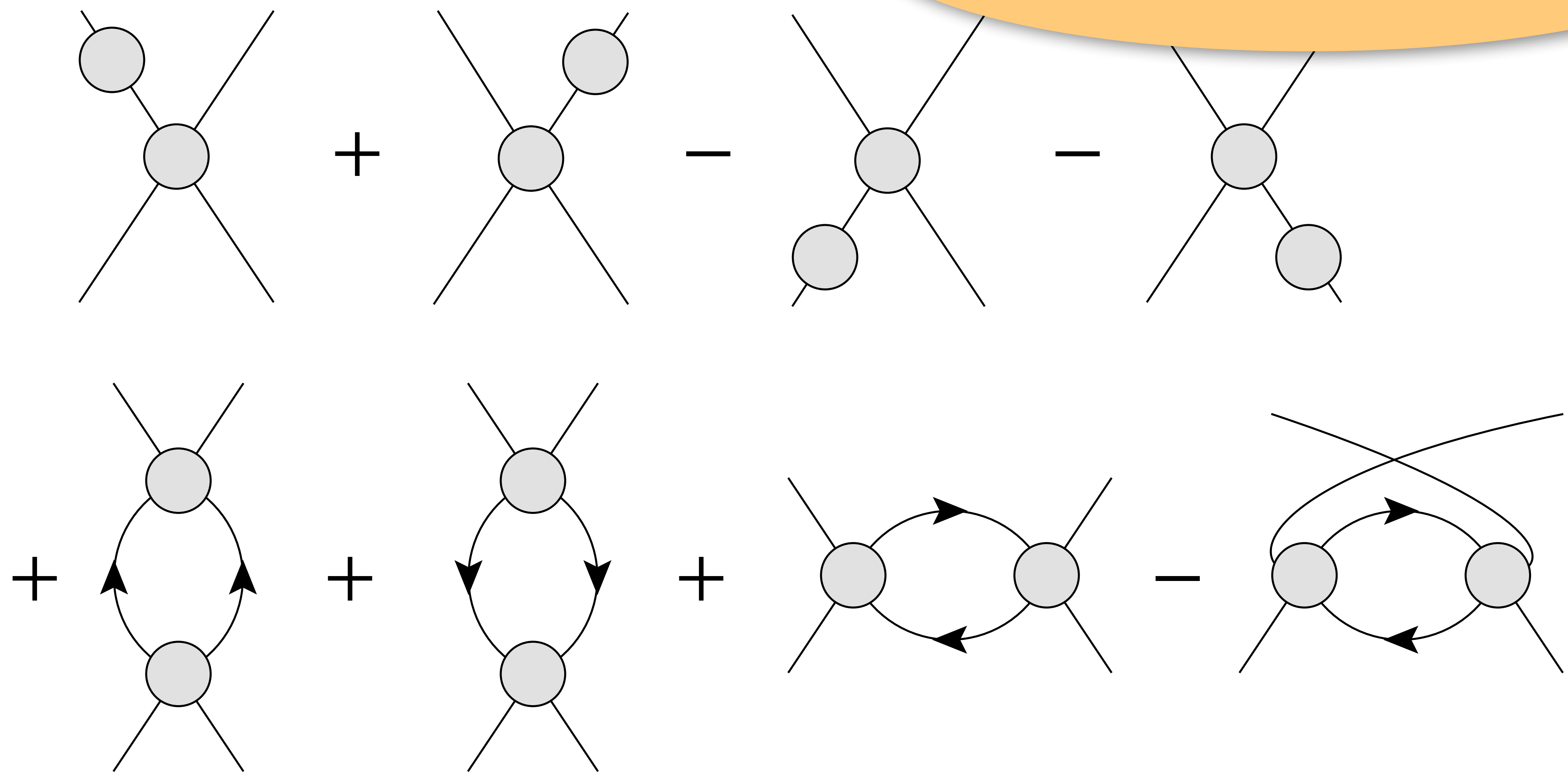
IM-SRG(2): truncate ops. at two-body level

IM-SRG(2) Flow Equations

2-body Flow

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

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



s channel

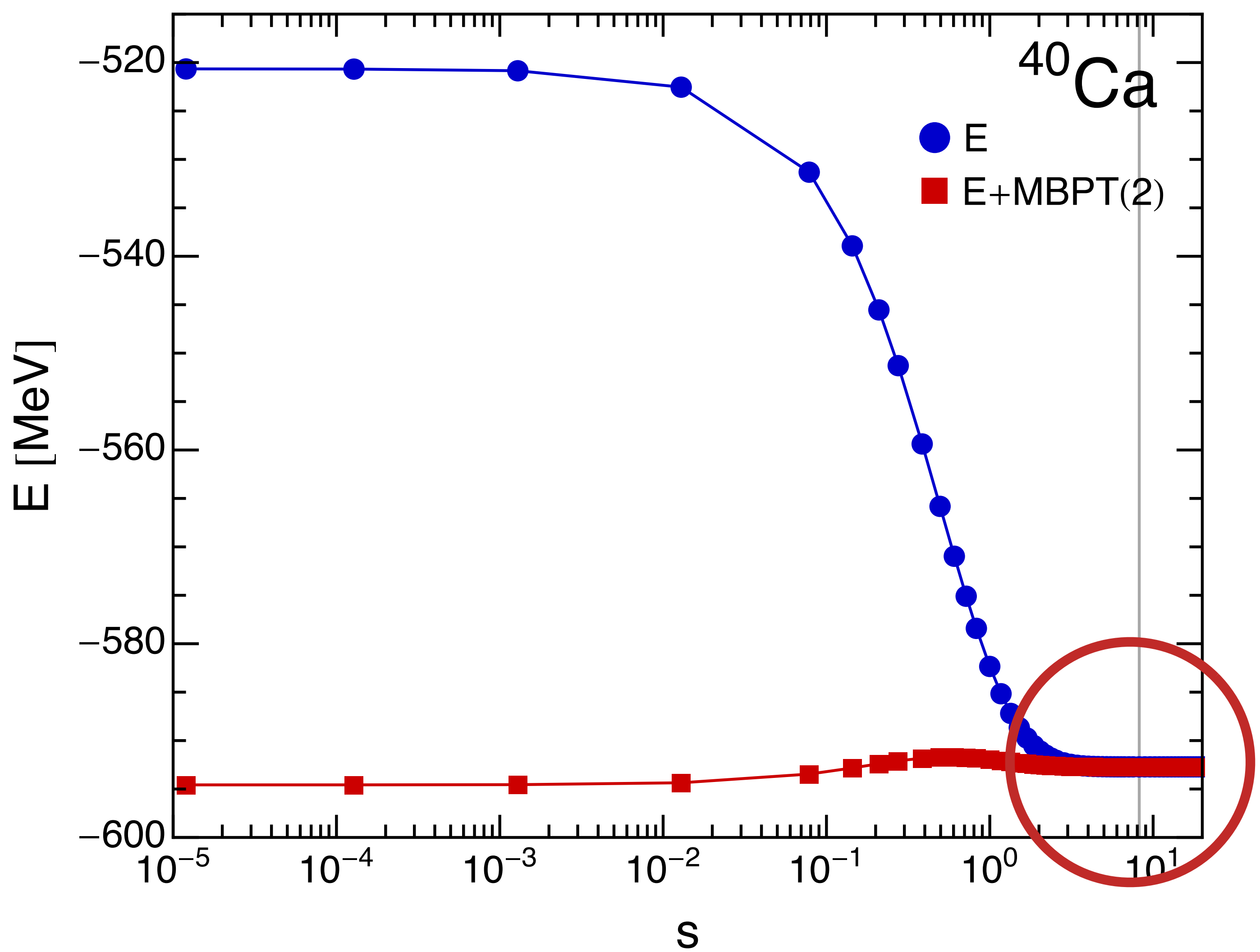
ladders

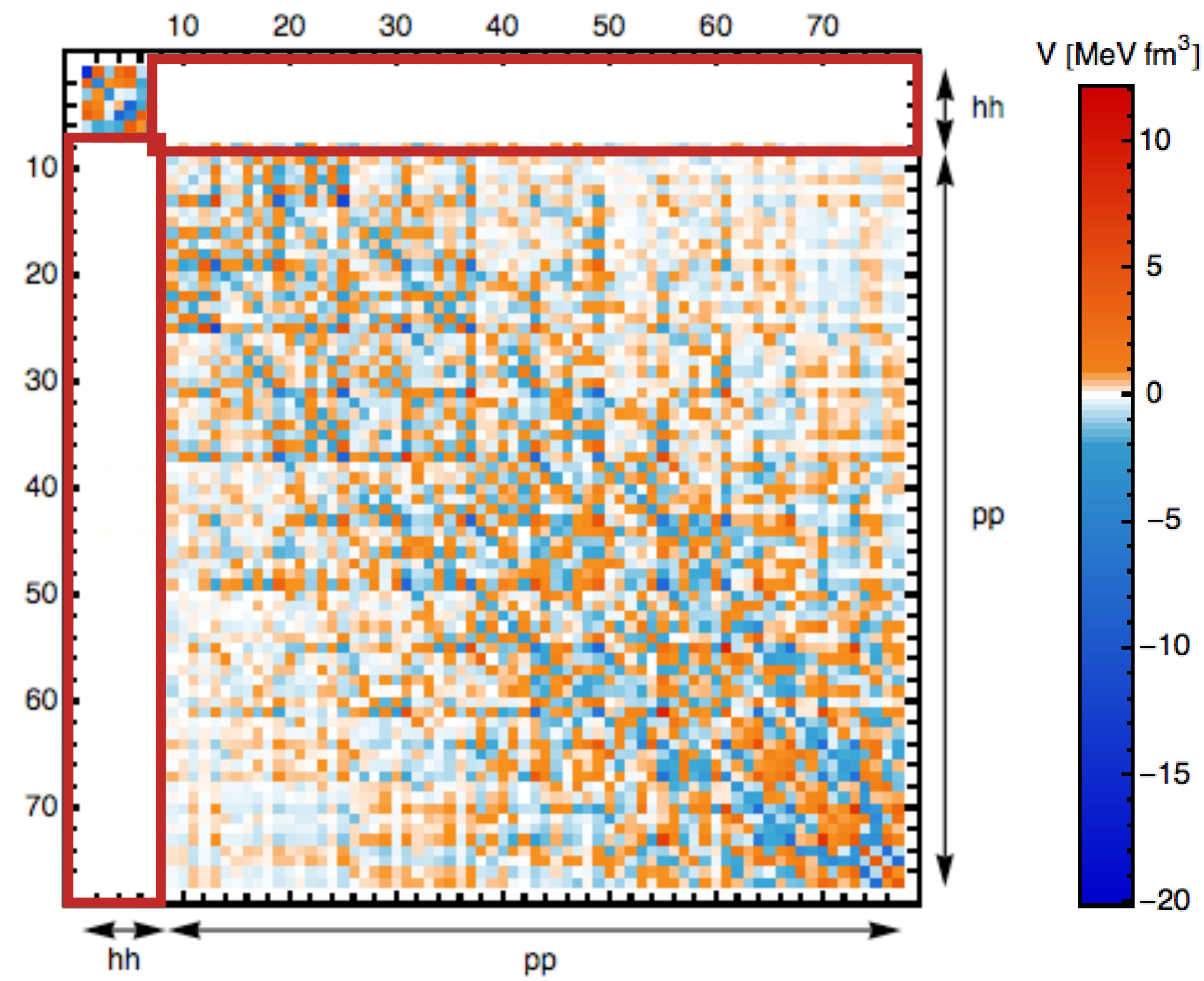
t channel

u channel

rings

Decoupling





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

non-perturbative resummation of MBPT series (correlations)

off-diagonal couplings are rapidly driven to zero

Multi-Reference IM-SRG

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)

Multi-Reference IM-SRG

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

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

$$\rho^{kl}_{mn} = \lambda^{kl}_{mn} + \lambda^k_m \lambda^l_n - \lambda^k_n \lambda^l_m$$
$$\rho^{ijk}_{lmn} = \lambda^{ijk}_{lmn} + \lambda^i_l \lambda^{jk}_{mn} + \lambda^i_l \lambda^j_m \lambda^k_n + \text{permutations}$$

$$\cdots$$

- irreducible densities give rise to additional contractions:

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

$$\cdots$$

MR-IM-SRG Flow Equations

0-body flow:

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

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

1-body flow:

$$\frac{d}{ds}f^1_2 = \sum_a\left(\eta^1_a f^a_2 - f^1_a\eta^a_2\right) + \sum_{ab}\left(\eta^a_b\Gamma^{b1}_{a2} - f^a_b\eta^{b1}_{a2}\right)(n_a - n_b)$$

$$+ \frac{1}{2}\sum_{abc}\left(\eta^{1a}_{bc}\Gamma^{bc}_{2a} - \Gamma^{1a}_{bc}\eta^{bc}_{2a}\right)(n_a\bar{n}_b\bar{n}_c + \bar{n}_a n_b n_c)$$

$$+\frac{1}{4}\sum_{abcde}\left(\eta^{1a}_{bc}\Gamma^{de}_{2a} - \Gamma^{1a}_{bc}\eta^{de}_{2a}\right)\lambda^{de}_{bc} + \sum_{abcde}\left(\eta^{1a}_{bc}\Gamma^{be}_{2d} - \Gamma^{1a}_{bc}\eta^{be}_{2d}\right)\lambda^{ae}_{cd}$$

$$-\frac{1}{2}\sum_{abcde}\left(\eta^{1a}_{2b}\Gamma^{cd}_{ae} - \Gamma^{1a}_{2b}\eta^{cd}_{ae}\right)\lambda^{cd}_{be} + \frac{1}{2}\sum_{abcde}\left(\eta^{1a}_{2b}\Gamma^{bc}_{de} - \Gamma^{1a}_{2b}\eta^{bc}_{de}\right)\lambda^{ac}_{de}$$

MR-IM-SRG 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 identical to closed-shell case
- numerical scaling: $O(N^6)$

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(N^4)

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

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

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

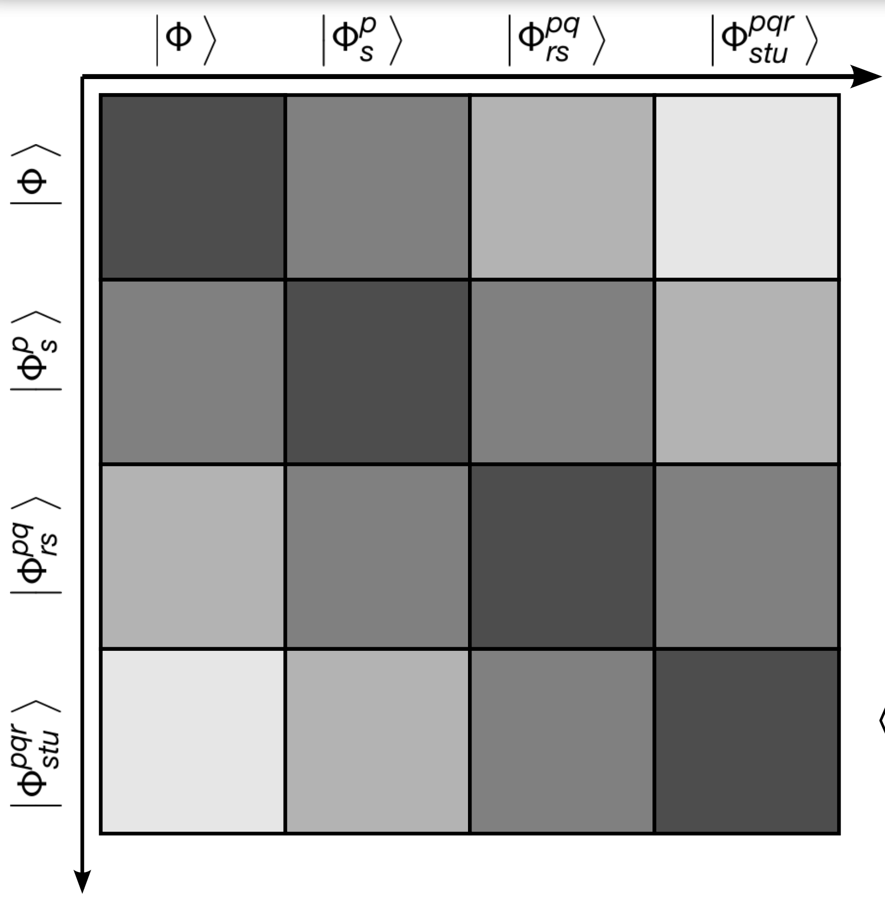
➡ exploit structure of specific reference states:

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

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

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

Decoupling Revisited



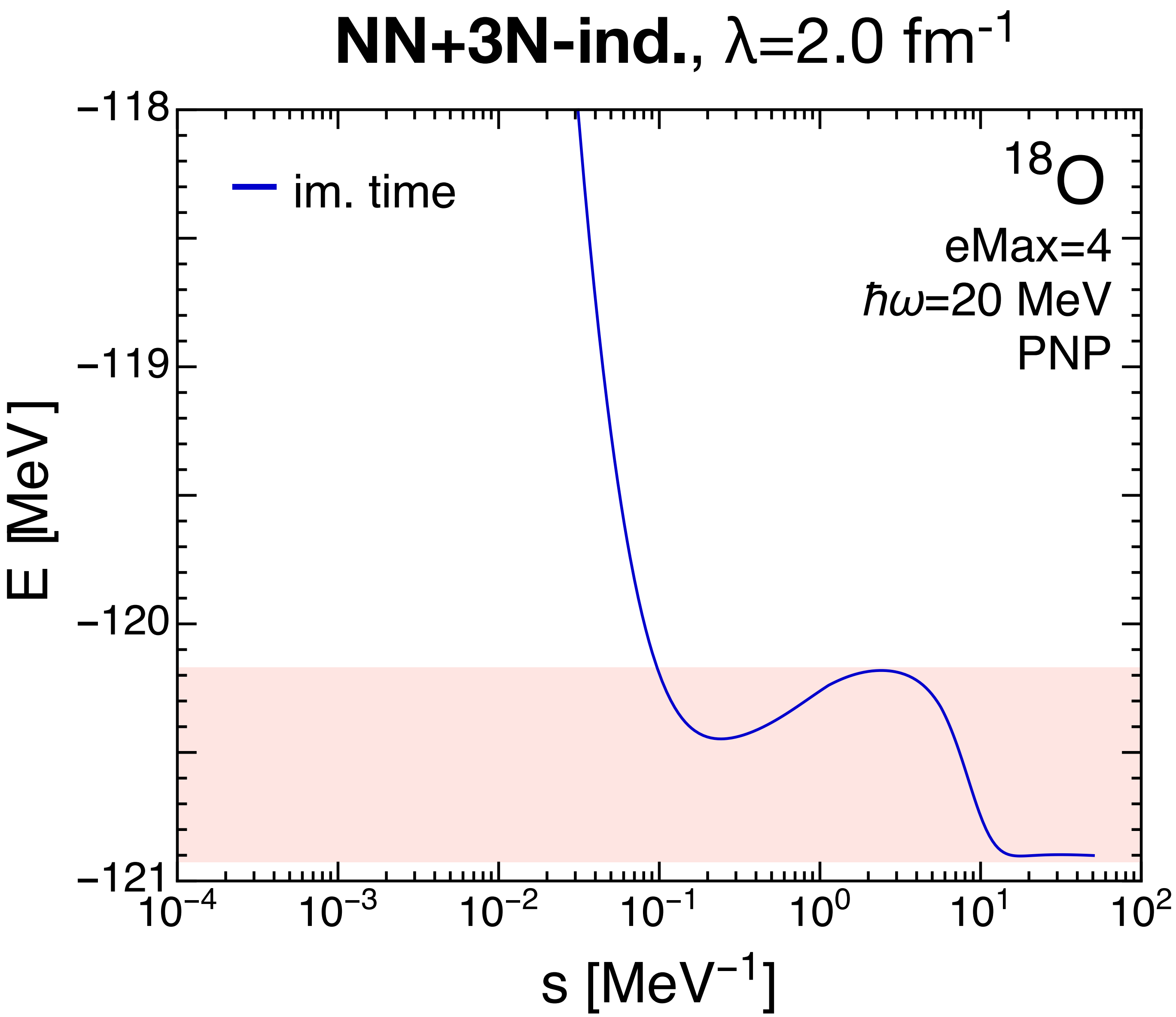
$$\left\langle {}^{p}_{s} \middle| H \middle| \Phi \right\rangle \sim \bar{n}_p n_s f^{p}_{s}\,, \sum_{kl} f^{k}_{l} \lambda^{sk}_{pl}, \sum_{klmn} \Gamma^{kl}_{mn} \lambda^{skl}_{pmn}, \ldots$$

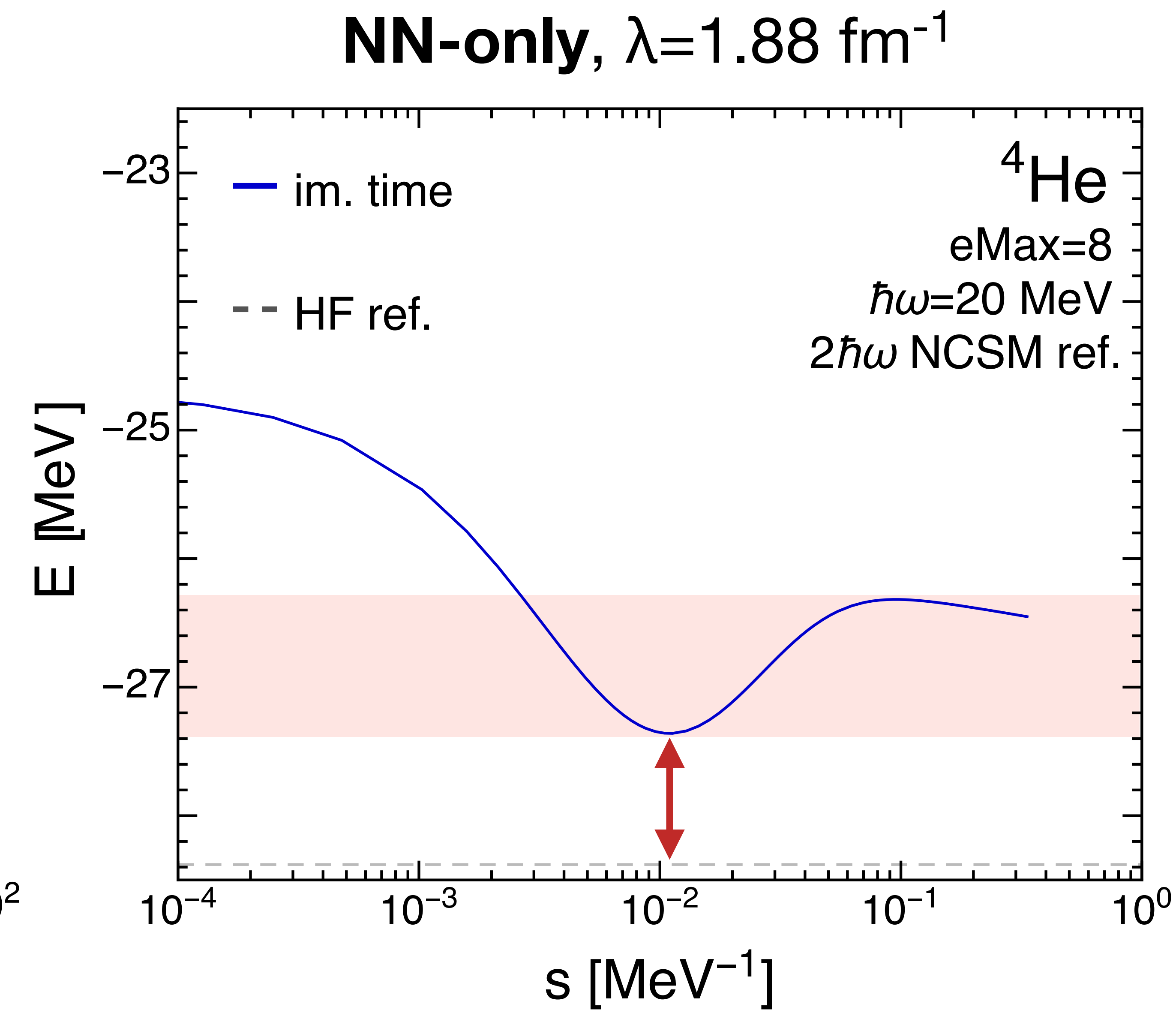
$$\left\langle {}^{pq}_{st} \middle| H \middle| \Phi \right\rangle \sim \bar{n}_p \bar{n}_q n_s n_t \Gamma^{pq}_{st}\,, \sum_{kl} \Gamma^{pk}_{sl} \lambda^{tk}_{ql}, \sum_{kl} f^{k}_{l} \lambda^{stk}_{pql}, \sum_{klmn} \Gamma^{kl}_{mn} \lambda^{stkl}_{pqmn}, \ldots$$

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

- 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





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

Brillouin Generator

- consider unitary variations of the energy functional

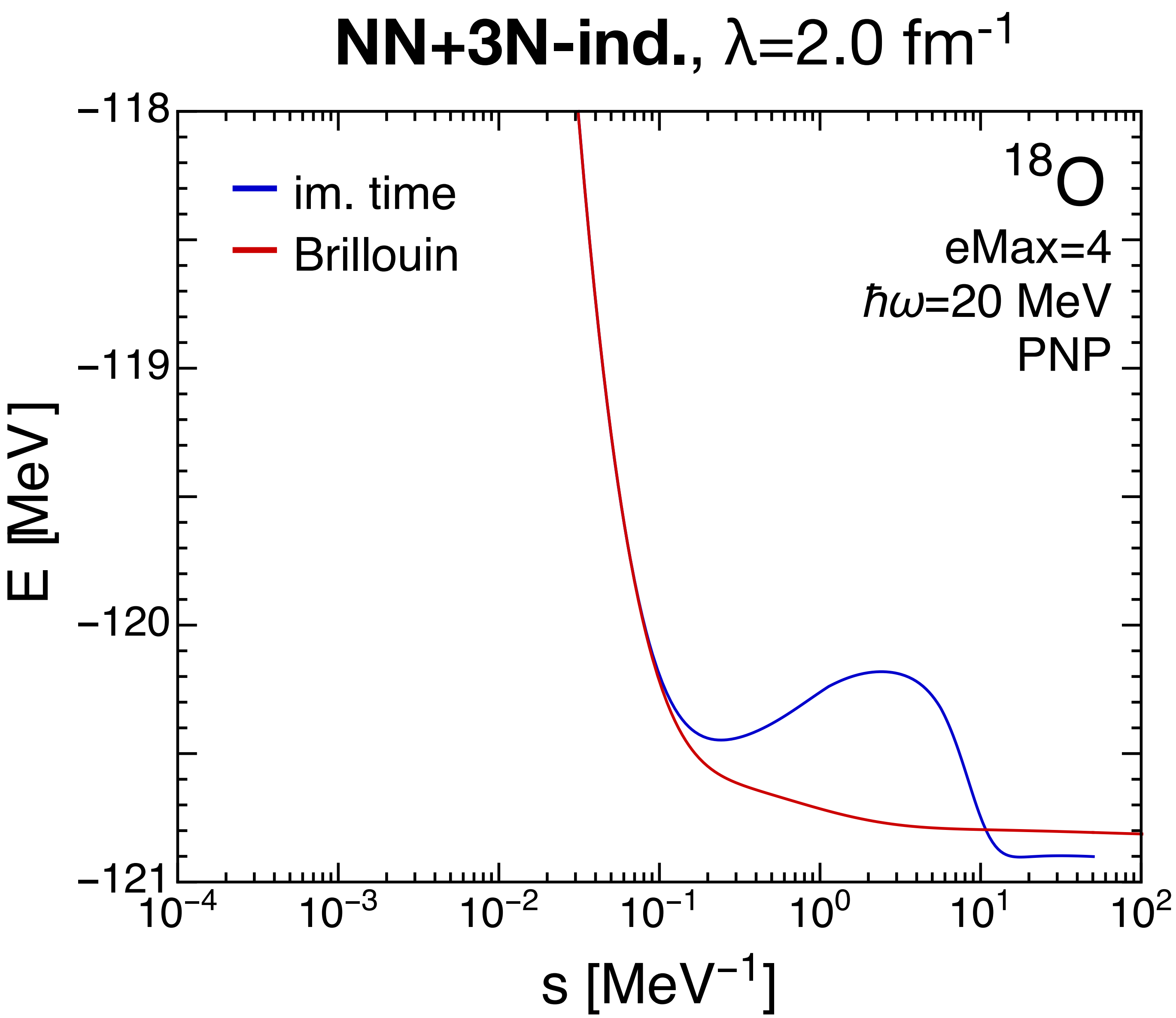
$$E(s) = \langle \Phi | H(s) | \Phi \rangle$$

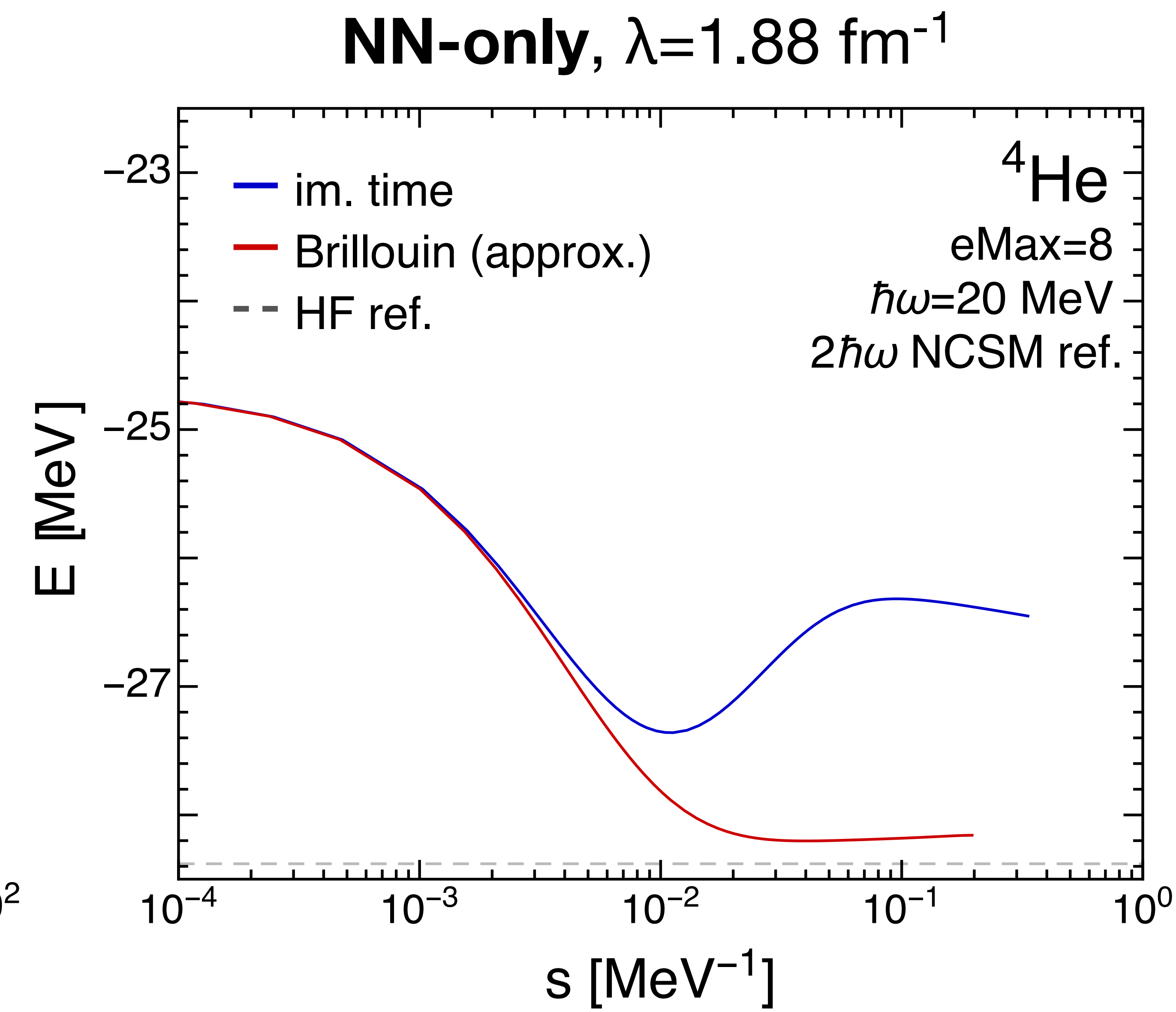
- define generator as the residual of the irreducible Brillouin condition (= gradient of E)

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

- 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

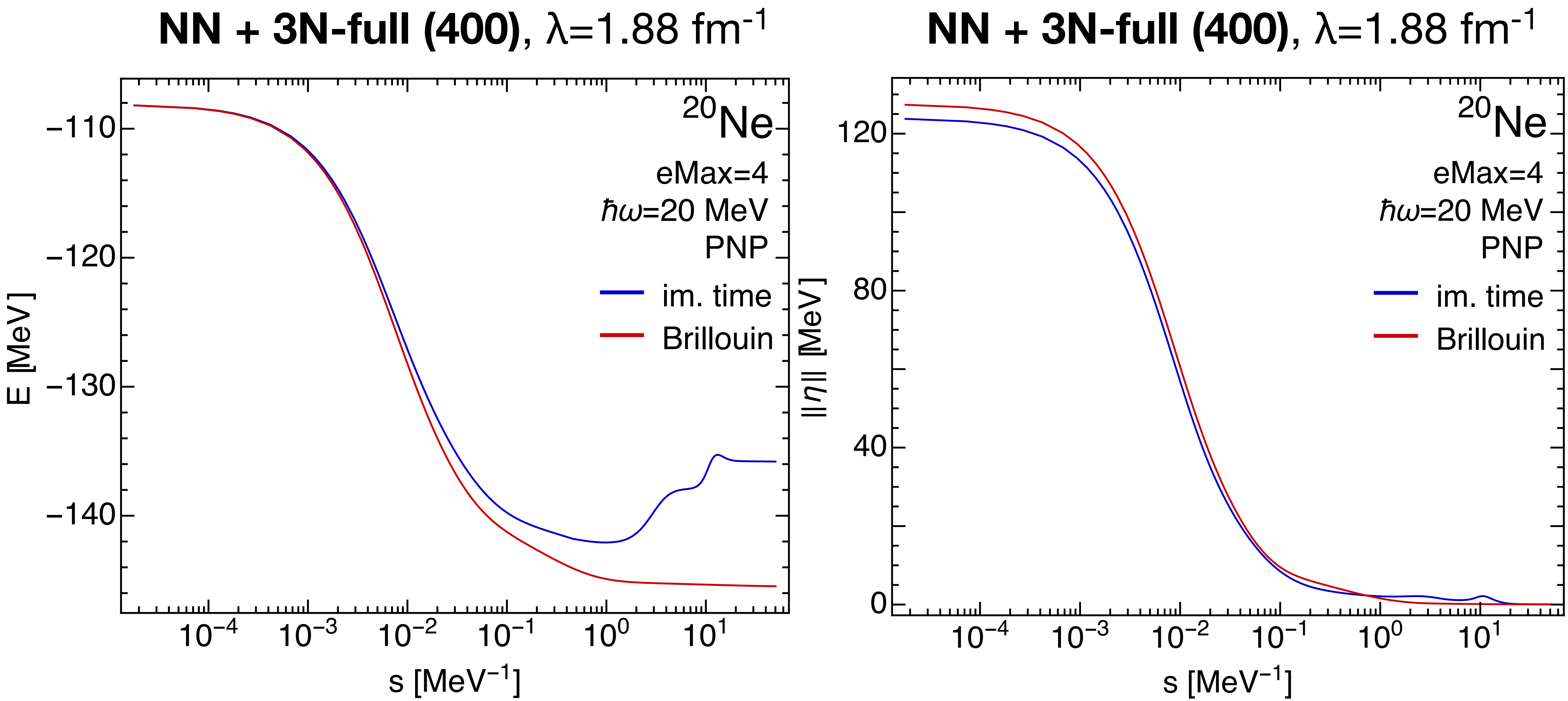
Brillouin Generator





➡ energy & norm of Brillouin generator decay monotonically
(approx. for ^{4}He: 2B "particle-hole"-like term switched off, 3B density not yet included)

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

Ground States of Closed and Open-Shell Nuclei

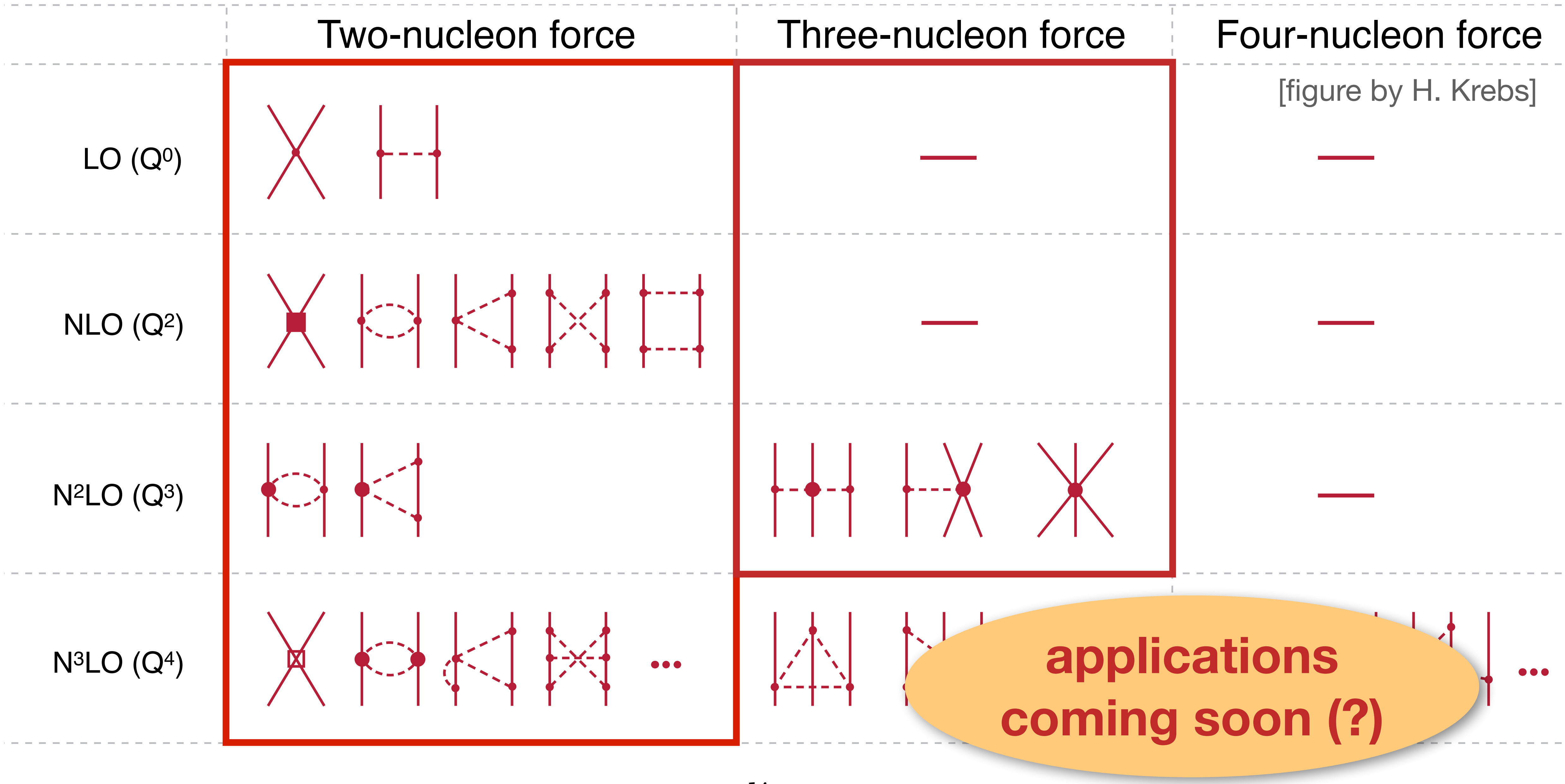
H. H., in preparation

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)

Interactions from Chiral EFT



- organization in powers $(Q/\Lambda_\chi)^\nu$ allows systematic improvement
- low-energy constants fit to NN, 3N data (future: from Lattice QCD (?))
- consistent NN, 3N, ... interactions & operators (electromagnetic & weak transitions, etc.)

Hamiltonians

Initial Hamiltonian

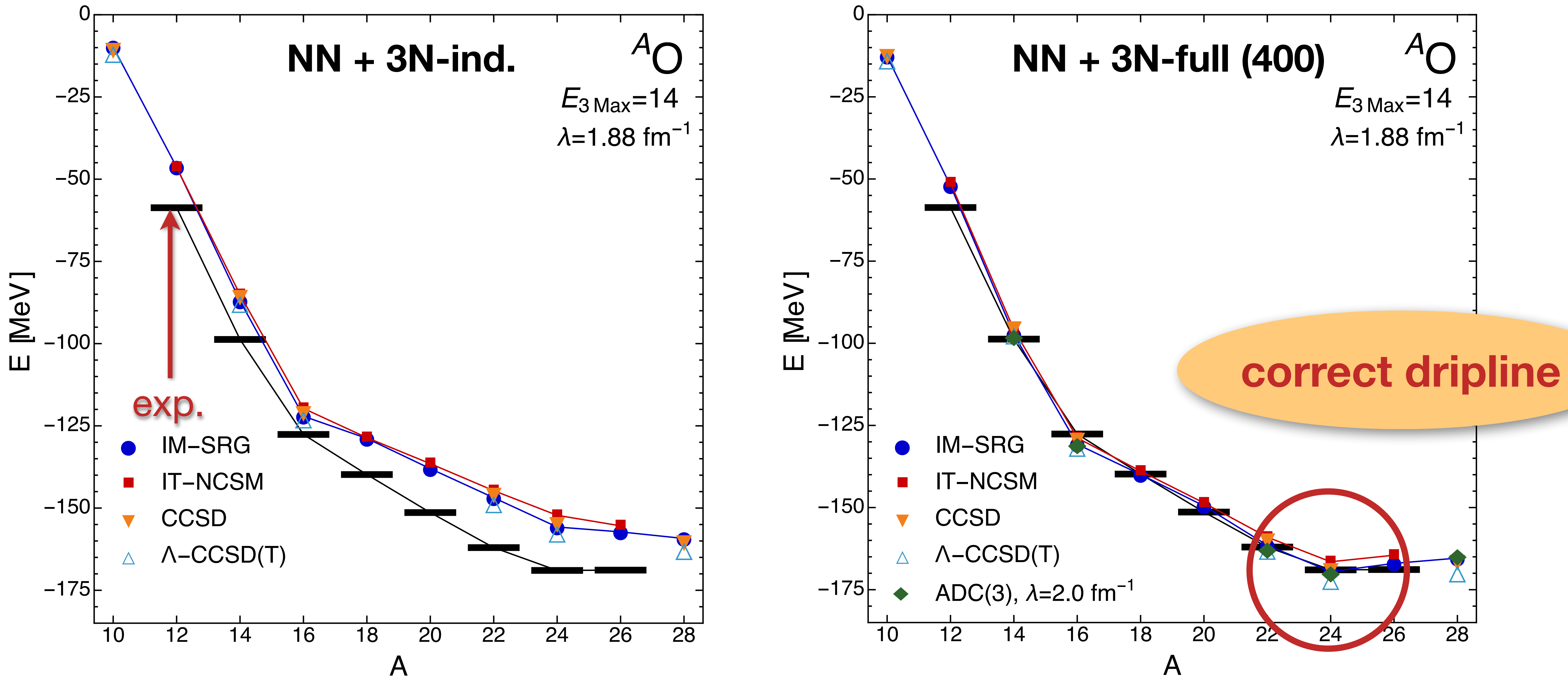
- NN: chiral interaction at N^3LO (Entem & Machleidt)
- 3N: chiral interaction at N^2LO (c_D, c_E fit to ^3H, ^4He energies, β decay)

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

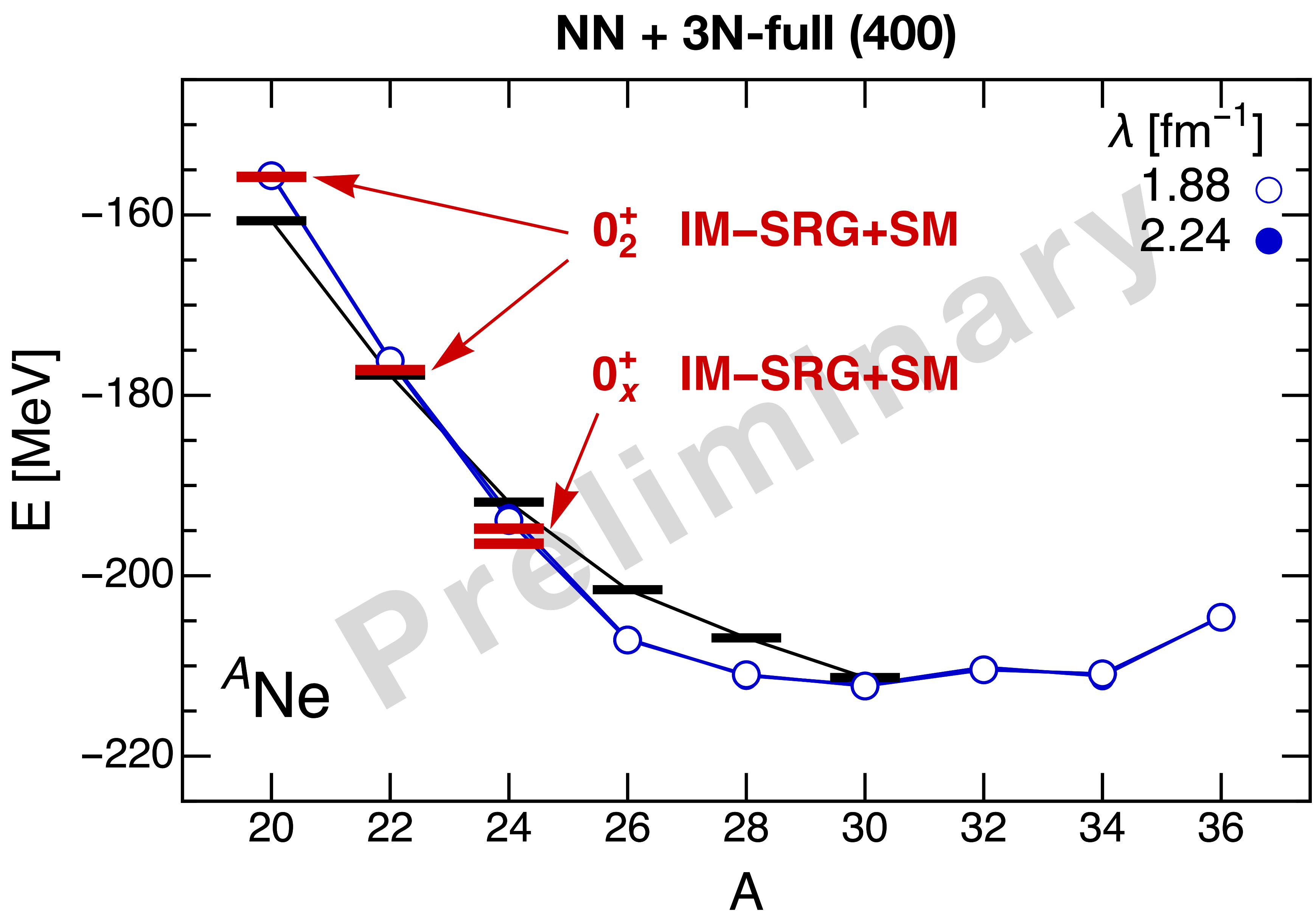
Results: Oxygen Chain

*HH et al., 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

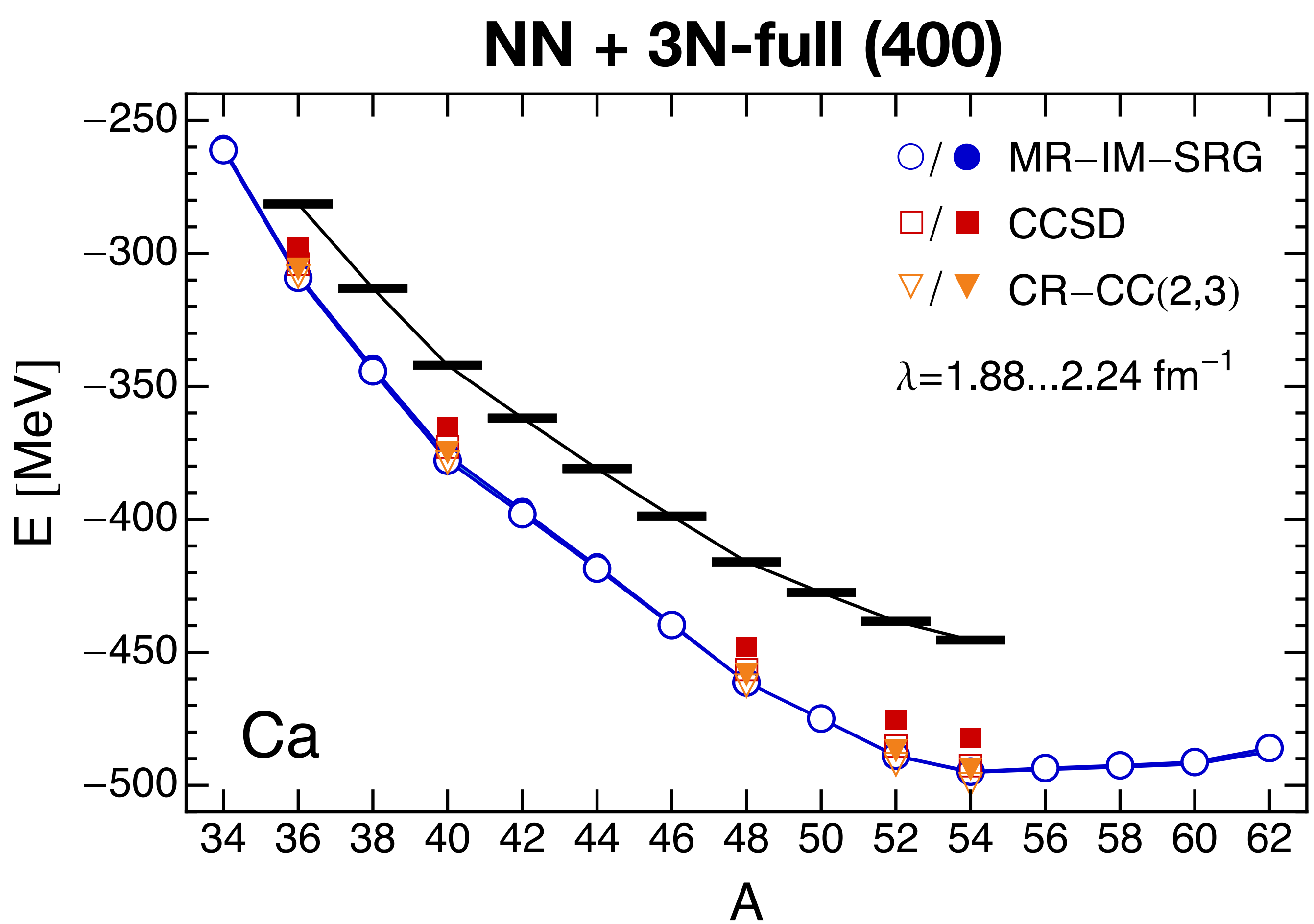
Neon Isotopes

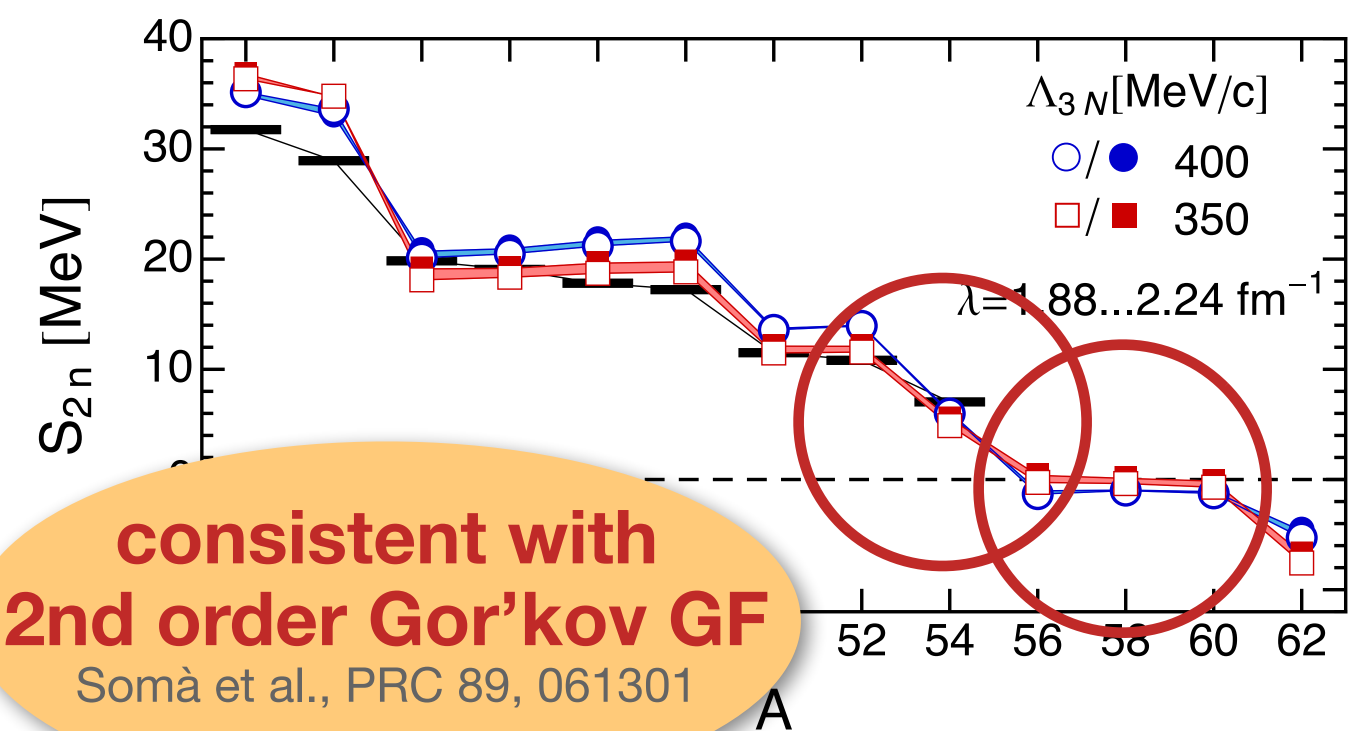


➡ MR-IM-SRG selects excited 0^+ state with spherical intrinsic structure (symmetry constrained)

Two-Neutron Separation Energies

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





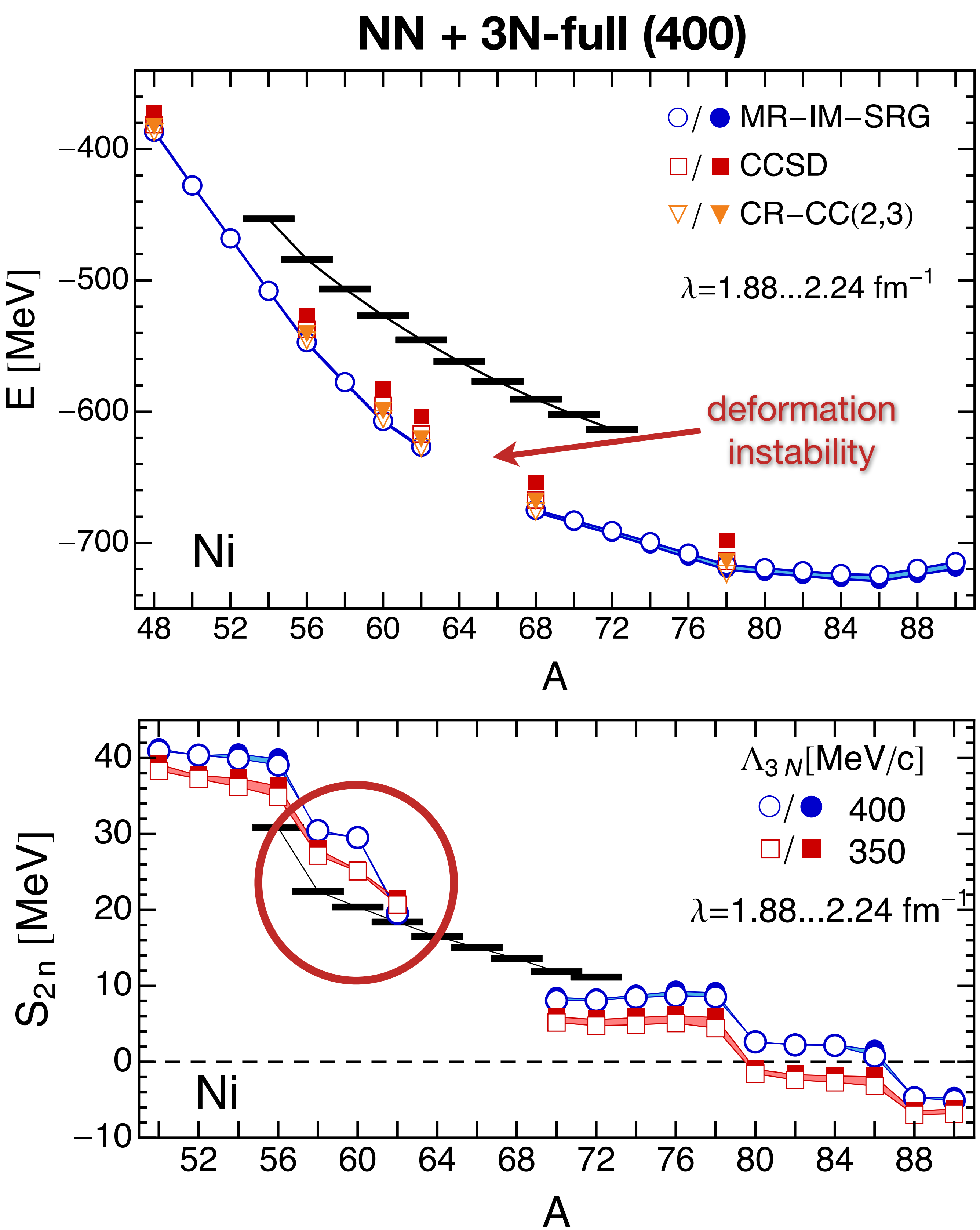
consistent with 2nd order Gor'kov GF

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

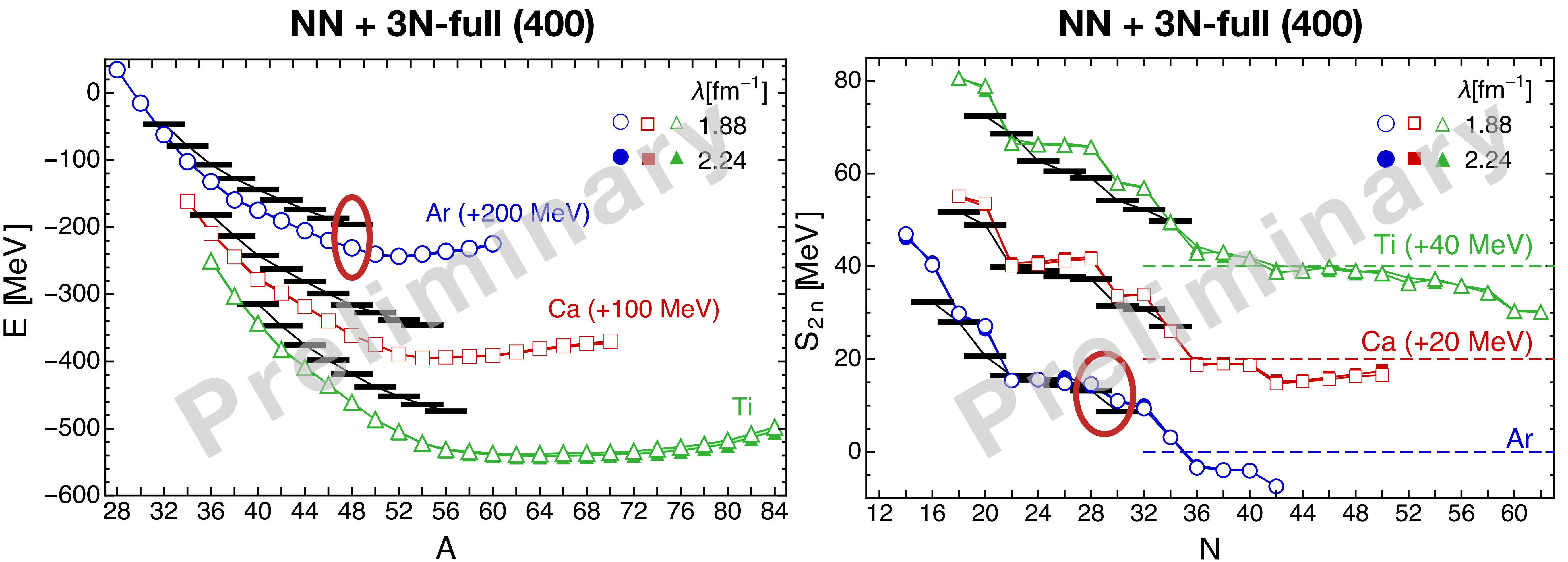
Two-Neutron Separation Energies

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



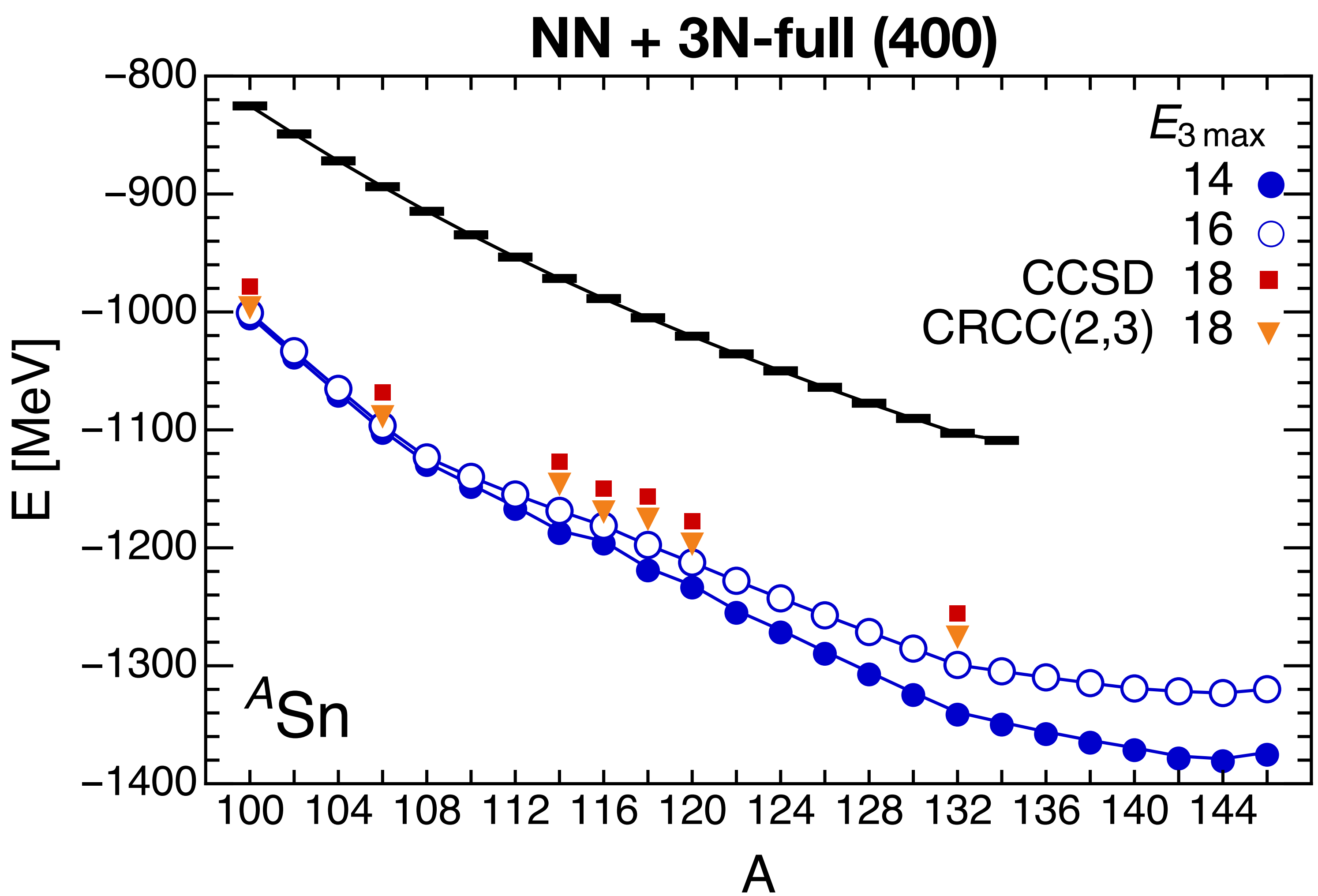
- flat trends for g. s. energies and S_{2n} (similar to Ca)
- deformation instability in ^{64,66}Ni calculations - issue with “shell” structure
- further evidence from 3N cutoff variation
- no continuum coupling yet, other S_{2n} uncertainties < 1MeV

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 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., T. D. Morris, A. Schwenk, and K. Tuskiyama, to appear in Phys. Rept.

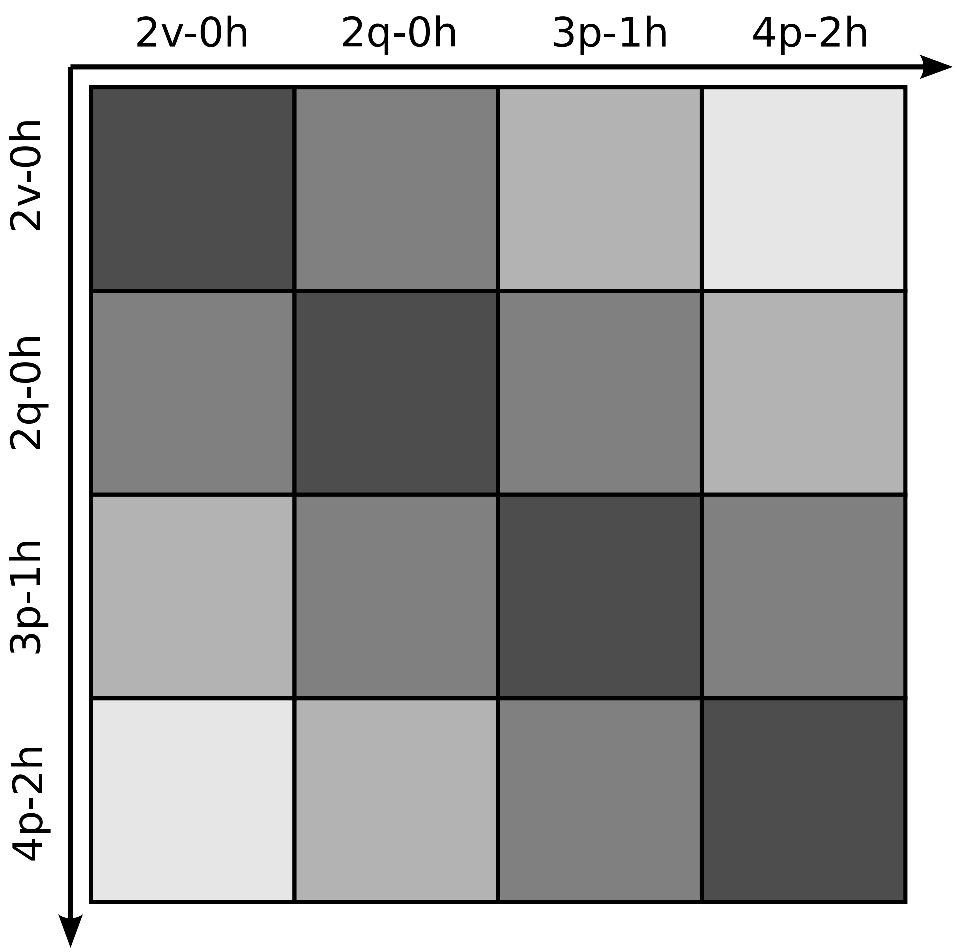
S. K. Bogner, H. H., J. D. Holt, S. R. Stroberg, A. Schwenk, in preparation

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)

also see talk by J. D. Holt (week 2)

Valence Space Decoupling

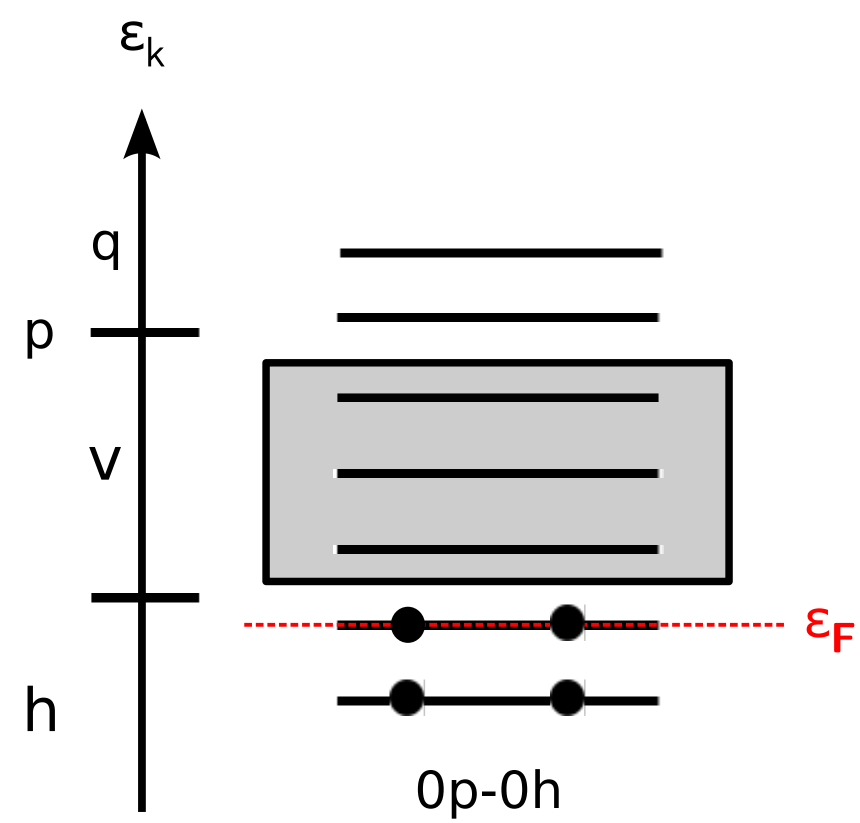


$\langle i | H | j \rangle$

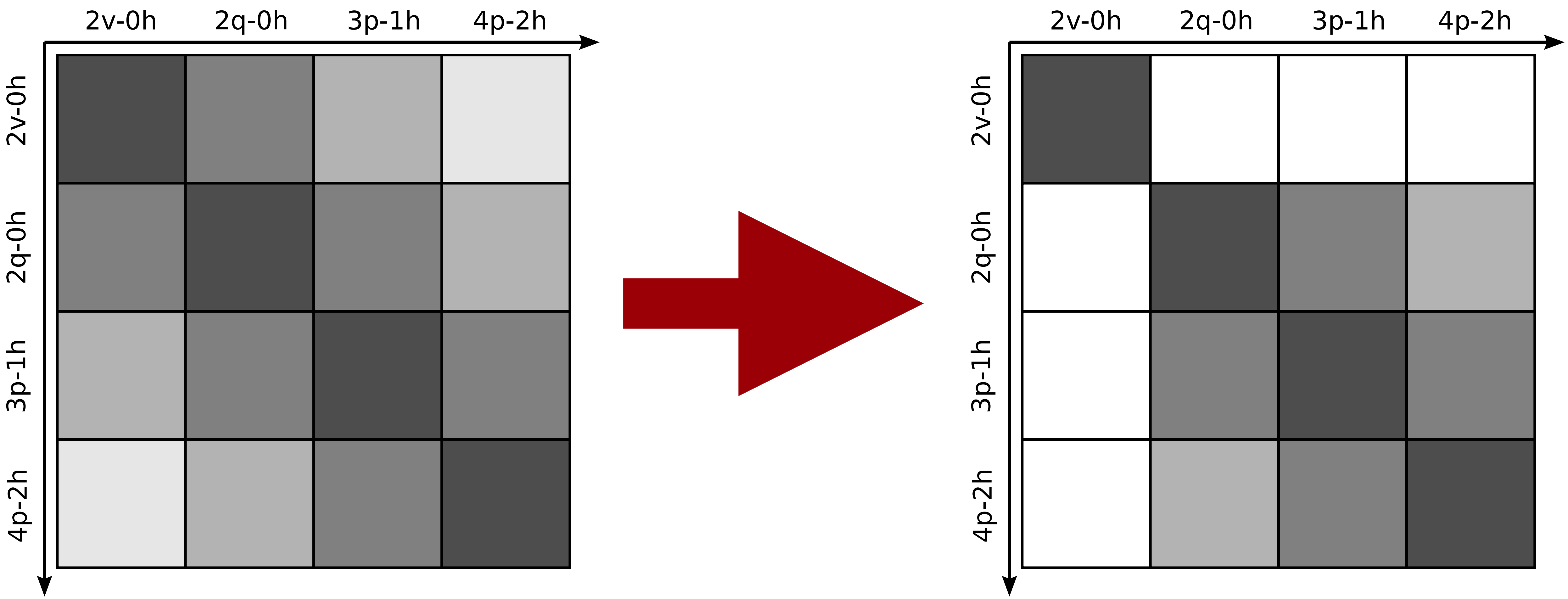
non-valence particle states

valence particle states

hole states (core)



Valence Space Decoupling



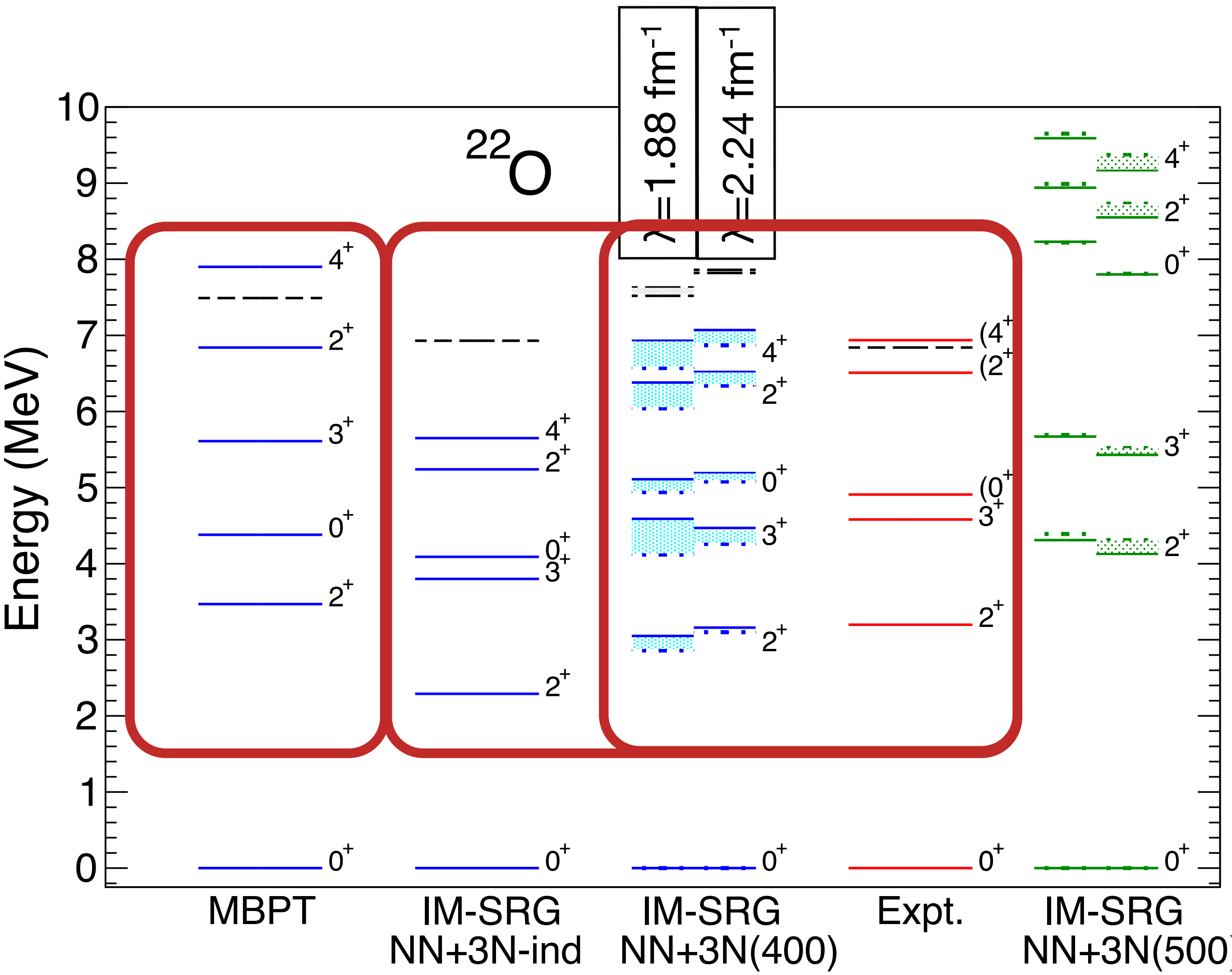
$\langle i | H | j \rangle$ $\qquad$ $\langle i | H(\infty) | j \rangle$

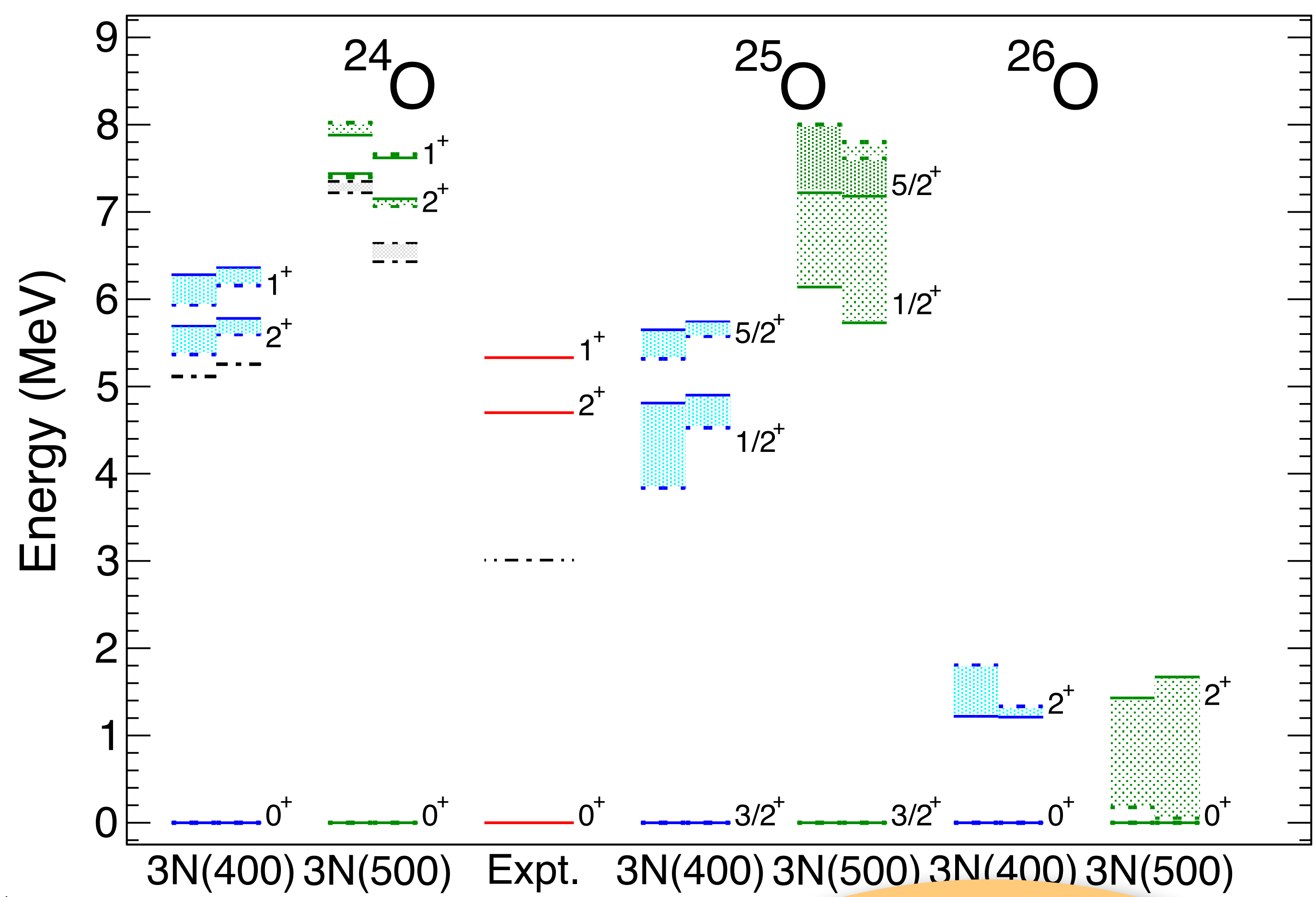
- construct generator from off-diagonal Hamiltonian

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

From Oxygen...

S. K. Bogner, HH, et al., PRL **113**, 142501 (2014)





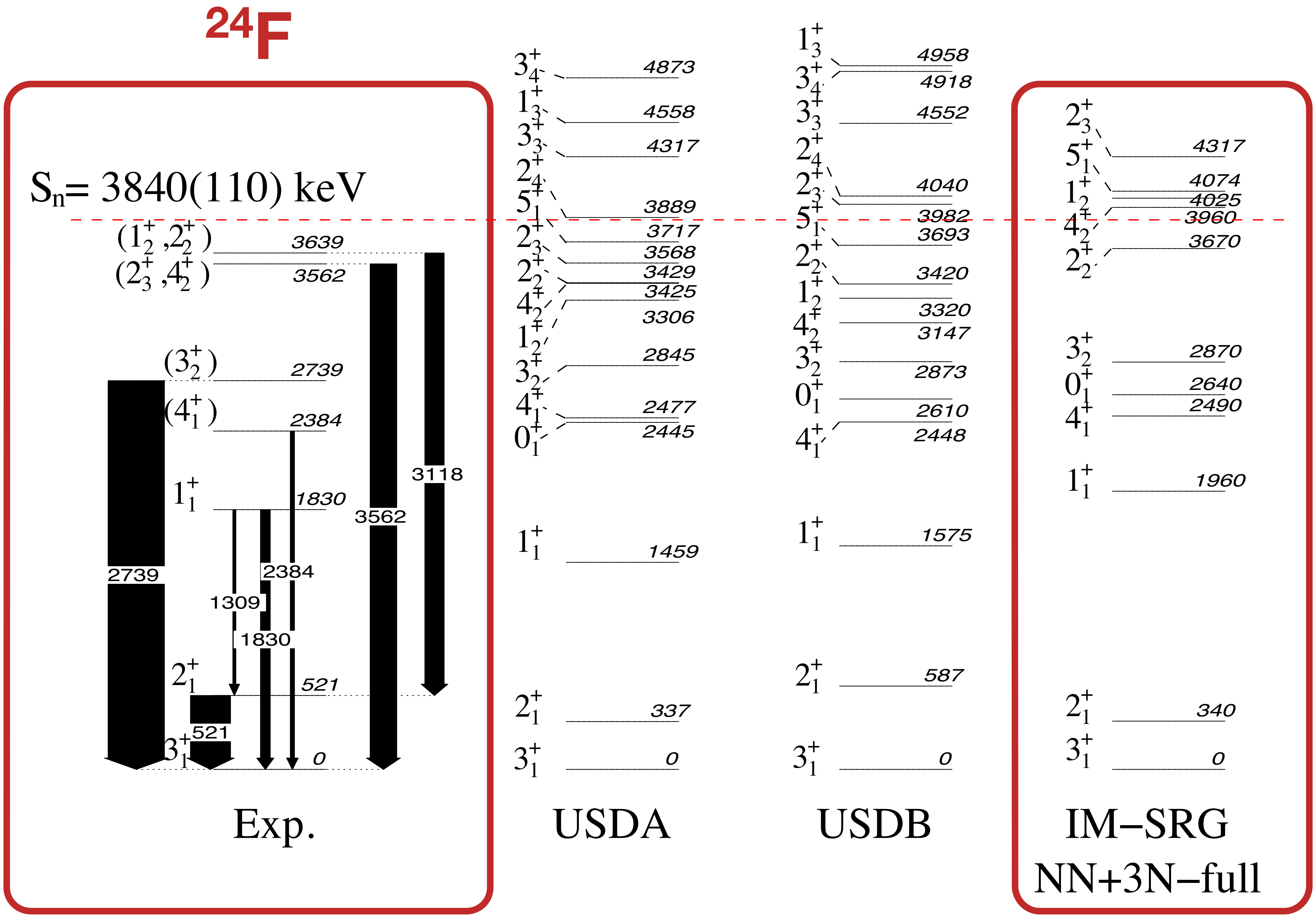
continuum lowers states by <1 MeV

shading: $\hbar\Omega$ variation

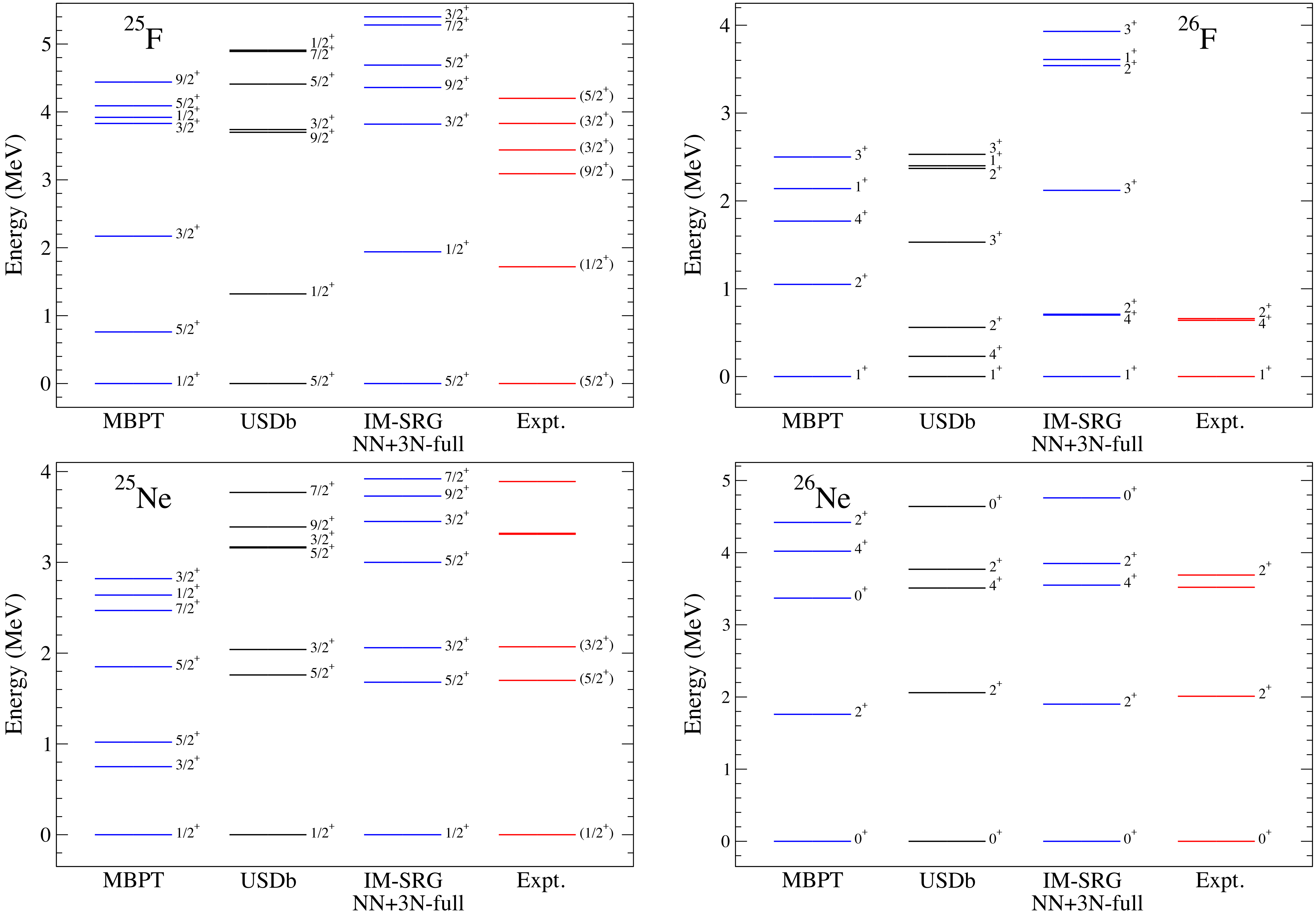
- **3N forces crucial**
- IM-SRG improves on finite-order MBPT effective interaction
- competitive with phenomenological calculations

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

L. Caceres et al., PRC **92**, 014327 (2015)

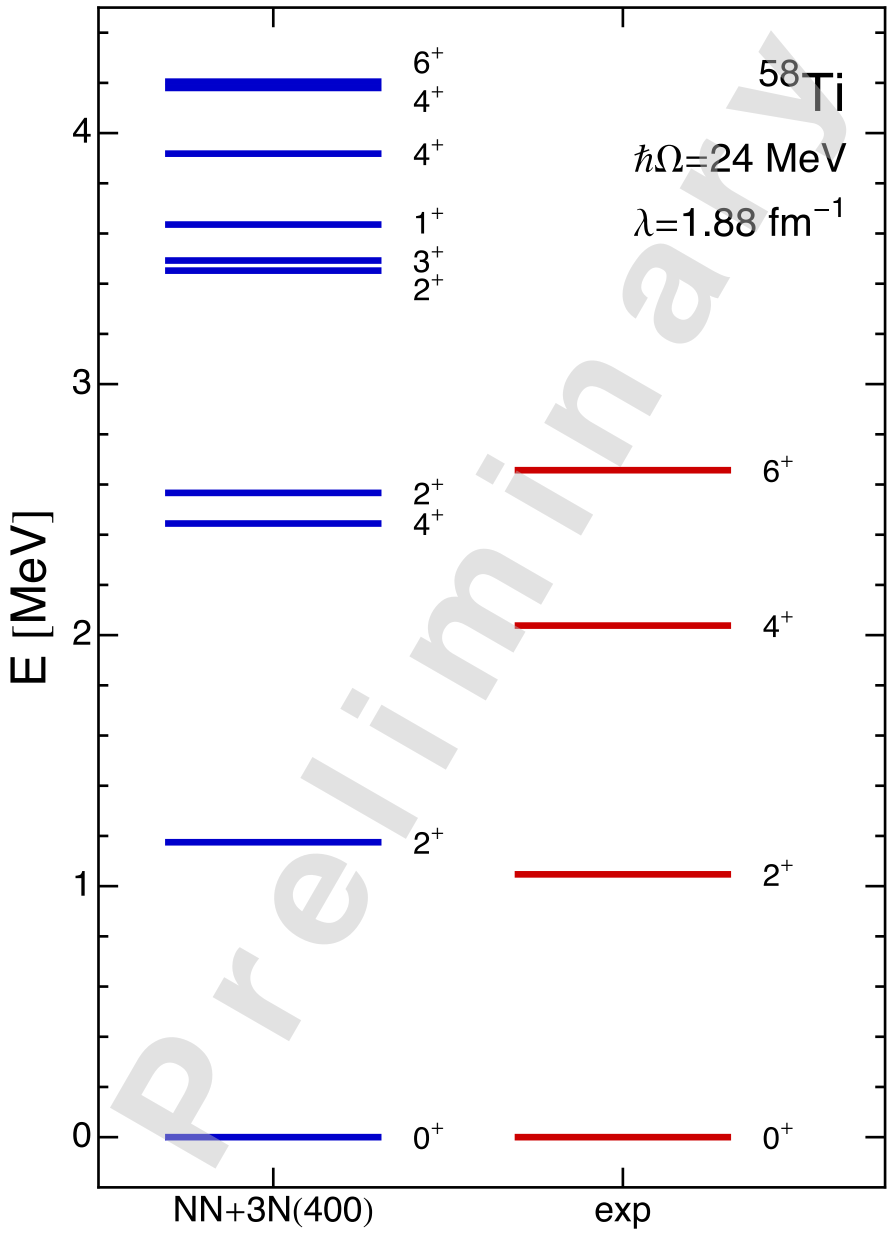


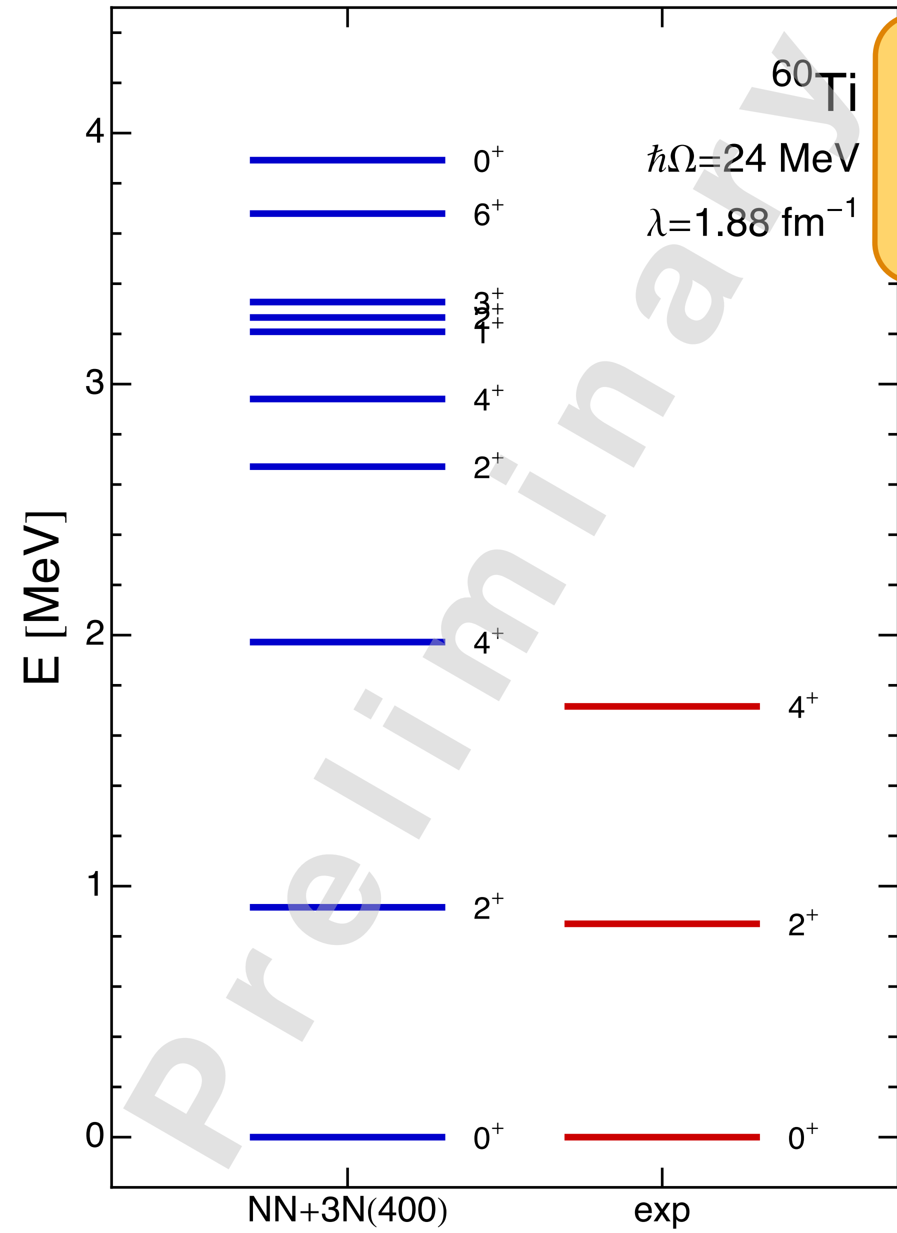
... Into the *sd*-Shell...



... And Beyond

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



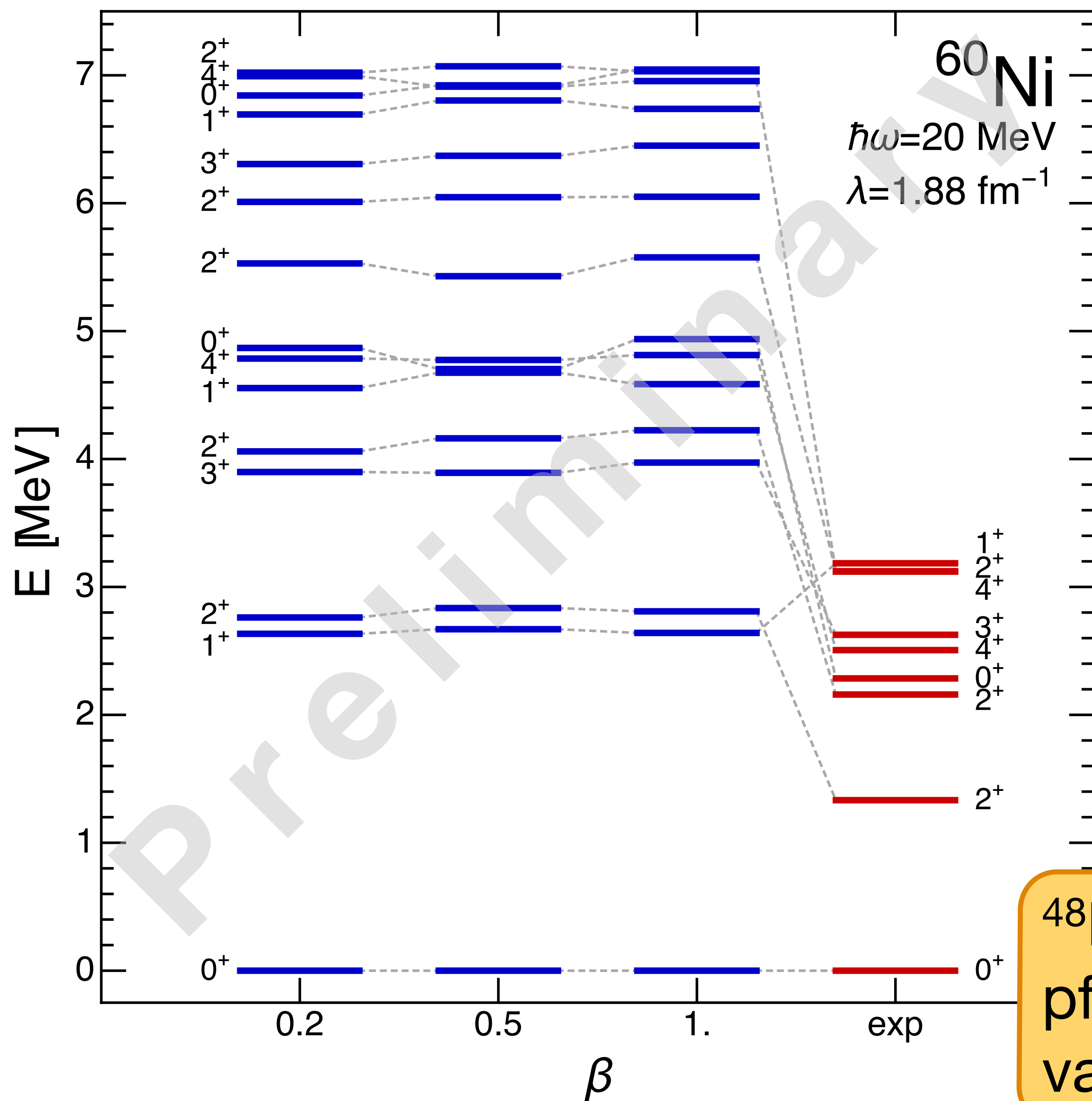


^{48}Ca core, $\nu pf_{5/2}$, πpf valence space

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

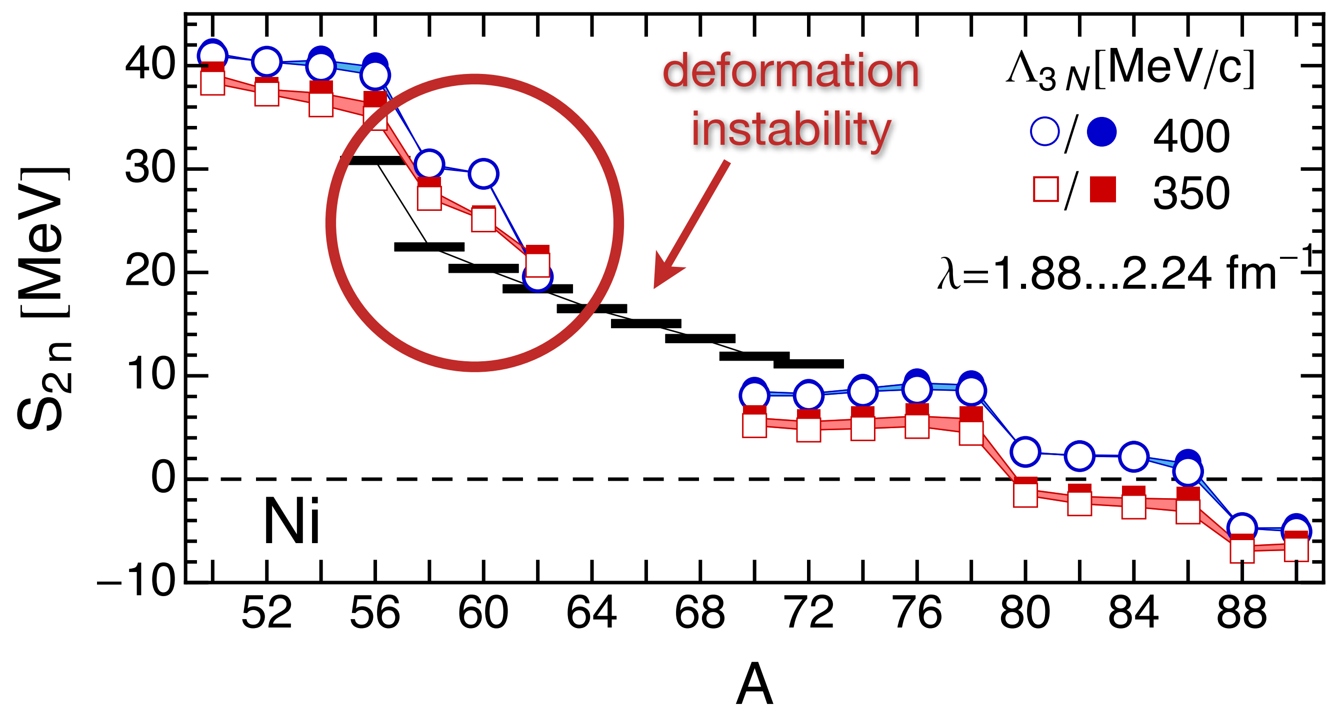
Multi-Shell Interactions

NN + 3N-full(400)



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

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



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

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

Next Steps

Magnus Series Formulation

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

- construct unitary transformation explicitly:

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

- flow equation for Magnus operator :

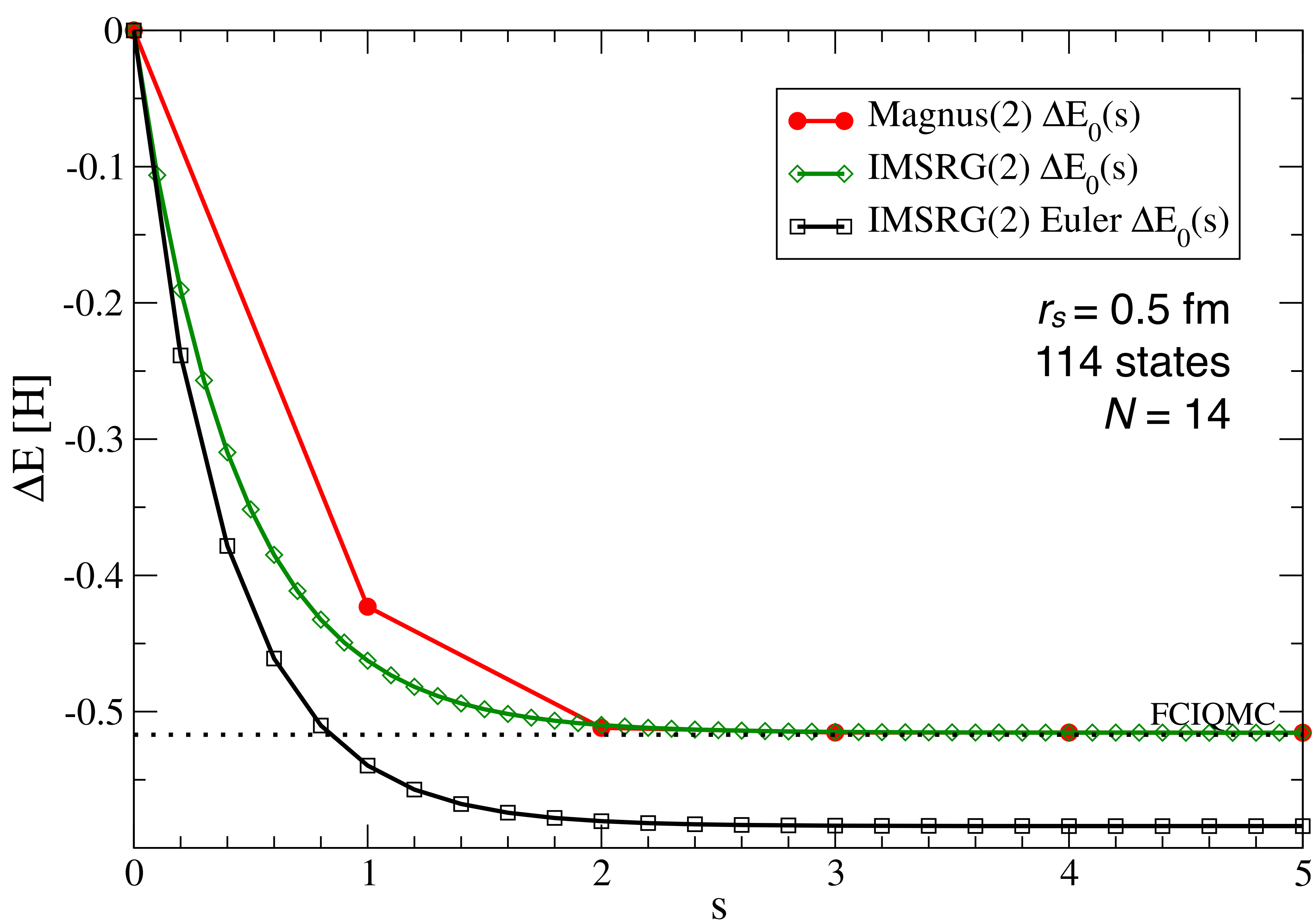
$$\frac{d}{ds}\Omega = \sum_{k=0}^{\infty} \frac{B_k}{k!} \mathrm{ad}_{\Omega}^{k}(\eta) \;, \quad \mathrm{ad}_{\Omega}(O) = [\Omega, O]$$

(B_k: Bernoulli numbers)

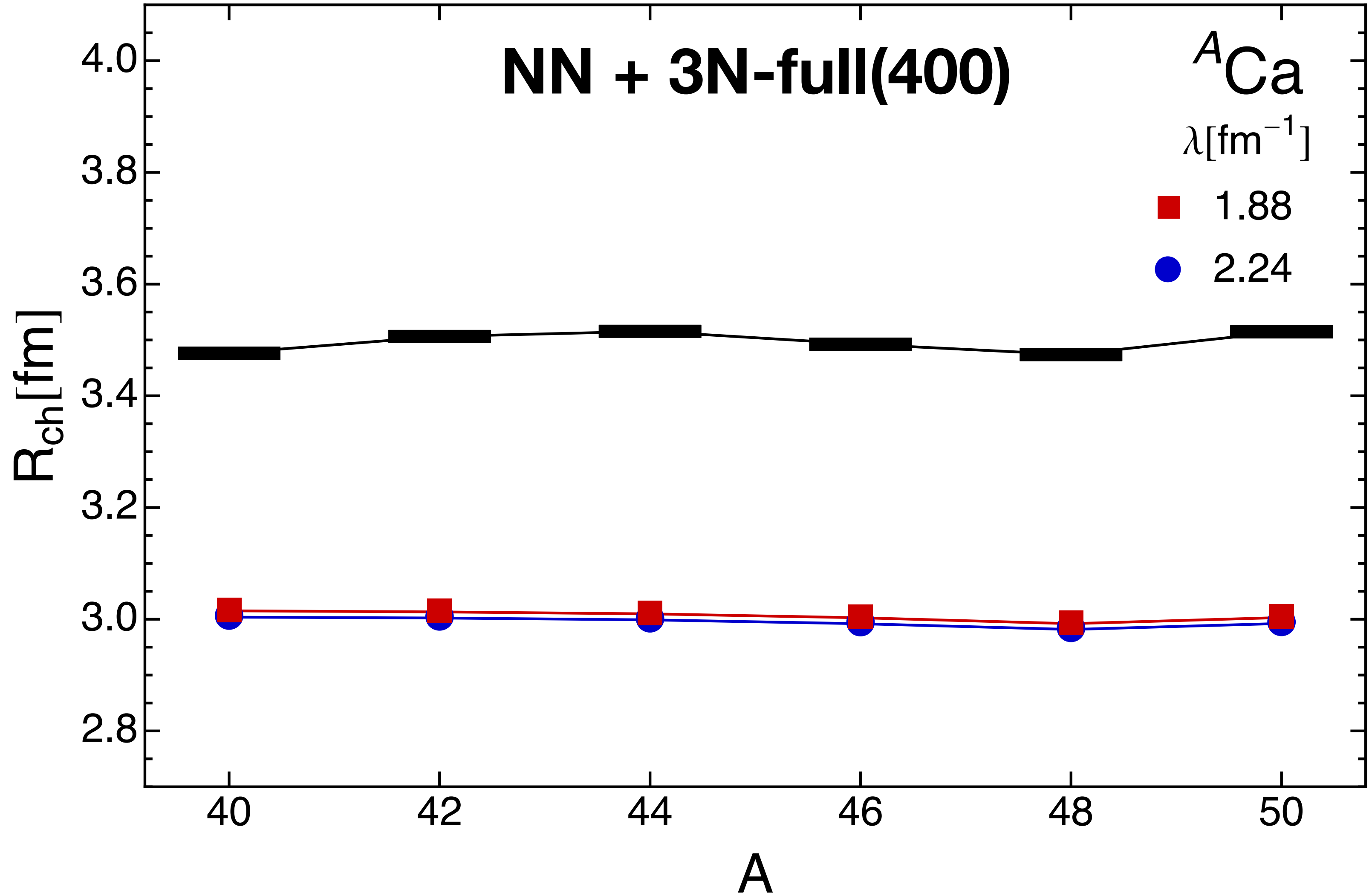
- construct $O(s) = U(s) O_0 U^{\dagger}(s)$ using Baker-Campbell-Hausdorff expansion (Hamiltonian + effective operators)
- generate systematic approximations to (MR-)IM-SRG(3)
- simple integrator sufficient (Euler!) - **unitarity built in**

Example: Homogenous Electron Gas

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

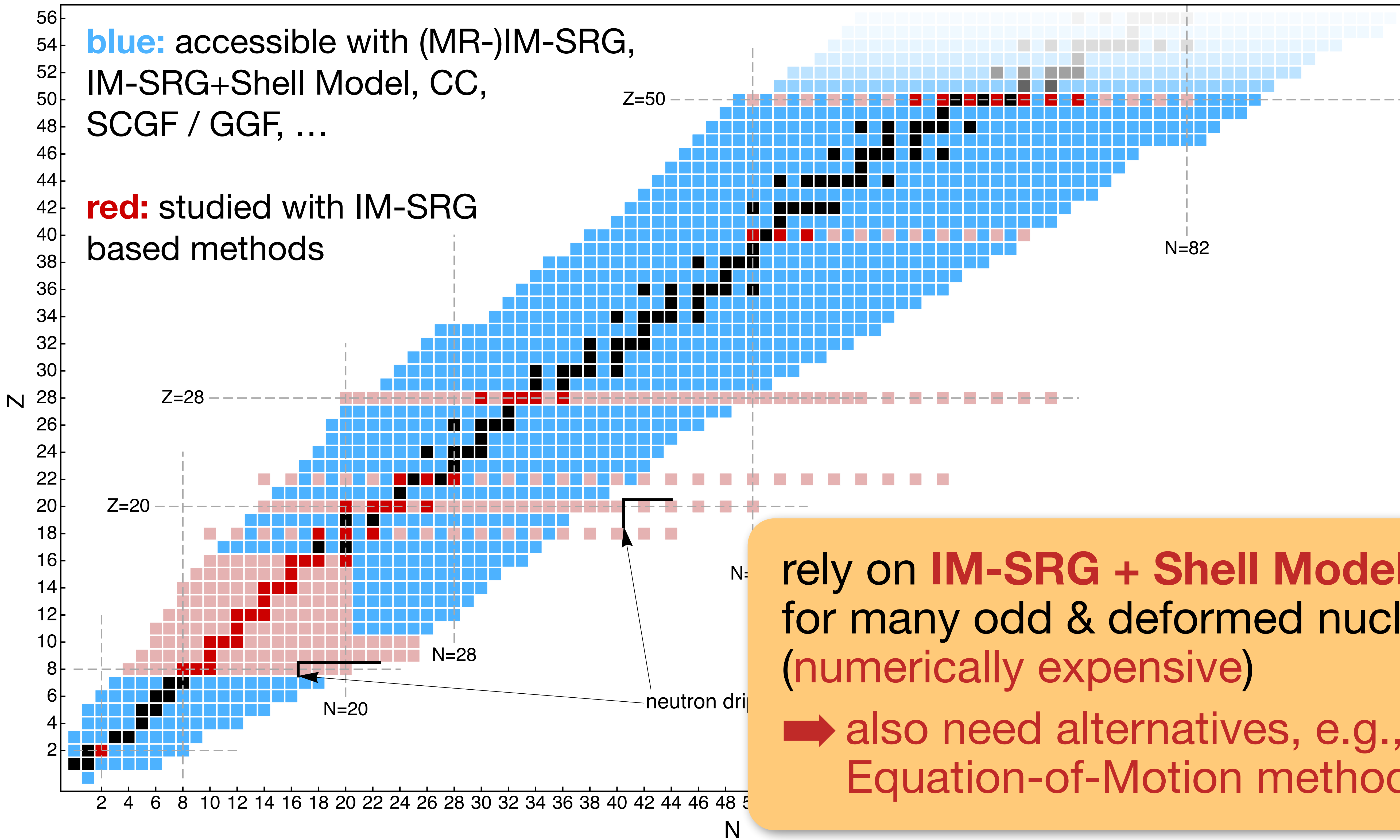


Effective Operators



- small radii: interaction issue (power counting, regulators, LECs, …), also consider currents?
- first applications for scalar operators (radii, electromagnetic monopole, …) in progress
- tensor operators under validation

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

Outlook

- 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^3LO, …)
- (Multi-Reference) Equation-of-Motion methods as an alternative to Shell Model (or CI)
- construction and validation of multi-shell valence interactions
- inclusion of continuum effects

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NERSC

NUCLEI
Nuclear Computational Low-Energy Initiative

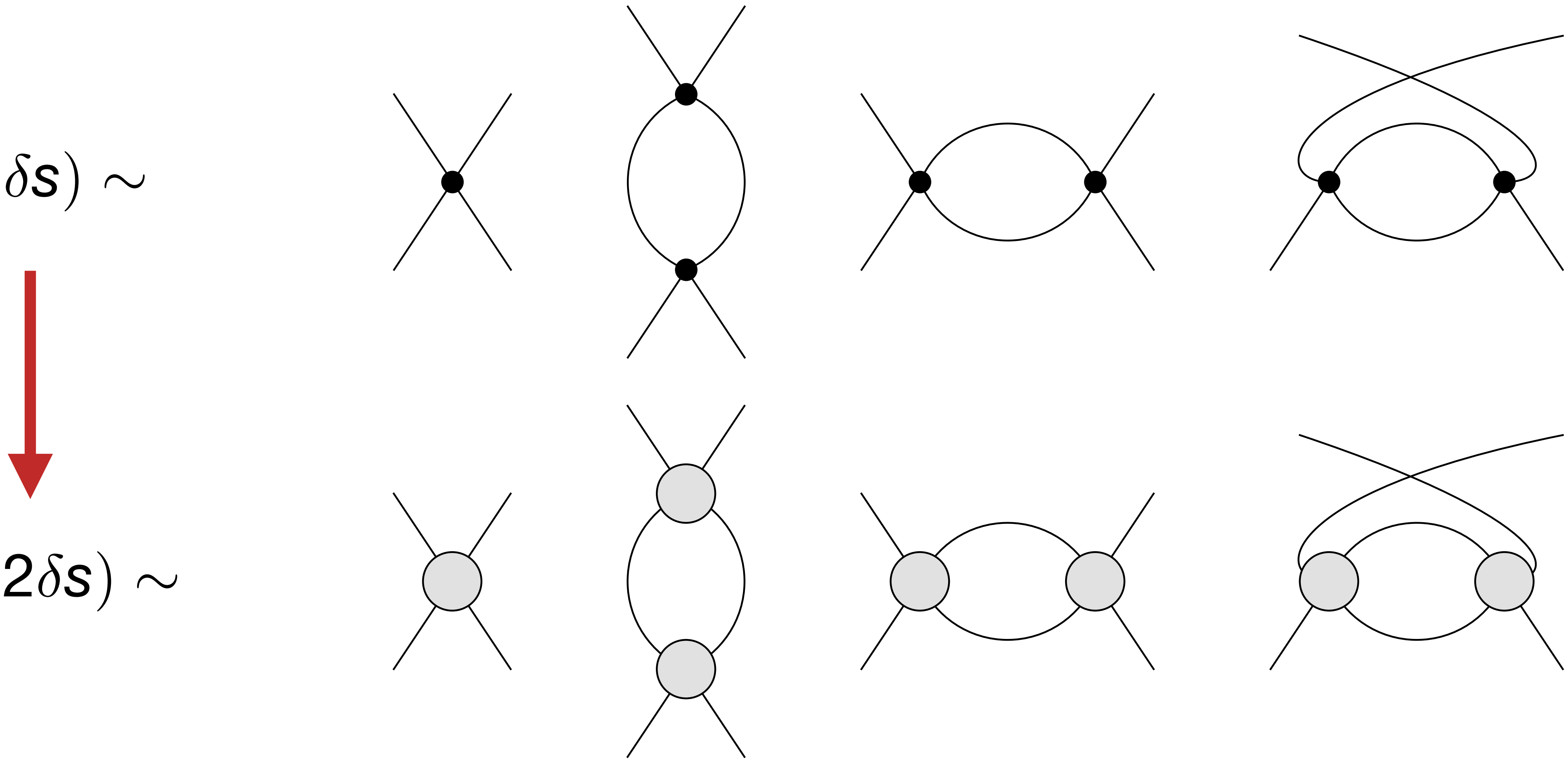
Ohio Supercomputer Center

ICER

Supplements

In-Medium SRG Flow: Diagrams

$\Gamma(\delta s) \sim$

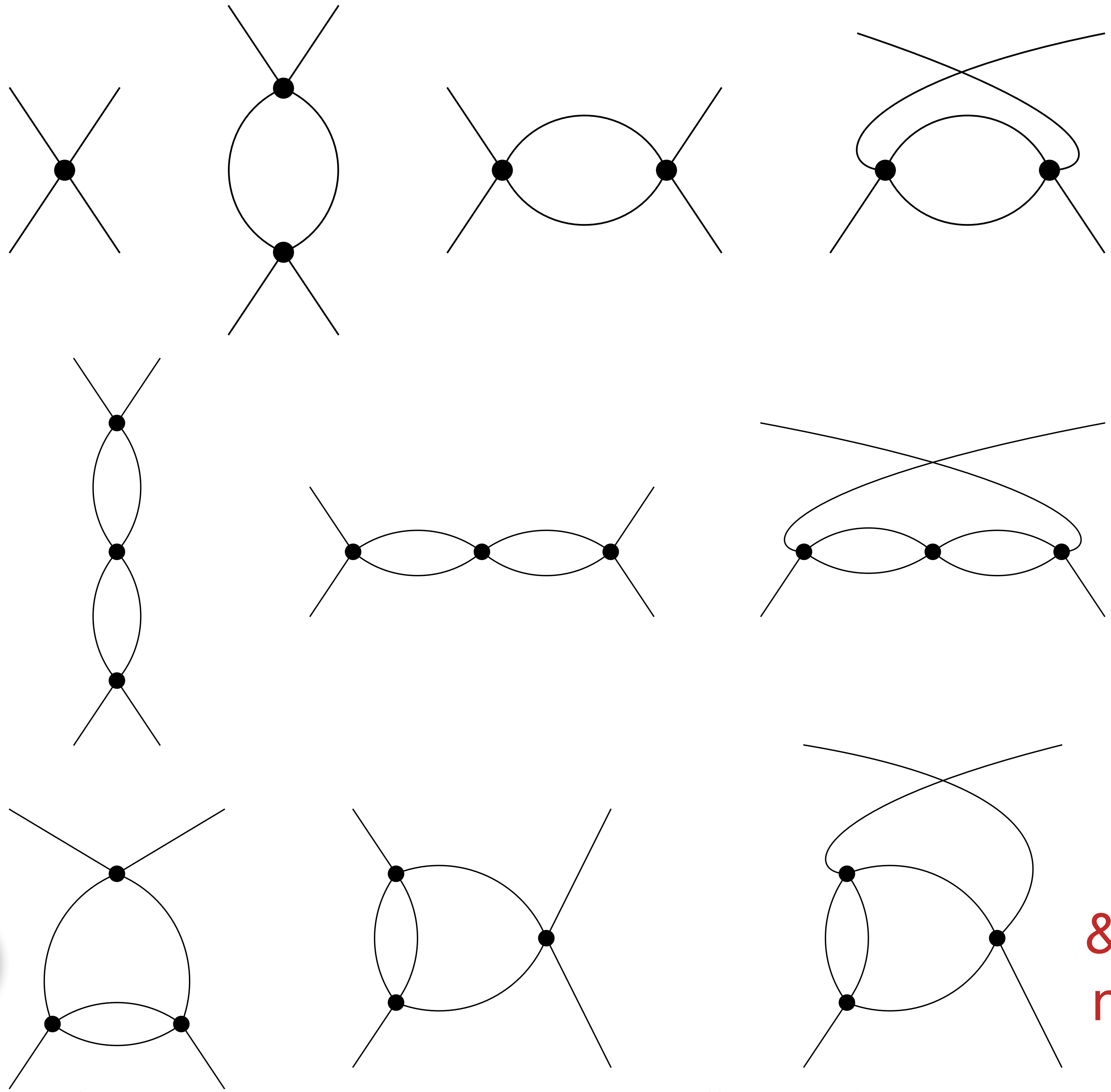


$\Gamma(2\delta s) \sim$

In-Medium SRG Flow: Diagrams

$\Gamma(\delta s) \sim$

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



non-perturbative resummation

& many more...

Particle-Number Projected HFB State

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

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

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

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

- 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

Equations-of-Motion for Excitations

- describe "excited states" based on reference state:

$$\left|\Psi_k\right\rangle \equiv R_k \left|\Psi_0\right\rangle$$

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

$$\left[H(\infty), R_k\right] = \omega_k R_k\,, \quad \omega_k = E_k - E_0$$

- computational effort scales **polynomially**, vs. factorial scaling of Shell Model

- can exploit Multi-Reference capabilities (commutator formulation identical to flow equations)

➡ **complementary** to Shell Model

EOM Applications

- particle-hole excitations (TDA, RPA, Second RPA, ...)

$$R_k = \sum_{ph} R^{(k)}_{ph} :a^\dagger_p a_h: + \sum_{pp'hh'} R^{(k)}_{pp'hh'} :a^\dagger_p a^\dagger_{p'} a_{h'} a_h: + \ldots$$

➡ **giant resonances**

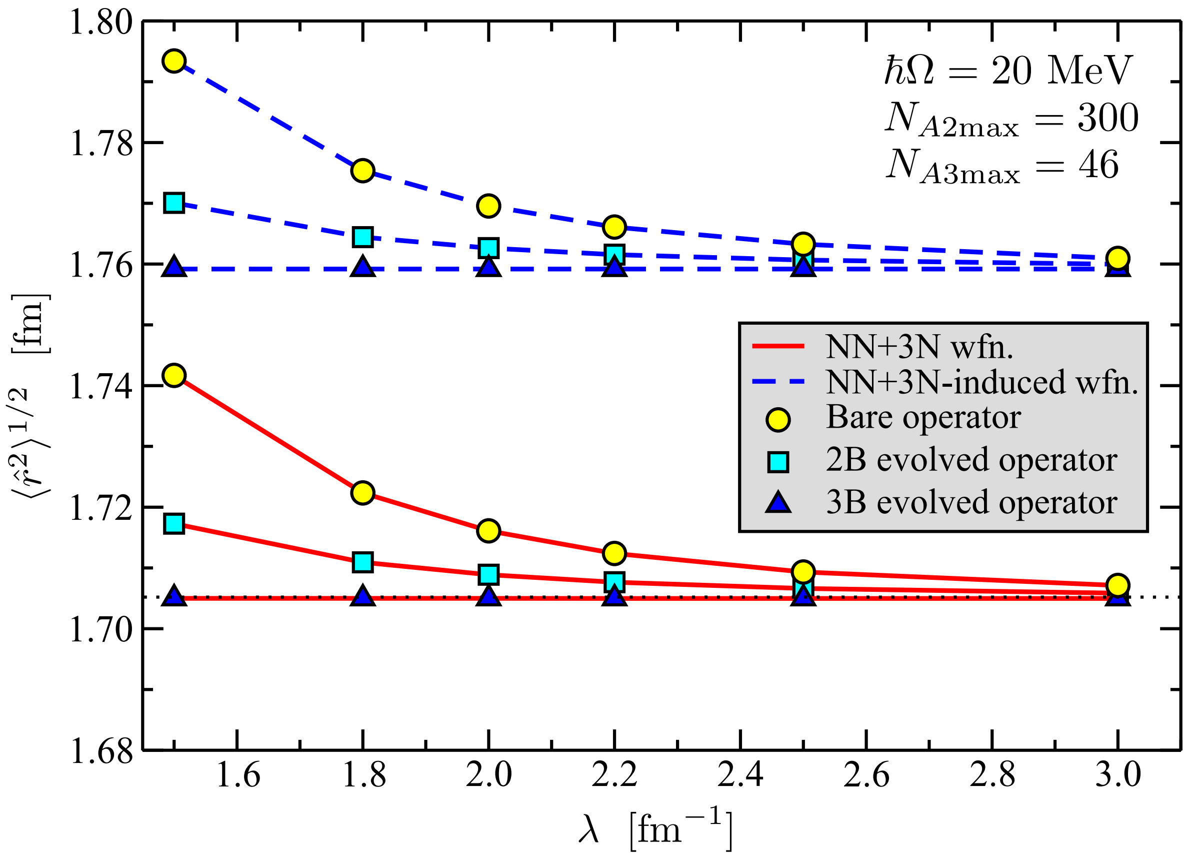
- particle attachment (analogous for removal):

$$R_k = \sum_{ph} R^{(k)}_{p} :a^\dagger_p: + \sum_{pp'h} R^{(k)}_{pp'h} :a^\dagger_p a^\dagger_{p'} a_h: + \ldots$$

➡ **ground and excited states in odd nuclei**

Effective Operators

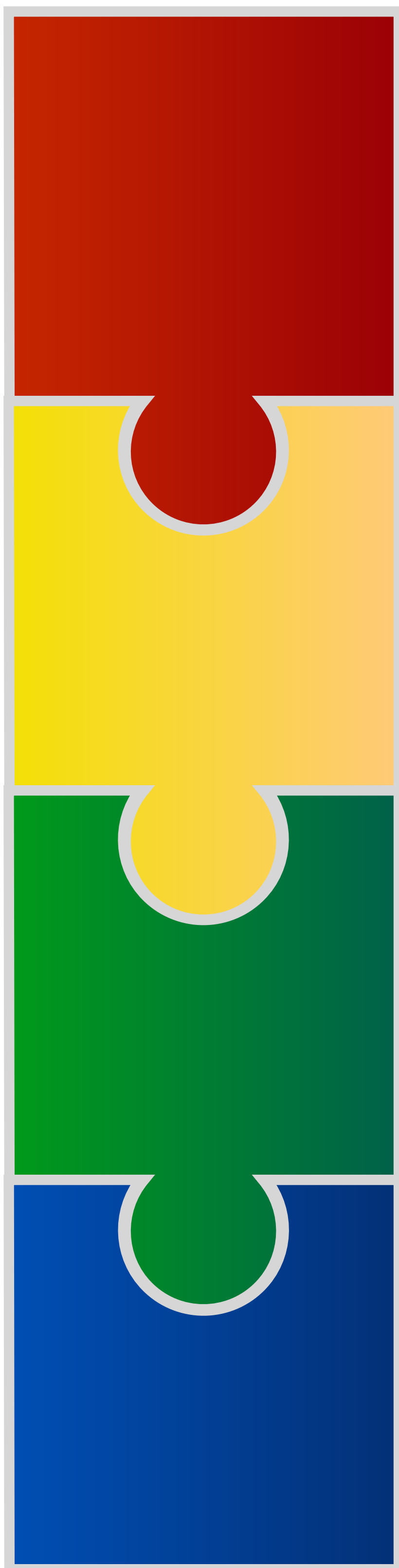
^{3}H rms matter radius



from: Schuster et al., PRC90, 011301 (2014)

- derive operators from chiral EFT, including currents
- optimize LECs together with interaction
- evolve to desired resolution scale
- evaluate operator (1B+2B +...) in IM-SRG (and Shell Model)
- (most) existing ab initio & Shell model codes lack capabilities for many-body observables

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)