

In-Medium SRG: Recent Developments and A Look Ahead

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Outline



- The In-Medium SRG
- Ground States of Closed- and Open-Shell Nuclei
- IM-SRG + Shell Model for Excited States
- Next Steps
- Conclusions

The In-Medium SRG

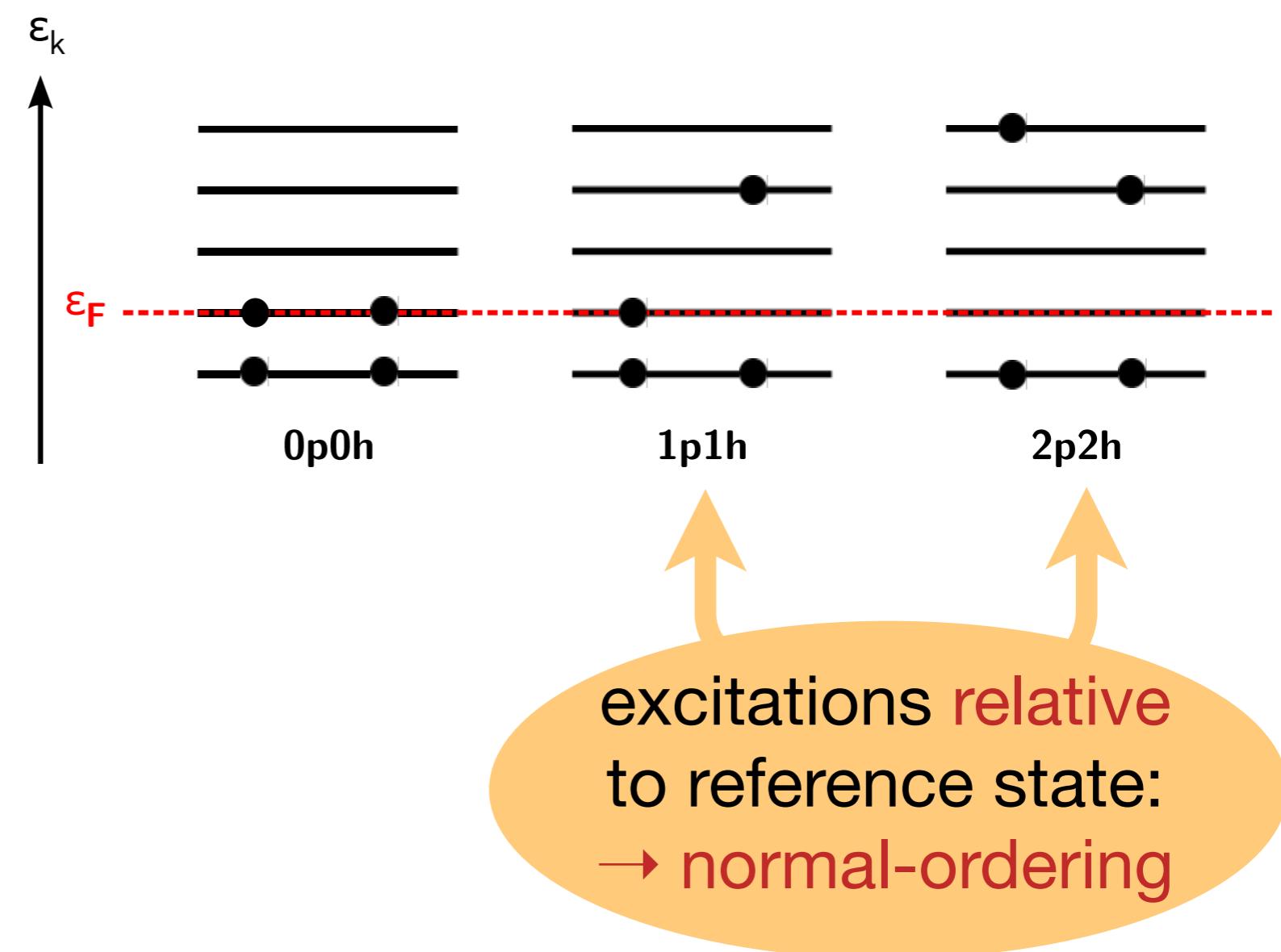
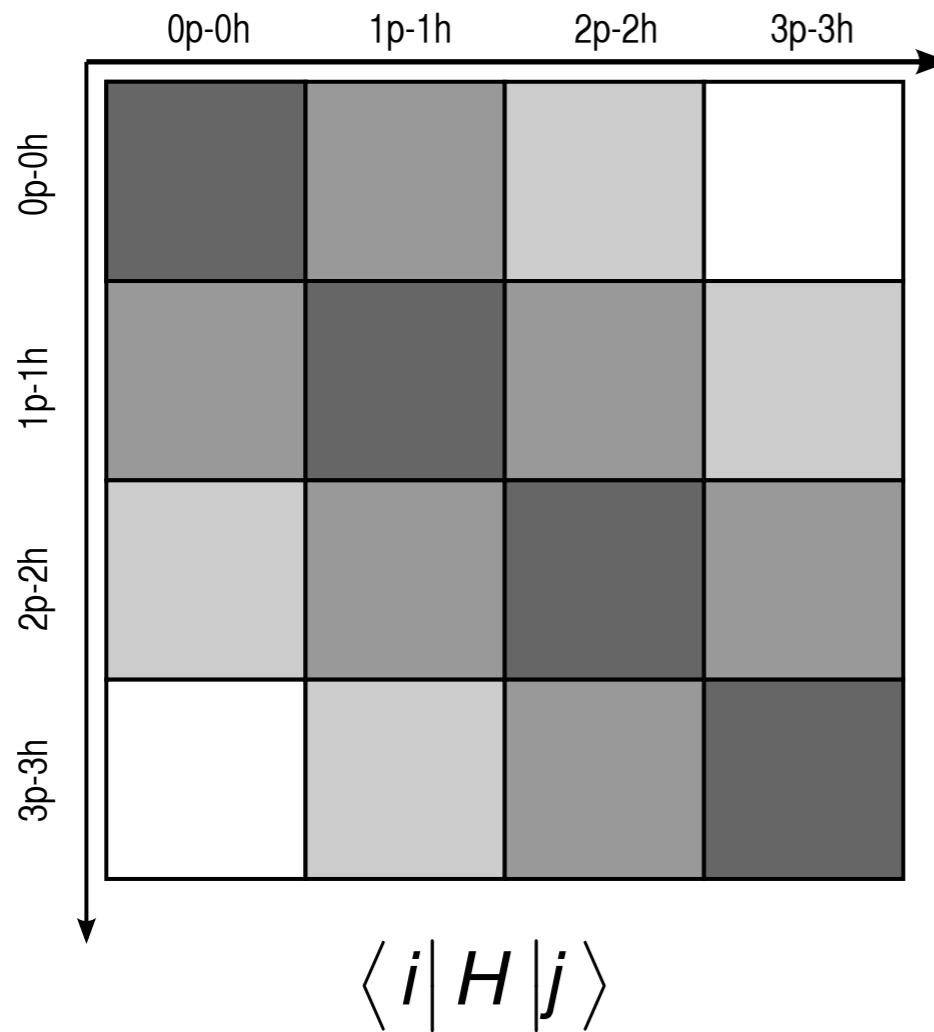
S. K. Bogner, H. H., T. Morris, A. Schwenk, and K. Tsukiyama, to appear in Phys. Rept.
H. H., S. K. Bogner, S. Binder, A. Calci, J. Langhammer, R. Roth, and A. Schwenk,
Phys. Rev. C **87**, 034307 (2013)
K. Tsukiyama, S. K. Bogner, and A. Schwenk, Phys. Rev. Lett. **106**, 222502 (2011)

Basic Concept

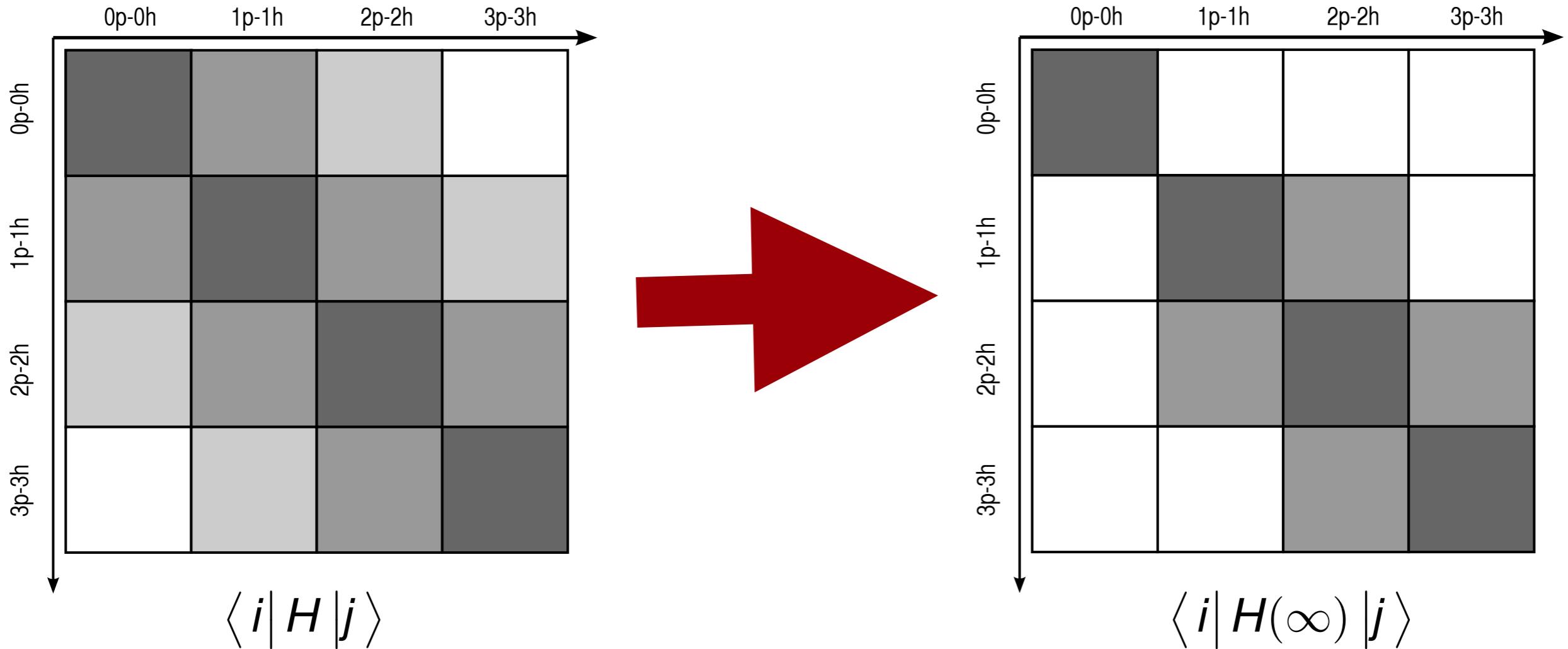
continuous unitary transformation of the Hamiltonian to band-diagonal form w.r.t. a given “uncorrelated” many-body basis

- **flow equation** for Hamiltonian $H(s) = U(s)HU^\dagger(s)$:
$$\frac{d}{ds}H(s) = [\eta(s), H(s)], \quad \eta(s) = \frac{dU(s)}{ds}U^\dagger(s) = -\eta^\dagger(s)$$
- choose $\eta(s)$ to achieve desired behavior, e.g.,
$$\eta(s) = [H_d(s), H_{od}(s)]$$
 to **suppress** (suitably defined) off-diagonal Hamiltonian
- **consistent evolution** for all **observables** of interest

Decoupling in A-Body Space



Decoupling in A-Body Space



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

Normal Ordering

- second quantization: $A_{I_1 \dots I_N}^{k_1 \dots k_N} = a_{k_1}^\dagger \dots a_{k_N}^\dagger a_{I_N} \dots a_{I_1}$

- particle- and hole density matrices:

$$\lambda_I^k = \langle \Phi | A_I^k | \Phi \rangle \rightarrow n_k \delta_I^k, \quad n_k \in \{0, 1\}$$

$$\xi_I^k = \lambda_I^k - \delta_I^k \quad \rightarrow -\bar{n}_k \delta_I^k \equiv -(1 - n_k) \delta_I^k$$

- define normal-ordered operators recursively:

$$A_{I_1 \dots I_N}^{k_1 \dots k_N} = :A_{I_1 \dots I_N}^{k_1 \dots k_N}: + \lambda_{I_1}^{k_1} :A_{I_2 \dots I_N}^{k_2 \dots k_N}: + \text{singles} \\ + \left(\lambda_{I_1}^{k_1} \lambda_{I_2}^{k_2} - \lambda_{I_2}^{k_1} \lambda_{I_1}^{k_2} \right) :A_{I_3 \dots I_N}^{k_3 \dots k_N}: + \text{doubles} + \dots$$

- algebra is simplified significantly because

$$\langle \Phi | :A_{I_1 \dots I_N}^{k_1 \dots k_N}: | \Phi \rangle = 0$$

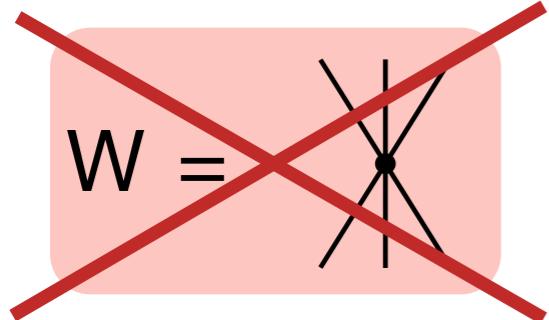
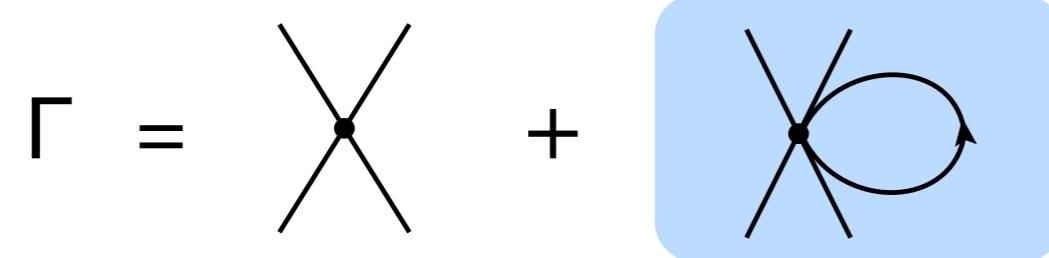
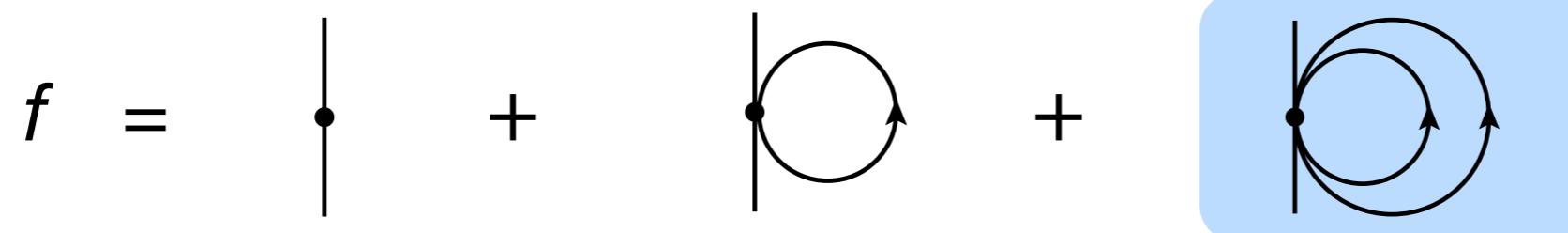
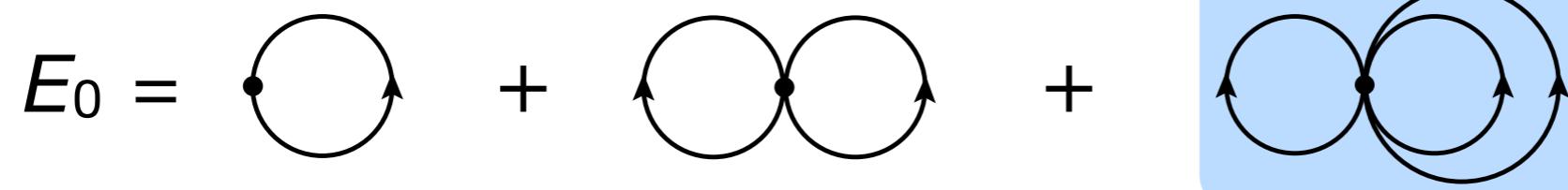
- Wick's theorem gives simplified expansions (fewer terms!) for products of normal-ordered operators

Normal-Ordered Hamiltonian



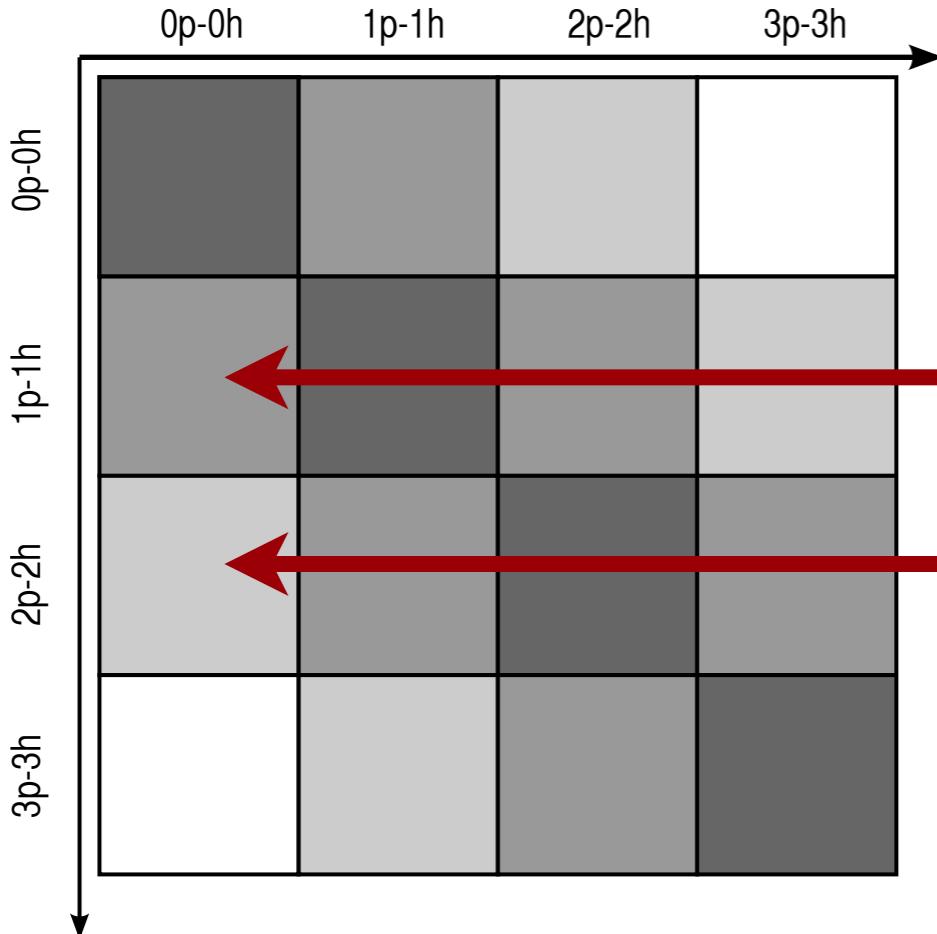
Normal-Ordered Hamiltonian

$$H = E_0 + \sum_{kl} f_l^k : A_l^k : + \frac{1}{4} \sum_{klmn} \Gamma_{mn}^{kl} : A_{mn}^{kl} : + \frac{1}{36} \sum_{ijklmn} W_{lmn}^{ijk} : A_{lmn}^{ijk} :$$



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

Choice of Generator



$$\langle \begin{matrix} p \\ h \end{matrix} | H | \Psi \rangle = \sum_{kl} f_l^k \langle \Psi | : A_p^h :: A_l^k : | \Psi \rangle = -n_h \bar{n}_p f_h^p$$

$$\langle \begin{matrix} pp' \\ hh' \end{matrix} | H | \Psi \rangle = \sum_{klmn} \Gamma_{mn}^{kl} \langle \Psi | : A_{pp'}^{hh'} :: A_{mn}^{kl} : | \Psi \rangle \sim \Gamma_{hh'}^{pp'}$$

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

$$H^{od} \equiv f^{od} + \Gamma^{od}, \quad f^{od} \equiv \sum_{ph} f_h^p : A_h^p : + \text{H.c.}, \quad \Gamma^{od} \equiv \sum_{pp'hh'} \Gamma_{hh'}^{pp'} : A_{hh'}^{pp'} : + \text{H.c.}$$

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

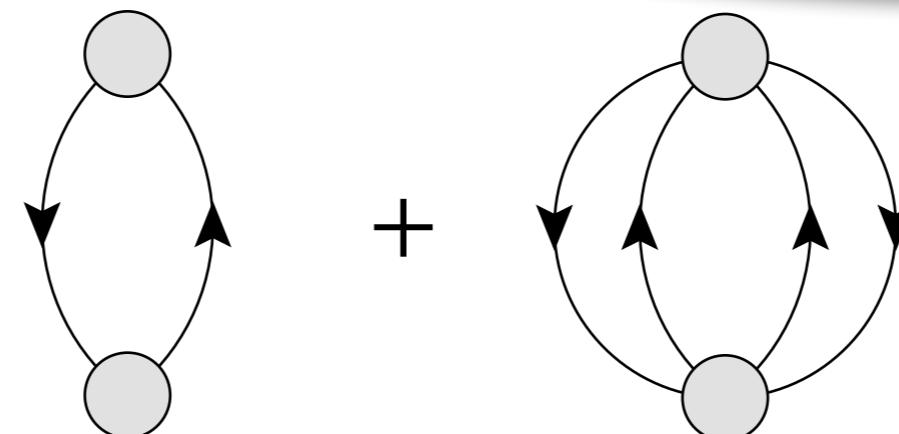
IM-SRG(2) Flow Equations



0-body Flow

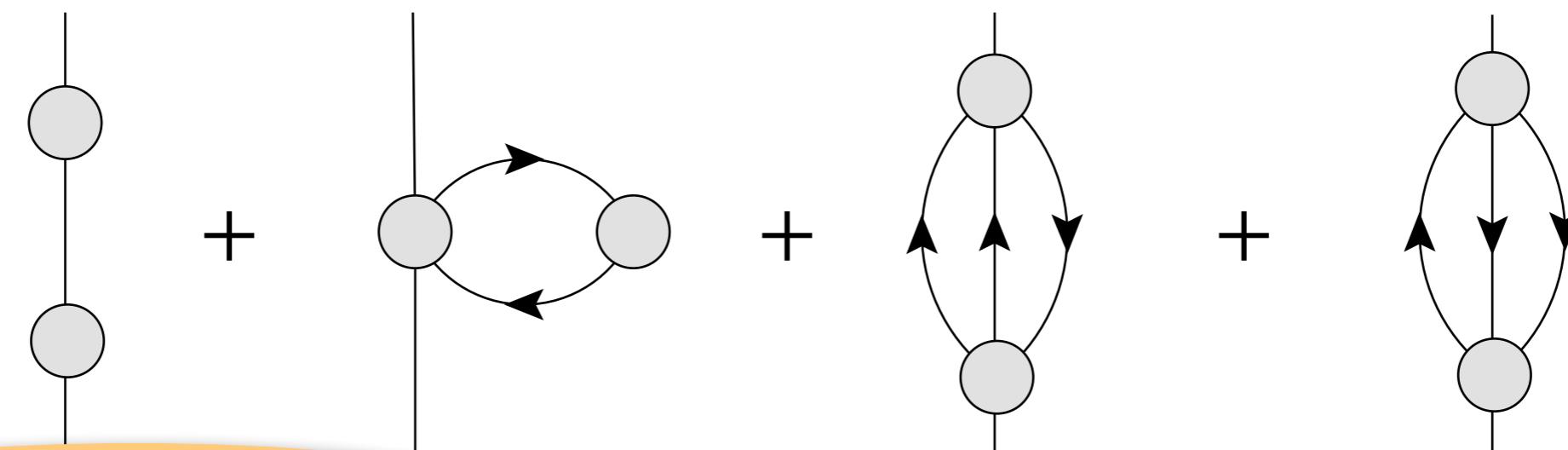
~ 2nd order MBPT for $H(s)$

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



1-body Flow

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



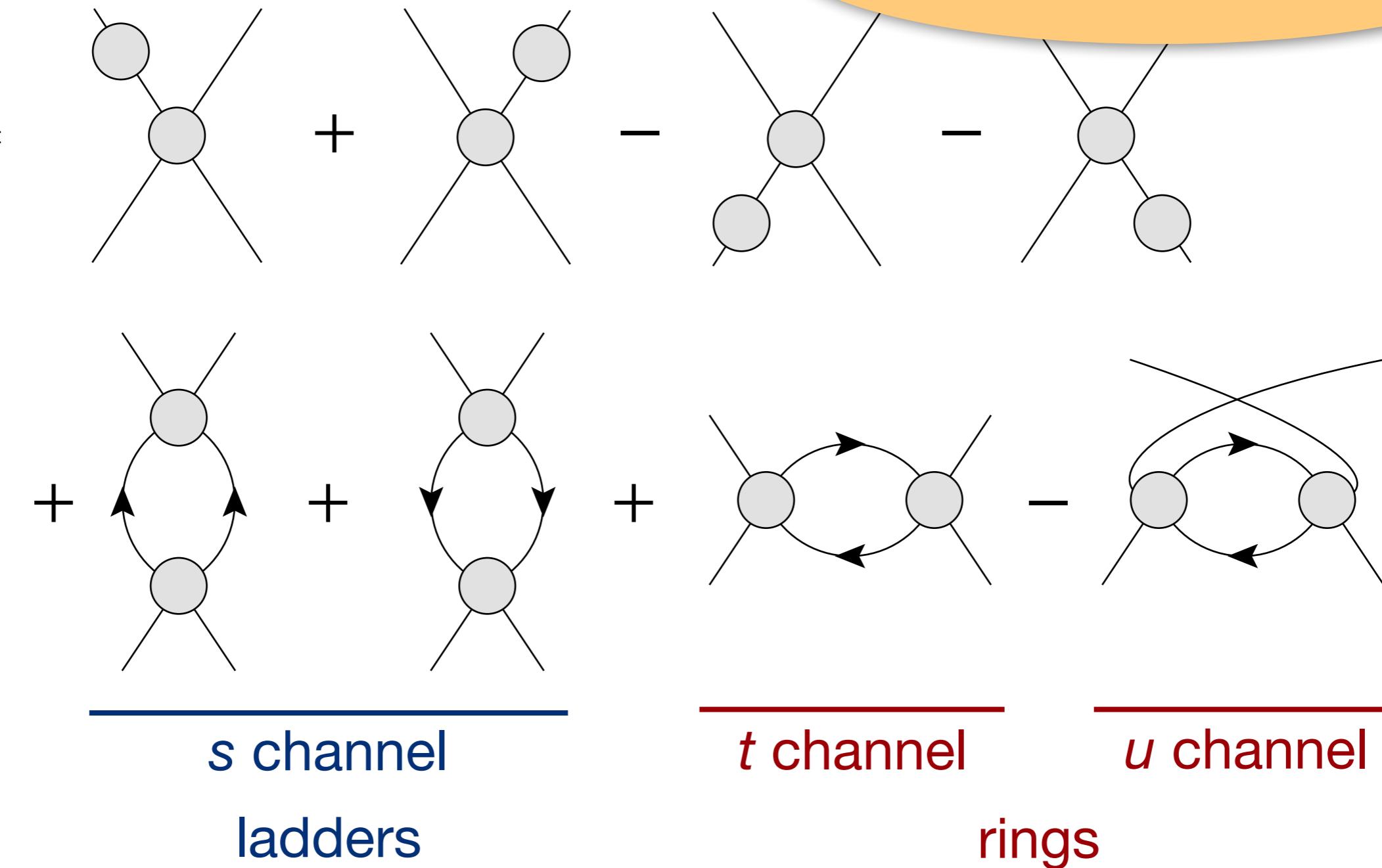
IM-SRG(2): truncate ops.
at two-body level

IM-SRG(2) Flow Equations



2-body Flow

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



Multi-Reference IM-SRG



- generalized Wick's theorem for arbitrary reference states (Kutzelnigg & Mukherjee)
- define irreducible n-body density matrices of reference state:

$$\rho_{mn}^{kl} = \lambda_{mn}^{kl} + \lambda_m^k \lambda_n^l - \lambda_n^k \lambda_m^l$$

$$\rho_{lmn}^{ijk} = \lambda_{lmn}^{ijk} + \lambda_l^i \lambda_{mn}^{jk} + \lambda_l^i \lambda_m^j \lambda_n^k + \text{permutations}$$

⋮ ⋮ ⋮

- irreducible densities give rise to additional contractions:

$$: A_{cd\dots}^{ab\dots} : A_{mn\dots}^{kl\dots} : \longrightarrow \lambda_{mn}^{ab}$$

$$: A_{cd\dots}^{ab\dots} : A_{mn\dots}^{kl\dots} :$$

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

⋮ ⋮ ⋮

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)

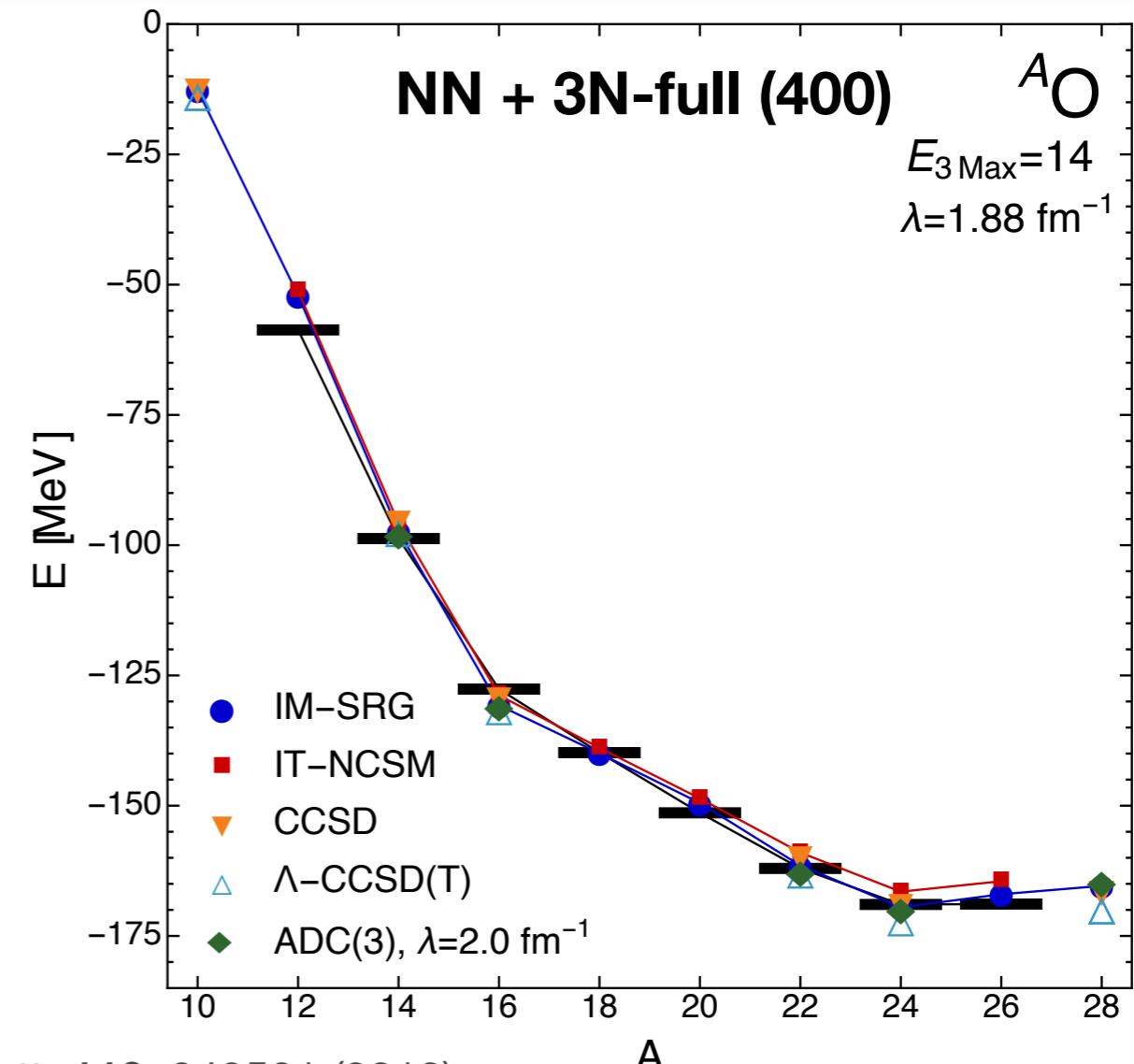
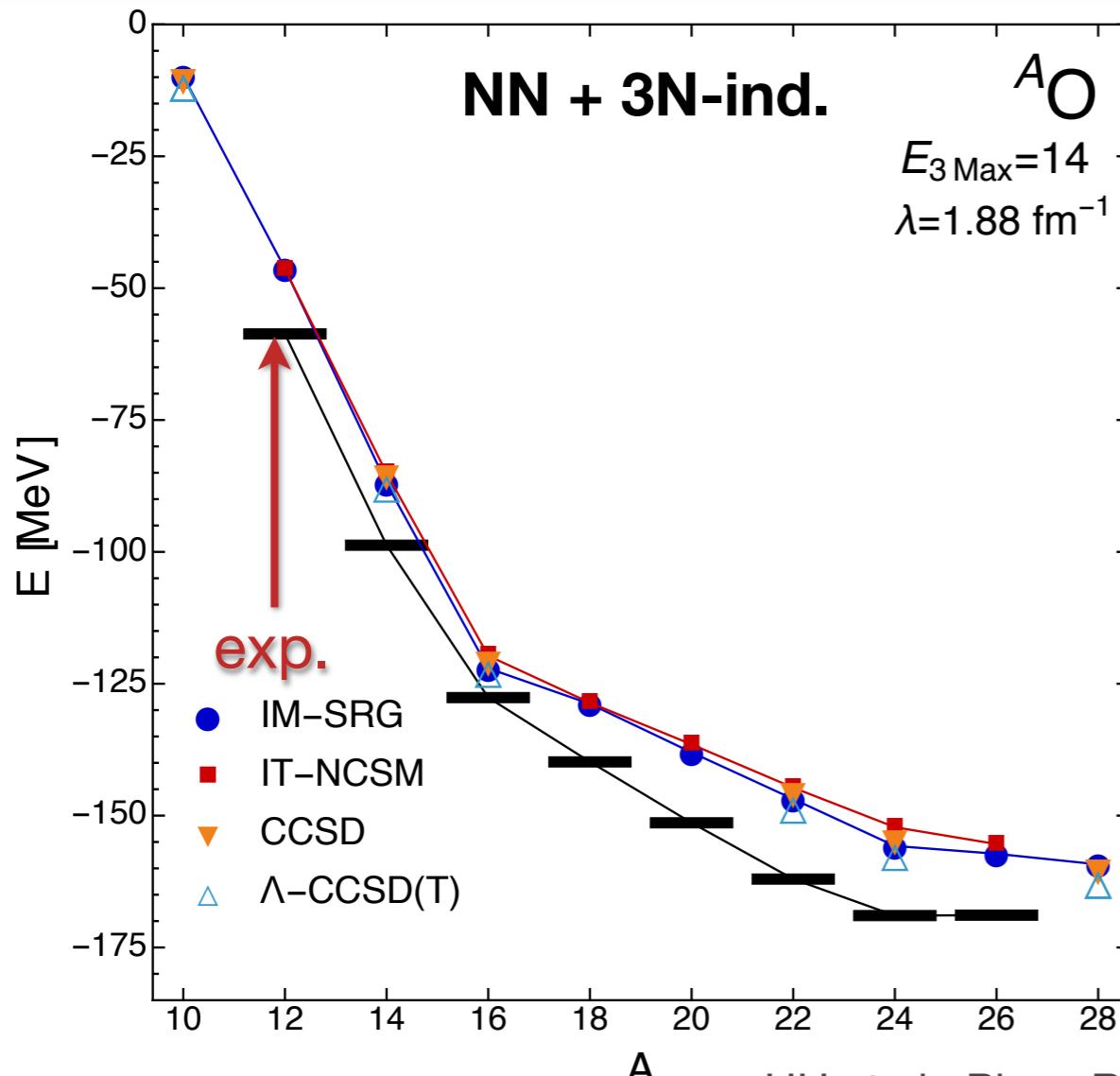
Initial Hamiltonian

- NN: chiral interaction at N³LO (Entem & Machleidt)
- 3N: chiral interaction at N²LO (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



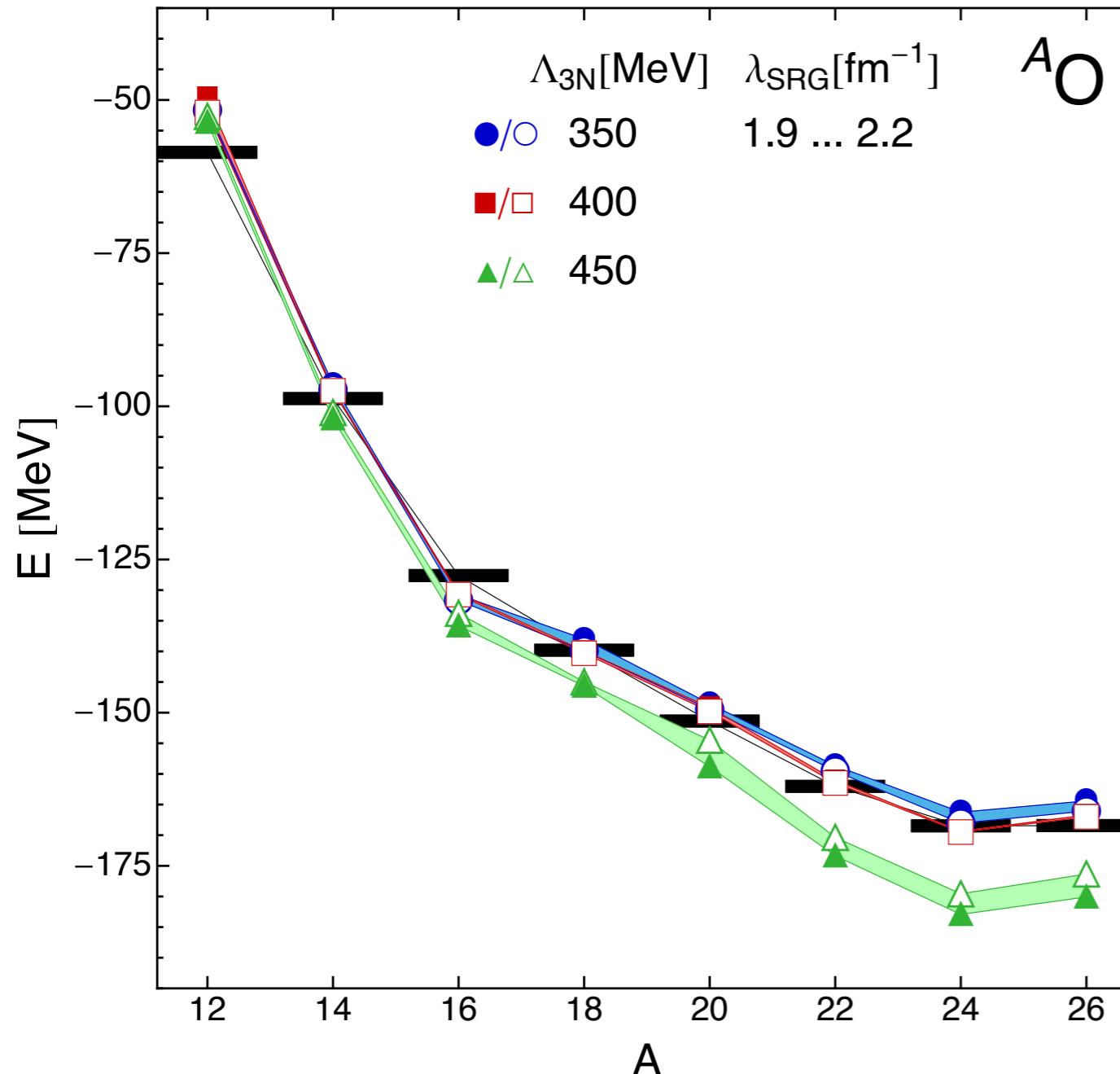
HH et al., Phys. Rev. Lett. **110**, 242501 (2013)

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

Variation of Scales

NN + 3N-full



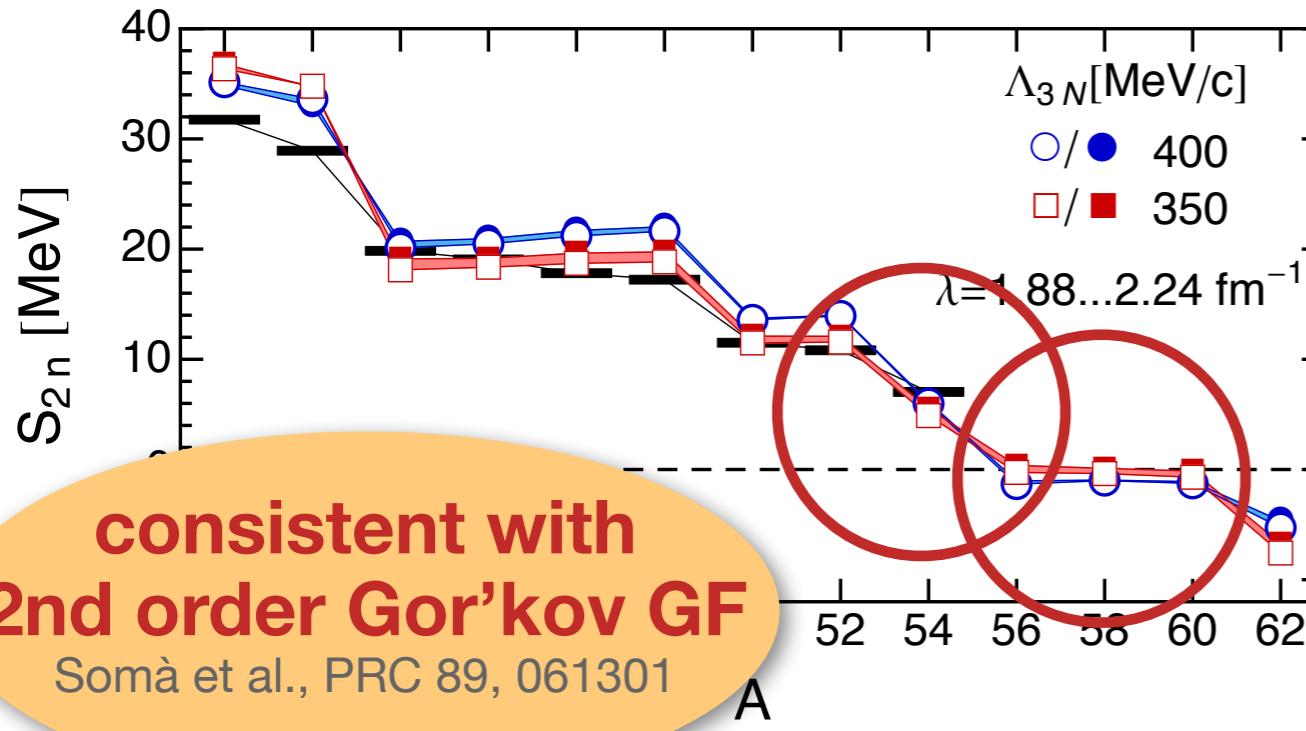
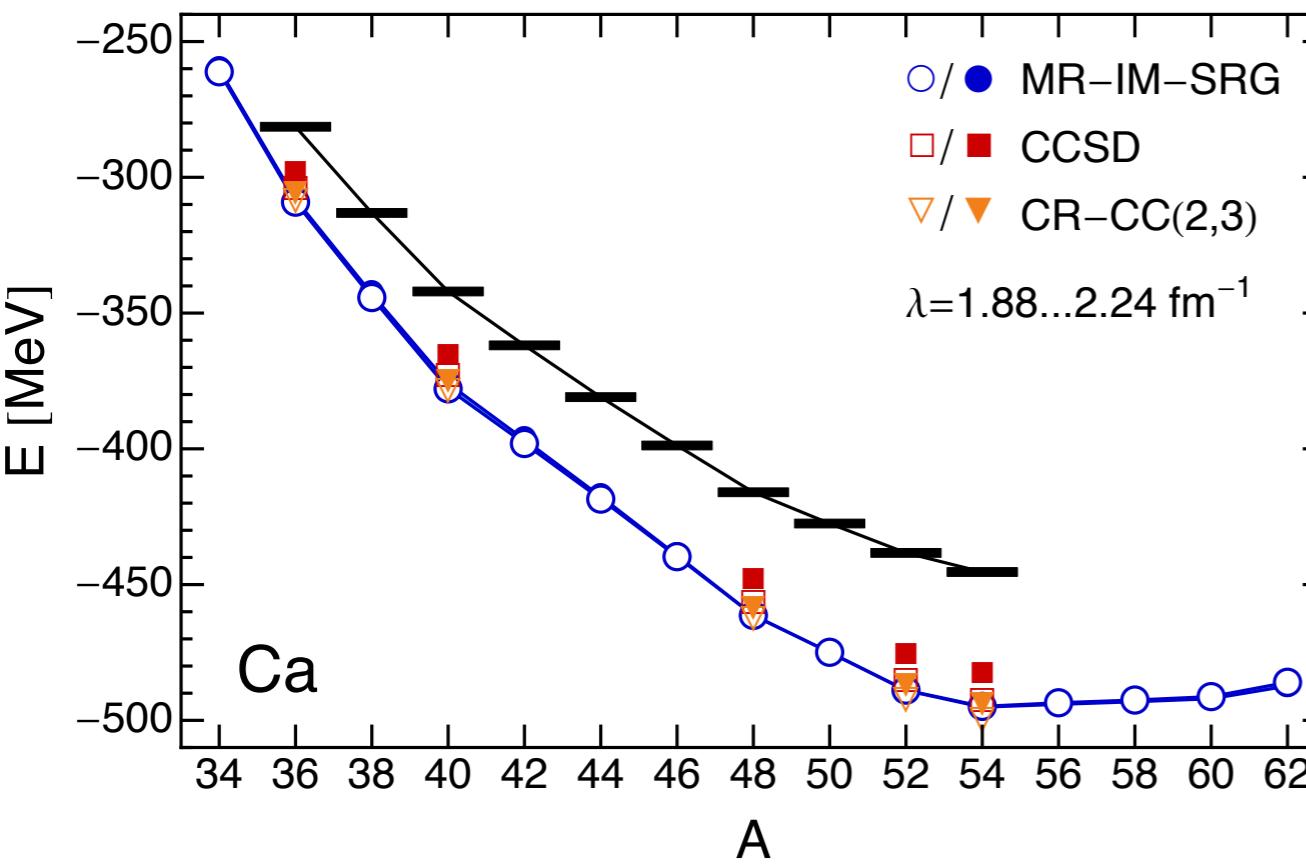
- variation of **initial 3N cutoff only**
- diagnostics for chiral interactions
- dripline at $A=24$ is robust under variations
- (leading) continuum effects too small to bind ^{26}O

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

Two-Neutron Separation Energies

PRC 90, 041302(R) (2014)

NN + 3N-full (400)



consistent with
2nd order Gor'kov GF

Somà et al., PRC 89, 061301

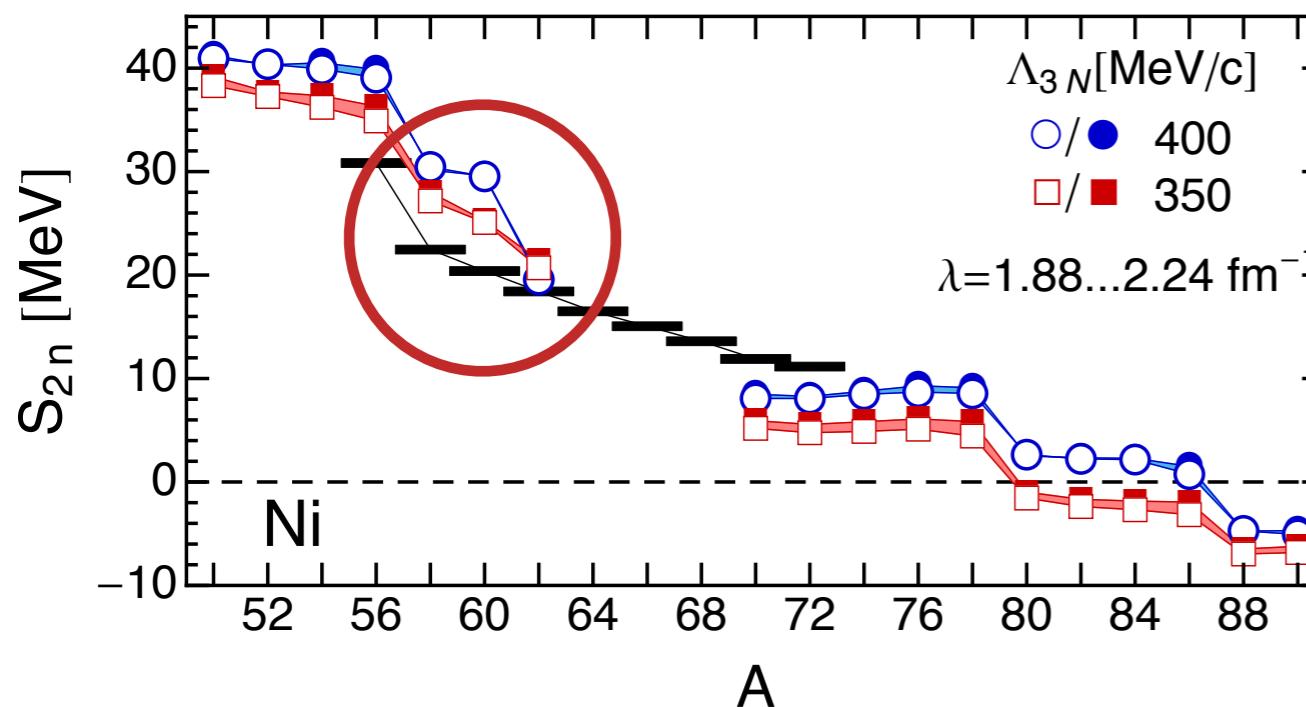
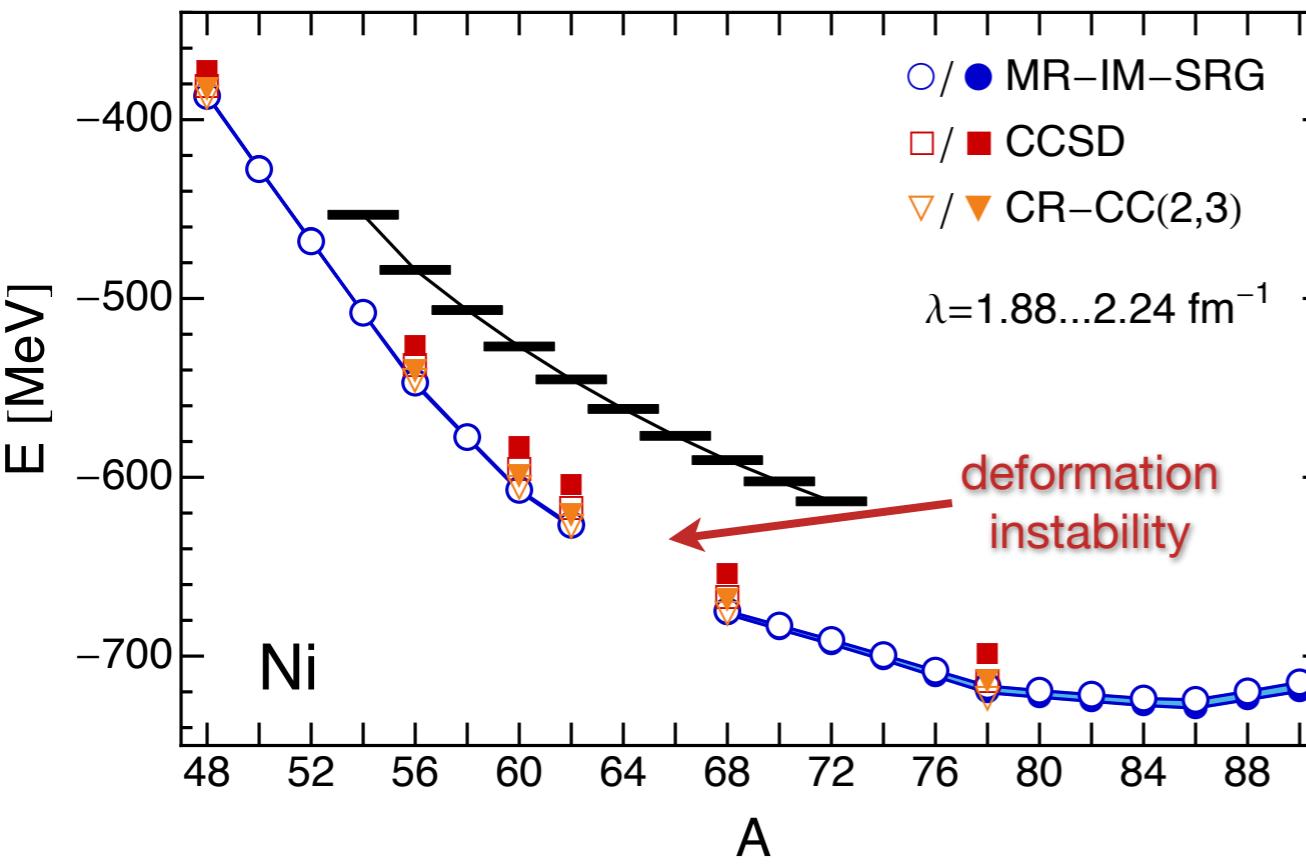
- differential observables (S_{2n} , spectra,...) filter out interaction components that cause overbinding
- predict flat trends for g.s. energies/ S_{2n} beyond ^{54}Ca
- await experimental data
- $^{52}\text{Ca}, ^{54}\text{Ca}$ robustly magic due to 3N interaction
- no continuum coupling yet, other S_{2n} uncertainties < 1 MeV

Two-Neutron Separation Energies



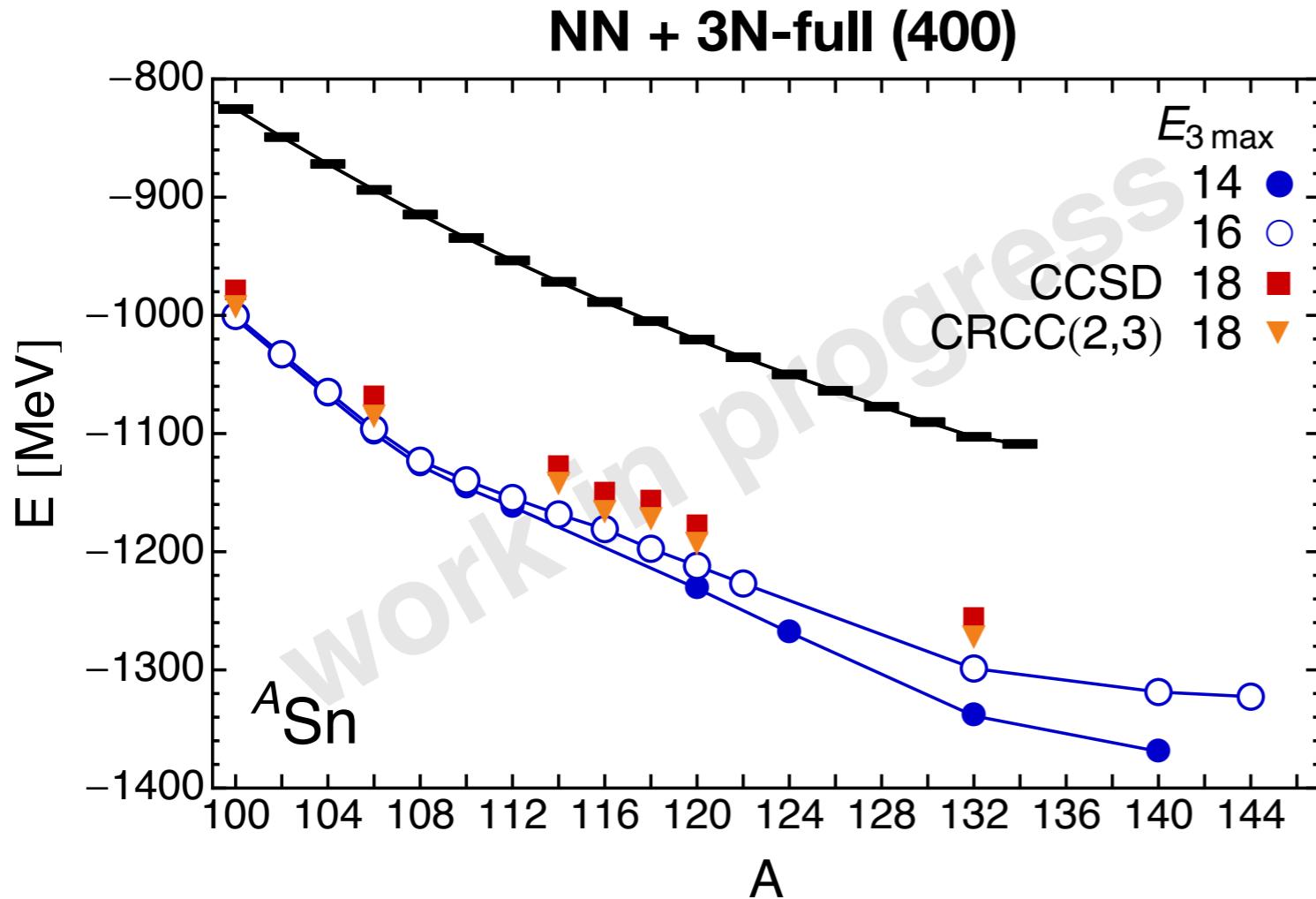
PRC 90, 041302(R) (2014)

NN + 3N-full (400)



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

The *Ab Initio* Mass Frontier: Tin



$E_{3\text{max}}$	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:

$$e_1 + e_2 + e_3 \leq E_{3\text{max}}$$
 $(e_{1,2,3} : \text{SHO energy quantum numbers})$
- need technical improvements to go further

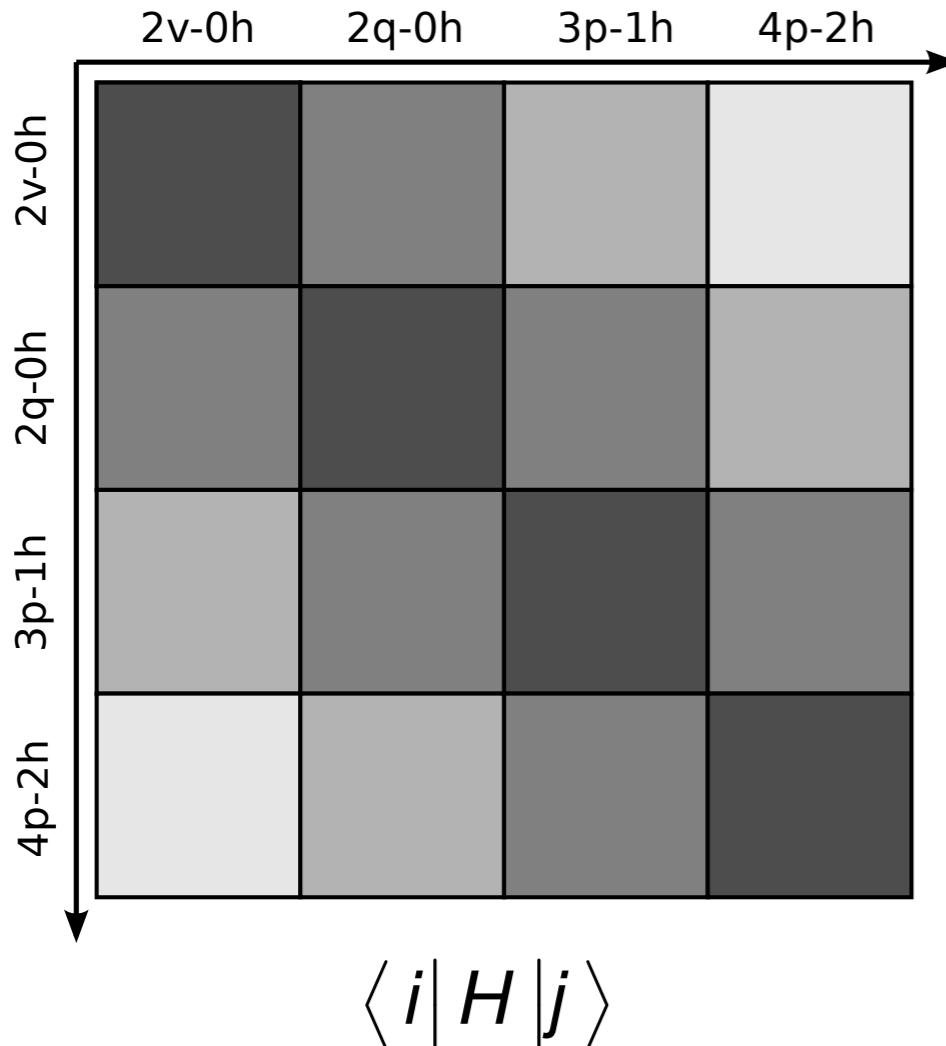
IM-SRG + Shell Model for Excited States

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)

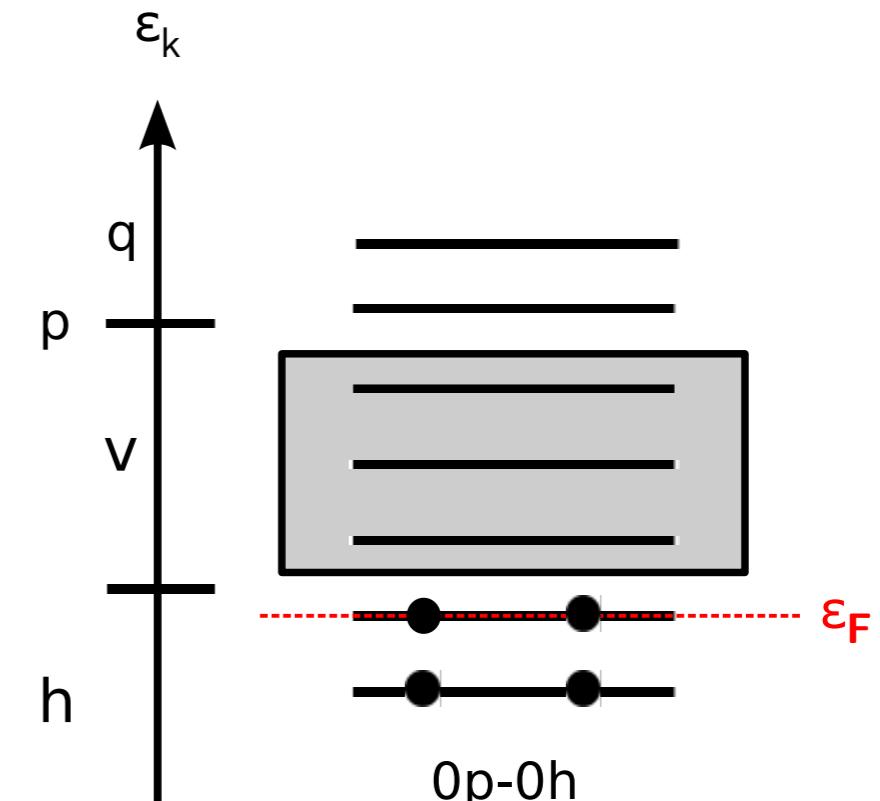
Valence Space Decoupling



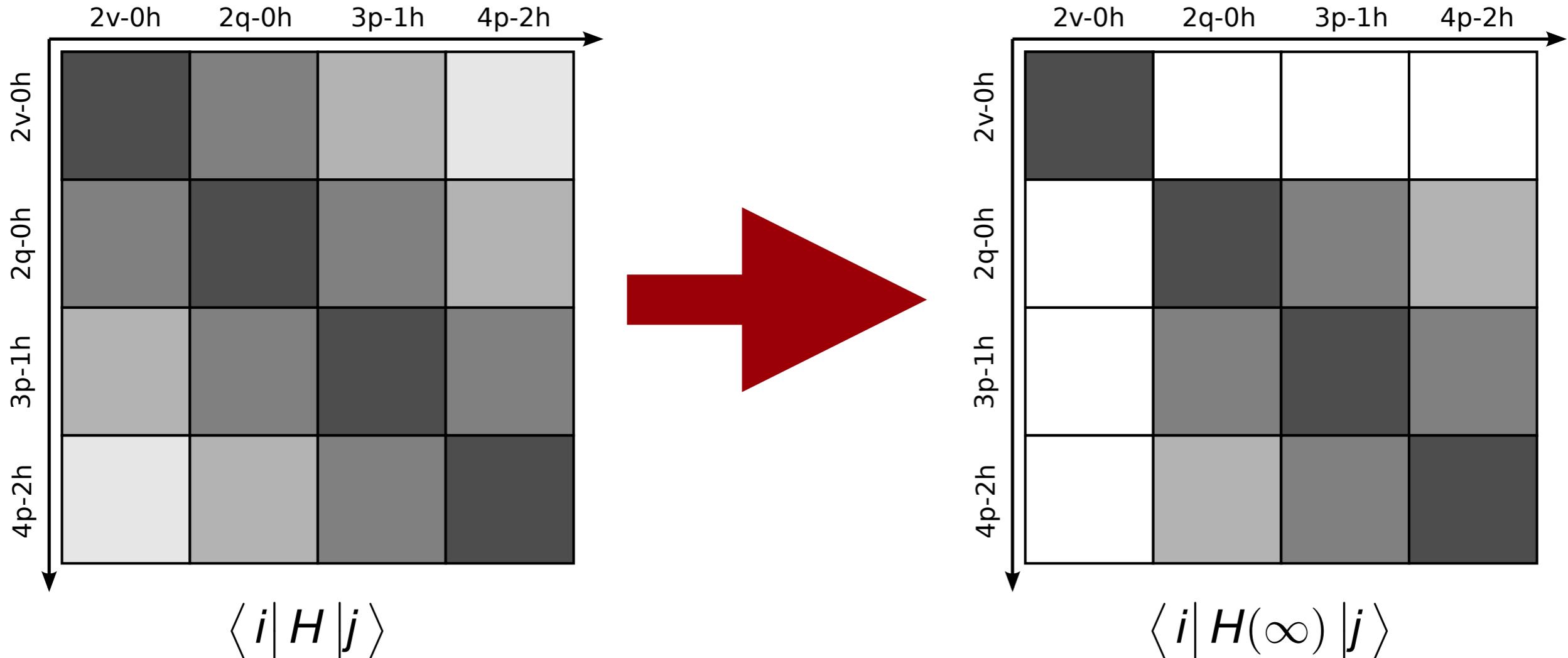
non-valence
particle states

valence
particle states

hole states
(core)



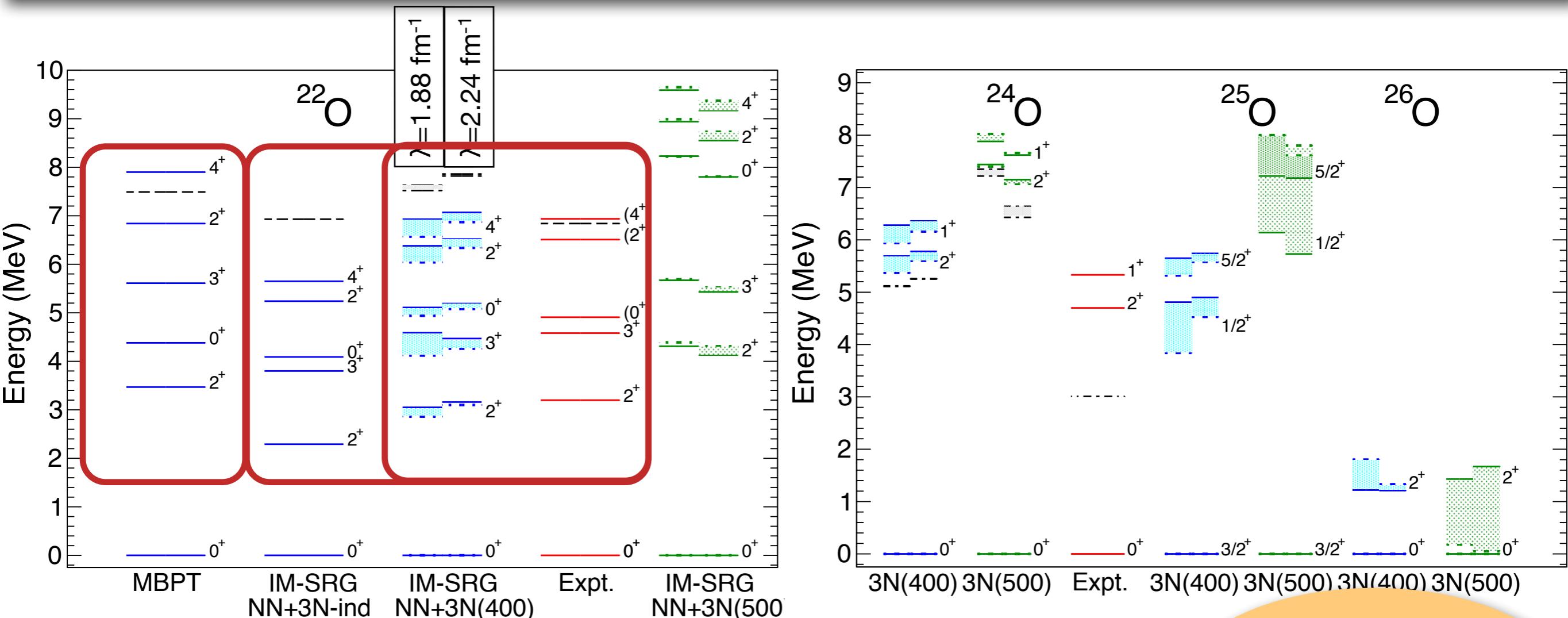
Valence Space Decoupling



- construct generator from off-diagonal Hamiltonian

$$\{H^{od}\} = \{\mathbf{f}_{h'}^h, \mathbf{f}_{p'}^p, f_h^p, \mathbf{f}_v^q, \Gamma_{hh'}^{pp'}, \Gamma_{hv}^{pp'}, \Gamma_{vv'}^{pq}\} \text{ & H.c.}$$

From Oxygen...



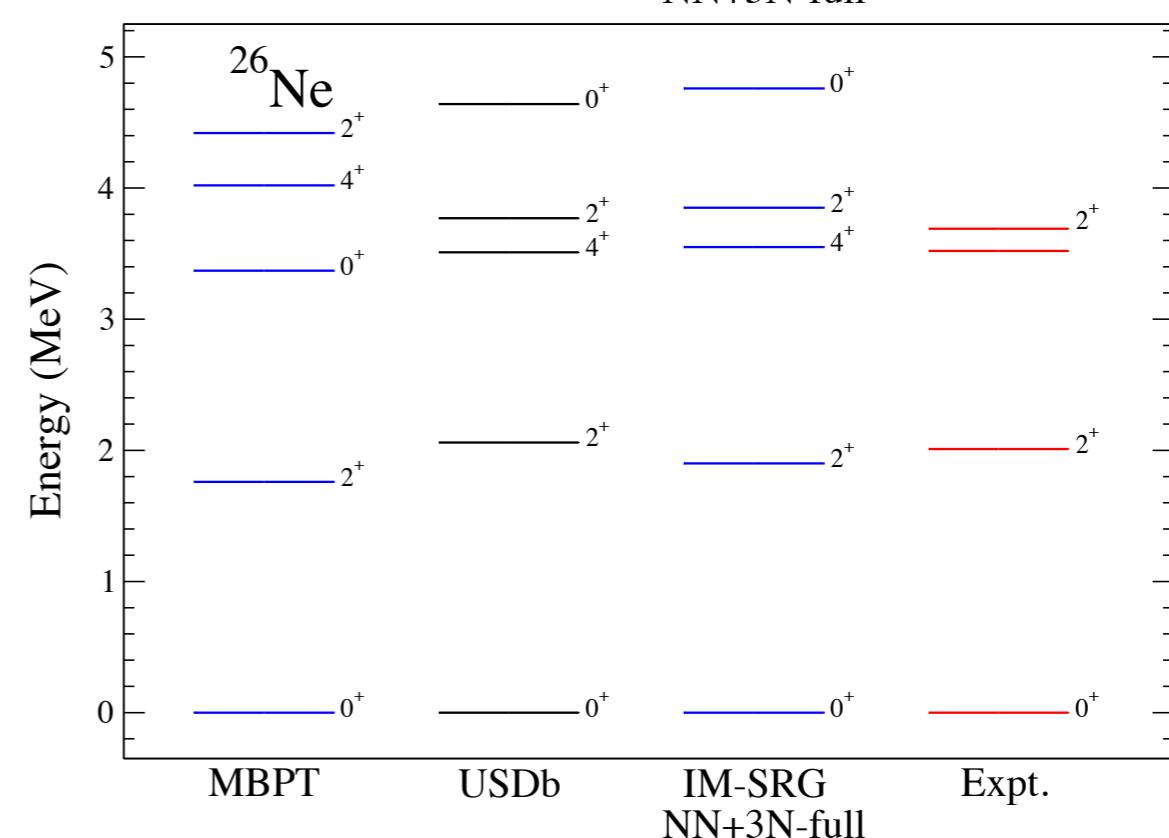
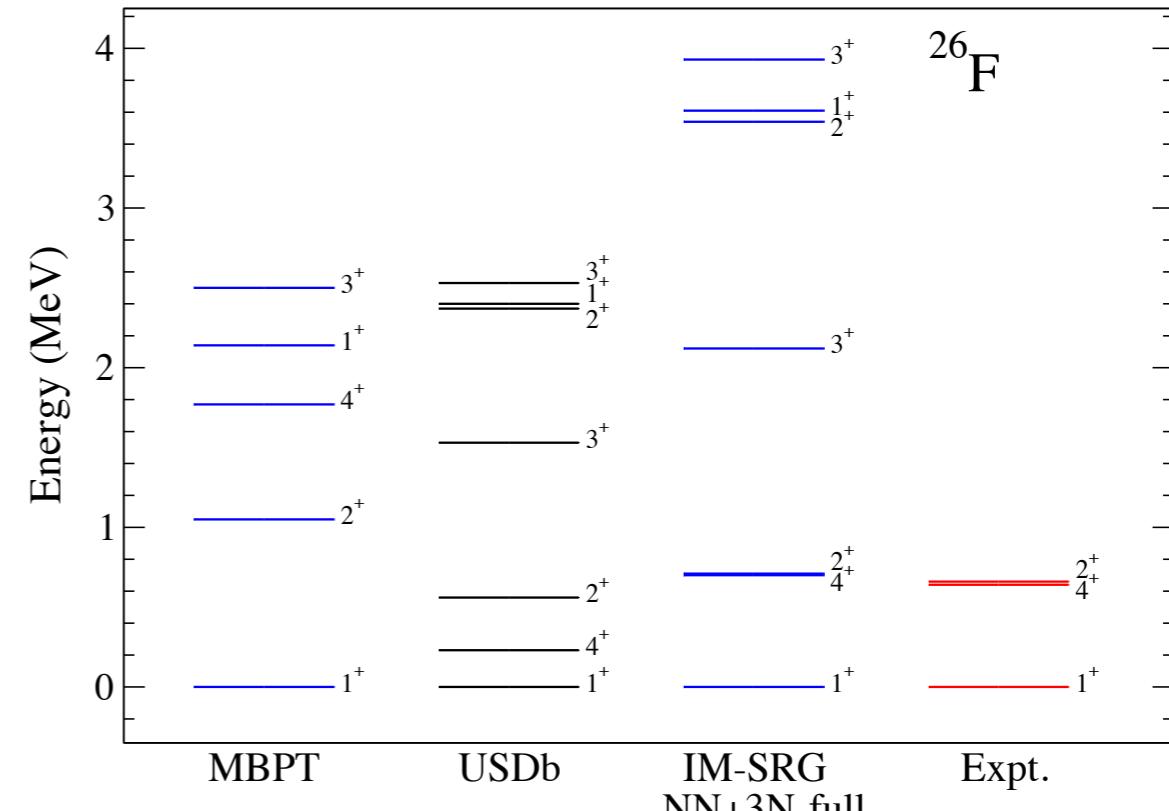
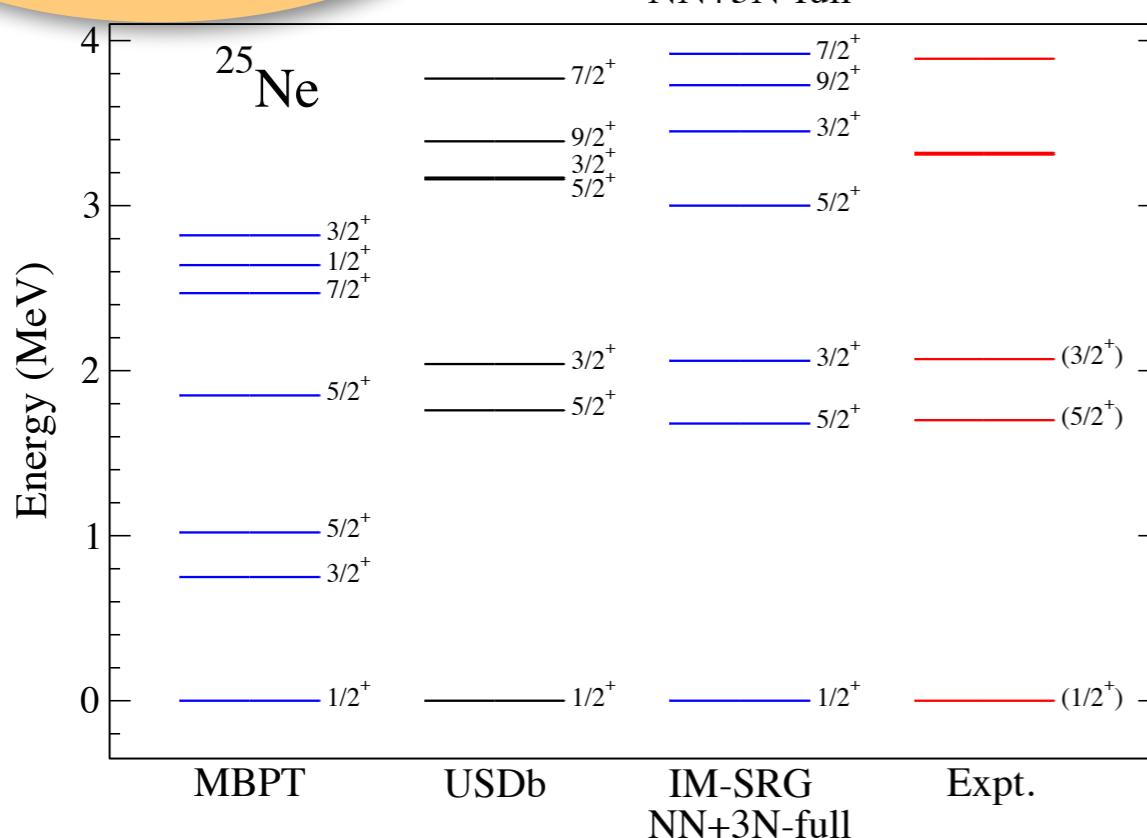
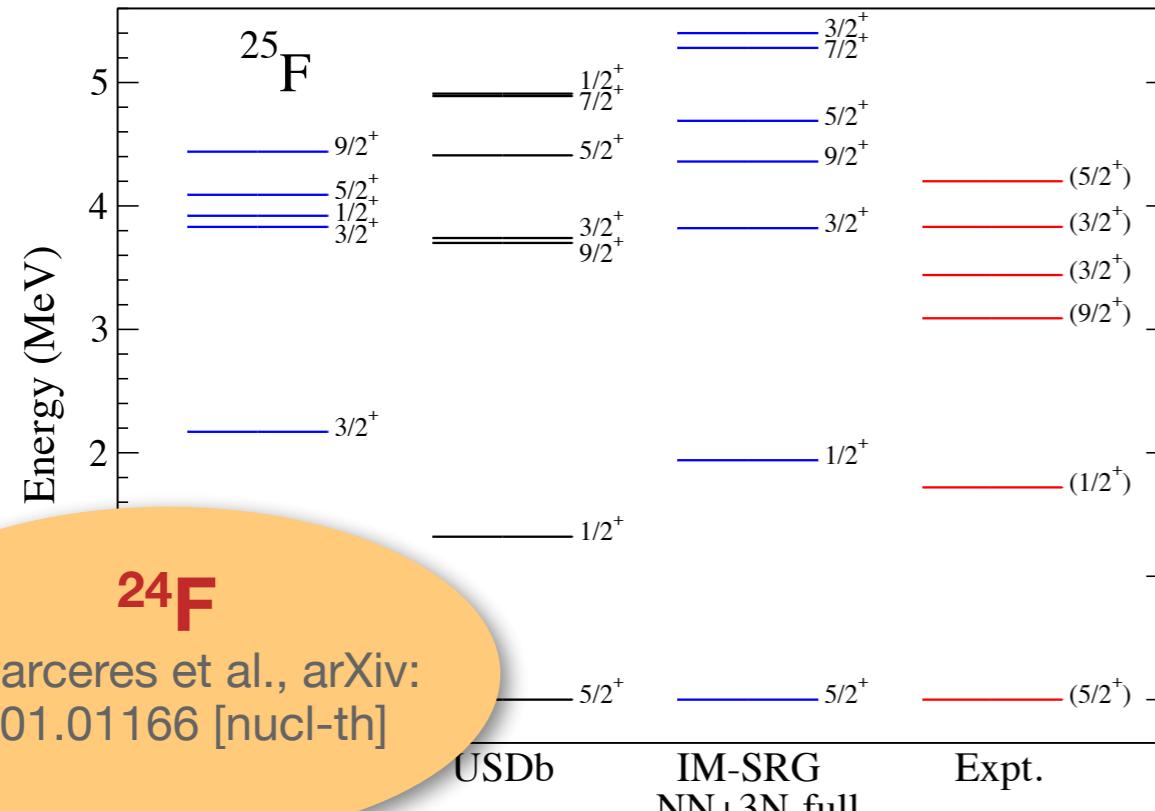
shading: $\hbar\Omega$ variation

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

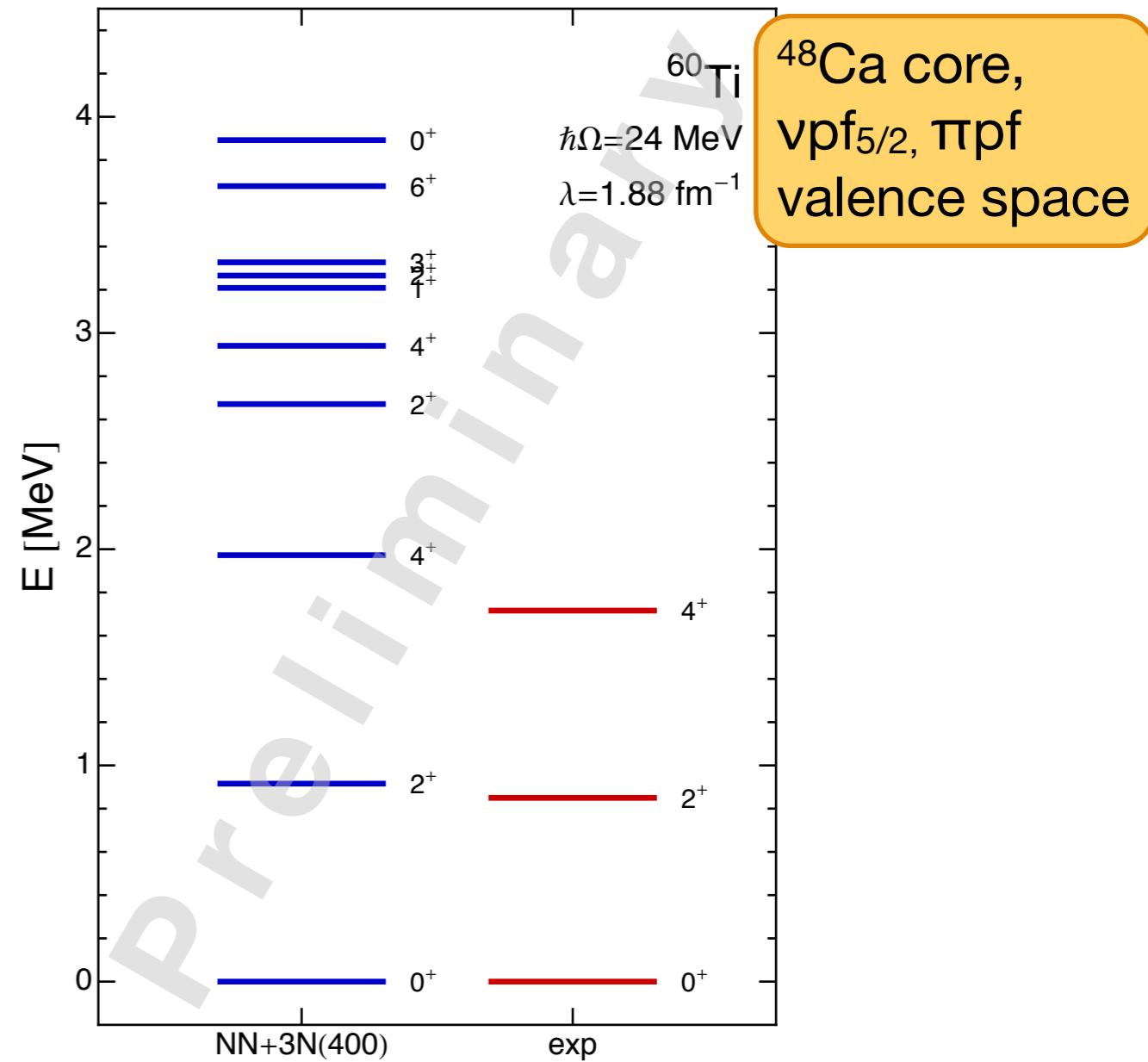
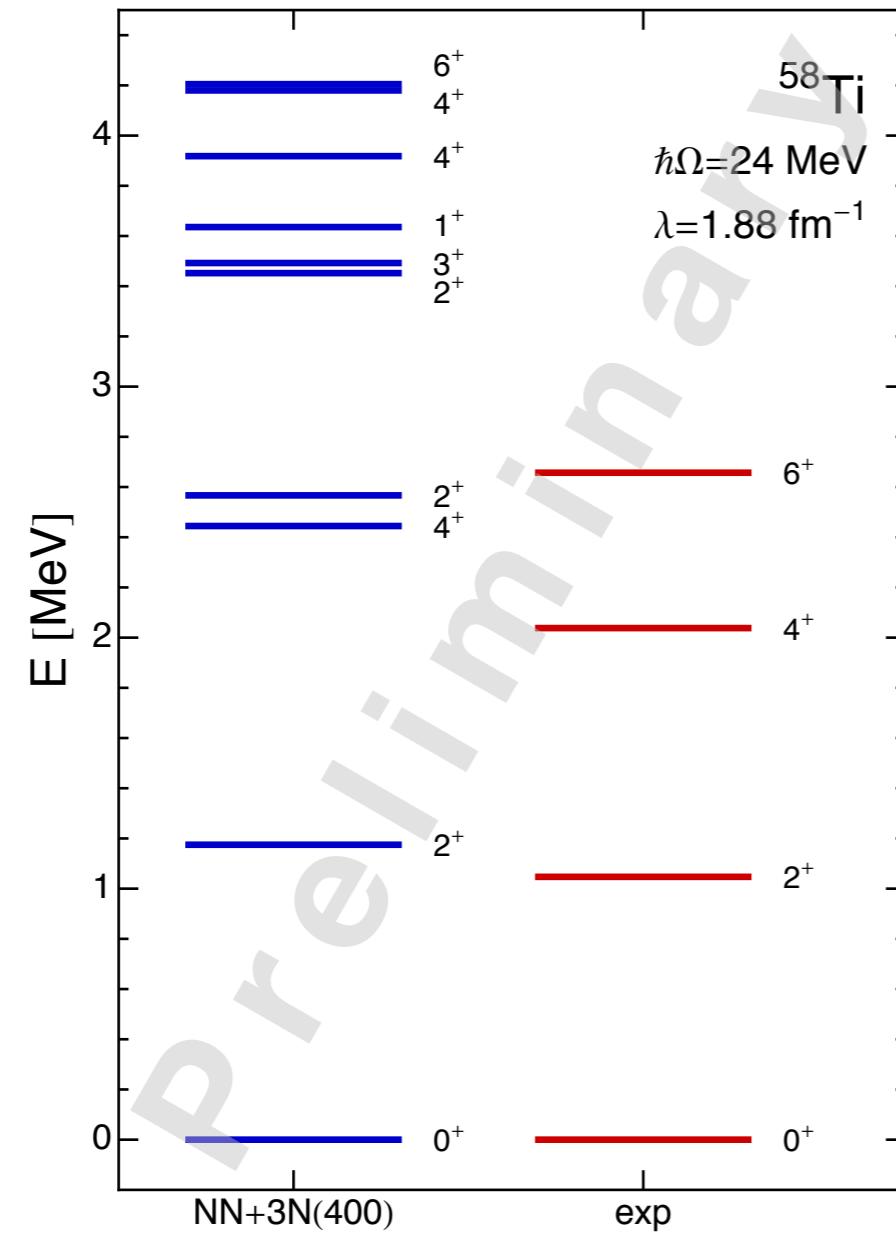
**continuum
lowers states
by <1 MeV**

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

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



... And Beyond

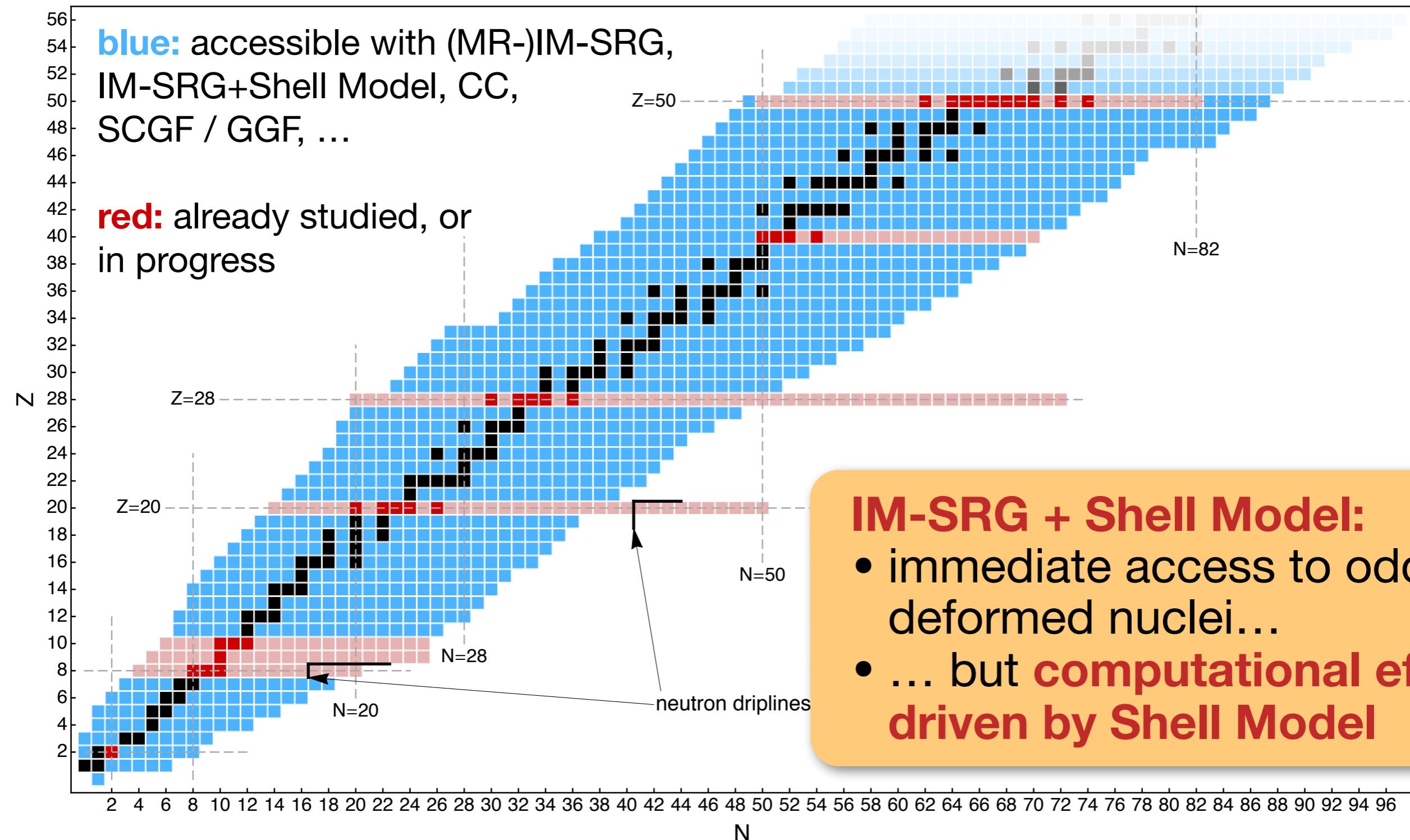


experimental data: A. Gade et al., Phys. Rev. Lett. **112**, 112503 (2014) and NNDC

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

Next Steps

Reach of Ab Initio Methods



Equations-of-Motion for Excitations



- describe “excited states” based on reference state:

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

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

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

- 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, ...)

$$R_k = \sum_{ph} R_{ph}^{(k)} : a_p^\dagger a_h : + \sum_{pp'hh'} R_{pp'hh'}^{(k)} : a_p^\dagger a_{p'}^\dagger a_{h'} a_h : + \dots$$

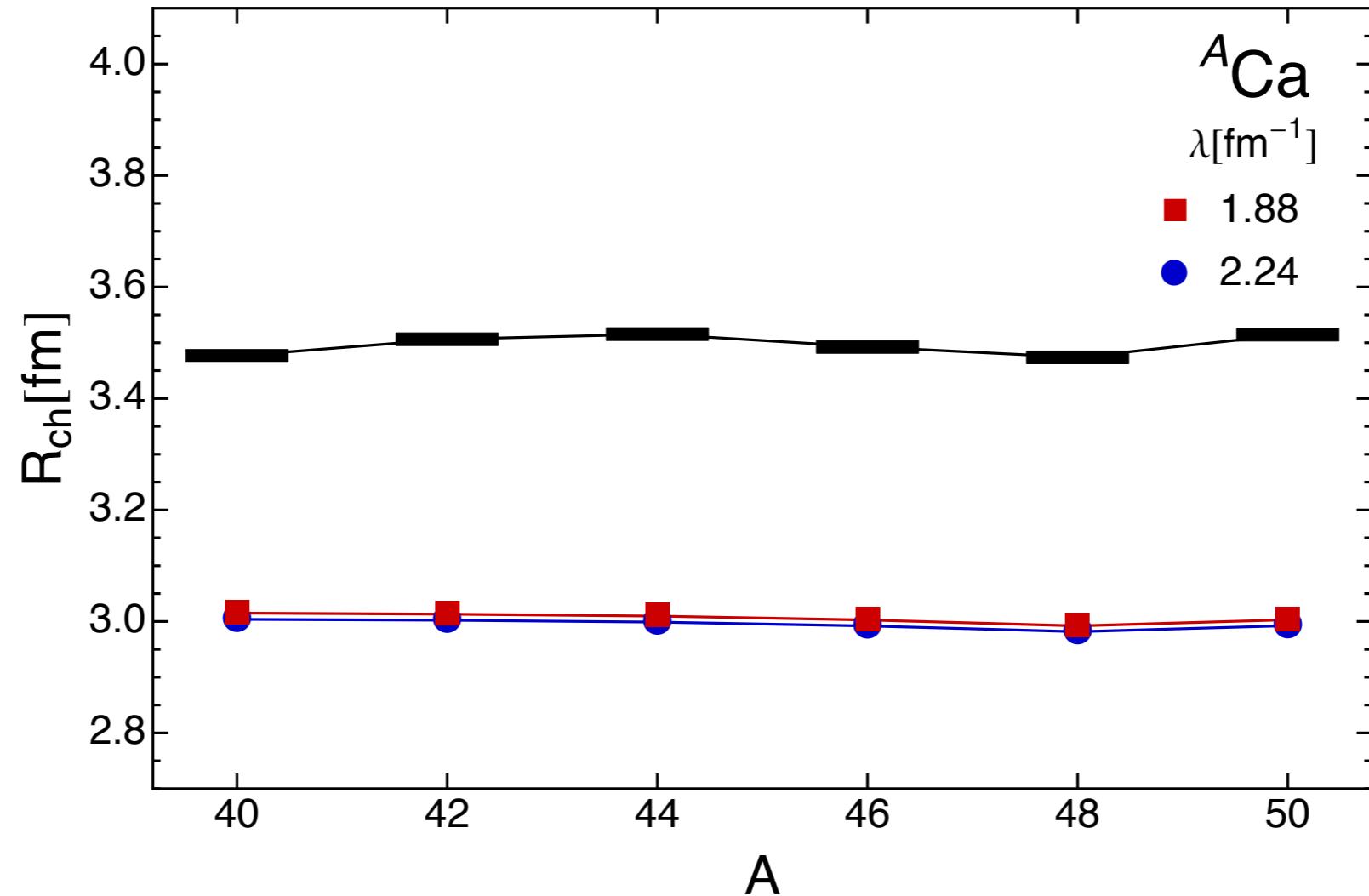
→ giant resonances

- particle attachment (analogous for removal):

$$R_k = \sum_{ph} R_p^{(k)} : a_p^\dagger : + \sum_{pp'h} R_{pp'h}^{(k)} : a_p^\dagger a_{p'}^\dagger a_h : + \dots$$

→ ground and excited states in odd nuclei

Effective Operators



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

Magnus Series Formulation



- construct unitary transformation explicitly:

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

also see talk
by R. Stroberg

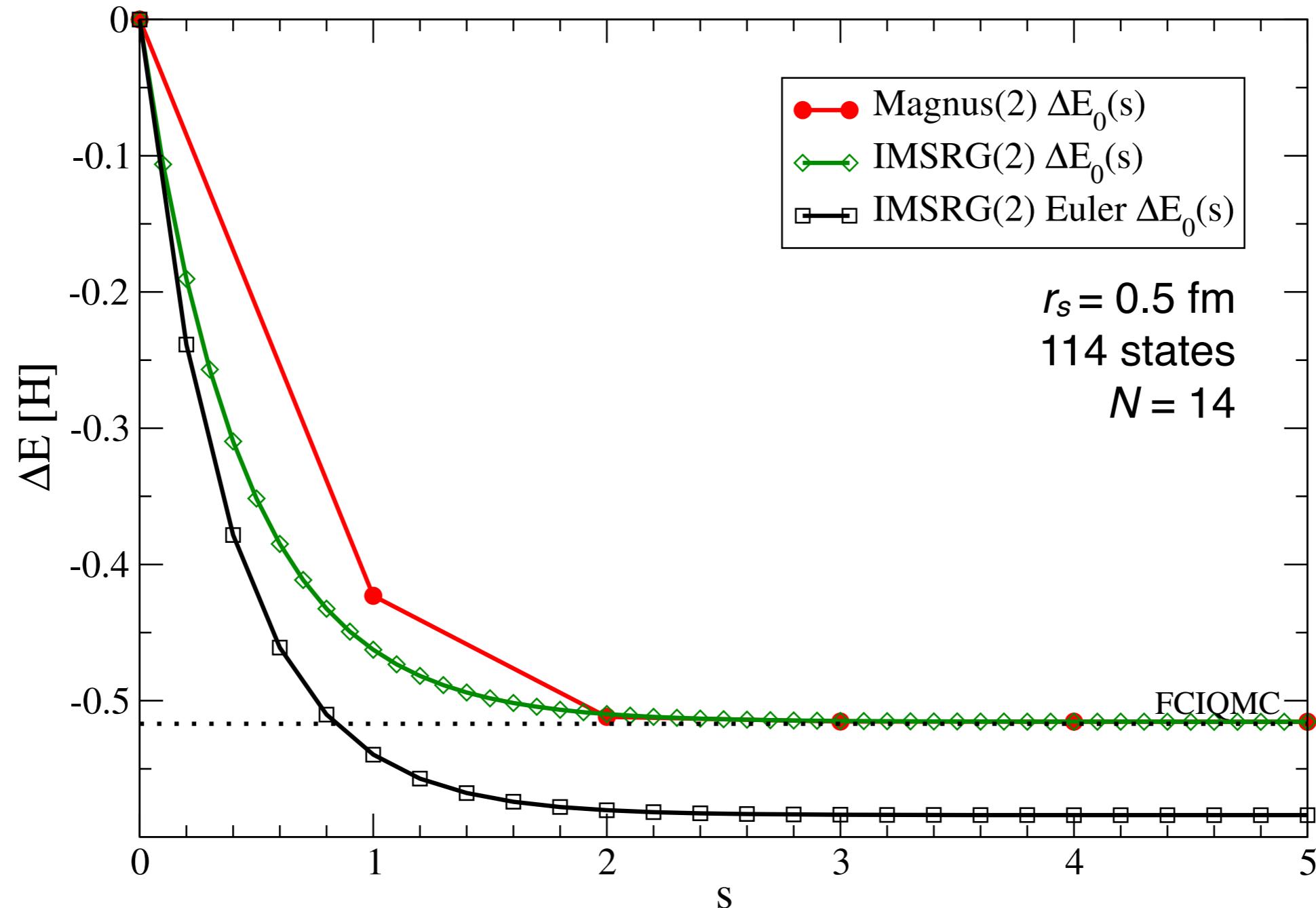
- flow equation for Magnus operator :

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

(B_k : Bernoulli numbers)

- construct $O(s) = U(s)O_0U^\dagger(s)$ 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, S. K. Bogner, in preparation

Conclusions

Conclusions



- IM-SRG is a powerful *ab initio* framework for closed- and open-shell, medium-mass & (heavy) nuclei
- derivation of Shell-Model interactions
 - immediate access to spectra, odd nuclei, intrinsic deformation (at Shell Model numerical cost)
- soon:
 - EOM for excited states
 - effective transition operators (see R. Stroberg's talk)
 - triples (everywhere)
- new perspectives for old (?) problems: evolution of long-range correlations, construction of density functionals...

Acknowledgments

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

E. Gebrerufael, K. Hebeler,
R. Roth, A. Schwenk, J. Simonis,
C. Stumpf, K. Vobig
TU Darmstadt, Germany

A. Calci, J. D. Holt, R. Stroberg
TRIUMF, Canada

S. Binder, K. Wendt
UT Knoxville & Oak Ridge National Laboratory

G. Papadimitriou
Iowa State University

R. Furnstahl, S. König, S. More,
R. Perry
The Ohio State University

P. Papakonstantinou
IBS / Rare Isotope Science Project, South Korea

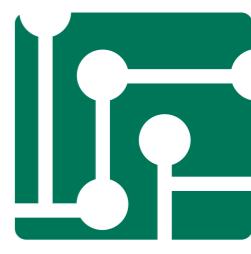
T. Duguet, V. Somà
CEA Saclay, France



NUCLEI
Nuclear Computational Low-Energy Initiative



Ohio Supercomputer Center



ICER

Supplements

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

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

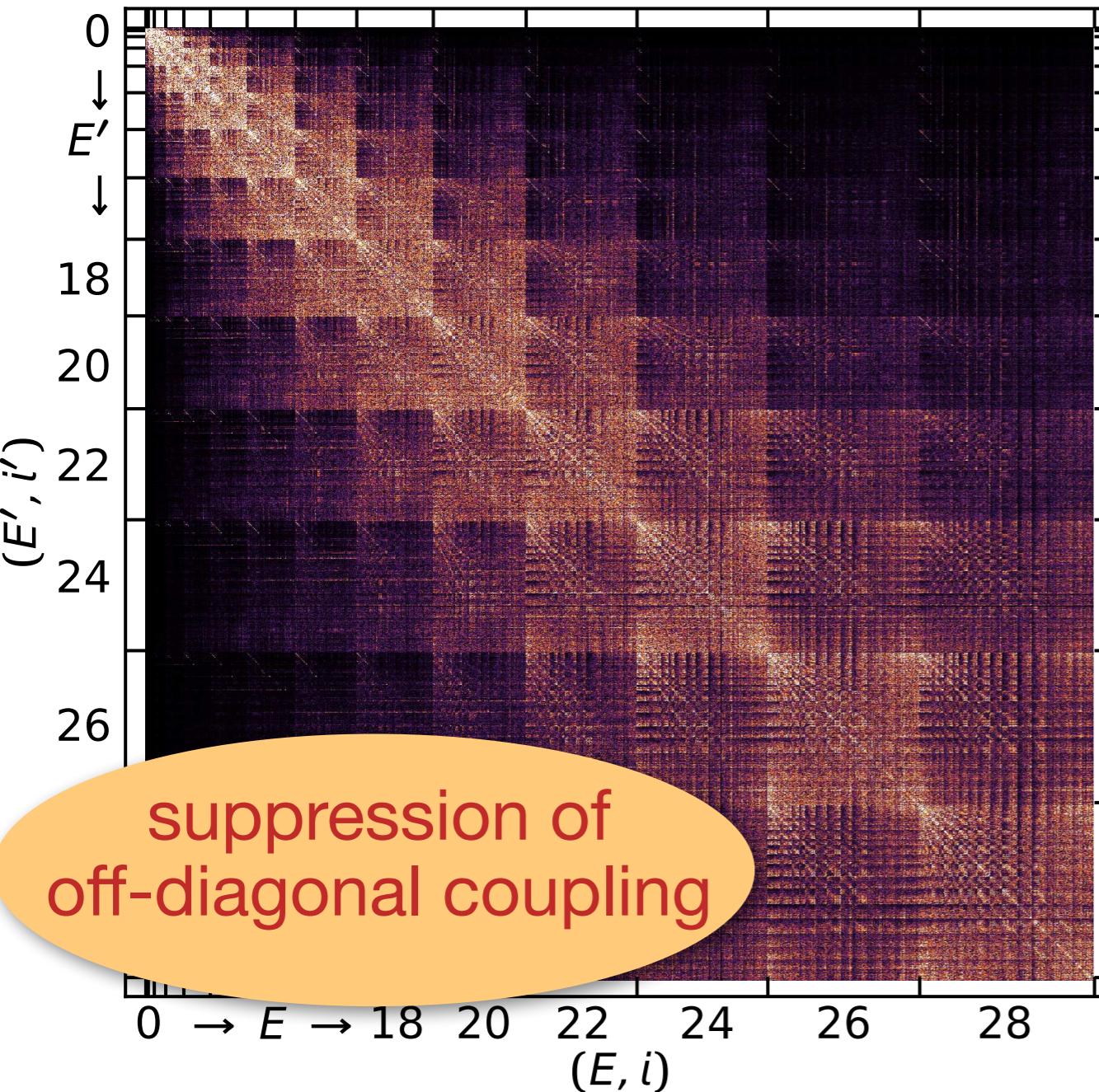
- state-of-the-art: evolve in three-body space, truncate induced four- and higher many-body forces
(Jurgenson, Furnstahl, Navratil, PRL 103, 082501; Hebeler, PRC 85, 021002; Wendt, PRC 87, 061001)
- **λ -dependence** of eigenvalues is a **diagnostic** for size of omitted induced interactions

SRG in Three-Body Space



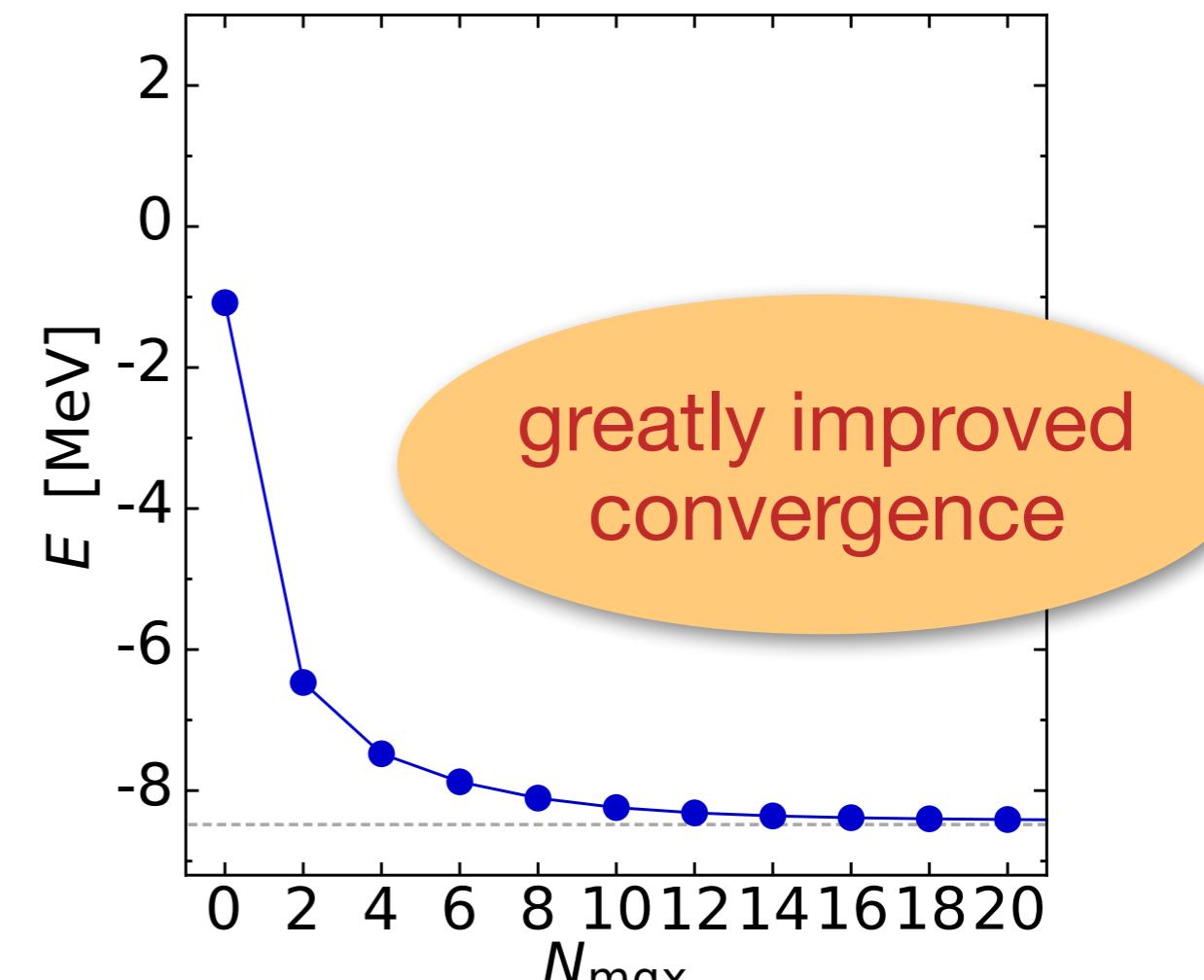
3B Jacobi-HO Matrix Elements

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



$$\lambda = 1.33 \text{ fm}^{-1}$$

^3H ground-state (NCSM)



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

Normal-Ordering & Wick's Theorem



- define elementary contractions of a one-body operator w.r.t. a given reference state as

$$A_I^k \equiv a_k^\dagger a_I, \quad \lambda_I^k \equiv \langle \Psi | A_I^k | \Psi \rangle, \quad \xi_I^k \equiv \lambda_I^k - \delta_I^k$$

- define normal-ordered operators recursively through **all possible internal contractions**:

$$\begin{aligned} A_{I_1 \dots I_N}^{k_1 \dots k_N} = & : A_{I_1 \dots I_N}^{k_1 \dots k_N} : + \lambda_{I_1}^{k_1} : A_{I_2 \dots I_N}^{k_2 \dots k_N} : + \text{singles} \\ & + \left(\lambda_{I_1}^{k_1} \lambda_{I_2}^{k_2} - \lambda_{I_2}^{k_1} \lambda_{I_1}^{k_2} \right) : A_{I_3 \dots I_N}^{k_3 \dots k_N} : + \text{doubles} + \dots \end{aligned}$$

- Wick's Theorem: products of normal-ordered operators can be expanded in terms of **external contractions** alone

$$\begin{aligned} : A_{m_1 \dots m_N}^{k_1 \dots k_N} :: A_{n_1 \dots n_N}^{l_1 \dots l_N} : = & (-1)^{N-1} \lambda_{n_1}^{k_1} : A_{m_1 \dots m_N n_2 \dots n_N}^{k_2 \dots k_N l_1 \dots l_N} : \\ & + (-1)^{N-1} \xi_{m_1}^{l_1} : A_{m_2 \dots m_N n_1 \dots n_N}^{k_1 \dots k_N l_2 \dots l_N} : + \dots \end{aligned}$$

Choice of Generator



- **Wegner:**

$$\eta' = [H^d, H^{od}]$$

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

$$\eta'' = \sum_{ph} \frac{f_h^p}{\Delta_h^p} : A_h^p : + \sum_{pp'hh'} \frac{\Gamma_{hh'}^{pp'}}{\Delta_{hh'}^{pp'}} : A_{hh'}^{pp'} : + \text{H.c.}$$

$\Delta_h^p, \Delta_{hh'}^{pp'}$: approx. 1p1h, 2p2h excitation energies

- **“imaginary time”:** (Morris, Bogner)

$$\eta''' = \sum_{ph} \text{sgn}(\Delta_h^p) f_h^p : A_h^p : + \sum_{pp'hh'} \text{sgn}(\Delta_{hh'}^{pp'}) \Gamma_{hh'}^{pp'} : A_{hh'}^{pp'} : + \text{H.c.}$$

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

In-Medium SRG Flow Equations



0-body Flow

$$\frac{dE}{ds} = \sum_{ab} (n_a - n_b) \left(\eta_b^a f_a^b - f_b^a \eta_a^b \right) + \frac{1}{4} \sum_{abcd} \left(\eta_{cd}^{ab} \Gamma_{ab}^{cd} - \Gamma_{cd}^{ab} \eta_{ab}^{cd} \right) n_a n_b \bar{n}_c \bar{n}_d$$

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

1-body Flow

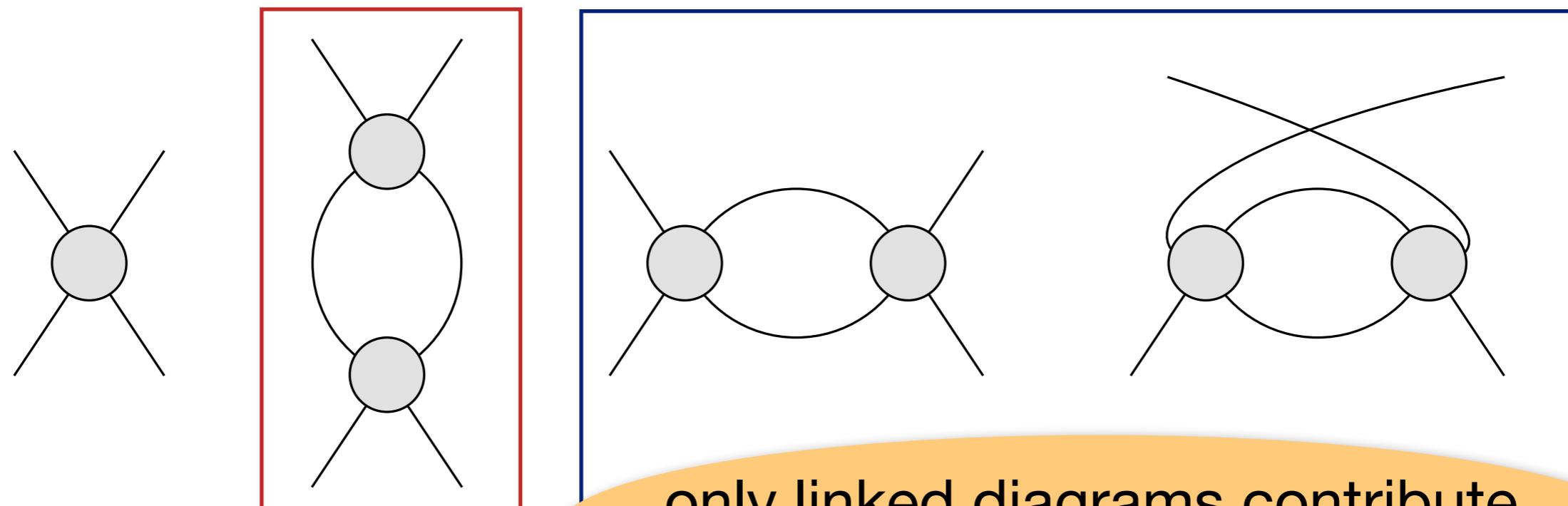
$$\begin{aligned} \frac{d}{ds} f_2^1 &= \sum_a \left(\eta_a^1 f_2^a - f_a^1 \eta_2^a \right) + \sum_{ab} \left(\eta_b^a \Gamma_{a2}^{b1} - f_b^a \eta_{a2}^{b1} \right) (n_a - n_b) \\ &\quad + \frac{1}{2} \sum_{abcdef} \left(\eta_{bc}^{1a} \Gamma_{2a}^{bc} - \Gamma_{bc}^{1a} \eta_{2a}^{bc} \right) (n_a \bar{n}_b \bar{n}_c + \bar{n}_a n_b n_c) \end{aligned}$$

In-Medium SRG Flow Equations



2-body Flow

$$\begin{aligned}\frac{d}{ds} \Gamma_{34}^{12} = & \sum_a \left(\eta_a^1 \Gamma_{34}^{a2} + \eta_a^2 \Gamma_{34}^{1a} - \eta_3^a \Gamma_{a4}^{12} - \eta_4^a \Gamma_{3a}^{12} - f_a^1 \eta_{34}^{a2} - f_a^2 \eta_{34}^{1a} + f_3^a \eta_{a4}^{12} + f_4^a \eta_{3a}^{12} \right) \\ & + \frac{1}{2} \sum_{ab} \underbrace{\left(\eta_{ab}^{12} \Gamma_{34}^{ab} - \Gamma_{ab}^{12} \eta_{34}^{ab} \right) (1 - n_a - n_b)}_{\text{linked diagrams}} \\ & + \sum_{ab} \underbrace{(n_a - n_b) \left(\left(\eta_{3b}^{1a} \Gamma_{4a}^{2b} - \Gamma_{3b}^{1a} \eta_{4a}^{2b} \right) - \left(\eta_{3b}^{2a} \Gamma_{4a}^{1b} - \Gamma_{3b}^{2a} \eta_{4a}^{1b} \right) \right)}_{\text{linked diagrams}}\end{aligned}$$

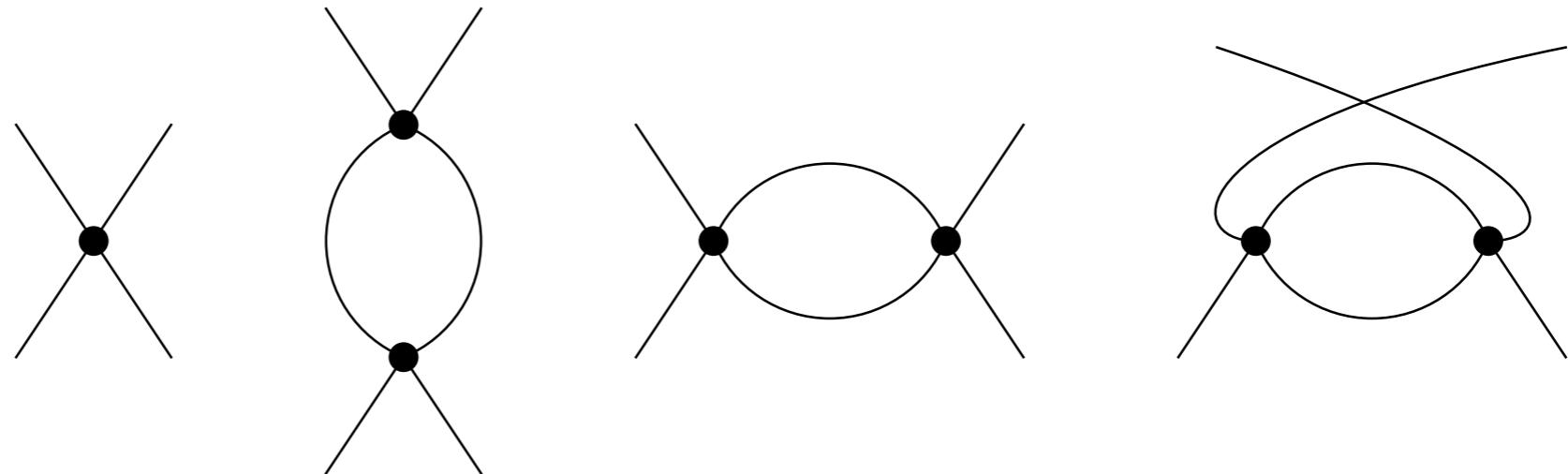


only linked diagrams contribute,
IM-SRG size-extensive

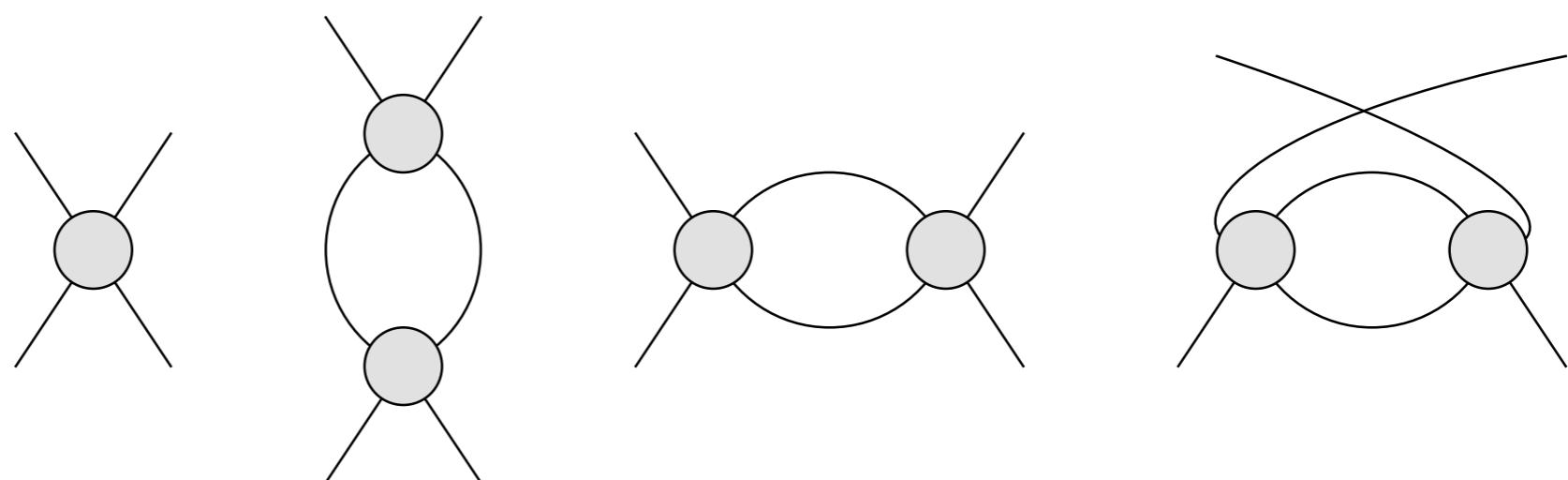
In-Medium SRG Flow: Diagrams



$\Gamma(\delta s) \sim$



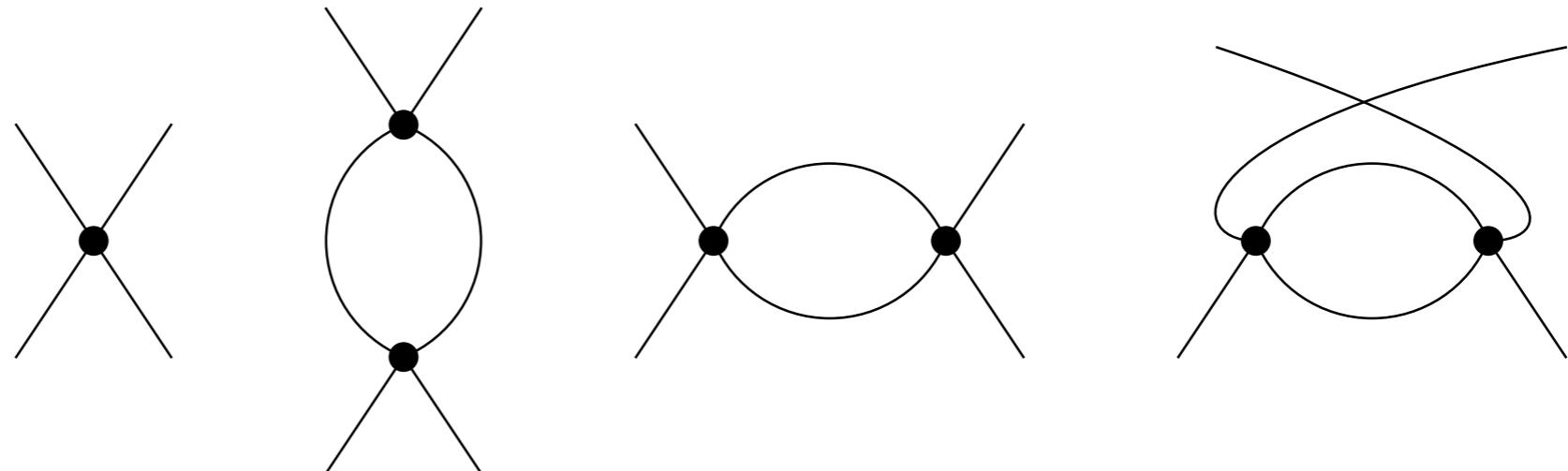
$\Gamma(2\delta s) \sim$



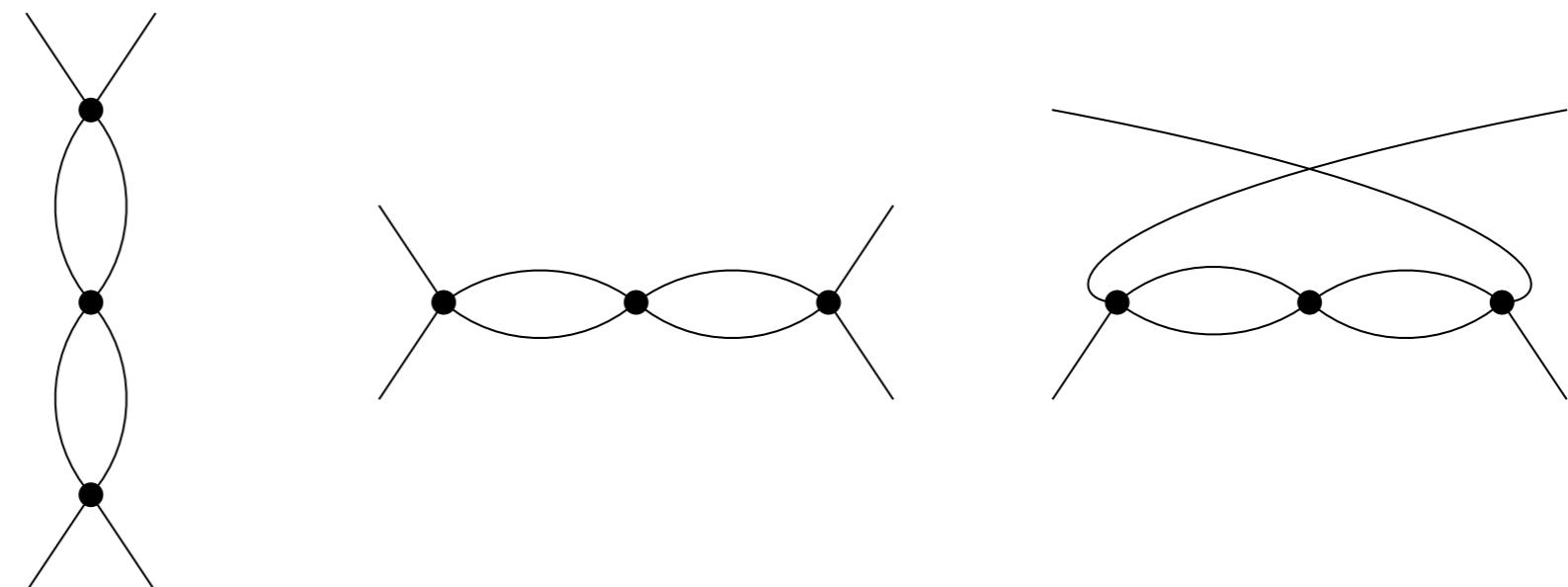
In-Medium SRG Flow: Diagrams



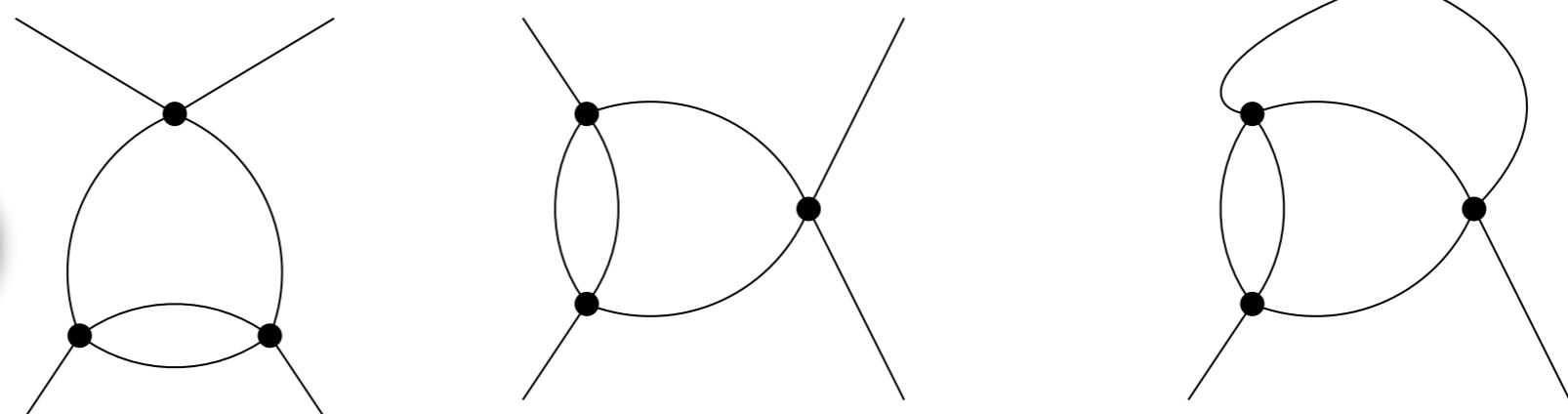
$$\Gamma(\delta s) \sim$$



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

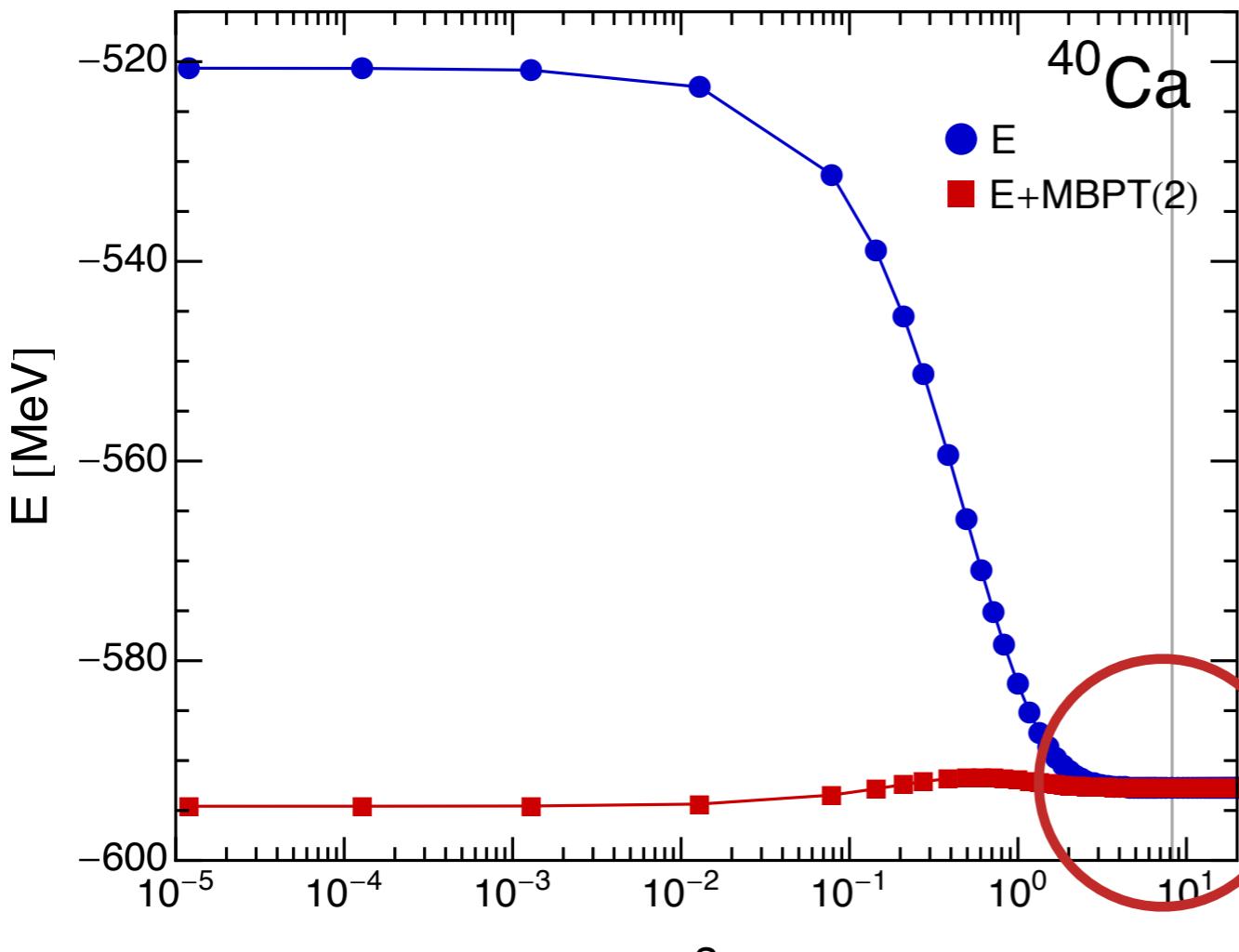


non-perturbative
resummation

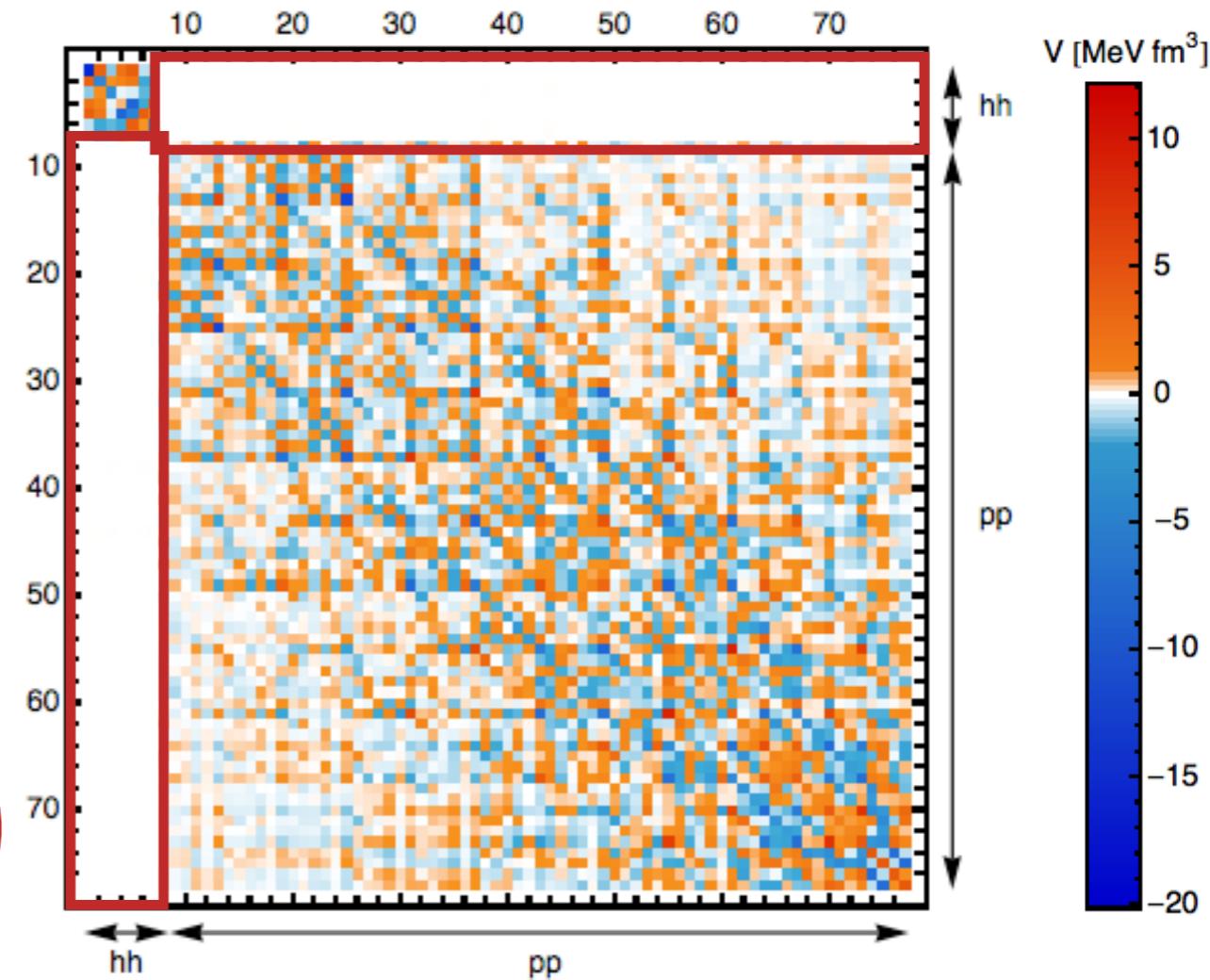


& many
more...

Decoupling

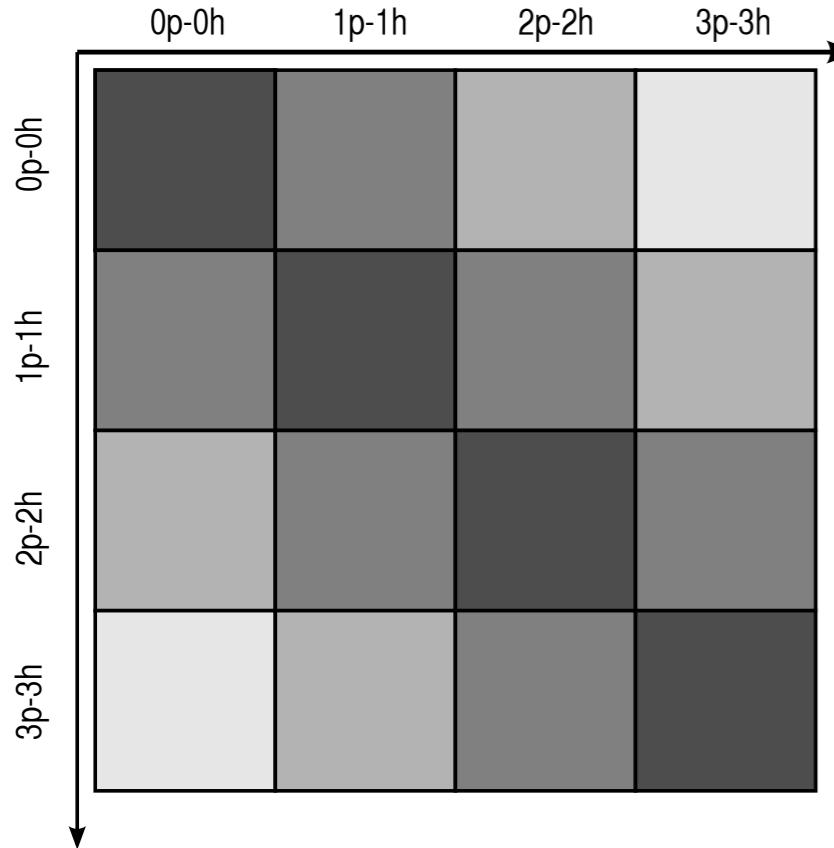


non-perturbative
resummation of MBPT series
(correlations)



off-diagonal couplings
are rapidly driven to zero

Decoupling



$$\langle \frac{p}{h} | H | \Psi \rangle \sim f_h^p, \sum_{kl} f_l^k \lambda_{pl}^{hk}, \sum_{klmn} \Gamma_{mn}^{kl} \lambda_{pmn}^{hkl}, \dots$$

$$\langle \frac{pp'}{hh'} | H | \Psi \rangle \sim \Gamma_{hh'}^{pp'}, \sum_{km} \Gamma_{hm}^{pk} \lambda_{p'm}^{h'k}, \sum_{kl} f_l^k \lambda_{pp'l}^{hh'k}, \sum_{klmn} \Gamma_{mn}^{kl} \lambda_{pp'mn}^{hh'kl}, \dots$$

$$\langle \frac{pp'p''}{hh'h'} | H | \Psi \rangle \sim \dots$$

- 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**:

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

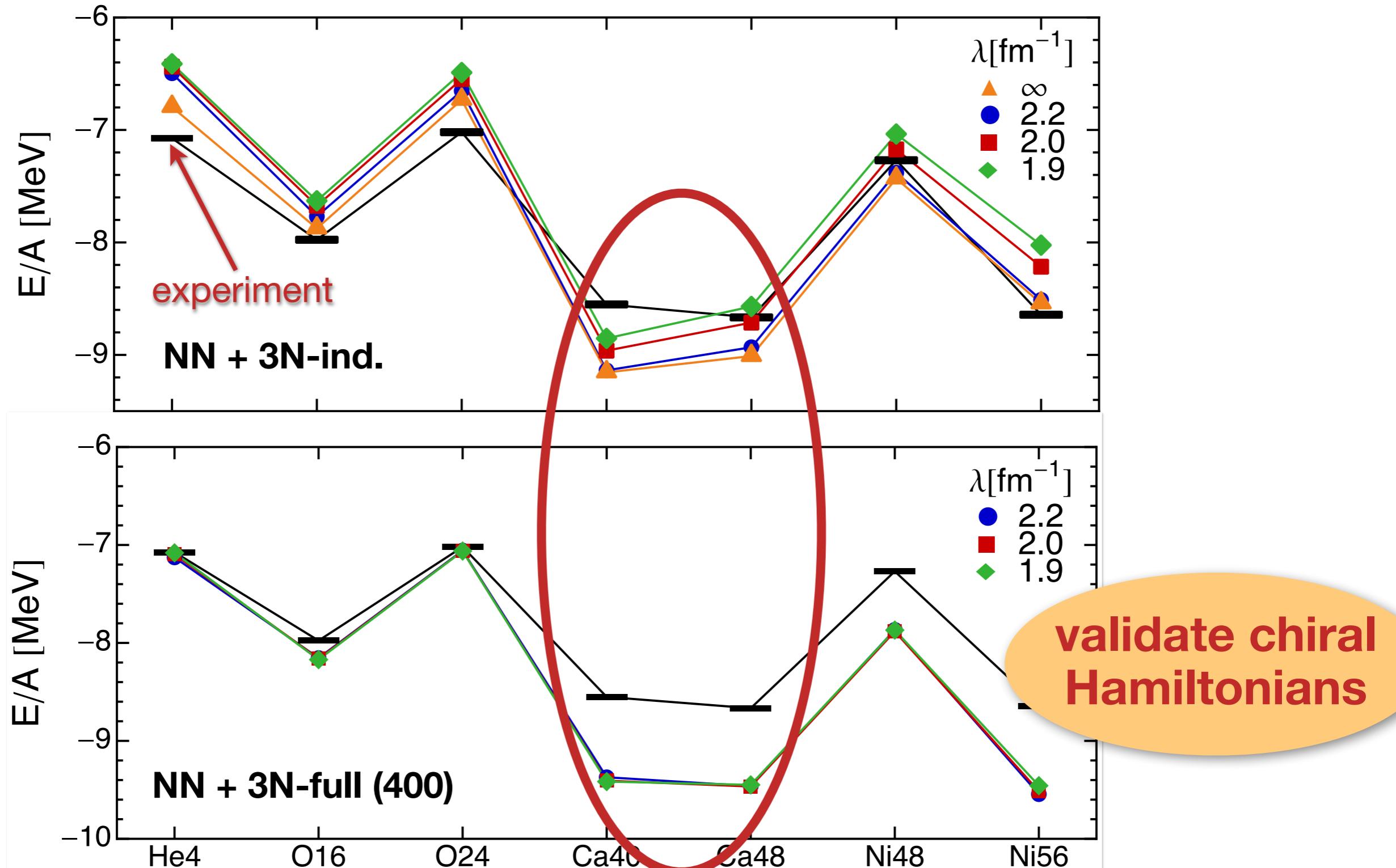
- calculate one- and two-body densities (**project only once**):

$$\lambda_I^k = \frac{\langle \Psi | A_I^k P_N | \Psi \rangle}{\langle \Psi | \Psi \rangle}, \quad \lambda_{mn}^{kl} = \frac{\langle \Psi | A_{mn}^{kl} P_N | \Psi \rangle}{\langle \Psi | \Psi \rangle} - \lambda_m^k \lambda_m^l + \lambda_n^k \lambda_m^l$$

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

$$\lambda_I^k = n_k \delta_I^k \quad (= v_k^2 \delta_I^k), \quad 0 \leq n_k \leq 1$$

Results: Closed-Shell Nuclei



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

H. Hergert - "Progress in Ab Initio Techniques in Nuclear Physics", TRIUMF, Vancouver, 02/19/2015

Multi-Reference Flow Equations



0-body flow:

$$\begin{aligned} \frac{dE}{ds} = & \sum_{ab} (n_a - n_b) \left(\eta_b^a f_a^b - f_b^a \eta_a^b \right) + \frac{1}{4} \sum_{abcd} \left(\eta_{cd}^{ab} \Gamma_{ab}^{cd} - \Gamma_{cd}^{ab} \eta_{ab}^{cd} \right) n_a n_b \bar{n}_c \bar{n}_d \\ & + \frac{1}{4} \sum_{abcd} \left(\frac{d}{ds} \Gamma_{cd}^{ab} \right) \lambda_{cd}^{ab} + \frac{1}{4} \sum_{abcdklm} \left(\eta_{cd}^{ab} \Gamma_{am}^{kl} - \Gamma_{cd}^{ab} \eta_{am}^{kl} \right) \lambda_{cdm}^{bkl} \end{aligned}$$

1-body flow:

$$\begin{aligned} \frac{d}{ds} f_2^1 = & \sum_a \left(\eta_a^1 f_2^a - f_a^1 \eta_2^a \right) + \sum_{ab} \left(\eta_b^a \Gamma_{a2}^{b1} - f_b^a \eta_{a2}^{b1} \right) (n_a - n_b) \\ & + \frac{1}{2} \sum_{abcdef} \left(\eta_{bc}^{1a} \Gamma_{2a}^{bc} - \Gamma_{bc}^{1a} \eta_{2a}^{bc} \right) (n_a \bar{n}_b \bar{n}_c + \bar{n}_a n_b n_c) \\ & + \frac{1}{4} \sum_{abcde} \left(\eta_{bc}^{1a} \Gamma_{2a}^{de} - \Gamma_{bc}^{1a} \eta_{2a}^{de} \right) \lambda_{bc}^{de} + \sum_{abcde} \left(\eta_{bc}^{1a} \Gamma_{2d}^{be} - \Gamma_{bc}^{1a} \eta_{2d}^{be} \right) \lambda_{cd}^{ae} \\ & - \frac{1}{2} \sum_{abcde} \left(\eta_{2b}^{1a} \Gamma_{ae}^{cd} - \Gamma_{2b}^{1a} \eta_{ae}^{cd} \right) \lambda_{be}^{cd} + \frac{1}{2} \sum_{abcde} \left(\eta_{2b}^{1a} \Gamma_{de}^{bc} - \Gamma_{2b}^{1a} \eta_{de}^{bc} \right) \lambda_{de}^{ac} \end{aligned}$$

Multi-Reference Flow Equations



2-body flow:

$$\begin{aligned}\frac{d}{ds} \Gamma_{34}^{12} = & \sum_a \left(\eta_a^1 \Gamma_{34}^{a2} + \eta_a^2 \Gamma_{34}^{1a} - \eta_3^a \Gamma_{a4}^{12} - \eta_4^a \Gamma_{3a}^{12} - f_a^1 \eta_{34}^{a2} - f_a^2 \eta_{34}^{1a} + f_3^a \eta_{a4}^{12} + f_4^a \eta_{3a}^{12} \right) \\ & + \frac{1}{2} \sum_{ab} \left(\eta_{ab}^{12} \Gamma_{34}^{ab} - \Gamma_{ab}^{12} \eta_{34}^{ab} \right) (1 - n_a - n_b) \\ & + \sum_{ab} (n_a - n_b) \left(\left(\eta_{3b}^{1a} \Gamma_{4a}^{2b} - \Gamma_{3b}^{1a} \eta_{4a}^{2b} \right) - \left(\eta_{3b}^{2a} \Gamma_{4a}^{1b} - \Gamma_{3b}^{2a} \eta_{4a}^{1b} \right) \right)\end{aligned}$$

2-body flow
unchanged