In-Medium SRG for Medium-Mass and Heavy Nuclei

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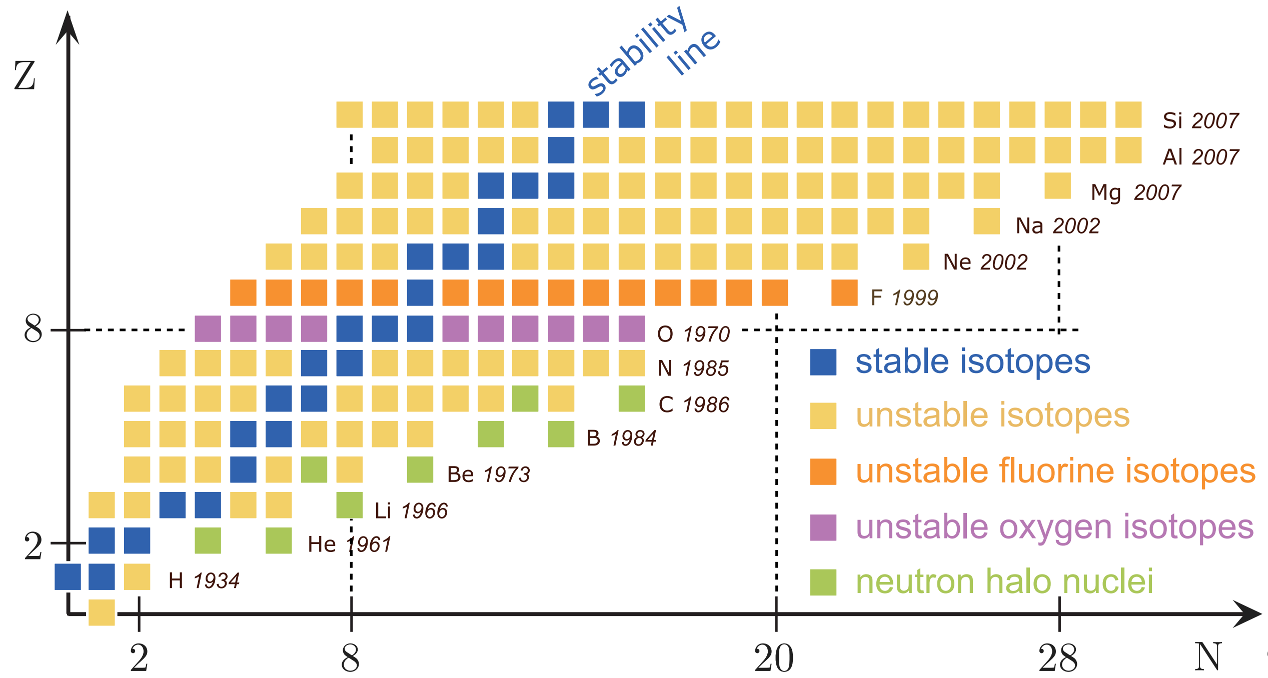
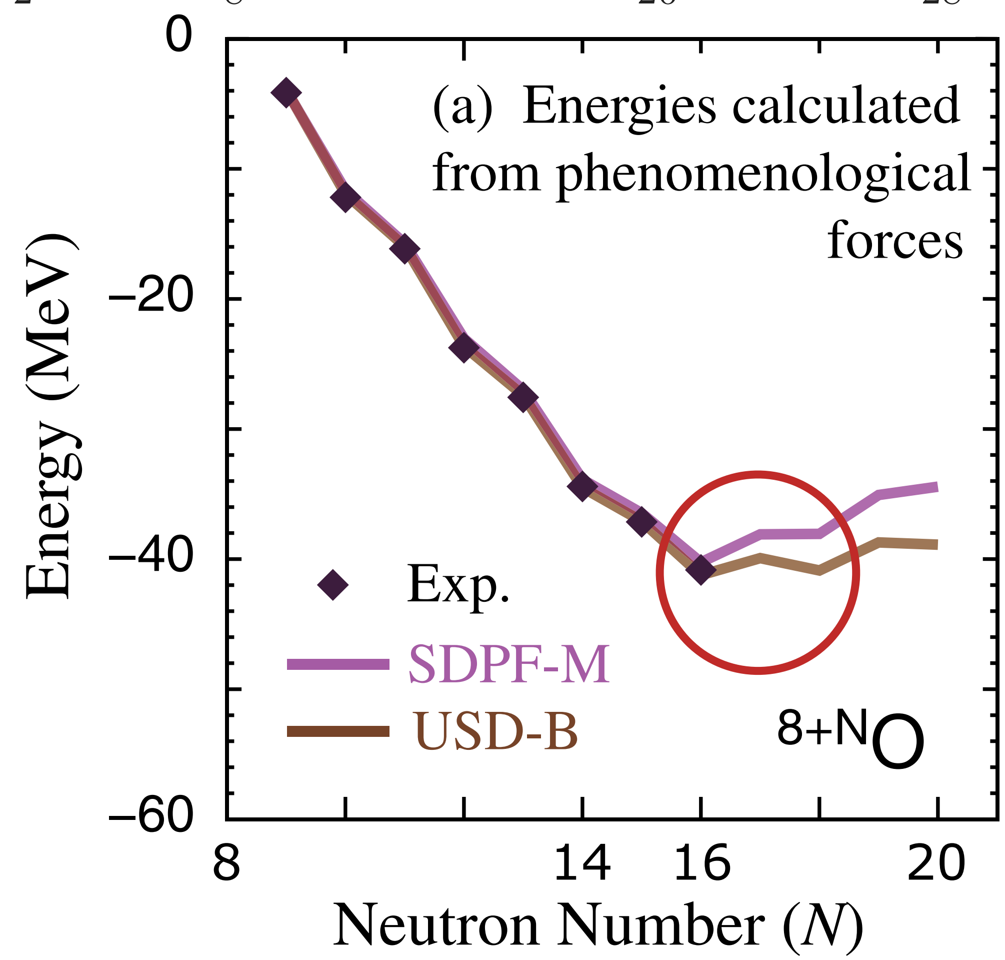
Why Ab Initio Nuclear Structure?

- Nuclear Many-Body Shell Model: oxygen drip line depends on interaction
- empirical interactions not interchangeable between many-body methods

- systematic improvements ?
- theoretical uncertainties ?
- systematic link to QCD ?





[T. Otsuka et al., Phys. Rev. Lett. 105, 032501 (2010)]

Outline

- Ingredients
  - Nuclear Interactions from Chiral EFT
  - (Free-Space) Similarity Renormalization Group
- In-Medium SRG and Applications
  - Ground-State Results
  - IM-SRG + Shell Model for Excited States
- Next Steps
- Conclusions

Ingredients:

Nuclear Interactions from Chiral Effective Field Theory

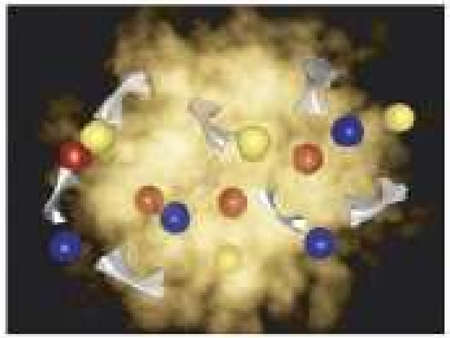
E. Epelbaum, H.-W. Hammer, and U.-G. Meissner, Rev. Mod. Phys. **81** (2009), 1773

Scales of the Strong Interaction

momentum transfer (resolution)

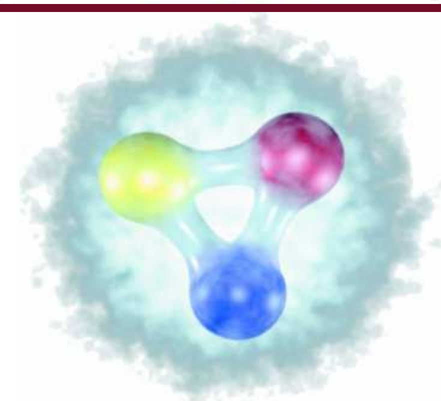
QCD

Chiral EFT

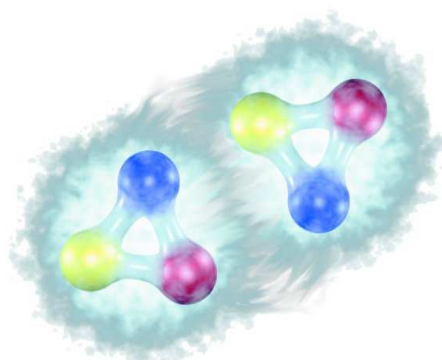


- quarks, gluons

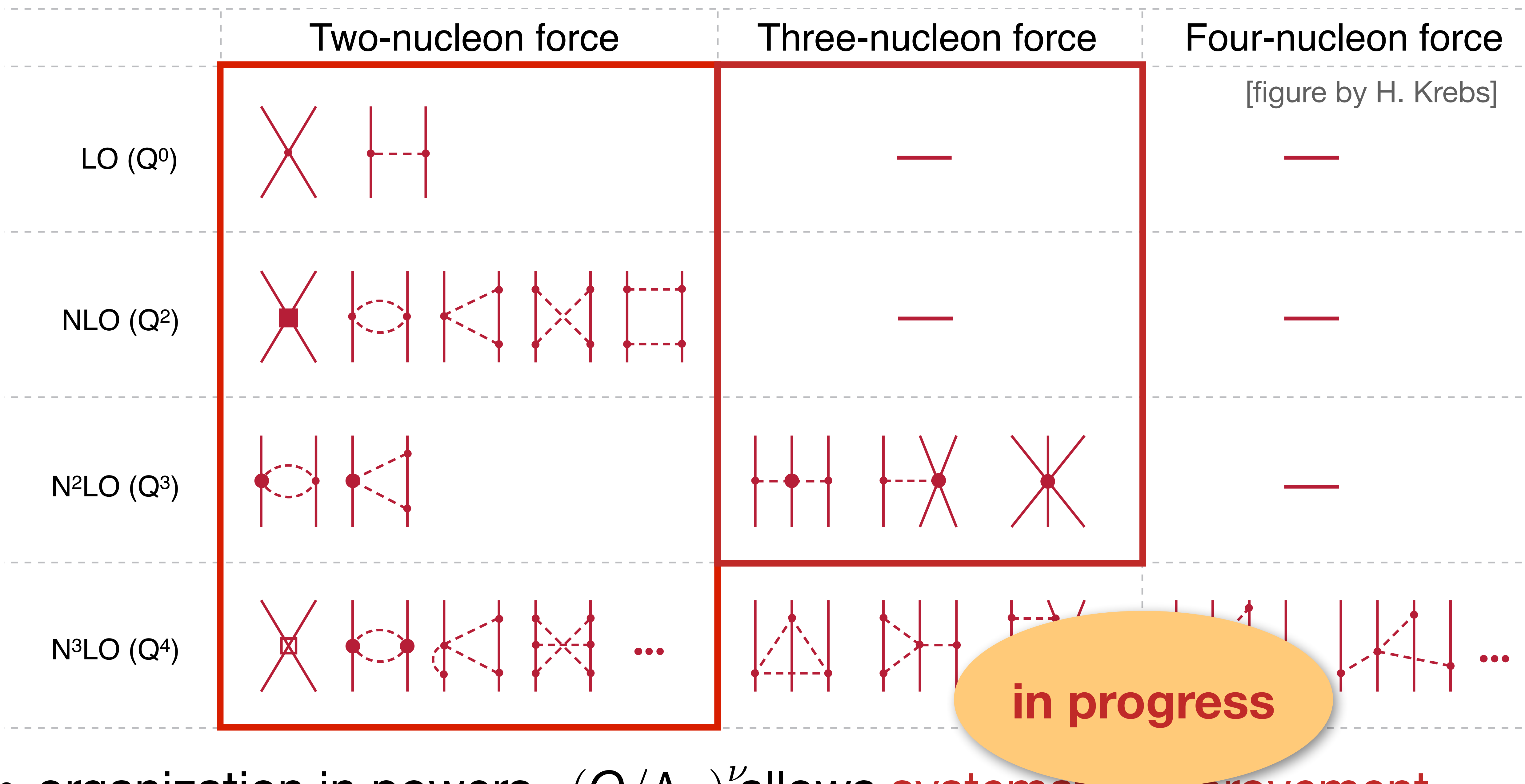
chiral symmetry



- pions, nucleons, ...
  - nuclear interactions
  - few-nucleon systems



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.)

Ingredients:

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

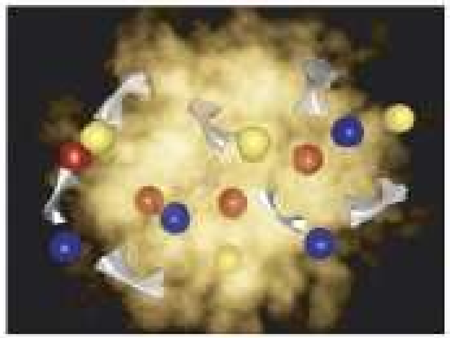
H. H. and R. Roth, Phys. Rev. **C75** (2007), 051001

Scales of the Strong Interaction

momentum transfer (resolution)

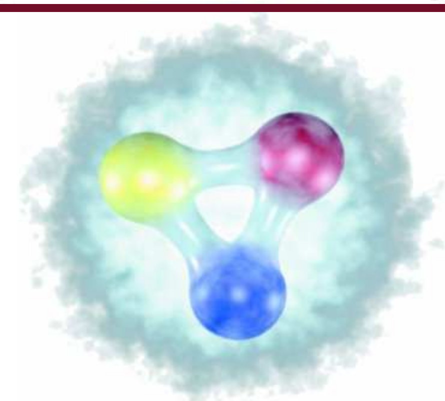
QCD

Chiral EFT

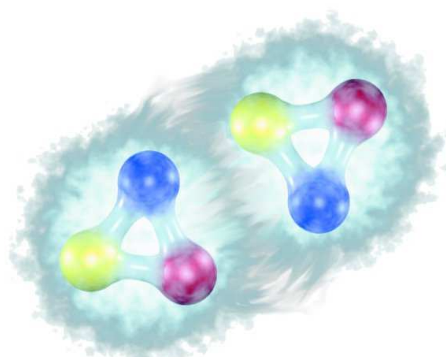


- quarks, gluons

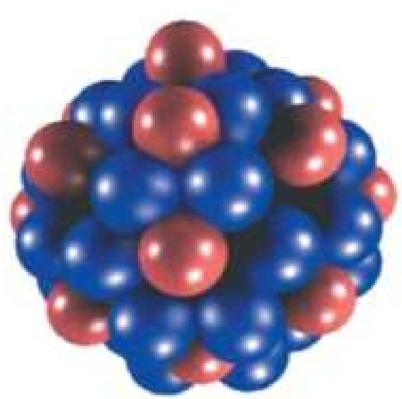
chiral symmetry



- pions, nucleons, ...
  - nuclear interactions
  - few-nucleon systems



(Which) Details necessary?



- finite nuclei
  - nuclear structure & reactions

Similarity Renormalization Group

Basic Concept

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

- evolved Hamiltonian

$$H(s) = U(s)HU^{\dagger}(s) \equiv T + V(s)$$

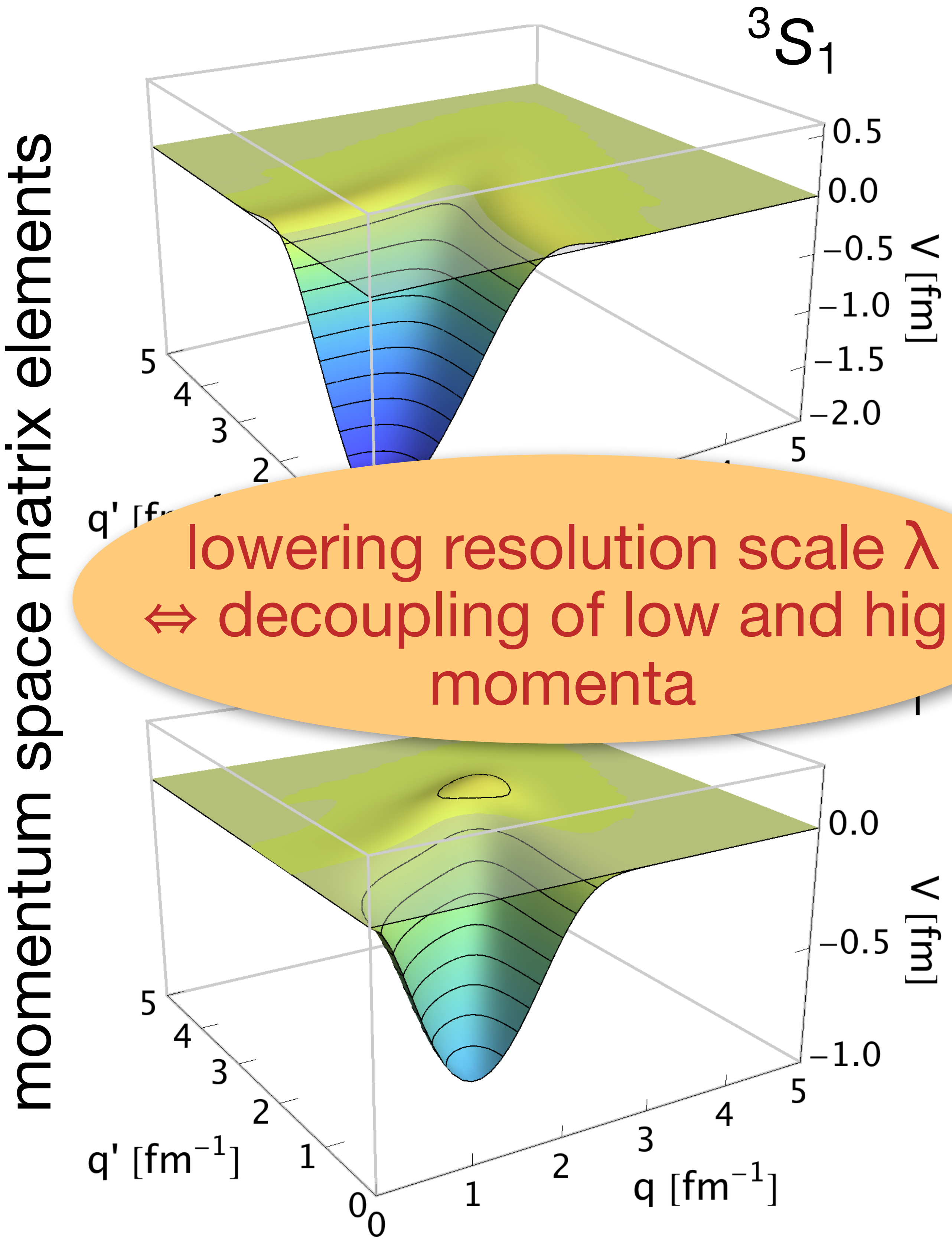
- flow equation:

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

- choose $\eta(s)$ to achieve desired behavior, e.g. decoupling of momentum or energy scales

- consistently evolve observables of interest

SRG in Two-Body Space



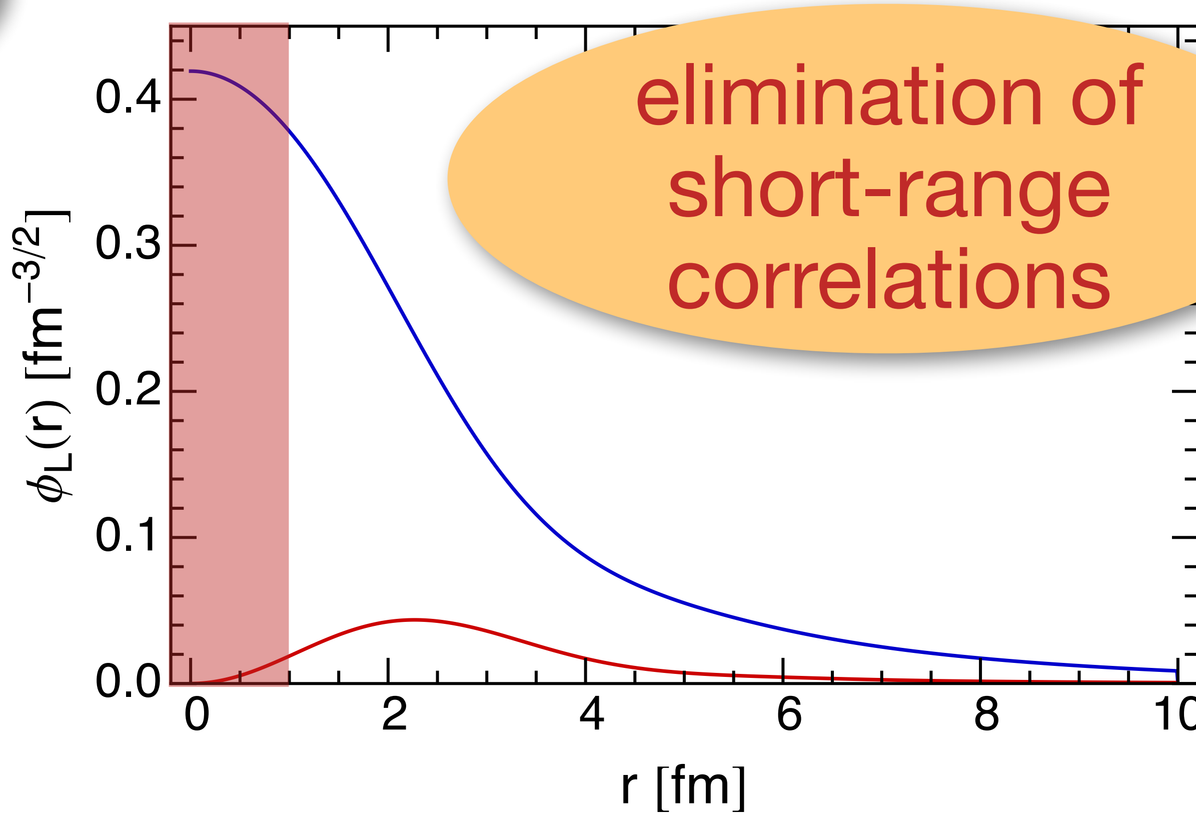
lowering resolution scale λ
⇔ decoupling of low and high momenta

λ = 1.8 fm^{-1}

$$\eta(\lambda) = 2\mu\left[T_{\text{rel}}, H(\lambda)\right]$$

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

deuteron wave function

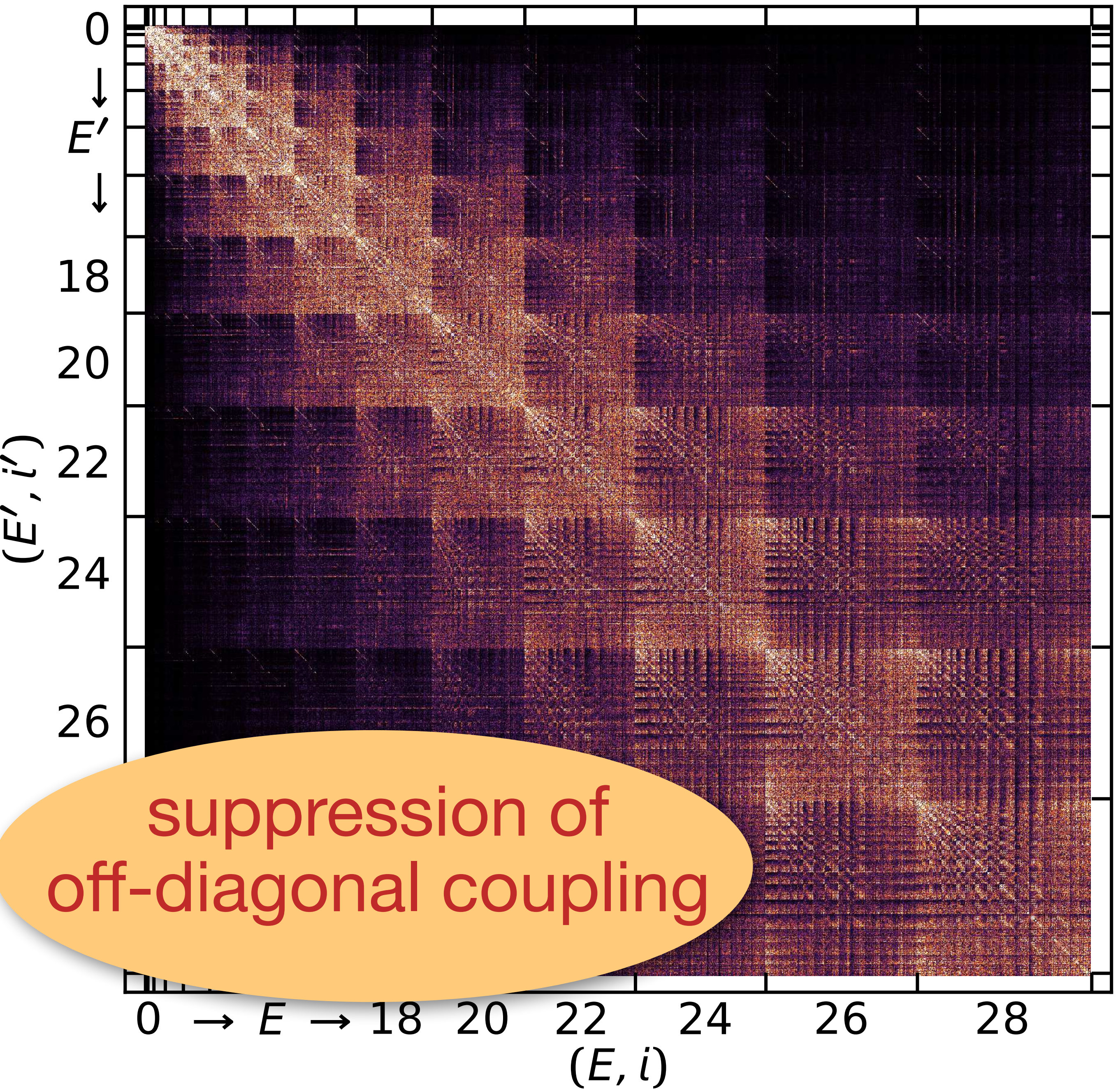


elimination of short-range correlations

SRG in Three-Body Space

3B Jacobi-HO Matrix Elements

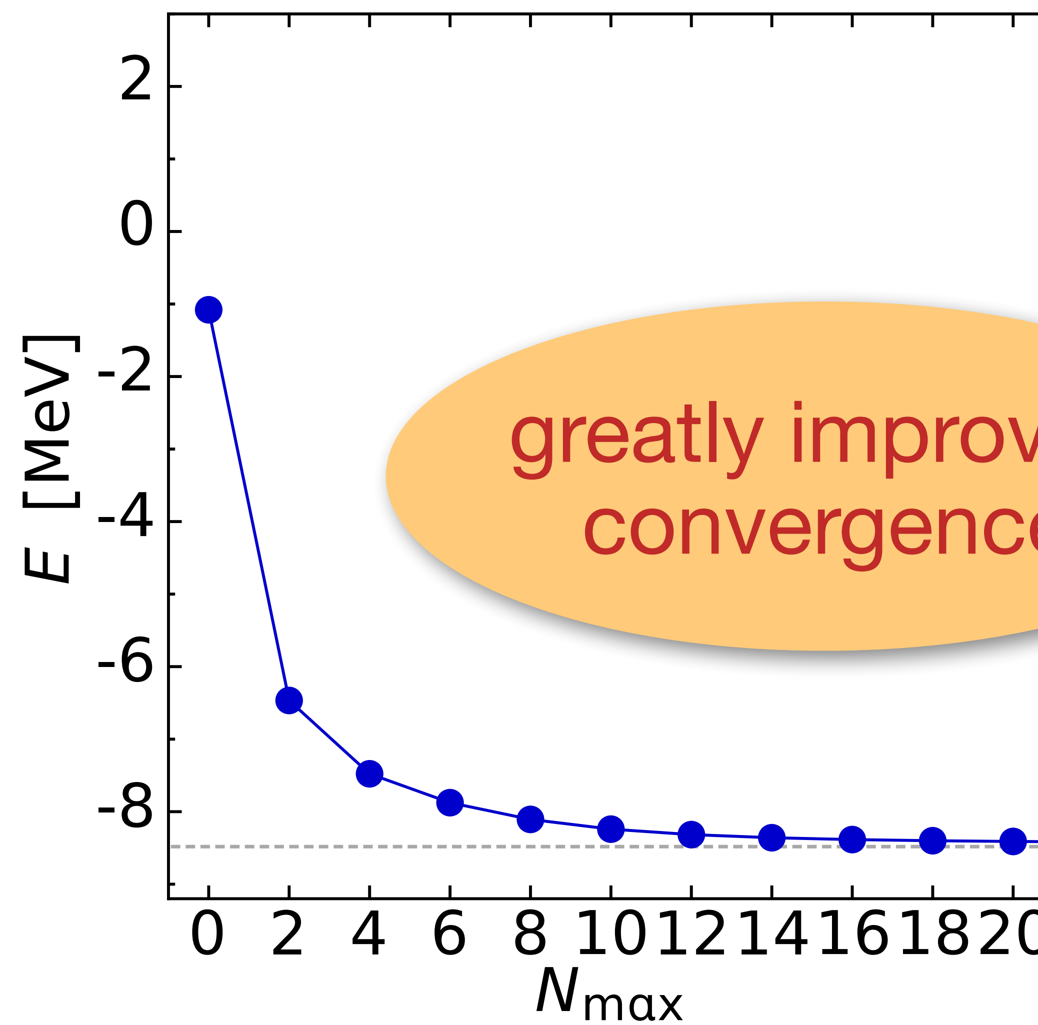
$J^\pi = \frac{1}{2}^+, T = \frac{1}{2}, \hbar\Omega = 28$ MeV



suppression of
off-diagonal coupling

λ = 1.33 fm^{-1}

^{3}H ground-state (NCSM)



greatly improved
convergence

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

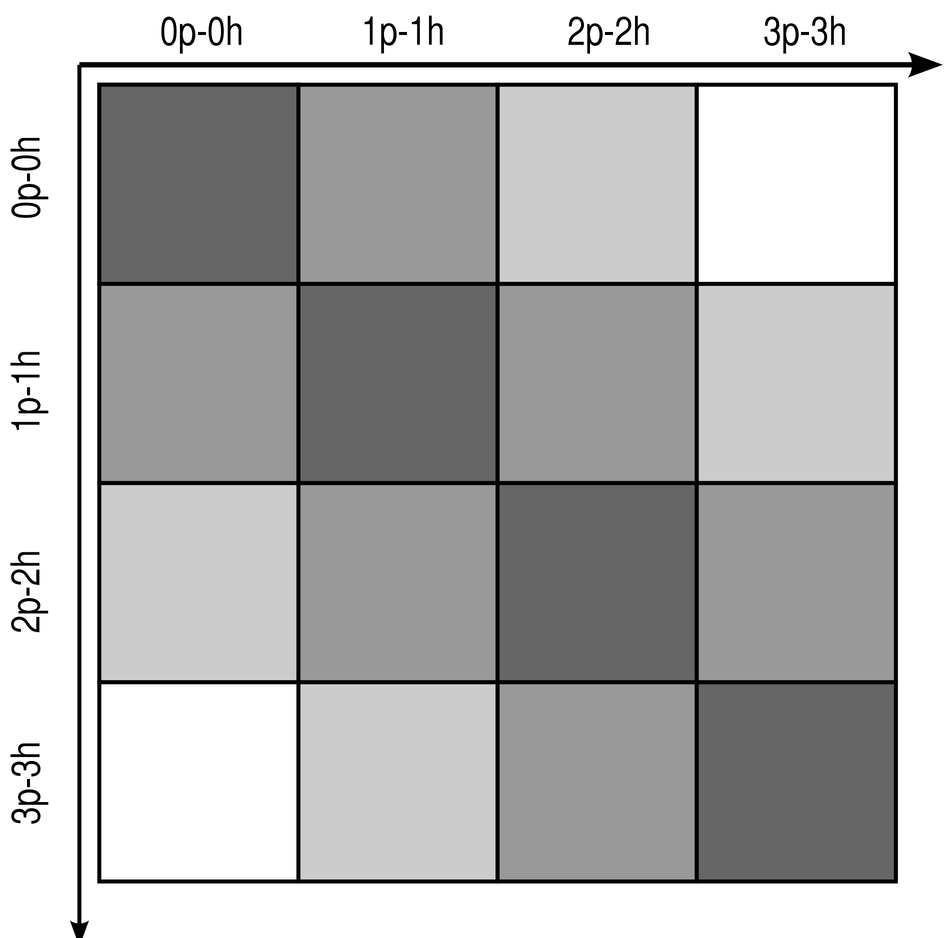
In-Medium SRG

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

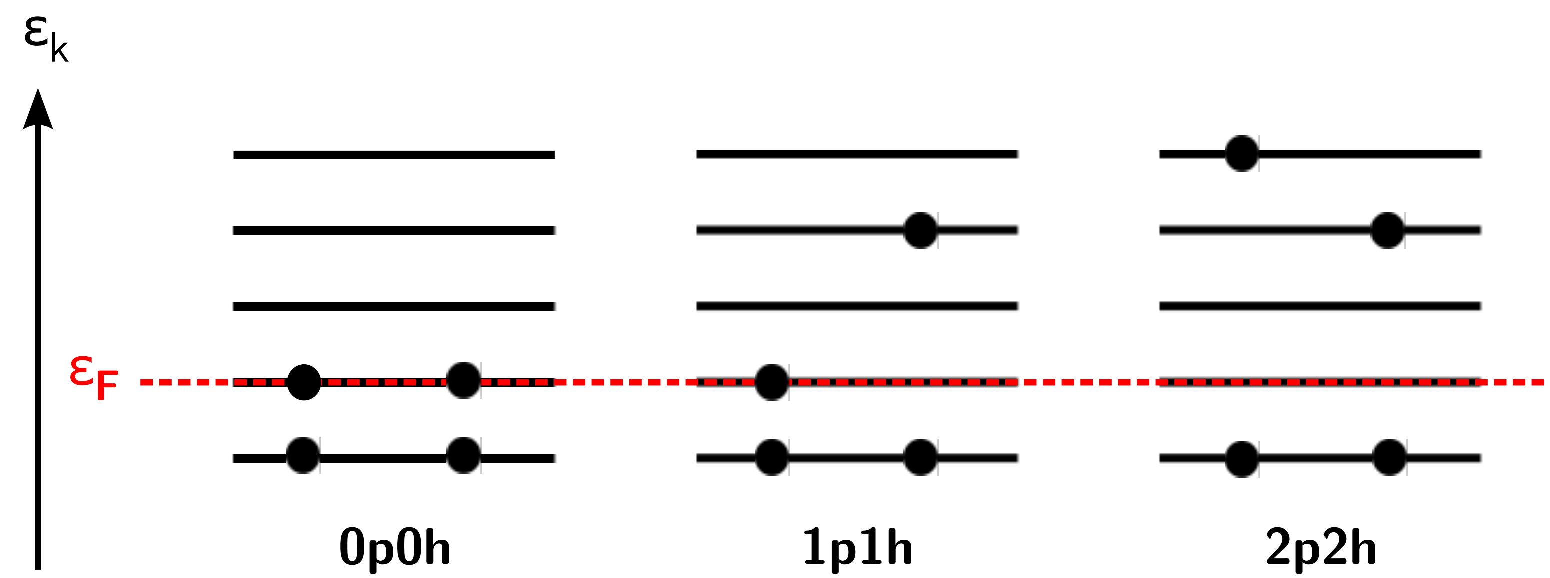
H. H., S. K. Bogner, S. Binder, A. Calci, J. Langhammer, R. Roth, and A. Schwenk, Phys. Rev. C **87**, 034307 (2013)

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

Decoupling in A-Body Space

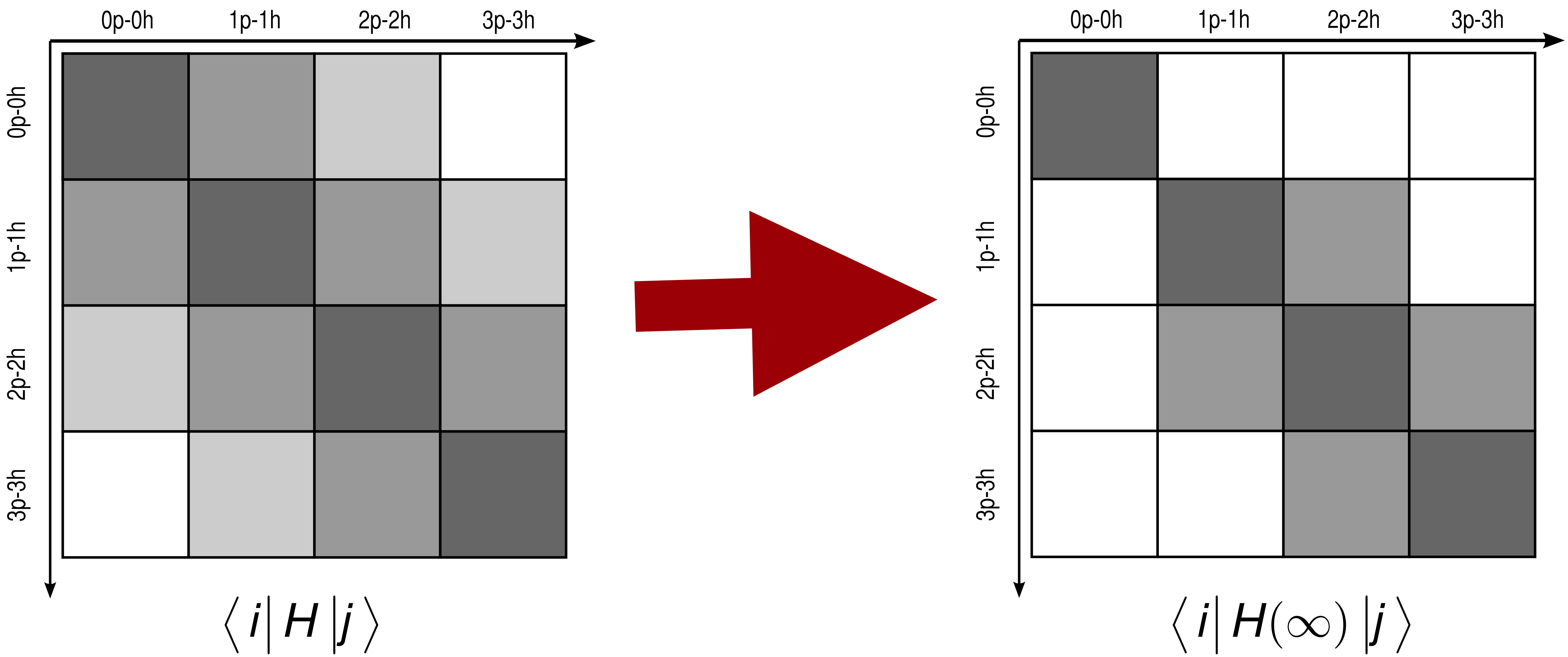


$\langle i | H | j \rangle$



excitations relative to reference state:
→ normal-ordering

Decoupling in A-Body Space



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

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

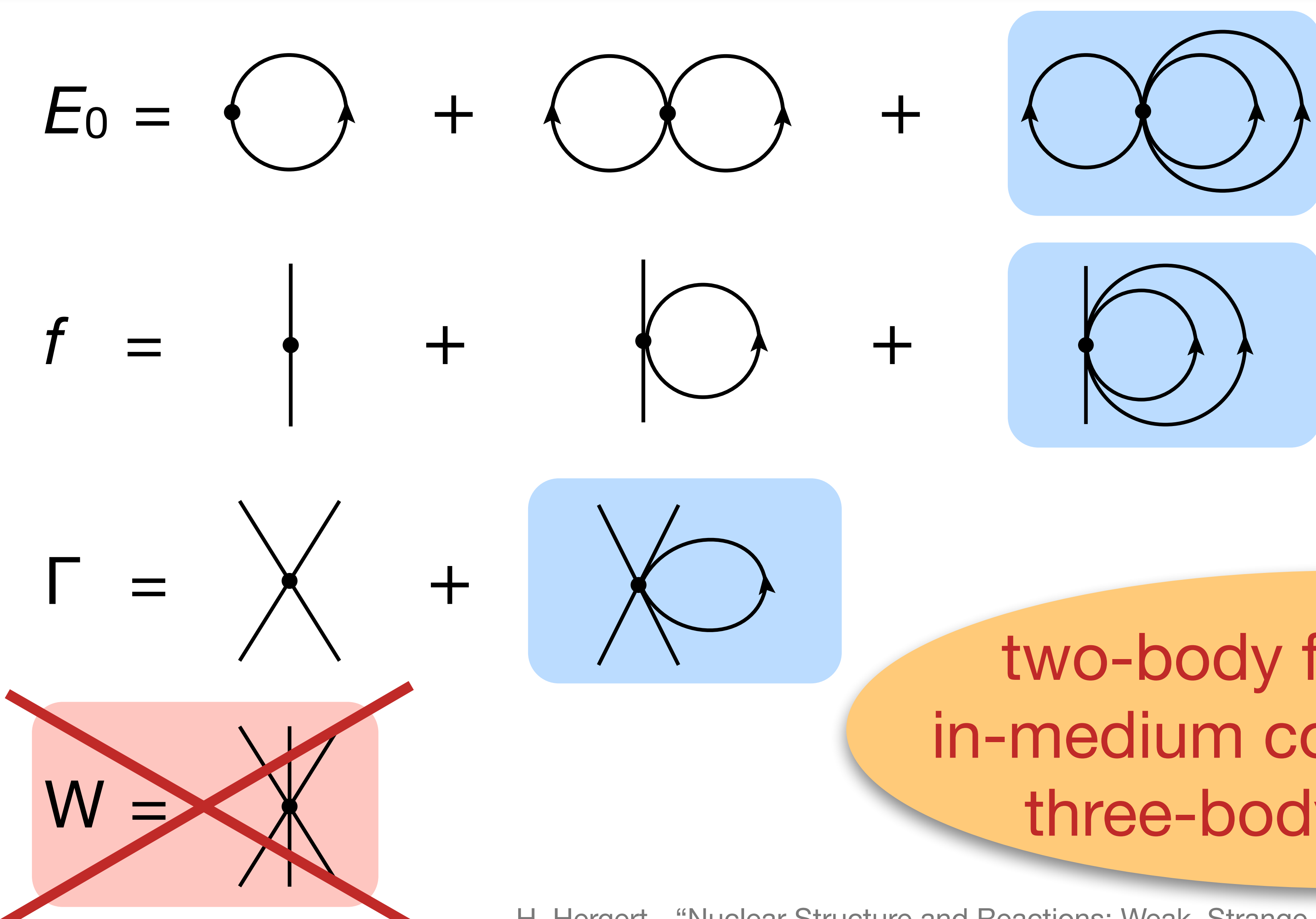
$$\left\langle \Phi \right| :A^{k_1\dots k_N}_{l_1\dots l_N}: \left| \Phi \right\rangle = 0$$

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

Normal-Ordered Hamiltonian

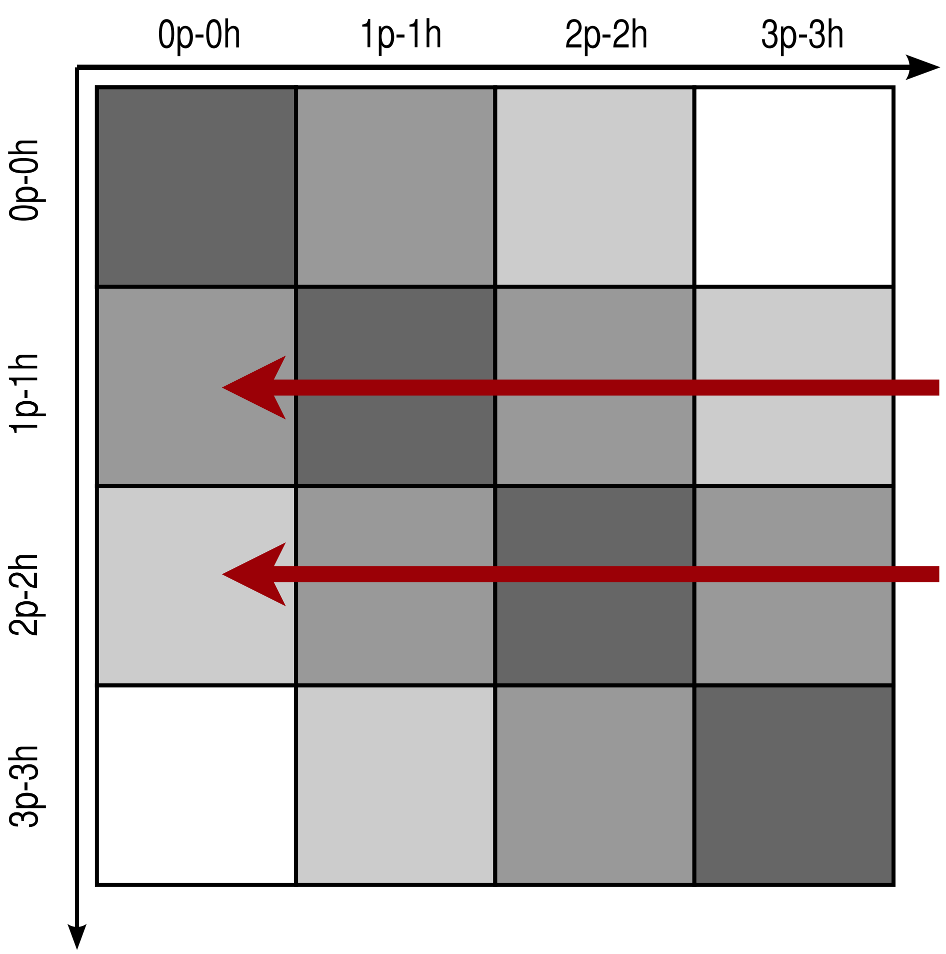
Normal-Ordered Hamiltonian

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



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

Choice of Generator



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

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

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

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

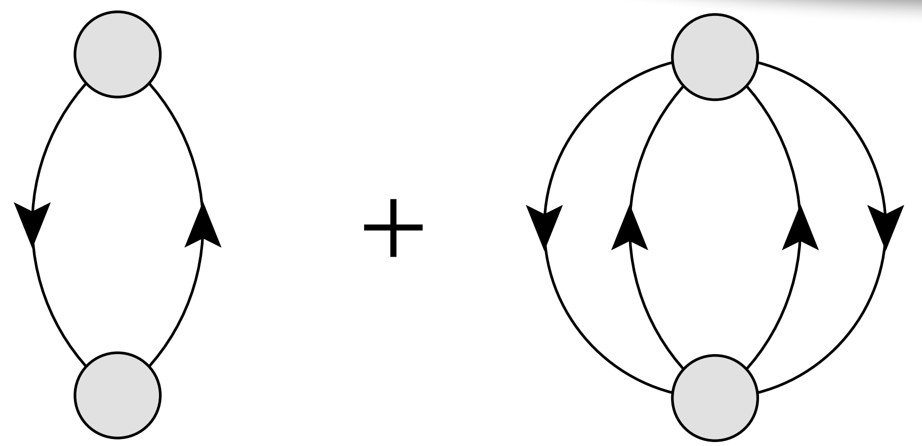
- construct generator, e.g., $\eta^{I} = \left[H^{d}, H^{od}\right]$ (Wegner-type)

IM-SRG(2) Flow Equations

0-body Flow

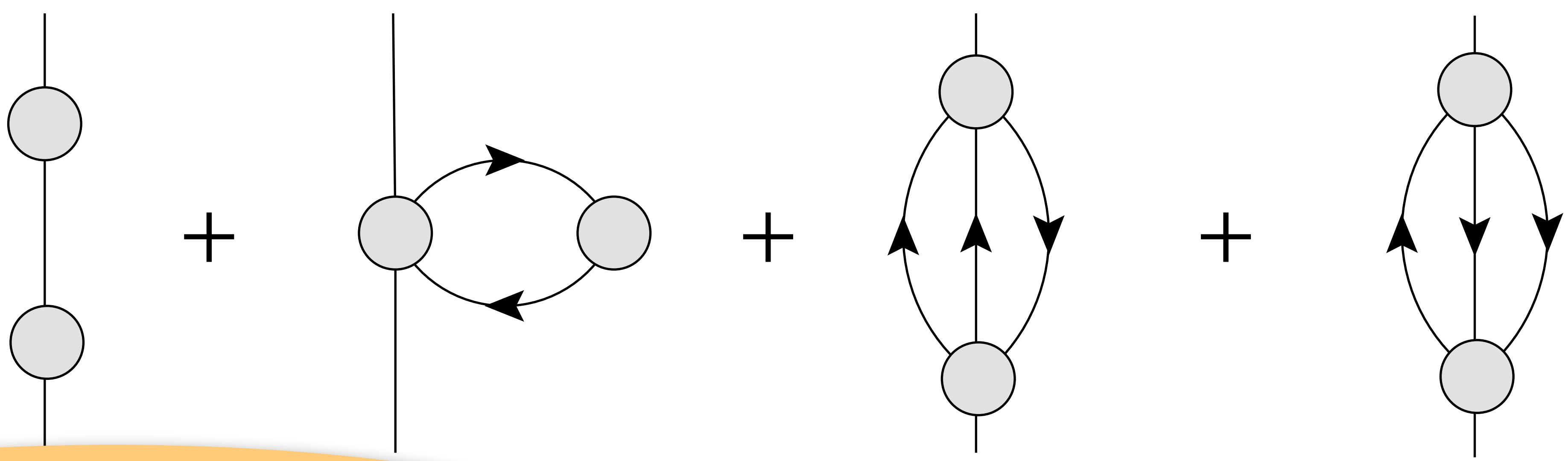
~ 2nd order MBPT for *H(s)*

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



1-body Flow

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



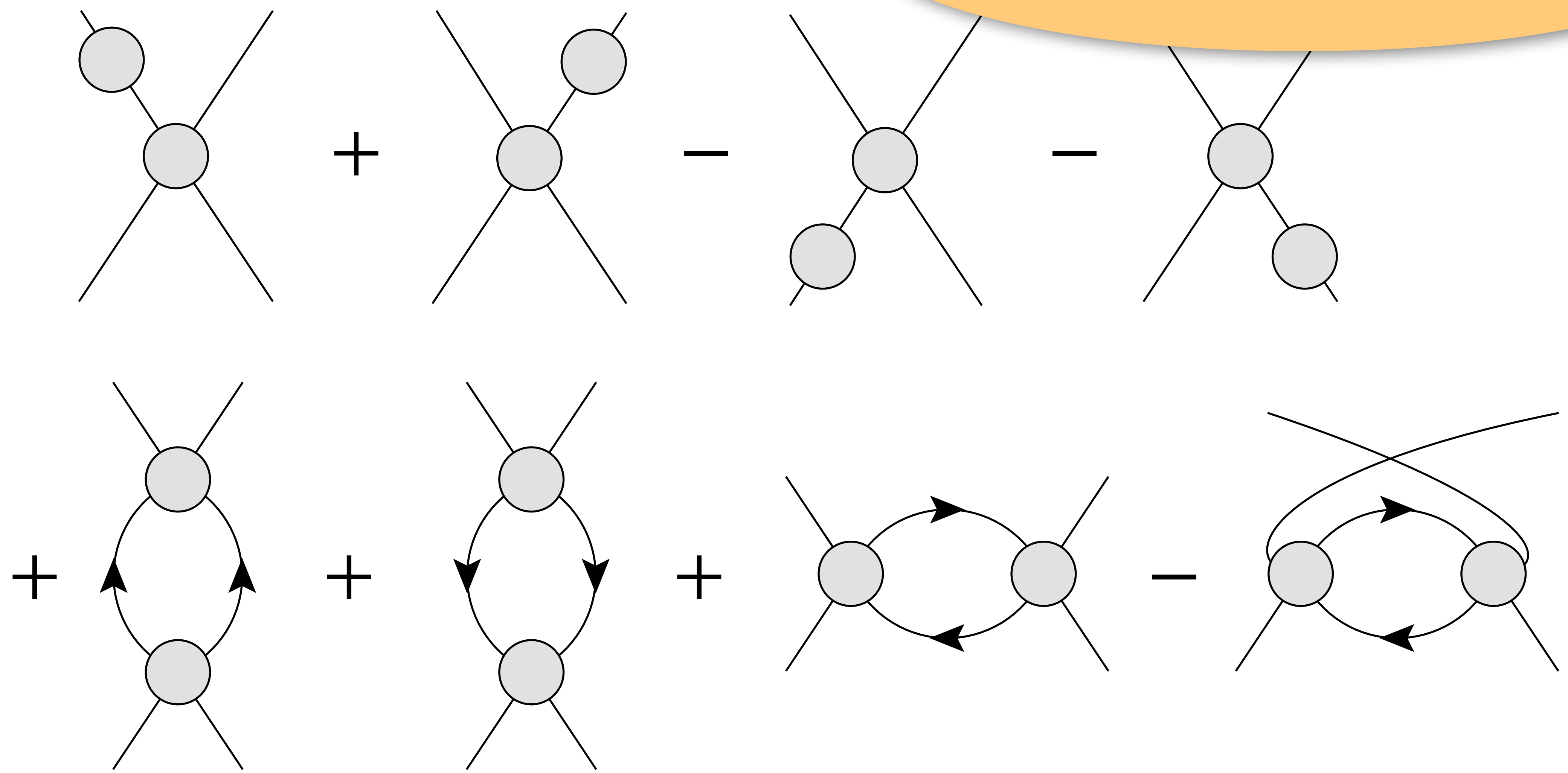
IM-SRG(2): truncate ops. at two-body level

IM-SRG(2) Flow Equations

2-body Flow

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

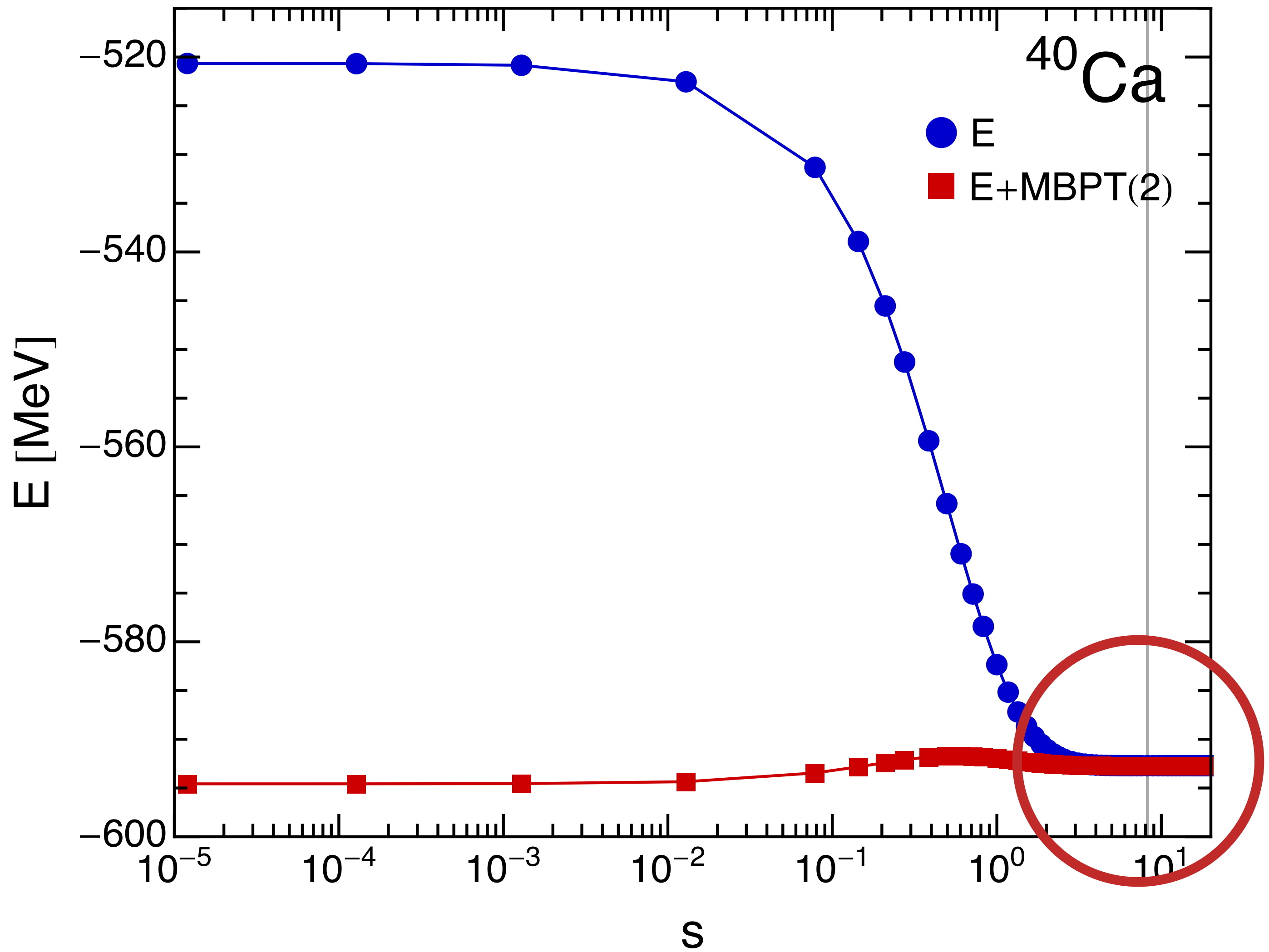
$$\frac{d\Gamma}{ds} =$$

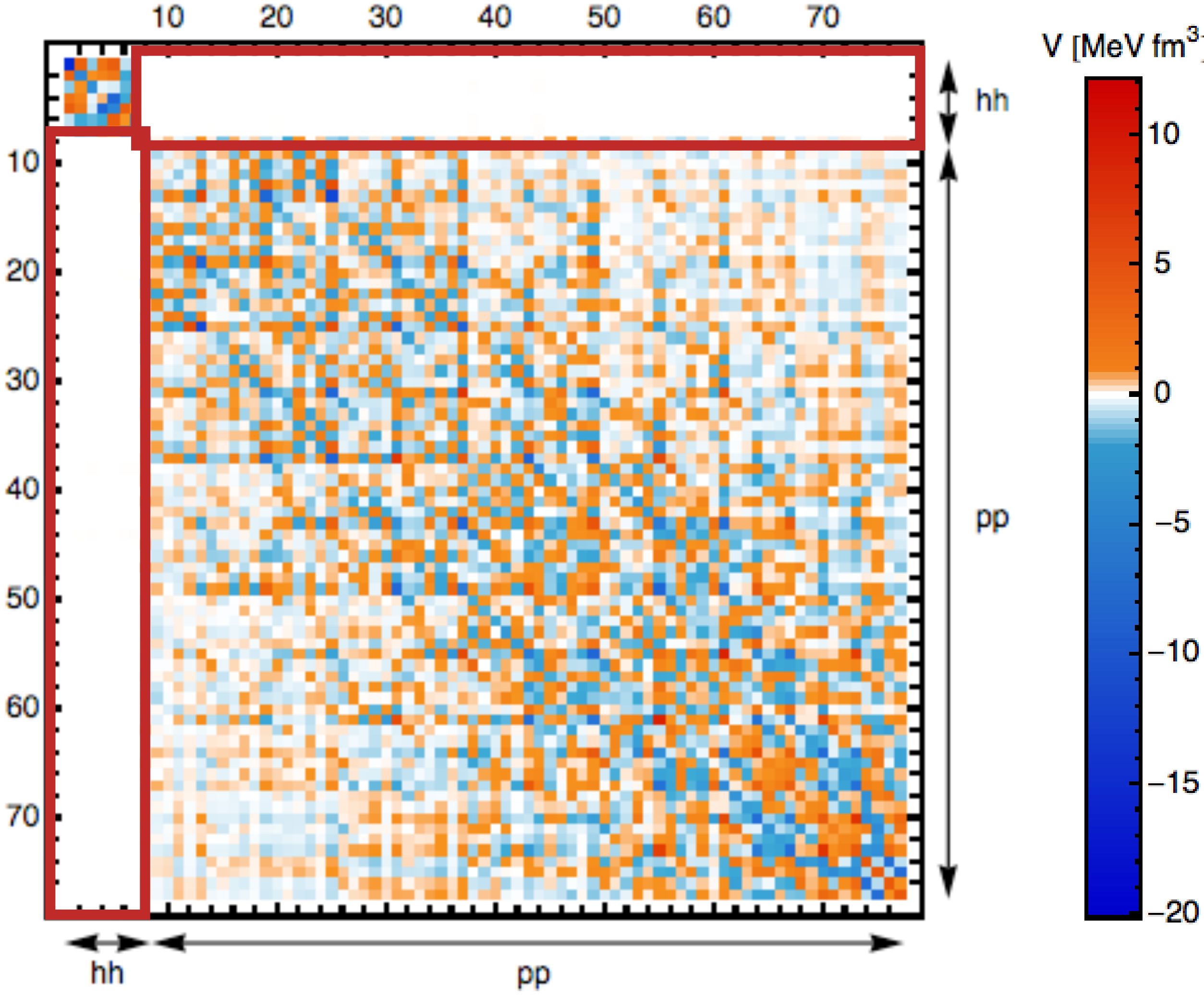


s channel — ladders

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

Applications:

Ground-State Results

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

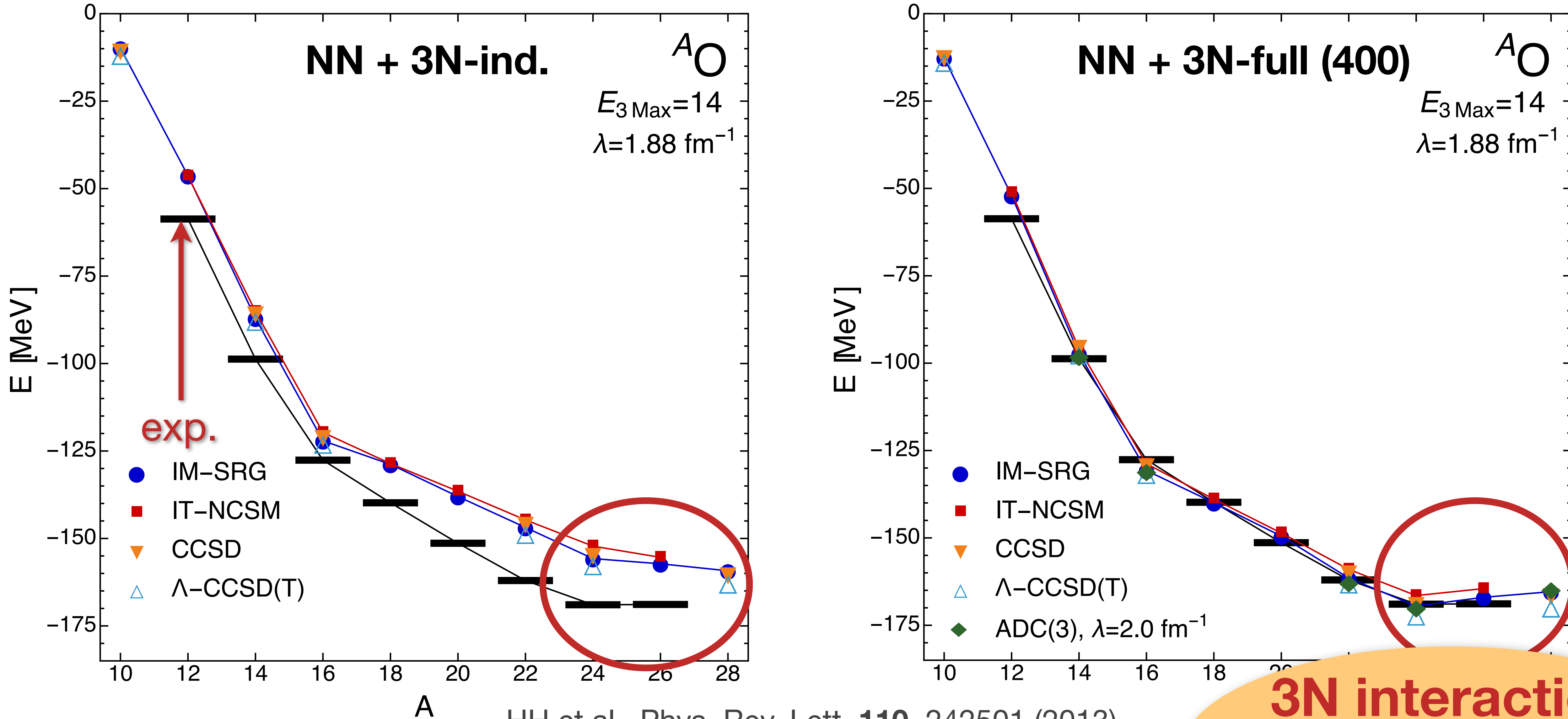
Initial Hamiltonian

- NN: chiral interaction at N^3LO (Entem & Machleidt)
- 3N: chiral interaction at N^2LO (c_D,c_E fit to ^3H energy & beta 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



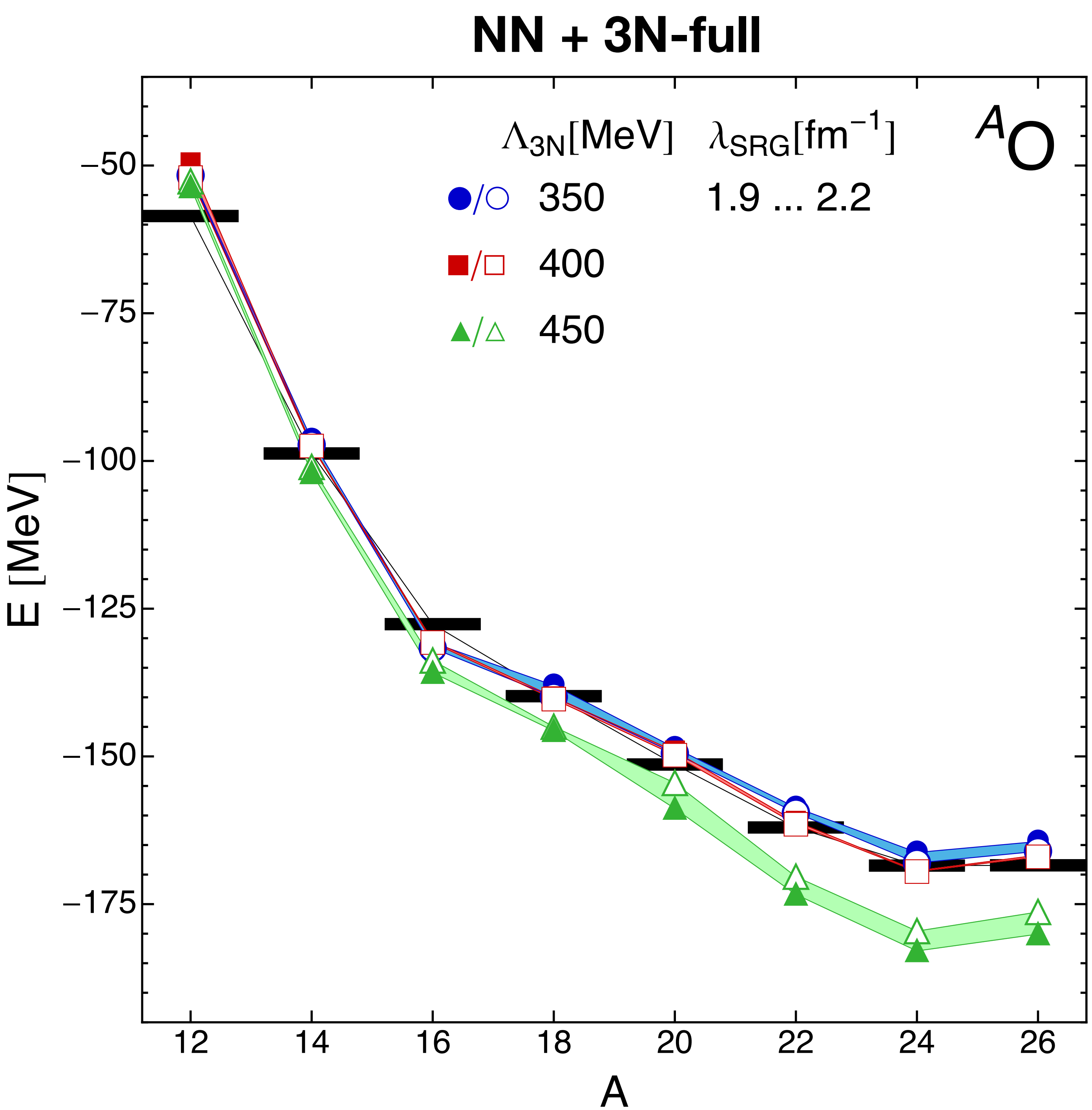
HH et al., Phys. Rev. Lett. **110**, 242501 (2013)

A. Cipollone et al., Phys. Rev. Lett. **111**, 242501 (2013) (C. Barbi

3N interaction completely fixed by A≤4 data

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

Variation of Scales

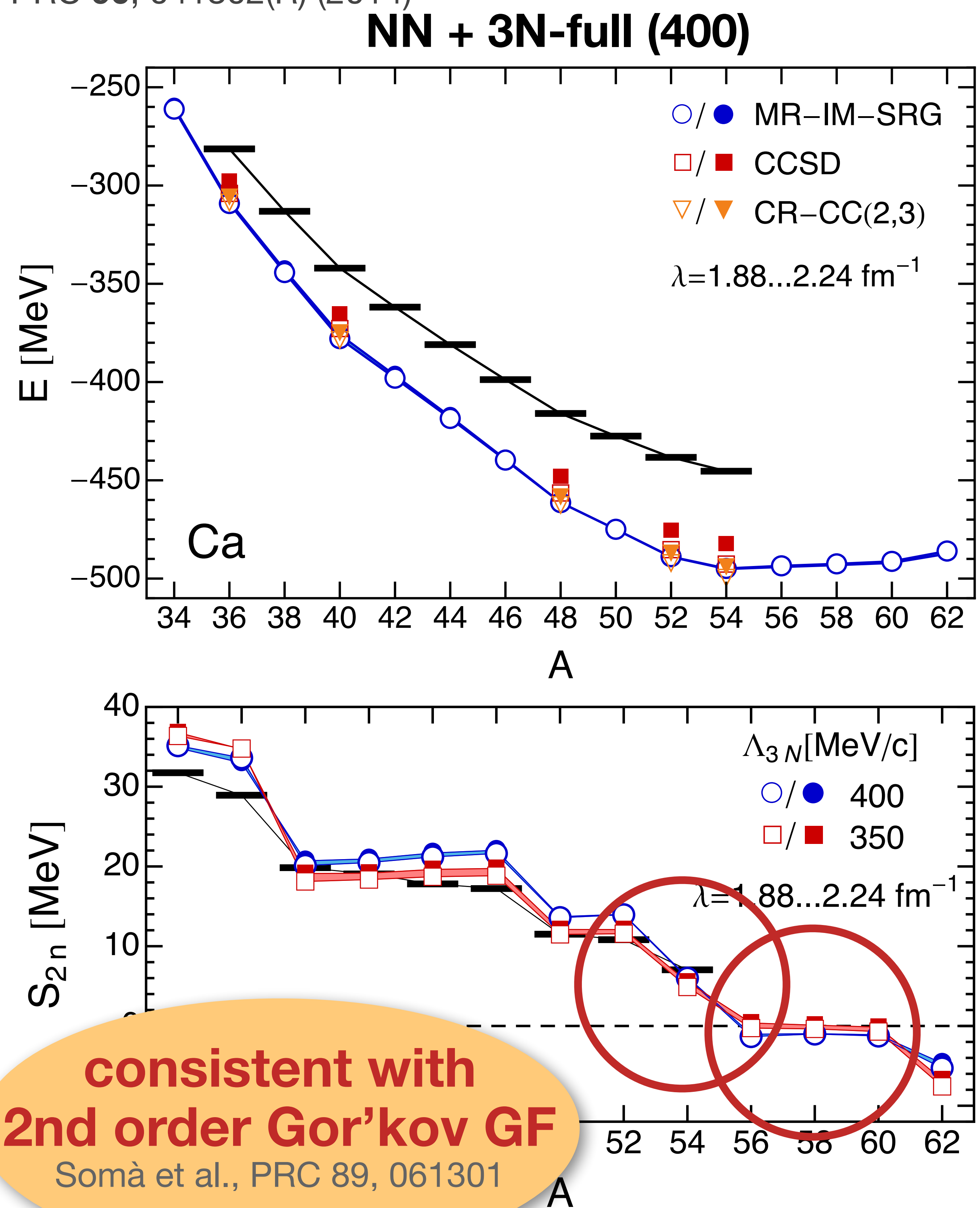


Phys. Rev. Lett. **110**, 242501 (2013)

- variation of initial 3N cutoff only
- diagnostics for chiral interactions
- dripline at A=24 is robust under variations
- (leading) continuum effects too small to bind ^{26}O

Two-Neutron Separation Energies

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

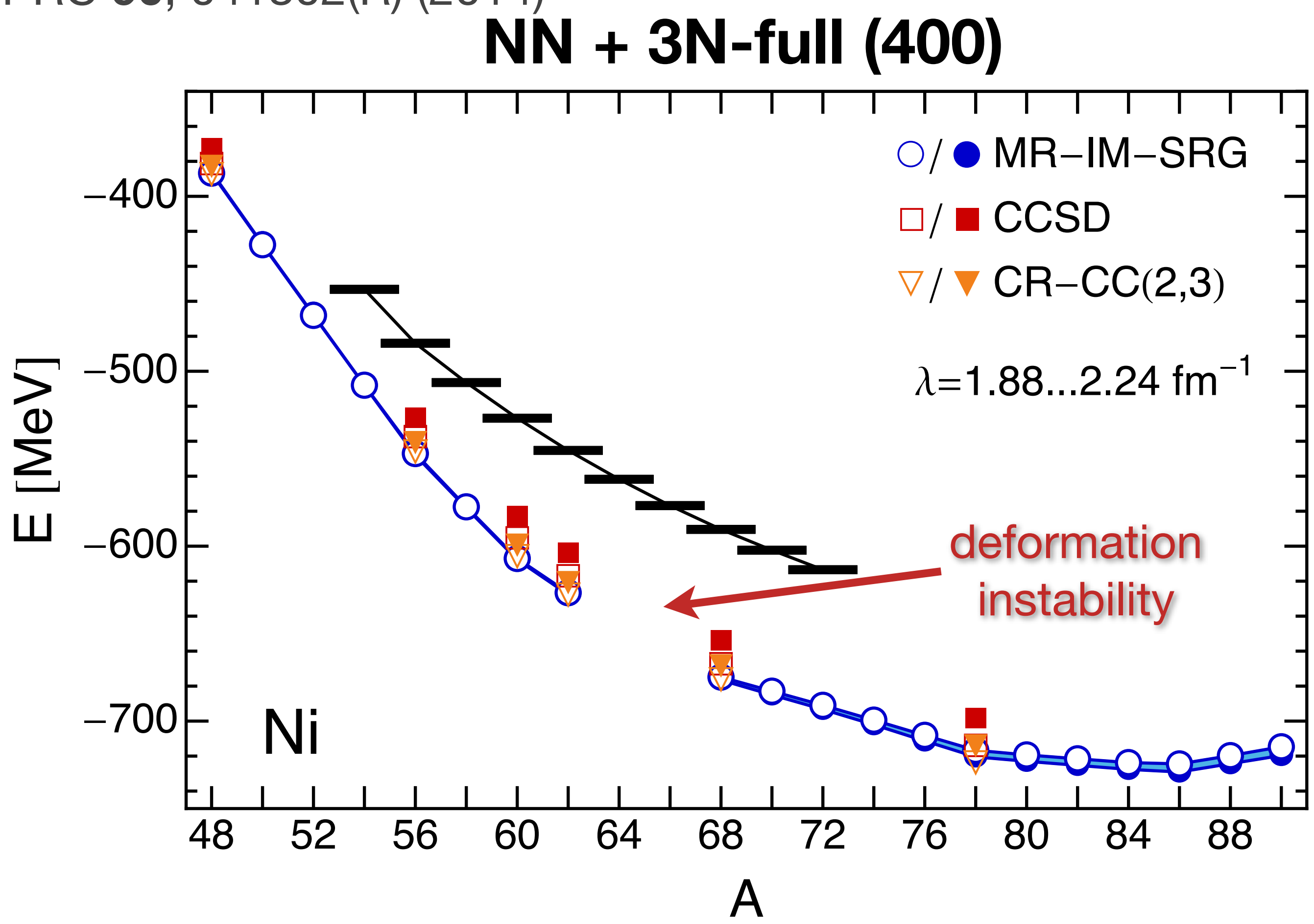


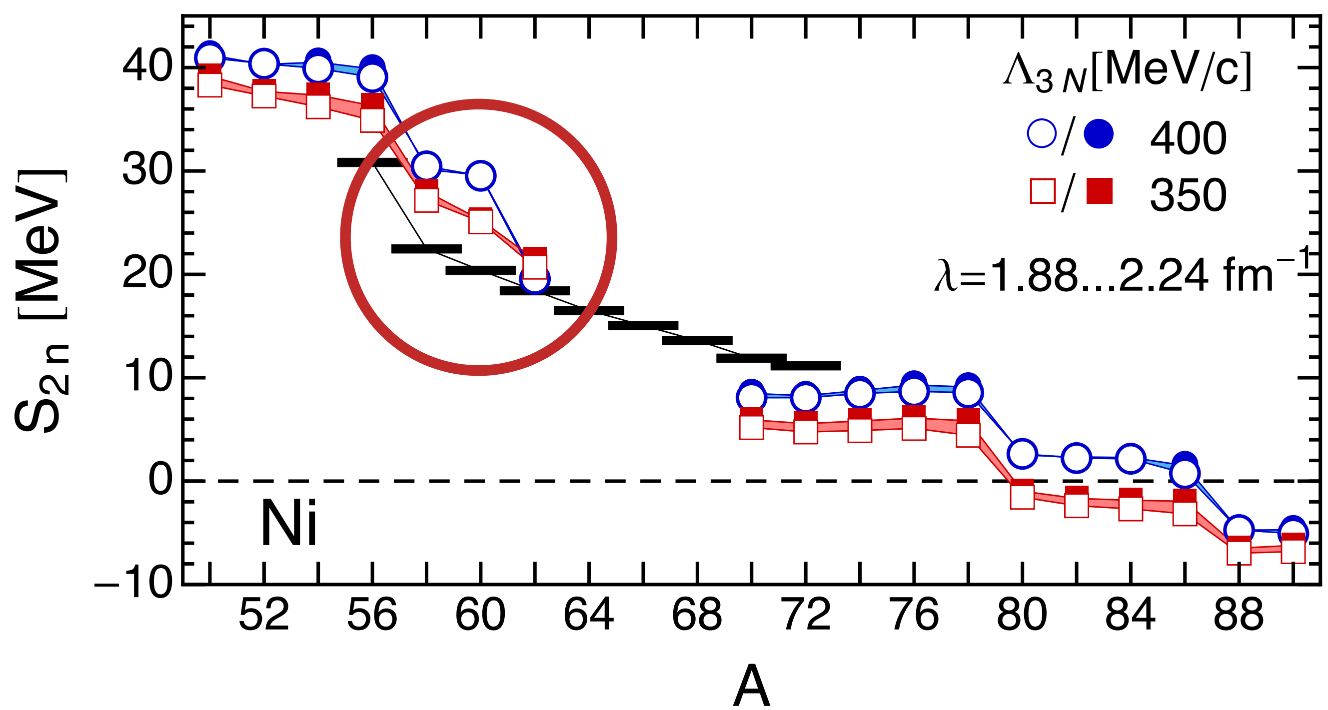
consistent with 2nd order Gor'kov GF
Somà et al., PRC 89, 061301

- 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

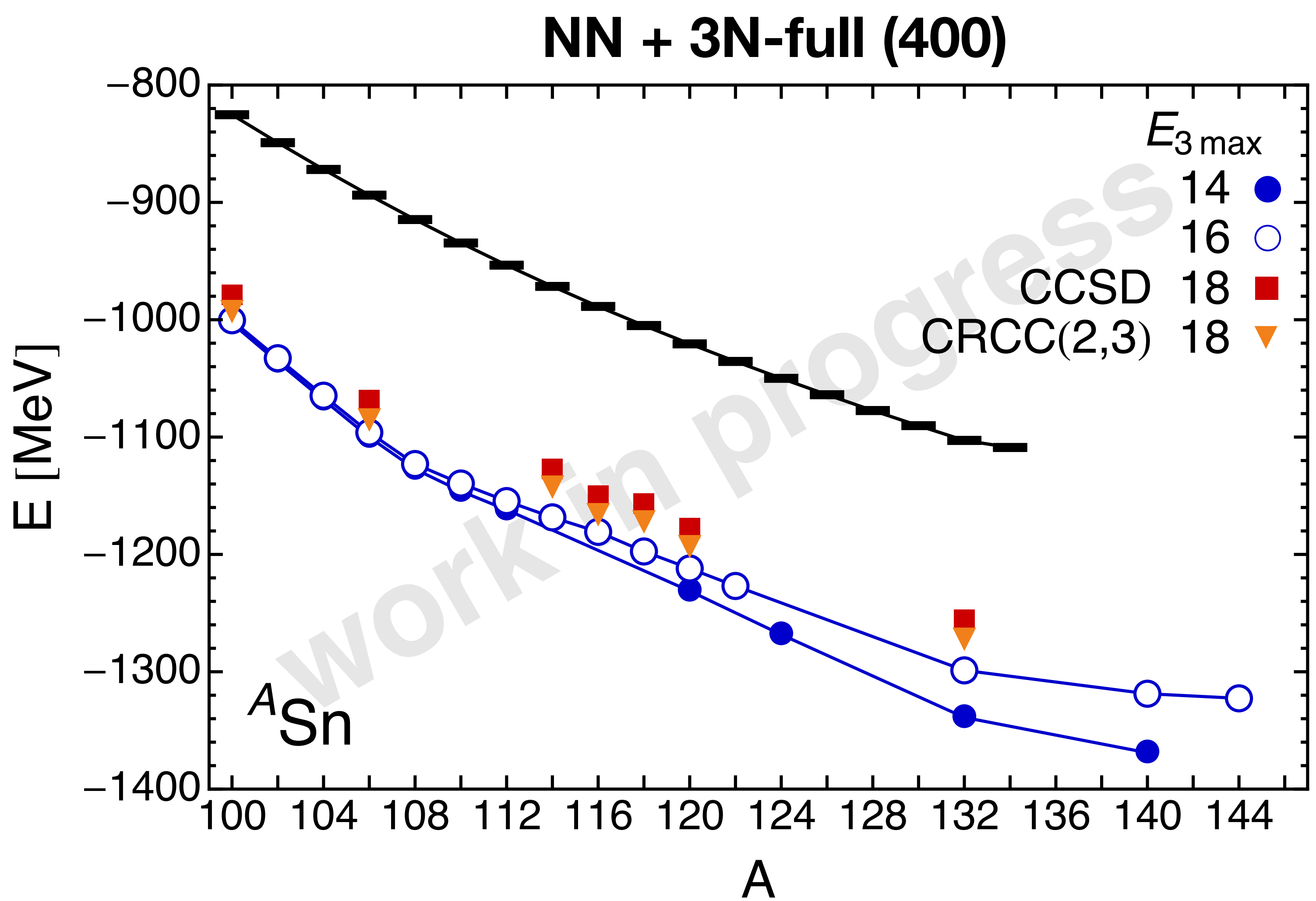
PRC **90**, 041302(R) (2014)





- 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

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

Applications:

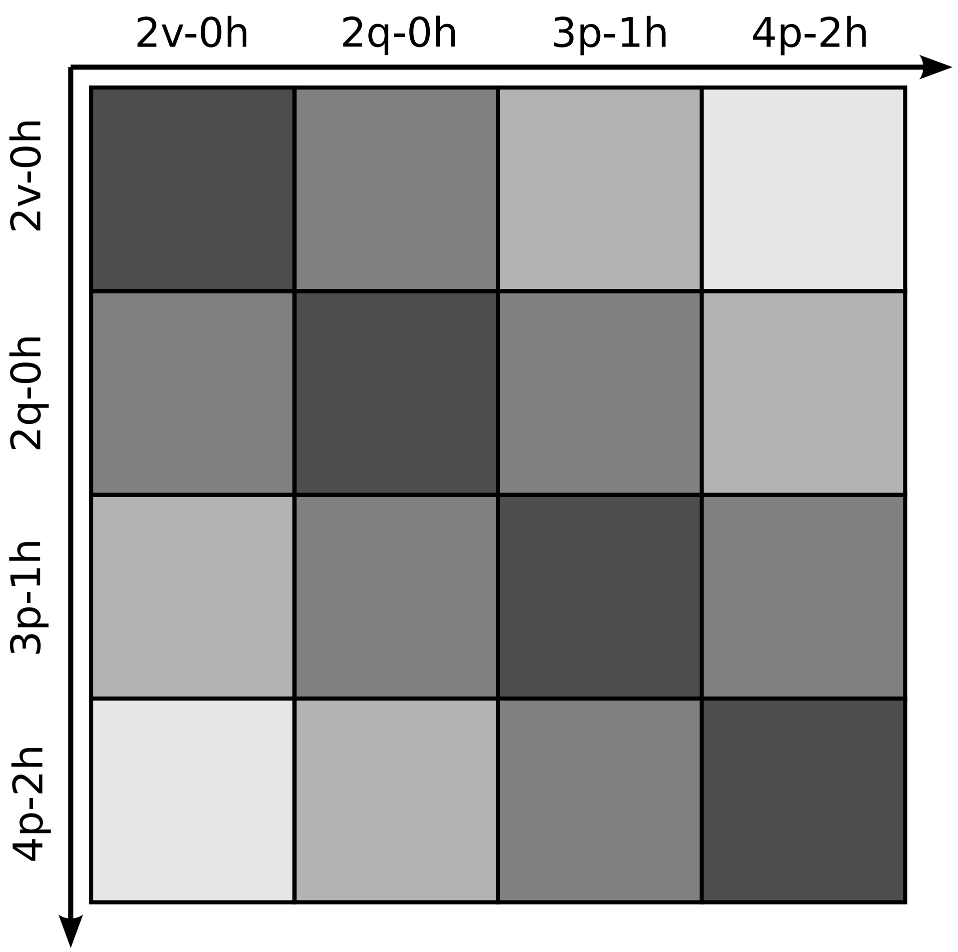
IM-SRG + Shell Model for Excited States

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

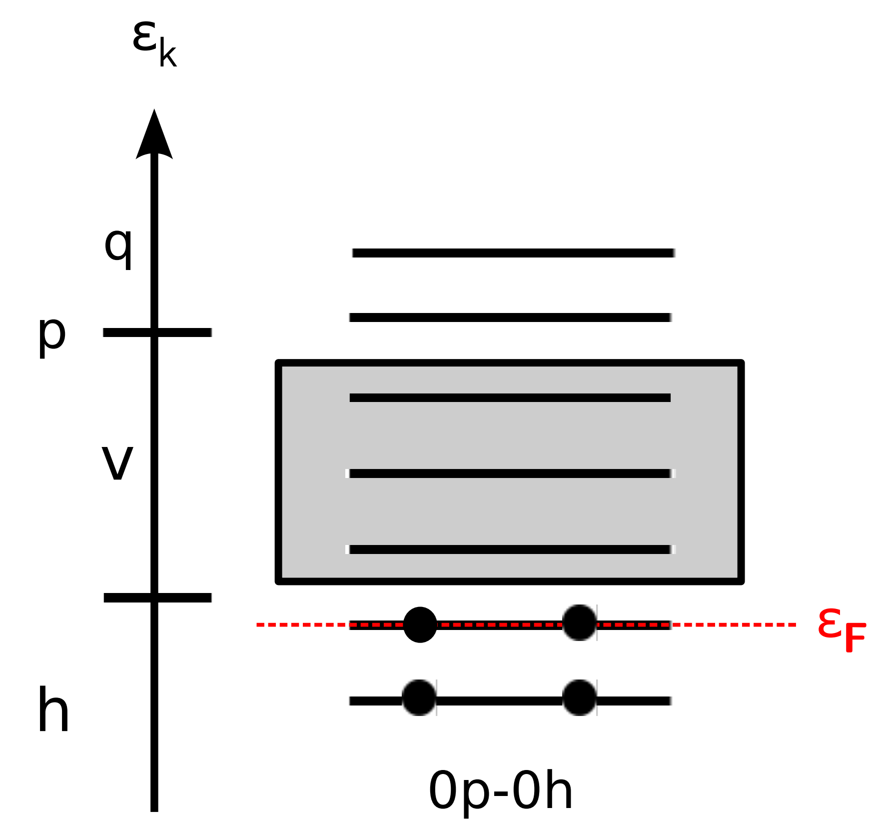


$\langle i | H | j \rangle$

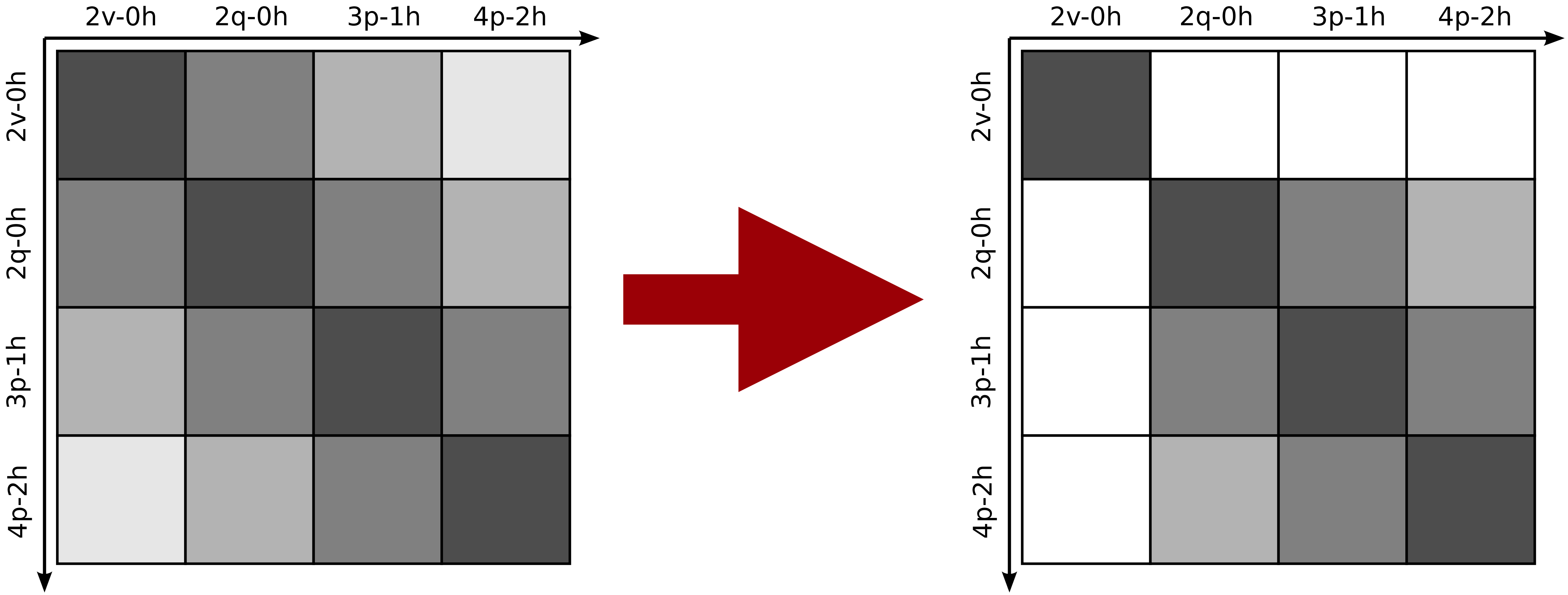
non-valence particle states

valence particle states

hole states (core)



Valence Space Decoupling

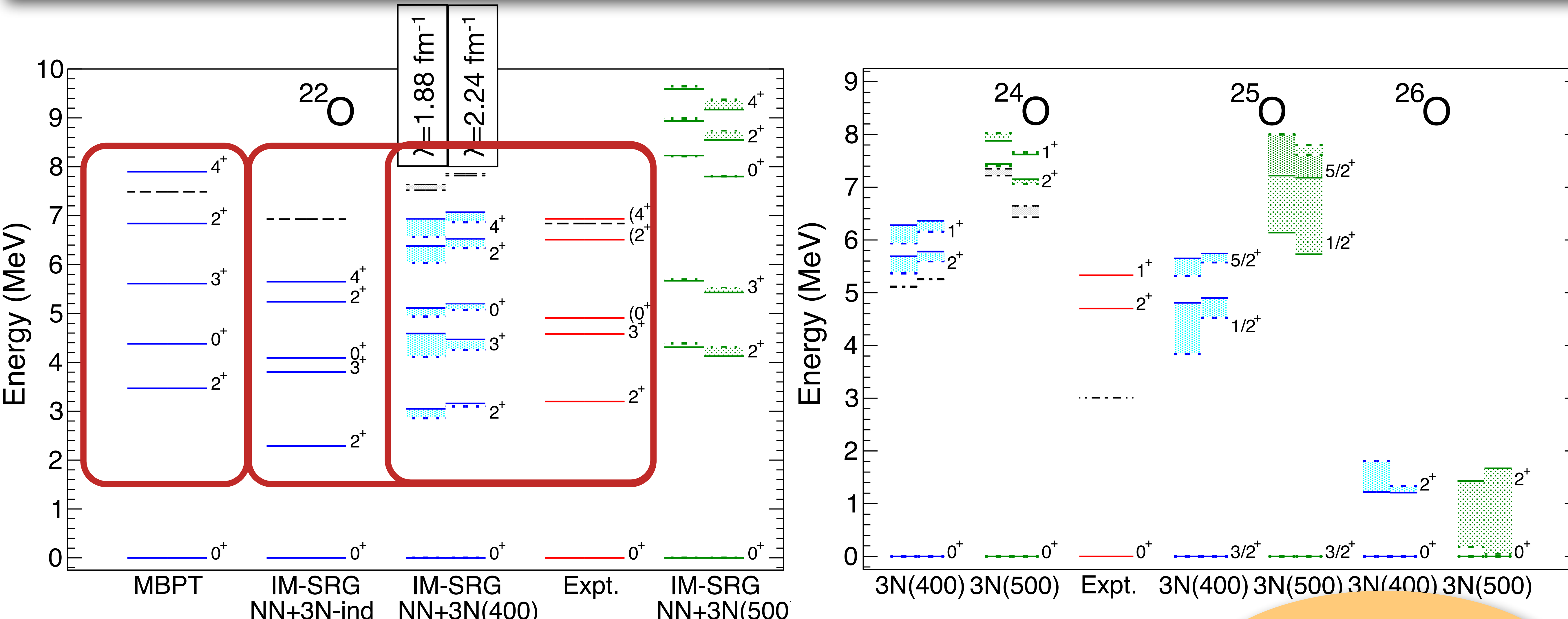


$\langle i | H | j \rangle$ $\quad\quad$ $\langle i | H(\infty) | j \rangle$

- 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...



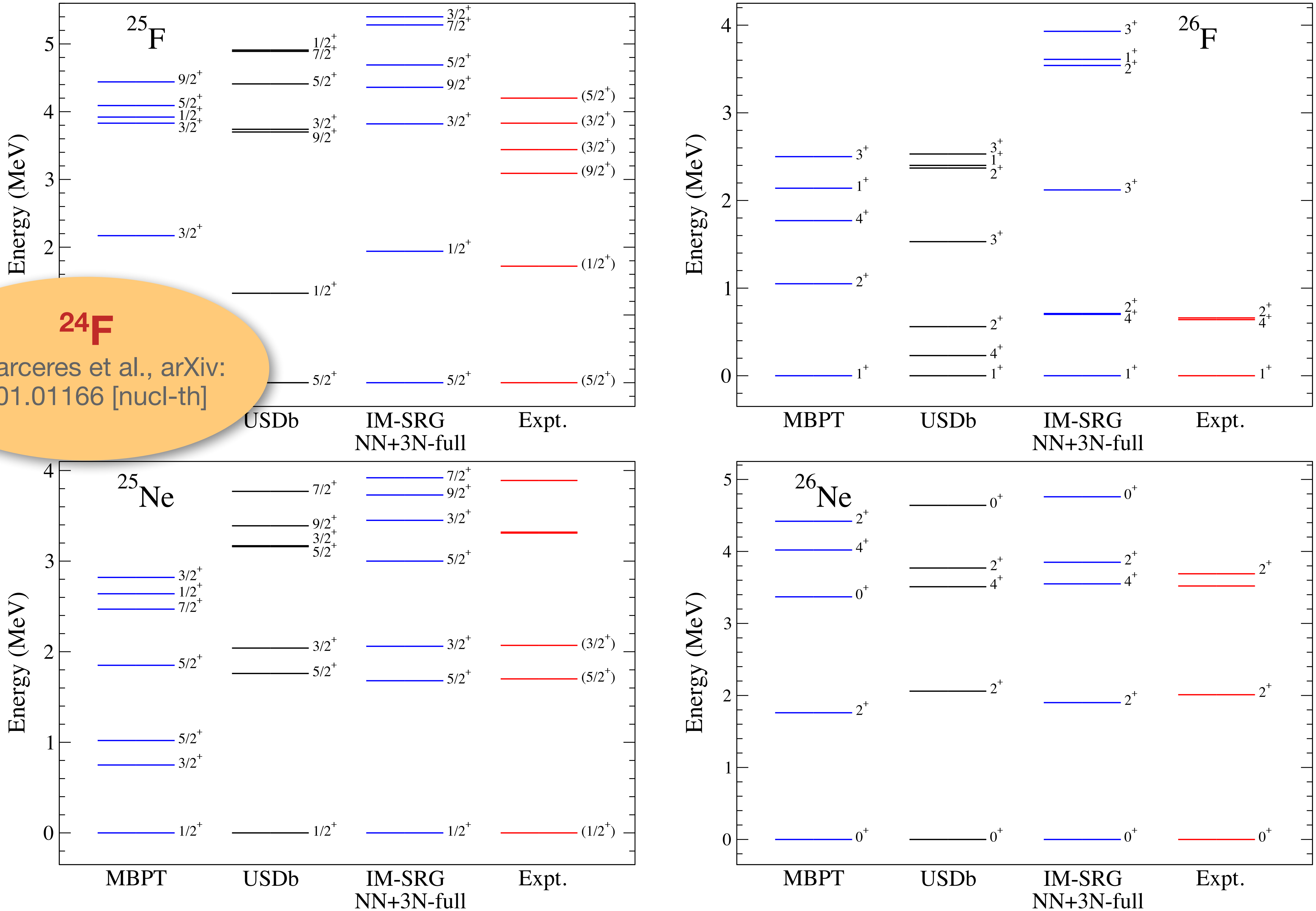
shading: $\hbar\Omega$ variation

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

continuum lowers states by <1 MeV

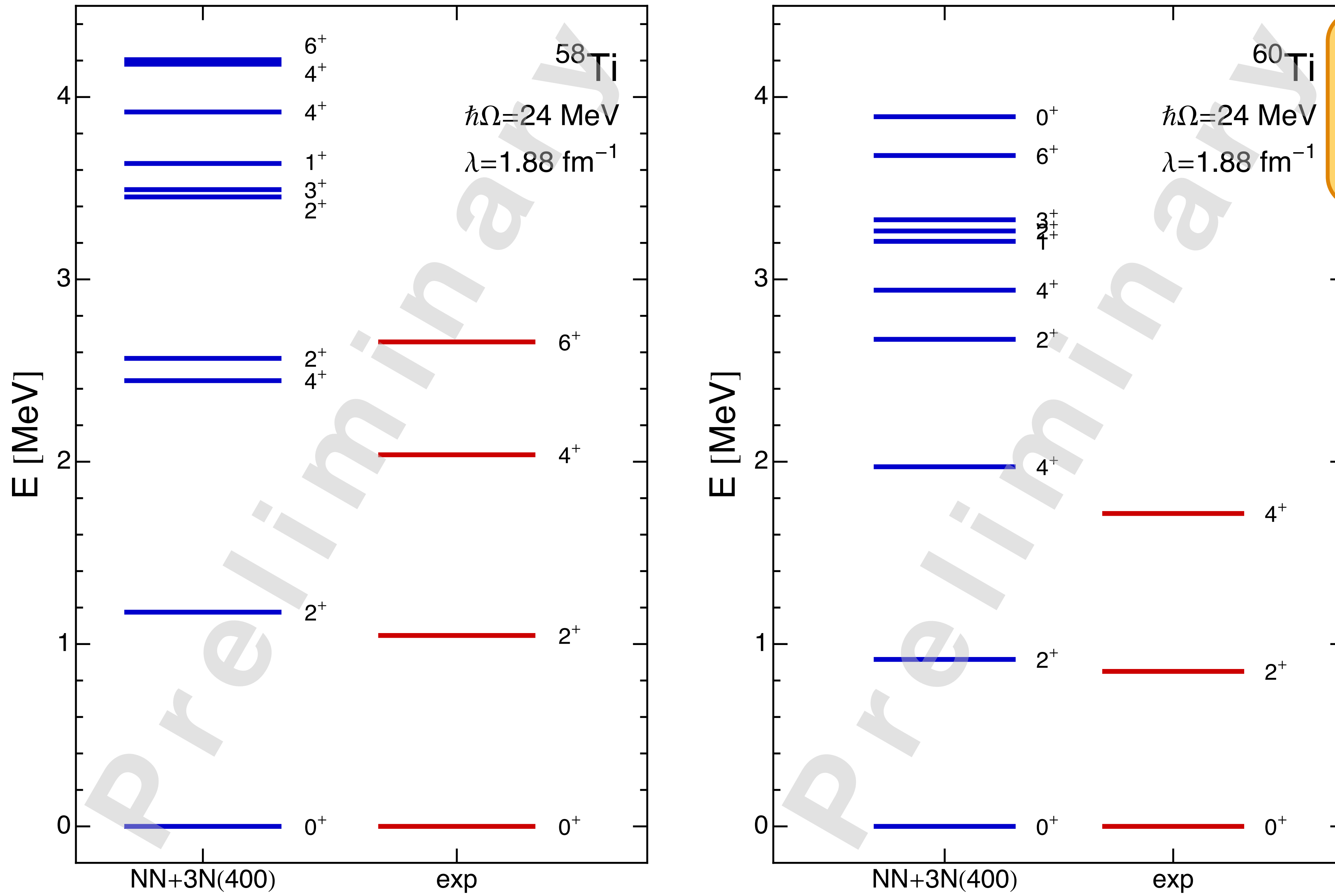
- **3N forces crucial**
- IM-SRG improves on finite-order MBPT effective interaction
- competitive with phenomenological calculations

... Into the *sd*-Shell



^{24}F
L. Carceres et al., arXiv: 1501.01166 [nucl-th]

Heavier Cores



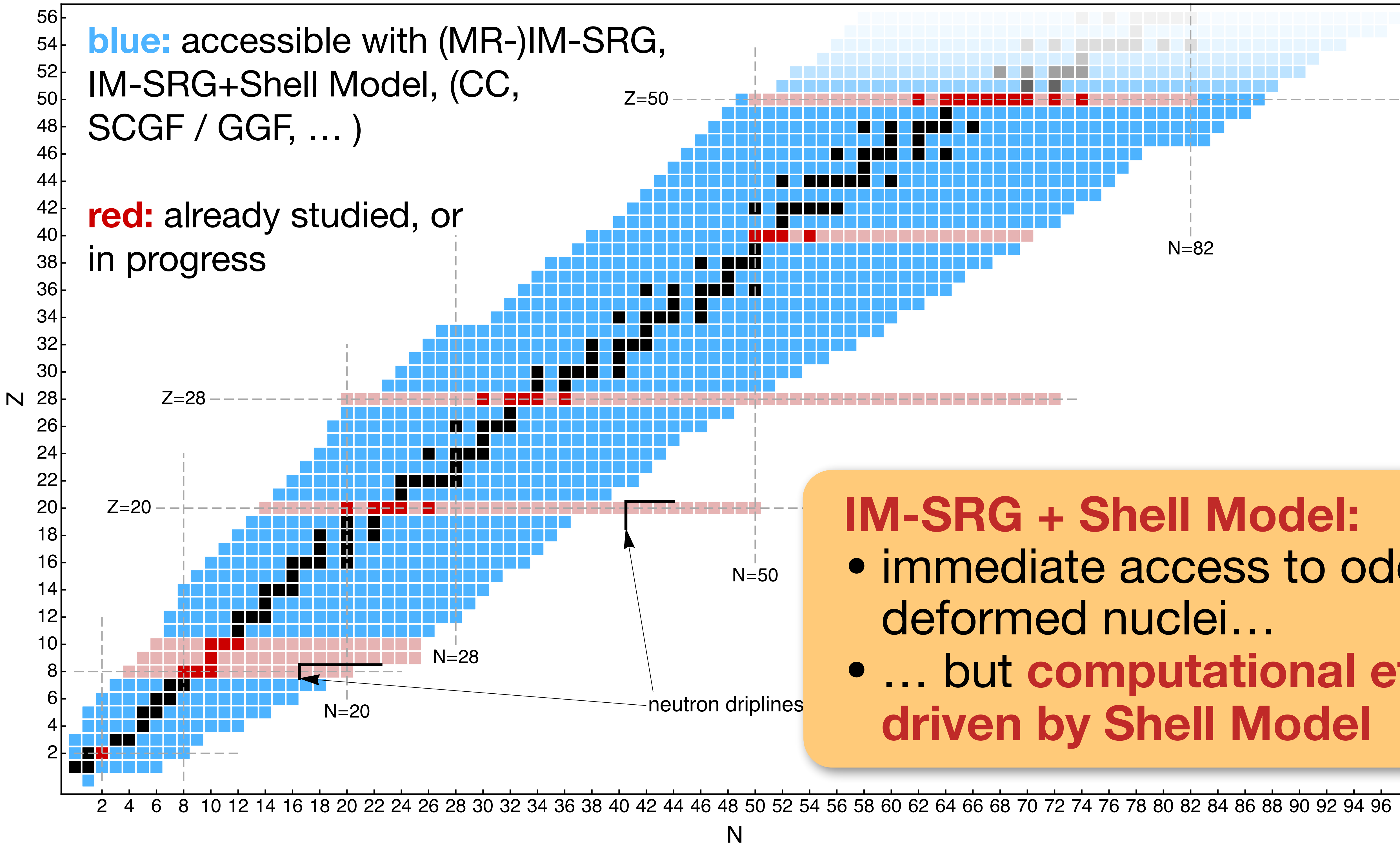
^{48}Ca core, $\nu pf_{5/2}$, πpf valence space

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

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

Next Steps

Reach of Ab Initio Methods



IM-SRG + Shell Model:

- immediate access to odd & deformed nuclei…
- … but **computational effort driven by Shell Model**

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, ...)

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

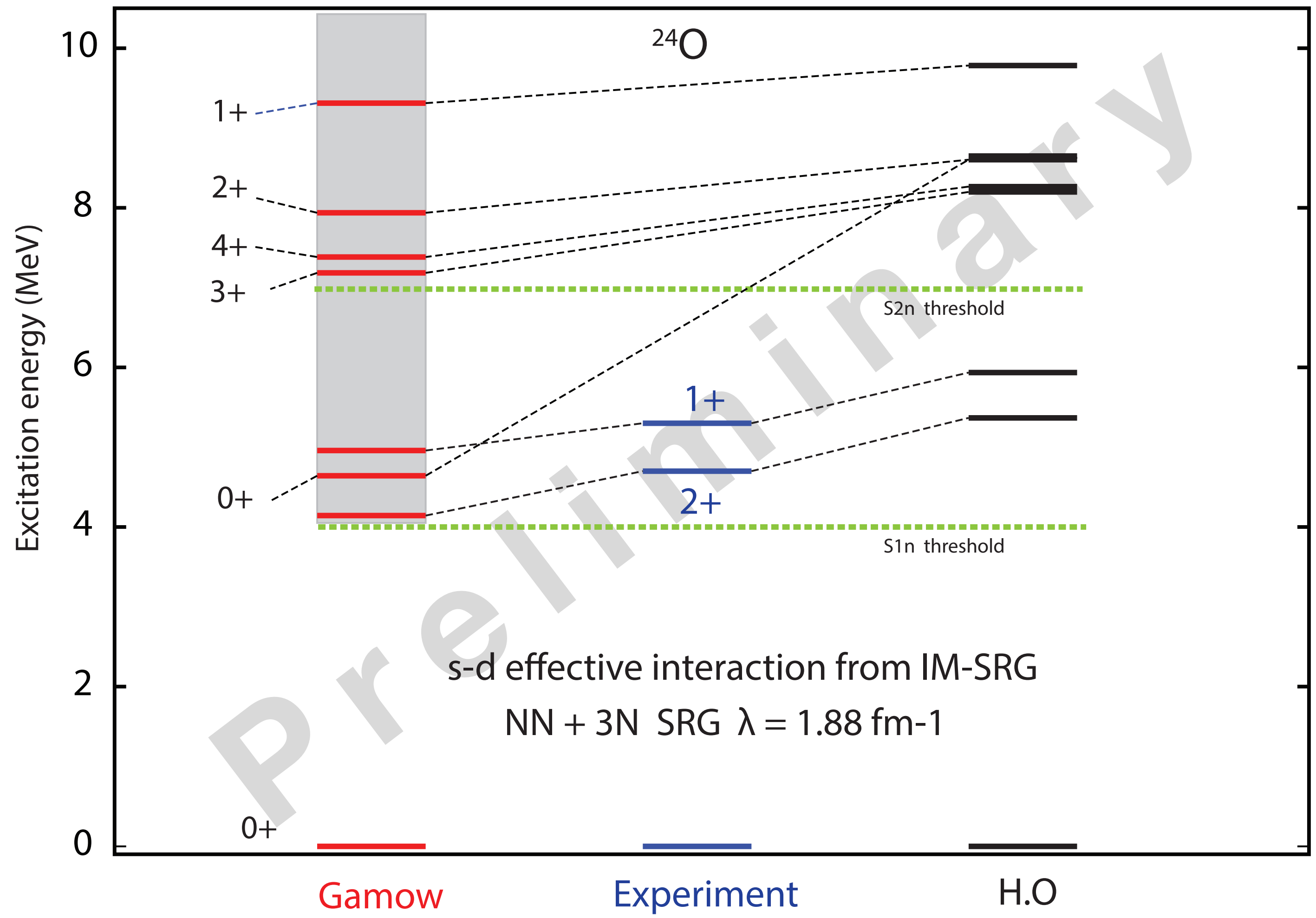
➡ **giant resonances**

- particle attachment (analogous for removal):

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

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

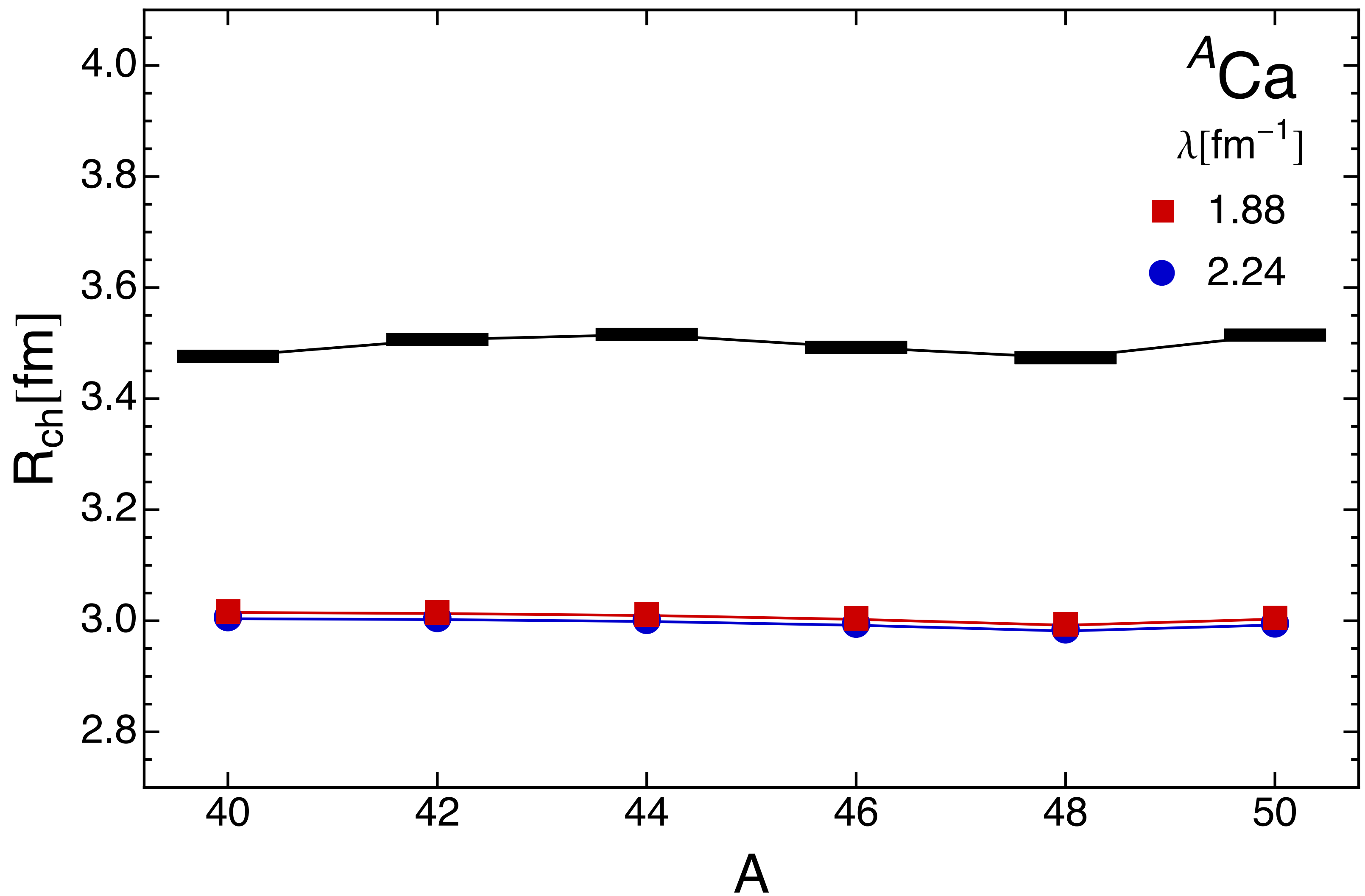
Continuum Effects



(with G. Papadimitriou, ISU)

- **Gamow Shell Model:** use Berggren s.p. basis containing bound, resonance, and scattering states
- first step: GSM calculations with IM-SRG interaction
- **future:** include continuum in IM-SRG evolution

Effective Operators



- small radii: interaction issue (power counting, regulators, LECs, …)? importance of currents?
- implementation of electromagnetic & weak transition operators in progress; aim for consistent treatment: chiral EFT, SRG, IM-SRG (& Shell Model code !)

Conclusions

Conclusions

- enormous progress in *ab initio* nuclear structure and reactions, driven by (S)RG and (chiral) EFT
  - stringent link to QCD
  - enhanced control over many-body methods, **uncertainty quantification**

- IM-SRG is a powerful *ab initio* framework for closed- and open-shell, medium-mass & (heavy) nuclei

  - allows derivation of Shell-Model interactions

  ➡ immediate access to spectra, odd nuclei, intrinsic deformation (at Shell Model numerical cost)

- new perspectives for old (?) problems: evolution of long-range correlations, construction of density functionals...

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Supplements

Induced Interactions

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

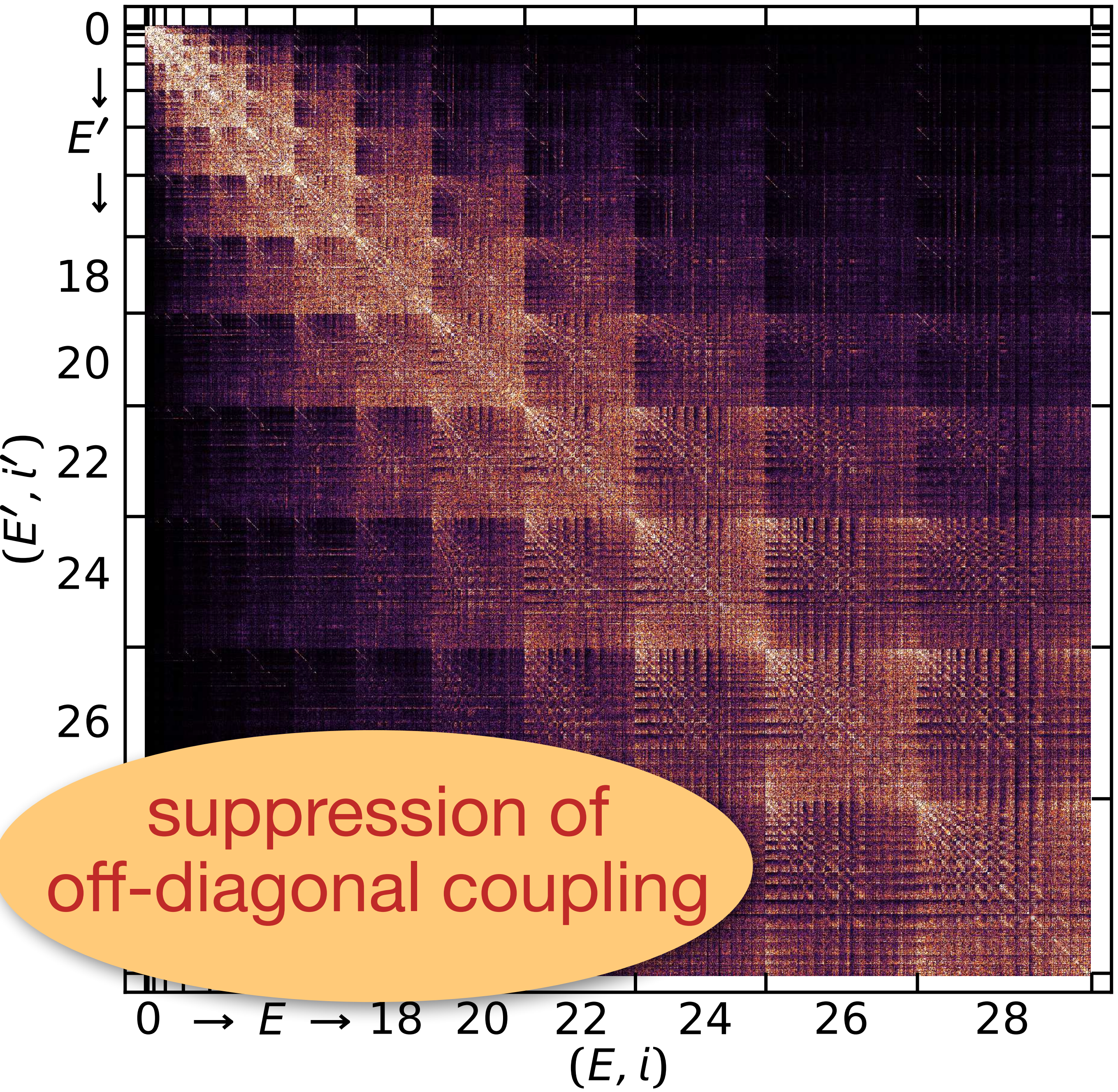
$$\frac{dH}{d\lambda} = [[\sum a^\dagger a, \sum \underbrace{a^\dagger a^\dagger aa}_{\text{2-body}}], \sum \underbrace{a^\dagger a^\dagger aa}_{\text{2-body}}] = \ldots + \sum \underbrace{a^\dagger a^\dagger a^\dagger aaa}_{\text{3-body}} + \ldots$$

- 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; Wendt, PRC 87, 061001)
- λ-dependence of eigenvalues is a diagnostic for size of omitted induced interactions

SRG in Three-Body Space

3B Jacobi-HO Matrix Elements

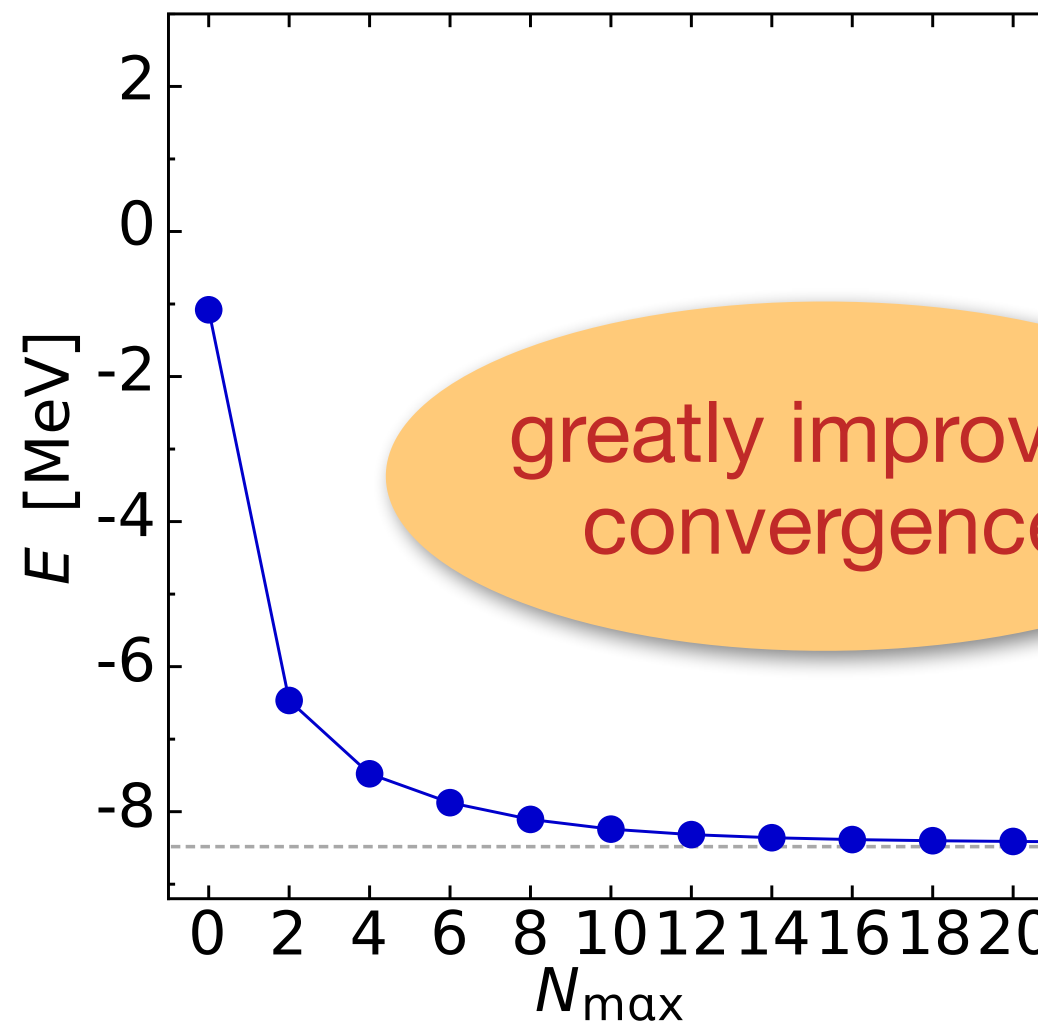
$J^\pi = \frac{1}{2}^+, T = \frac{1}{2}, \hbar\Omega = 28$ MeV



suppression of off-diagonal coupling

λ = 1.33 fm^{-1}

^{3}H ground-state (NCSM)



greatly improved convergence

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

Choice of Generator

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

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

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

- "imaginary time": (Morris, Bogner)

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

- 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 $\ll 1\%$

In-Medium SRG Flow Equations

0-body Flow

$$\frac{dE}{ds} = \sum_{ab}(n_a - n_b)\left(\eta^a_b f^b_a - f^a_b \eta^b_a\right) + \frac{1}{4}\sum_{abcd}\left(\eta^{ab}_{cd}\Gamma^{cd}_{ab} - \Gamma^{ab}_{cd}\eta^{cd}_{ab}\right) n_a n_b \bar{n}_c \bar{n}_d$$

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

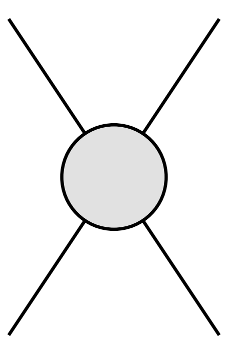
1-body Flow

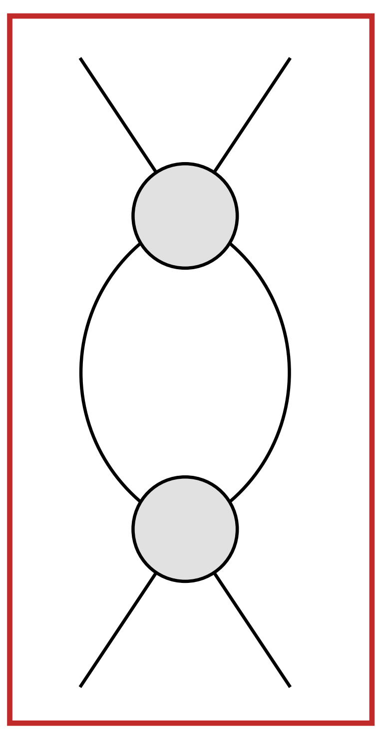
$$\frac{d}{ds} f^1_2 = \sum_{a}\left(\eta^1_a f^a_2 - f^1_a \eta^a_2\right) + \sum_{ab}\left(\eta^a_b \Gamma^{b1}_{a2} - f^a_b \eta^{b1}_{a2}\right)(n_a - n_b)$$
$$+ \frac{1}{2}\sum_{abcdef}\left(\eta^{1a}_{bc}\Gamma^{bc}_{2a} - \Gamma^{1a}_{bc}\eta^{bc}_{2a}\right)(n_a \bar{n}_b \bar{n}_c + \bar{n}_a n_b n_c)$$

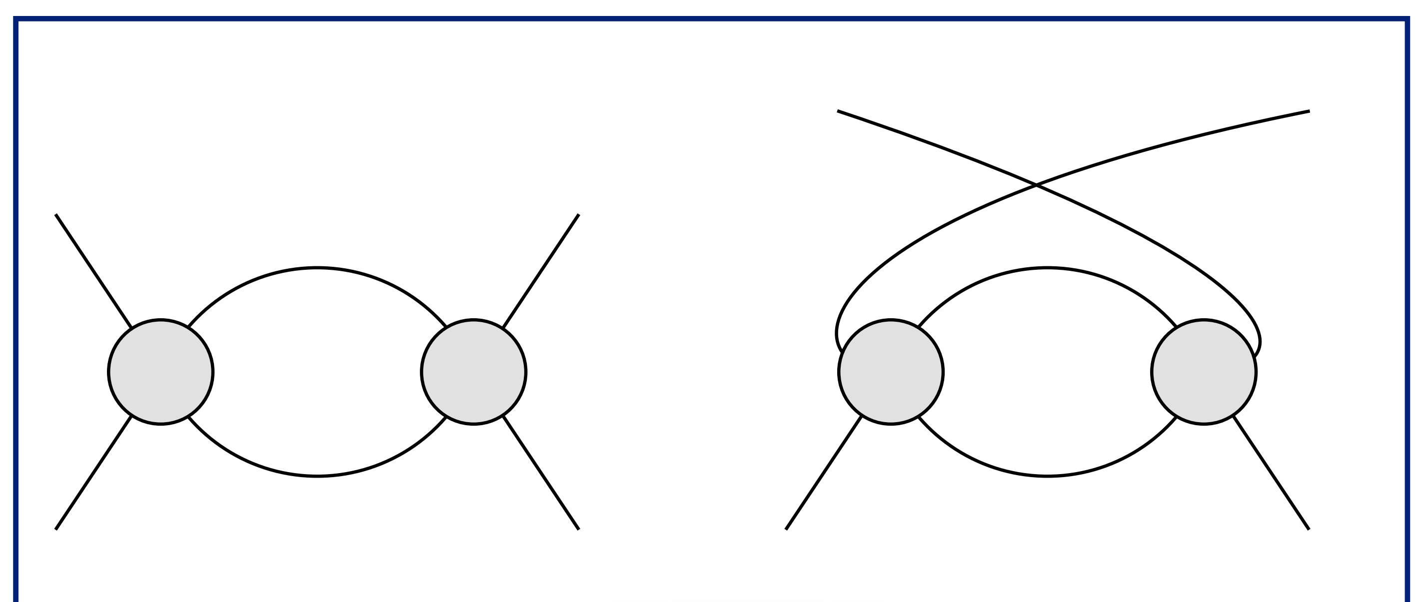
In-Medium SRG Flow Equations

2-body Flow

$$
\begin{aligned}
\frac{d}{ds}\Gamma^{12}_{34} = &\sum_a \left(\eta^1_a \Gamma^{a2}_{34} + \eta^2_a \Gamma^{1a}_{34} - \eta^a_3 \Gamma^{12}_{a4} - \eta^a_4 \Gamma^{12}_{3a} - f^1_a \eta^{a2}_{34} - f^2_a \eta^{1a}_{34} + f^a_3 \eta^{12}_{a4} + f^a_4 \eta^{12}_{3a}\right) \\
&+ \underline{\frac{1}{2}\sum_{ab}\left(\eta^{12}_{ab}\Gamma^{ab}_{34} - \Gamma^{12}_{ab}\eta^{ab}_{34}\right)(1 - n_a - n_b)} \\
&+ \underline{\sum_{ab}(n_a - n_b)\left(\left(\eta^{1a}_{3b}\Gamma^{2b}_{4a} - \Gamma^{1a}_{3b}\eta^{2b}_{4a}\right) - \left(\eta^{2a}_{3b}\Gamma^{1b}_{4a} - \Gamma^{2a}_{3b}\eta^{1b}_{4a}\right)\right)}
\end{aligned}
$$





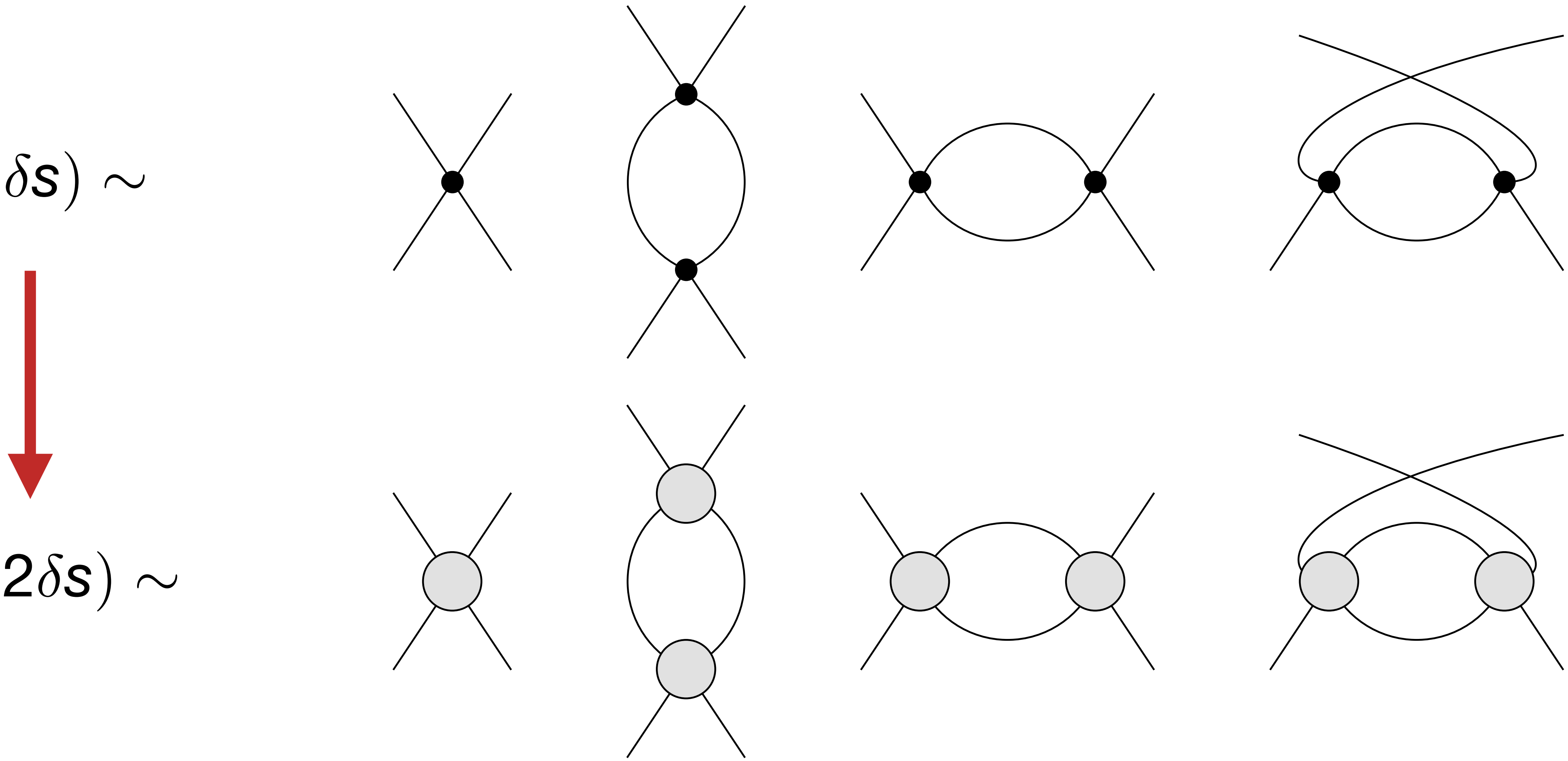


only linked diagrams contribute, IM-SRG size-extensive

In-Medium SRG Flow: Diagrams

$\Gamma(\delta s) \sim$

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



In-Medium SRG Flow: Diagrams

$\Gamma(\delta s) \sim$

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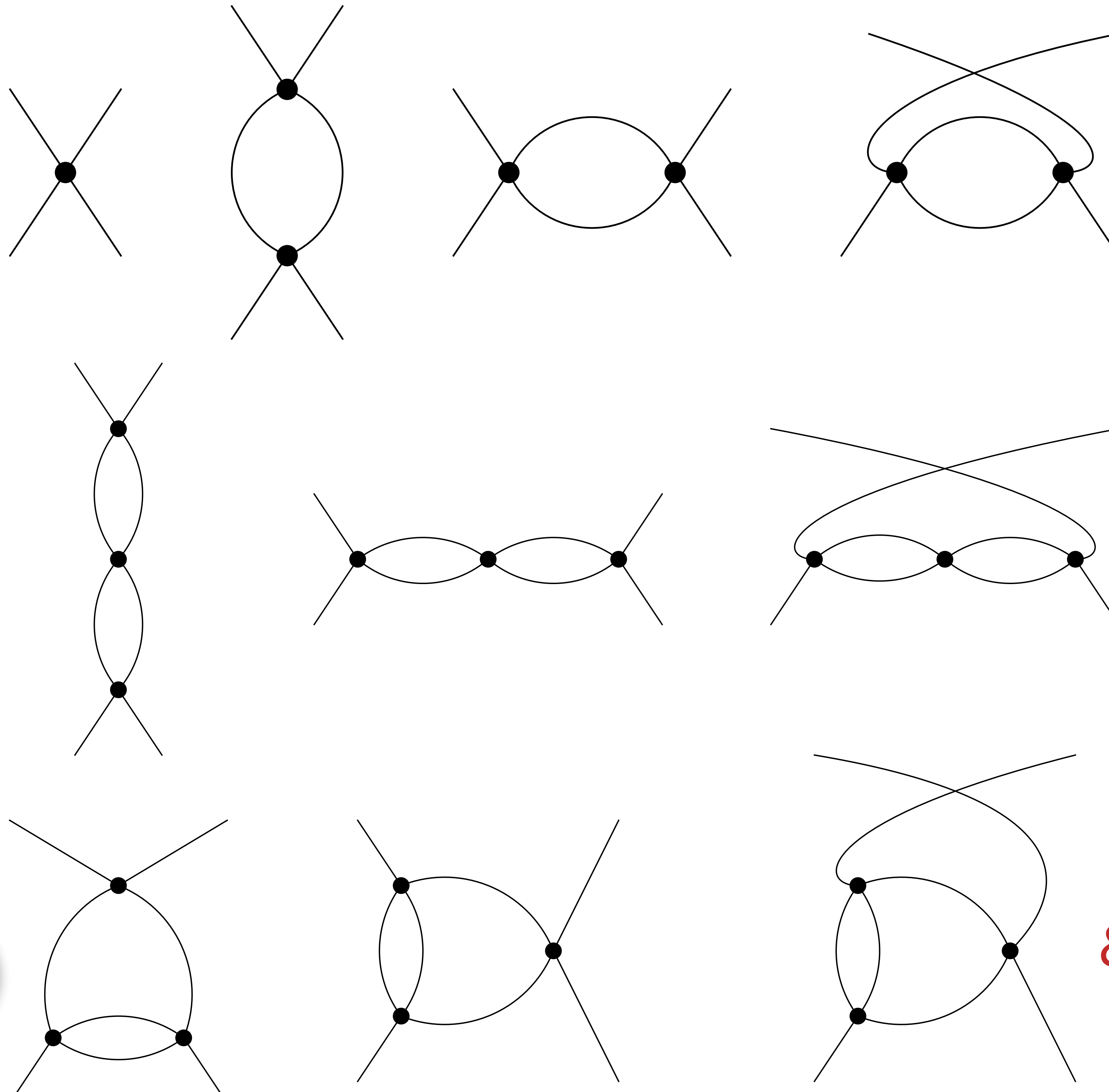


non-perturbative resummation

& many more...

Generalized Normal Ordering

- 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:

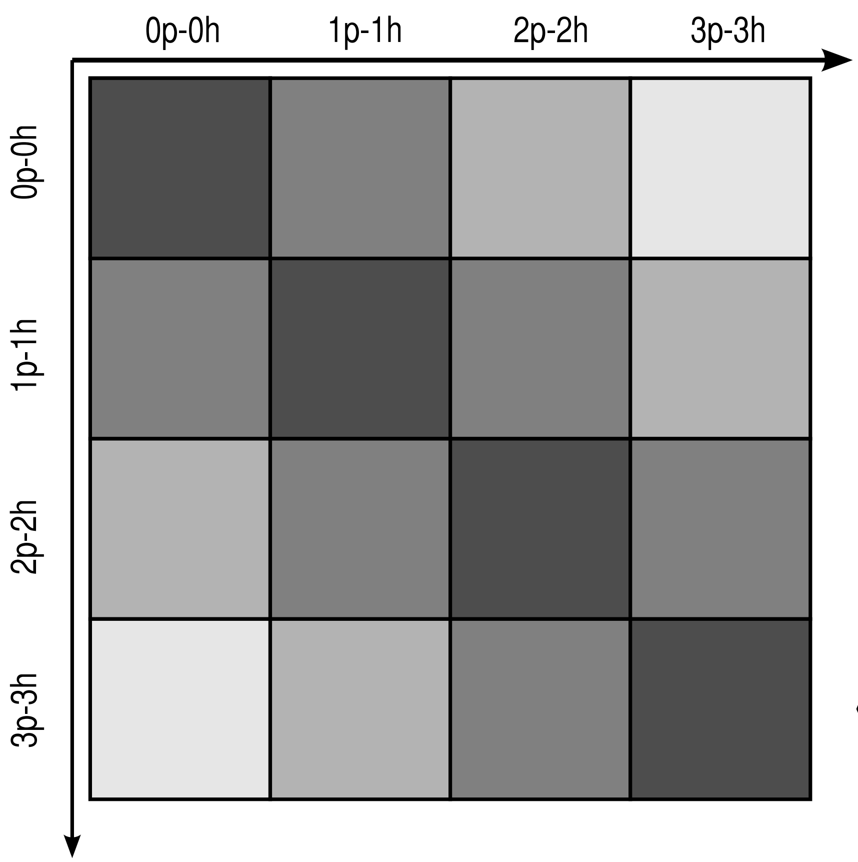
$$:A^{ab\ldots}_{cd\ldots}::A^{kl\ldots}_{mn\ldots}: \quad \longrightarrow \quad \lambda^{ab}_{mn}$$

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

$$\ldots$$

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

Decoupling



$$\left\langle {}^{p}_{h} \right| H \left| \Psi \right\rangle \sim f^{p}_{h},\ \sum_{kl} f^{k}_{l} \lambda^{hk}_{pl},\ \sum_{klmn} \Gamma^{kl}_{mn} \lambda^{hkl}_{pmn}, \ldots$$

$$\left\langle {}^{pp'}_{hh'} \right| H \left| \Psi \right\rangle \sim \Gamma^{pp'}_{hh'},\ \sum_{km} \Gamma^{pk}_{hm} \lambda^{h'k}_{p'm},\ \sum_{kl} f^{k}_{l} \lambda^{hh'k}_{pp'l},\ \sum_{klmn} \Gamma^{kl}_{mn} \lambda^{hh'kl}_{pp'mn}, \ldots$$

$$\left\langle {}^{pp'p''}_{hh'hh'} \right| H \left| \Psi \right\rangle \sim \ldots$$

- truncation in irreducible density matrices
  - 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

Particle-Number Projected HFB State

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

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

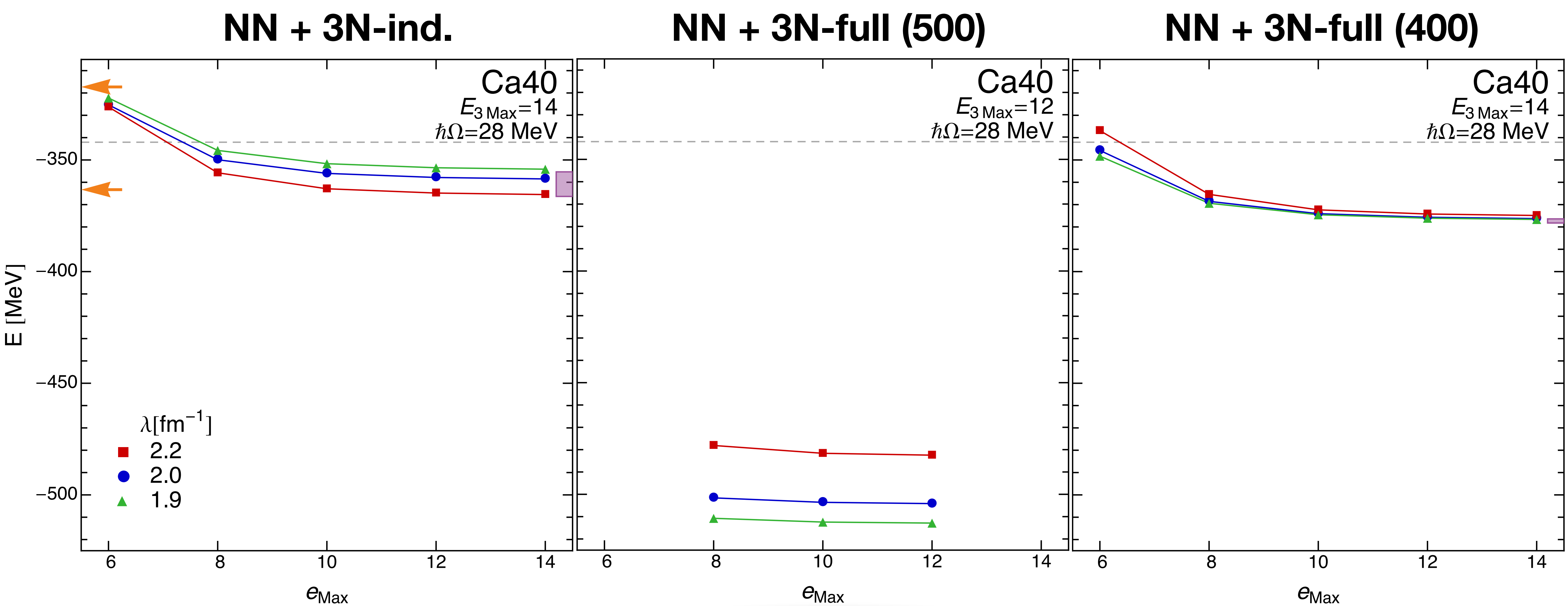
- calculate one- and two-body densities (project only once):

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

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

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

Results: Closed-Shell Nuclei

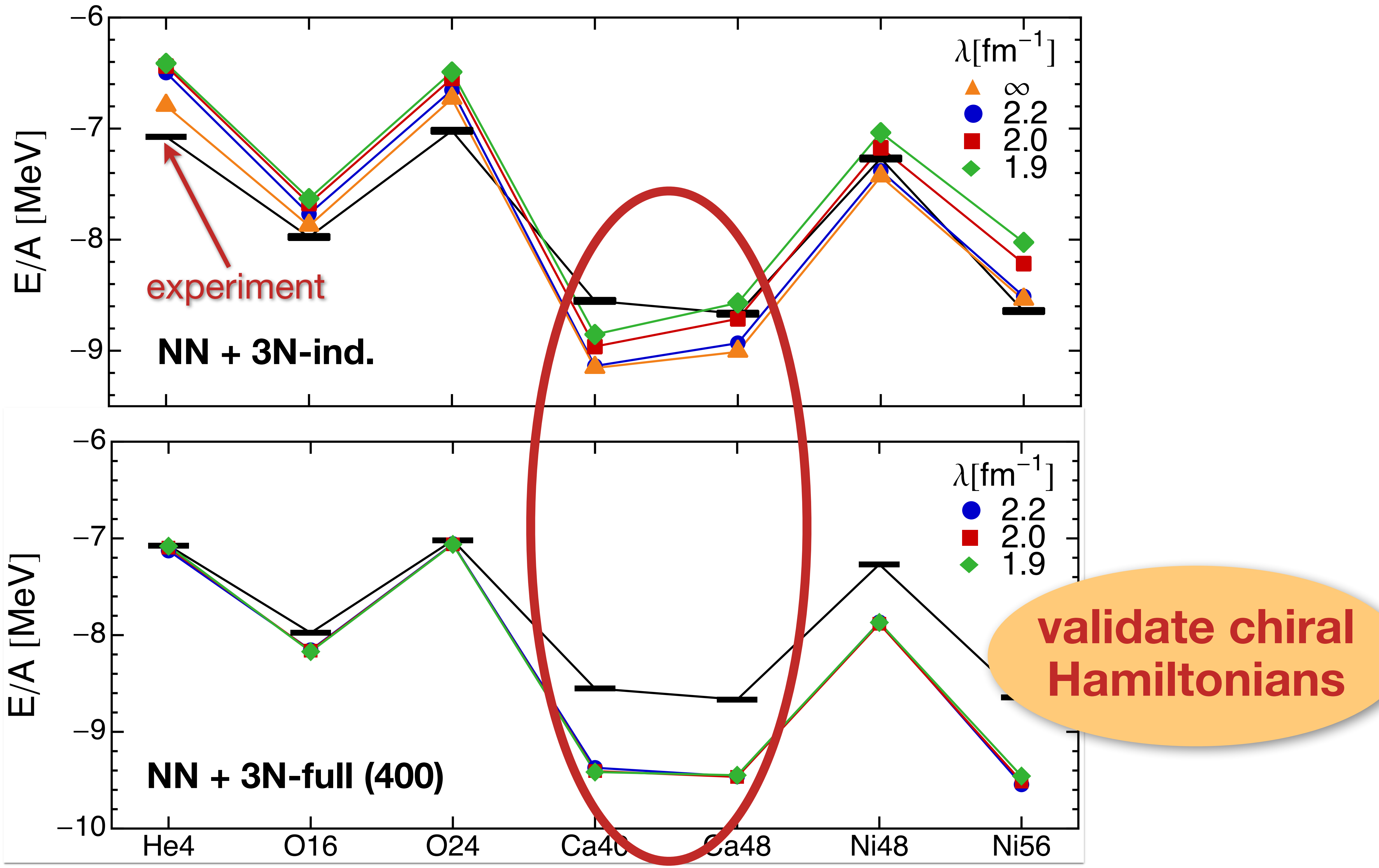


validate chiral Hamiltonians

CCSD/Λ-CCSD(T), $\lambda = \infty$, G. Hagen et al., PRL 109, 032502 (2012)

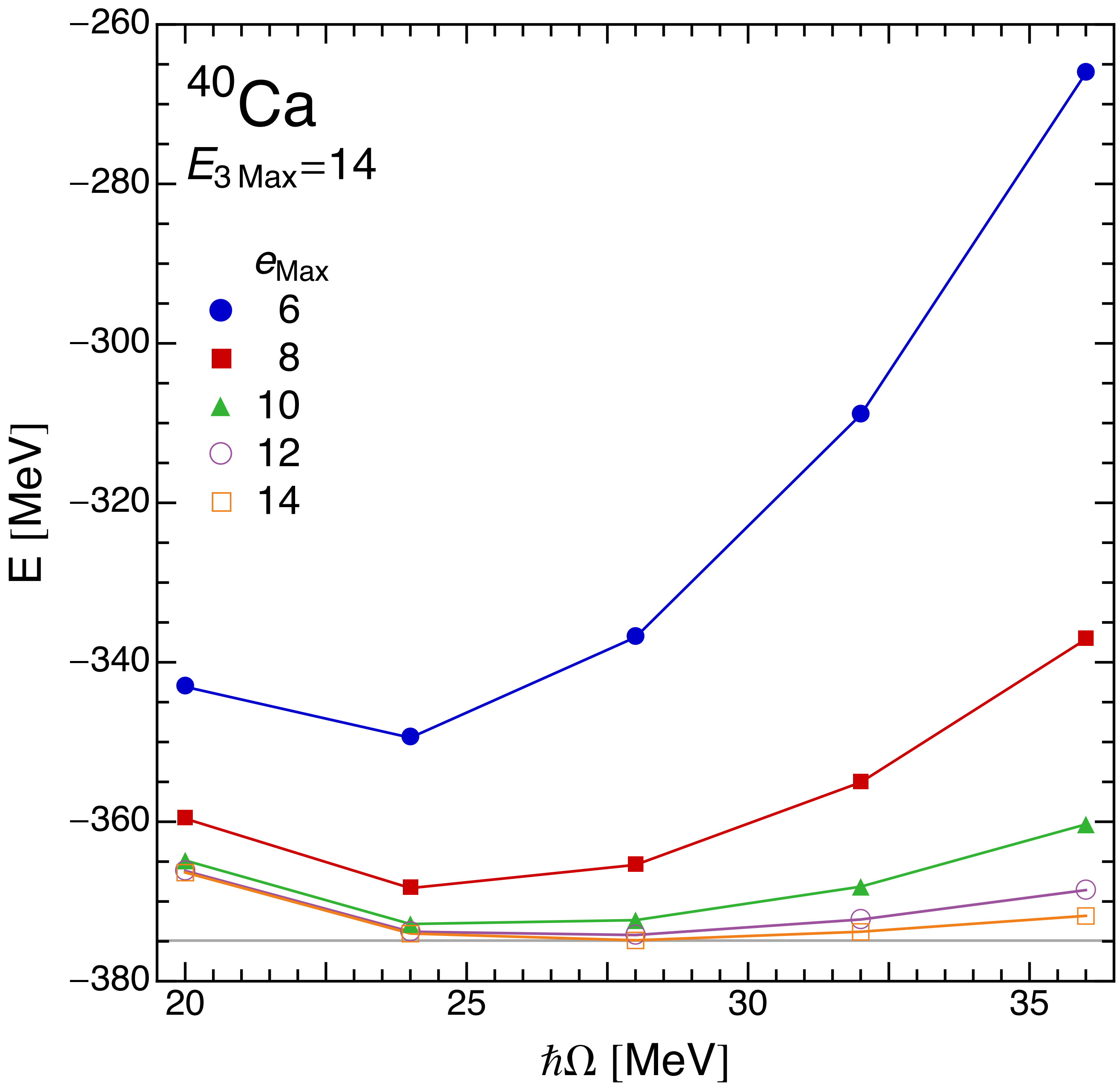
Λ-CCSD(T), $\lambda = 1.9 - 2.2$ fm^{-1} , S.Binder et al., arXiv:1211.4748 [nucl-th] & PRL 109, 052501 (2012)

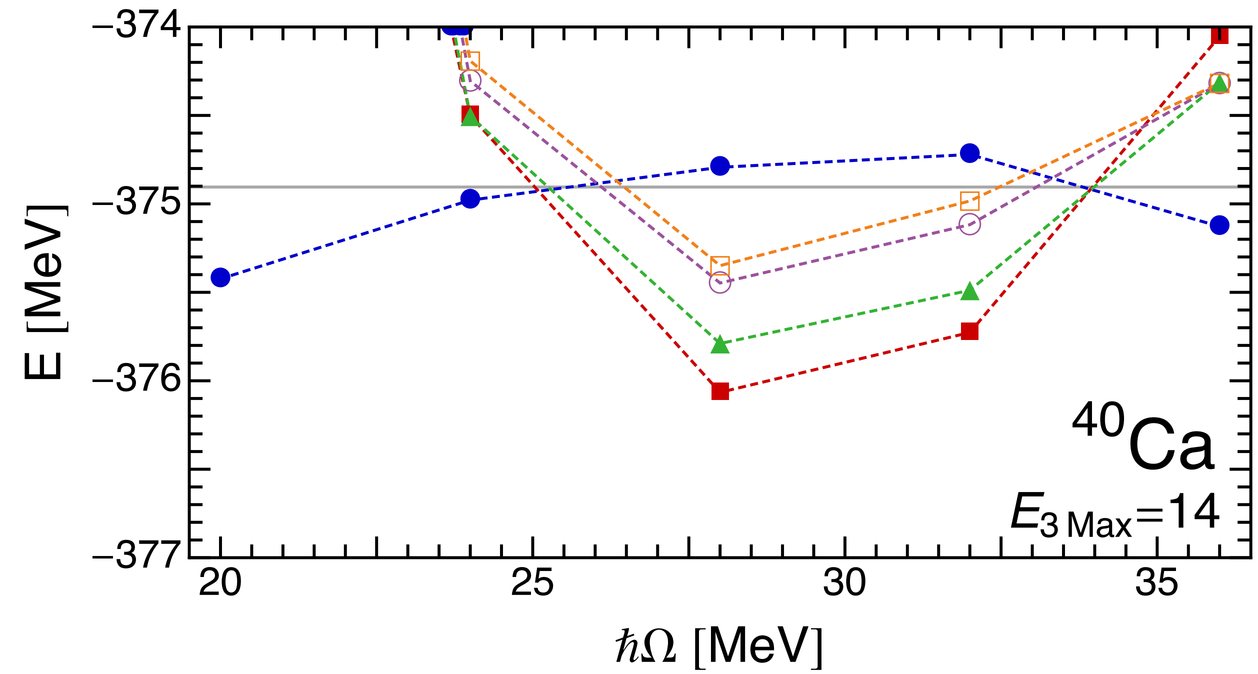
Results: Closed-Shell Nuclei



Phys. Rev. C **87**, 034307 (2013), arXiv: 1212.1190 [nucl-th]

Extrapolation





max./UV momentum:

$$\Lambda_{UV} = \sqrt{2m(e_{Max} + 3/2)\hbar\Omega}$$

radial extent:

$$L = \sqrt{2(e_{Max} + 3/2)\hbar/m\Omega}$$

simultaneous ultraviolet & infrared extrapolation:

$$E(\Lambda_{UV}, L) = E_\infty + A_0 \exp\left(-2\Lambda_{UV}^2/A_1^2\right) + A_2 \exp\left(-2k_\infty L\right)$$

(R. Furnstahl, G. Hagen & T. Papenbrock, PRC 86,031301 (2012))

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:

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

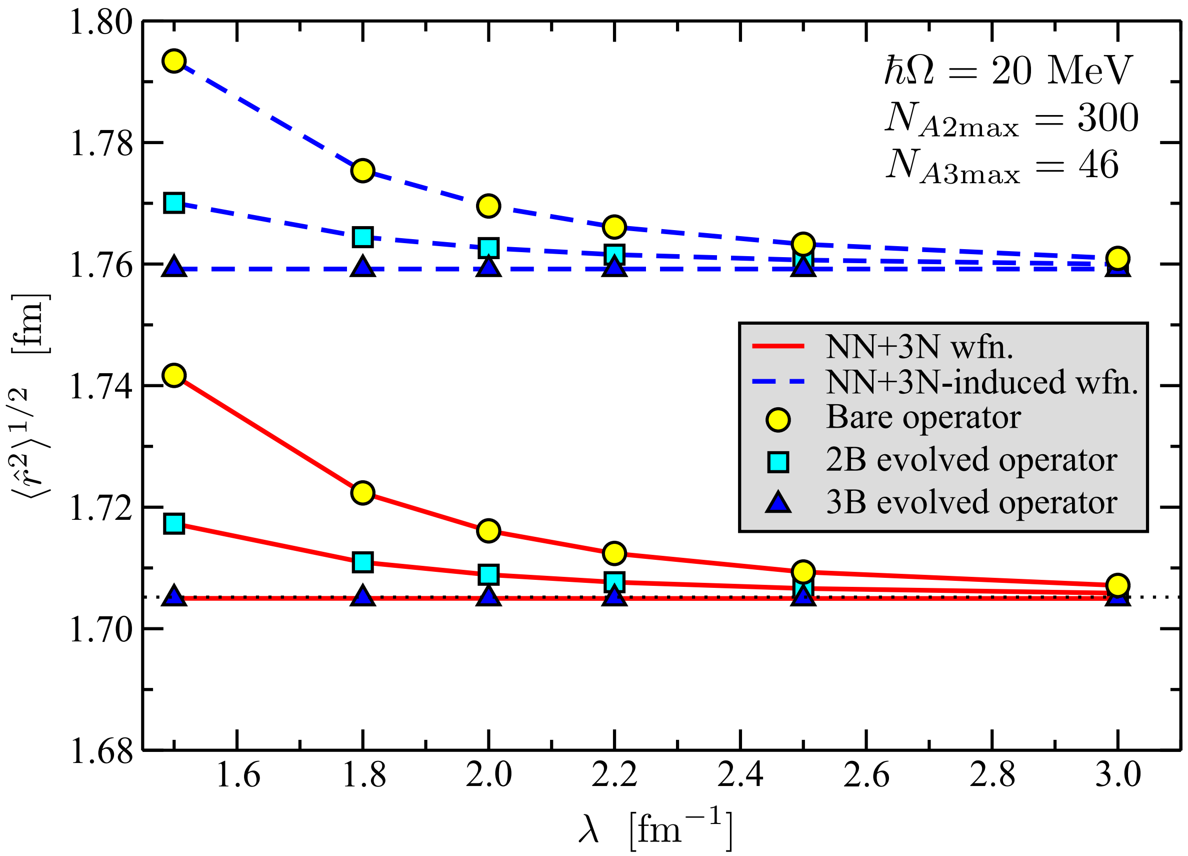
$$+ \frac{1}{2}\sum_{ab}\left(\eta^{12}_{ab}\Gamma^{ab}_{34} - \Gamma^{12}_{ab}\eta^{ab}_{34}\right)(1 - n_a - n_b)$$

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

2-body flow unchanged

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