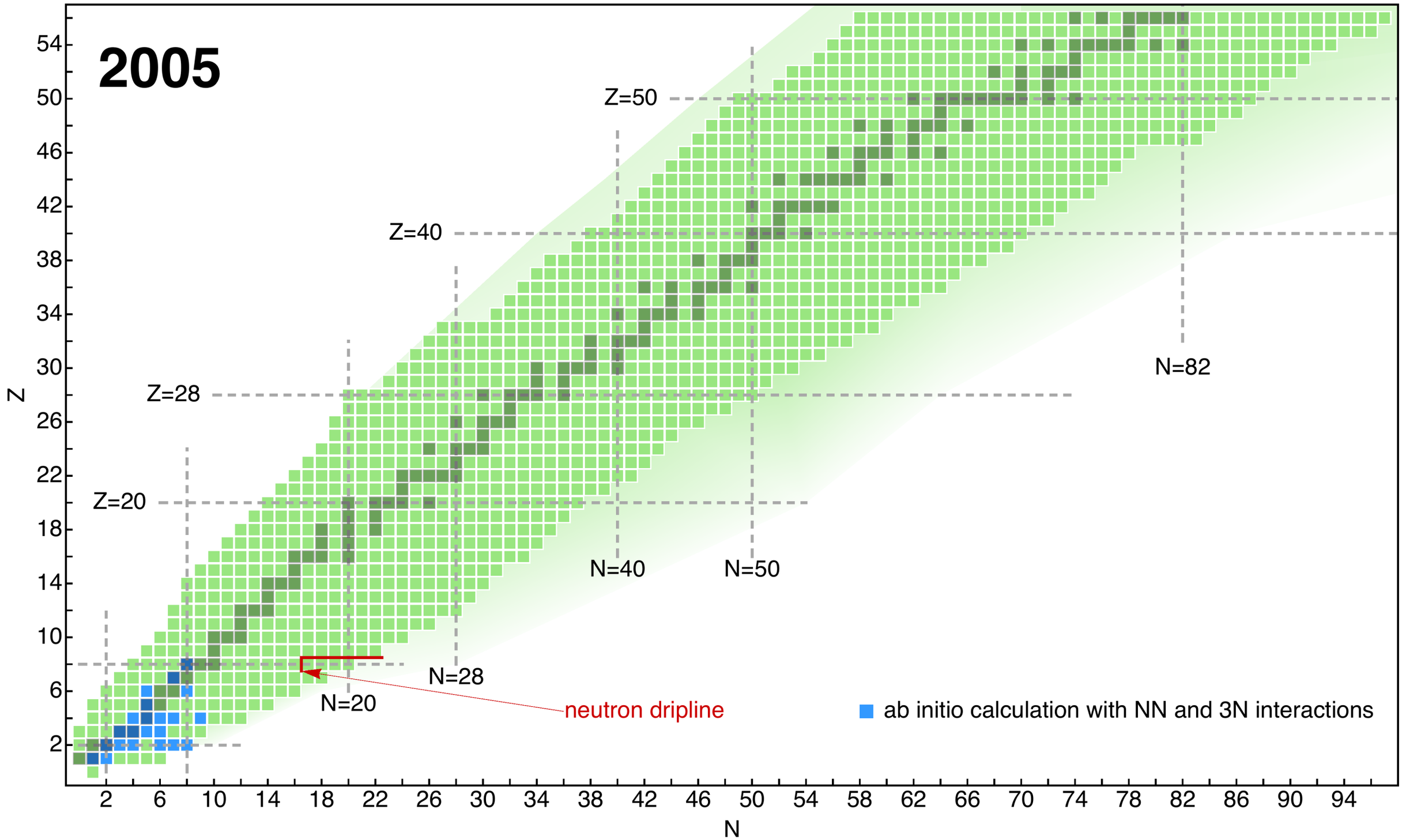
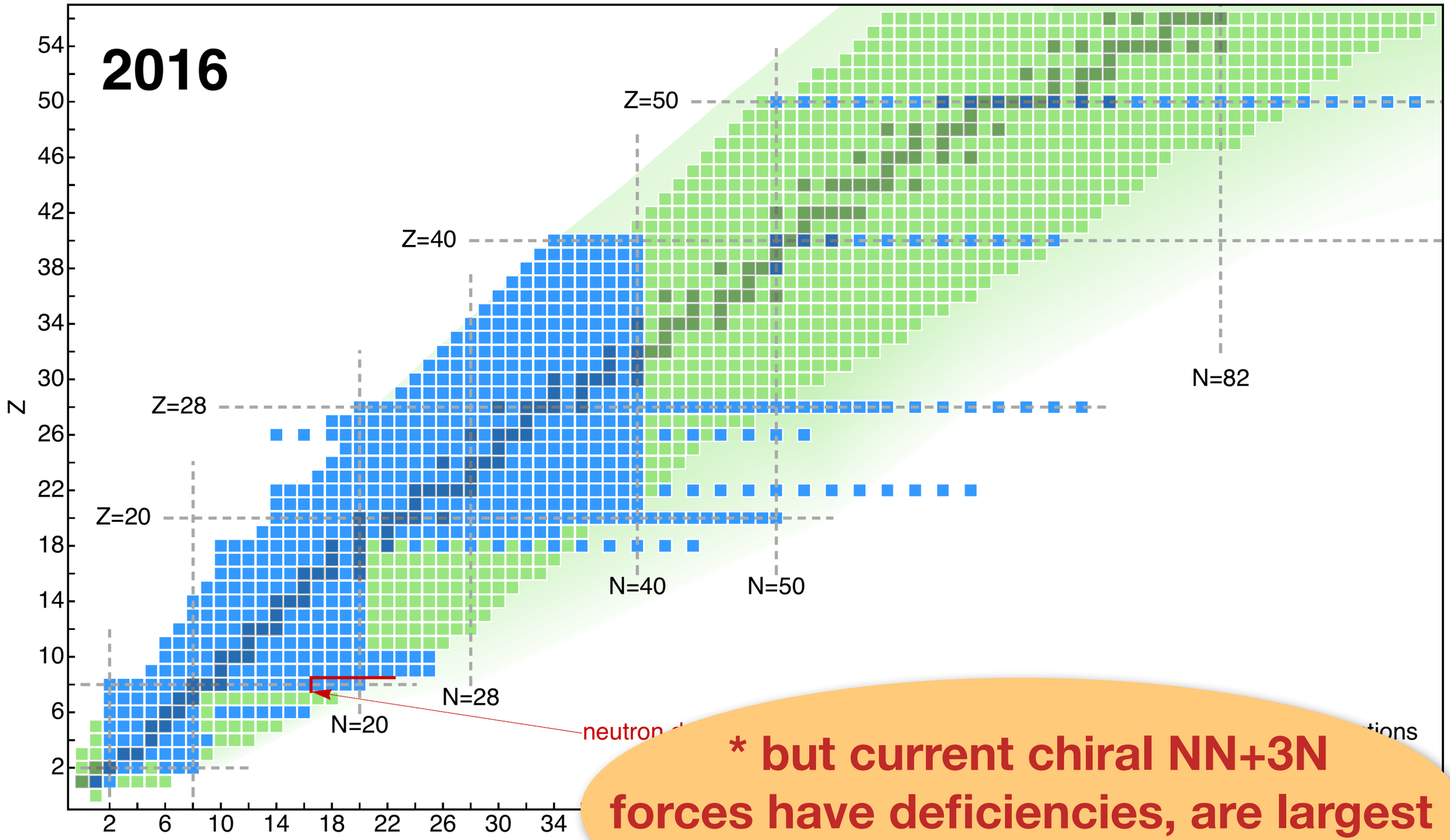
Novel *Ab Initio* Methods for Nuclei

Heiko Hergert
National Superconducting Cyclotron Laboratory
& Department of Physics and Astronomy
Michigan State University

Progress in *Ab Initio* Calculations



Progress in *Ab Initio* Calculations



*** but current chiral NN+3N forces have deficiencies, are largest source of uncertainty**

Progress in *Ab Initio* Calculations

- **Coupled Cluster**

  see talks by S. Binder, G. Hagen

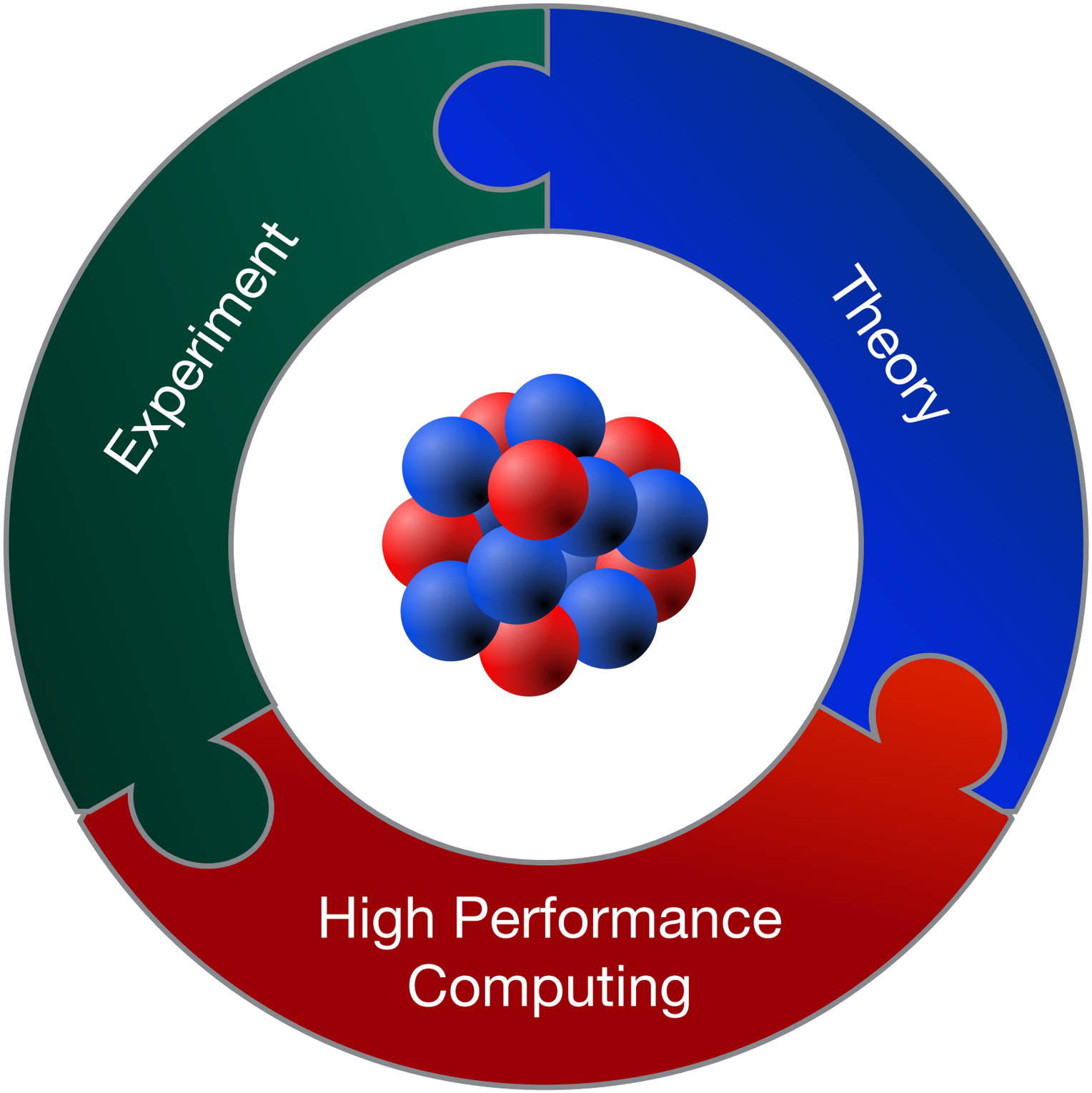
- **Self-Consistent Green's Functions**

  see talks by A. Carbone, C. Barbieri

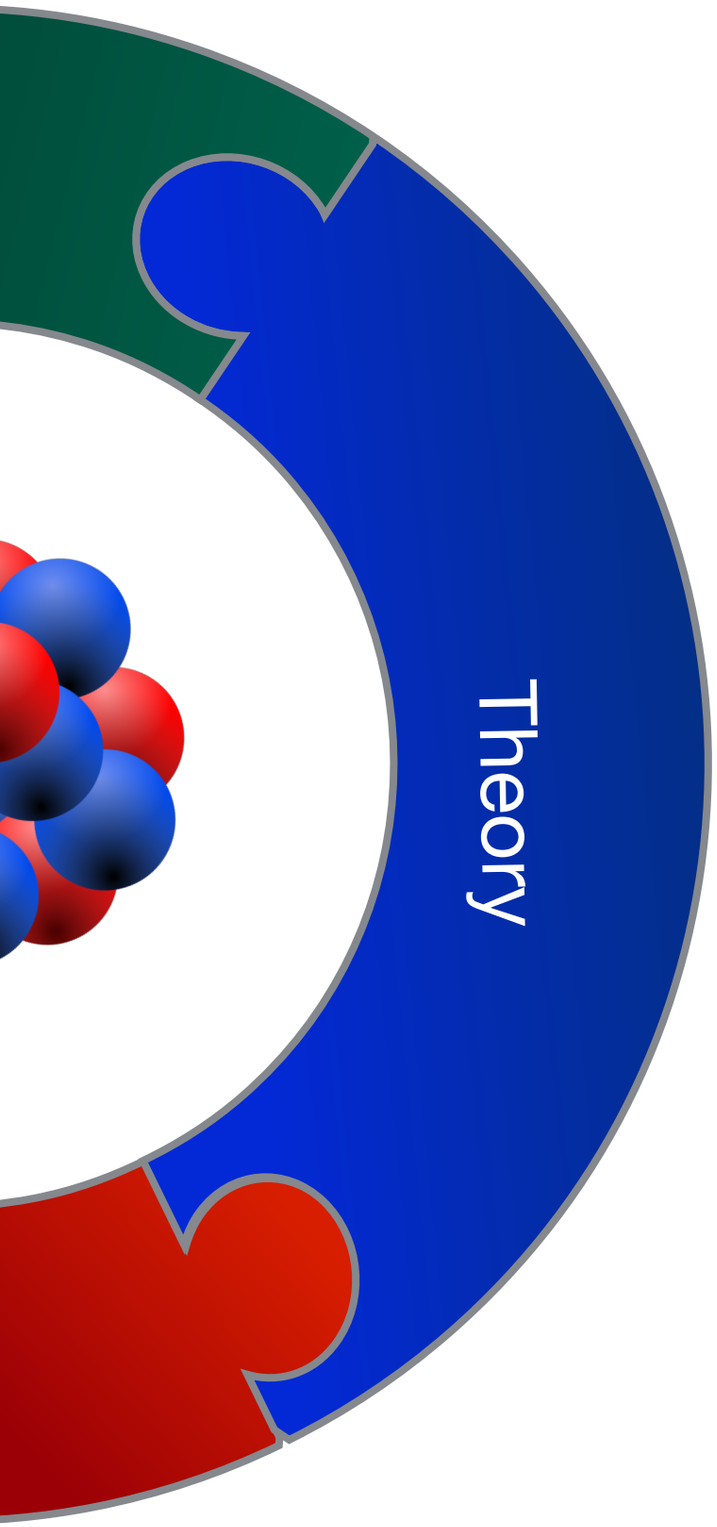
- **In-Medium Similarity Renormalization Group**

  also see talk by T. Morris

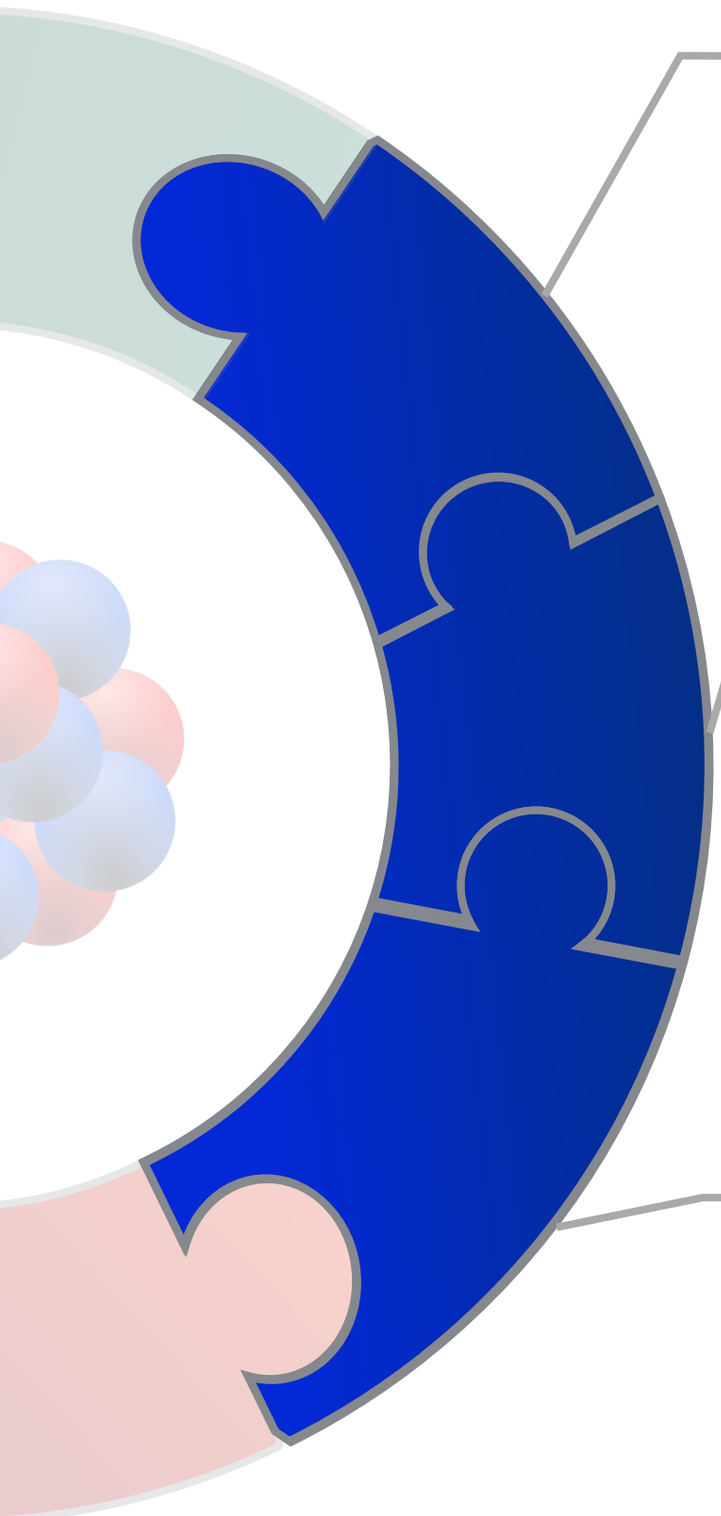
The Nuclear Many-Body Problem



The Nuclear Many-Body Problem

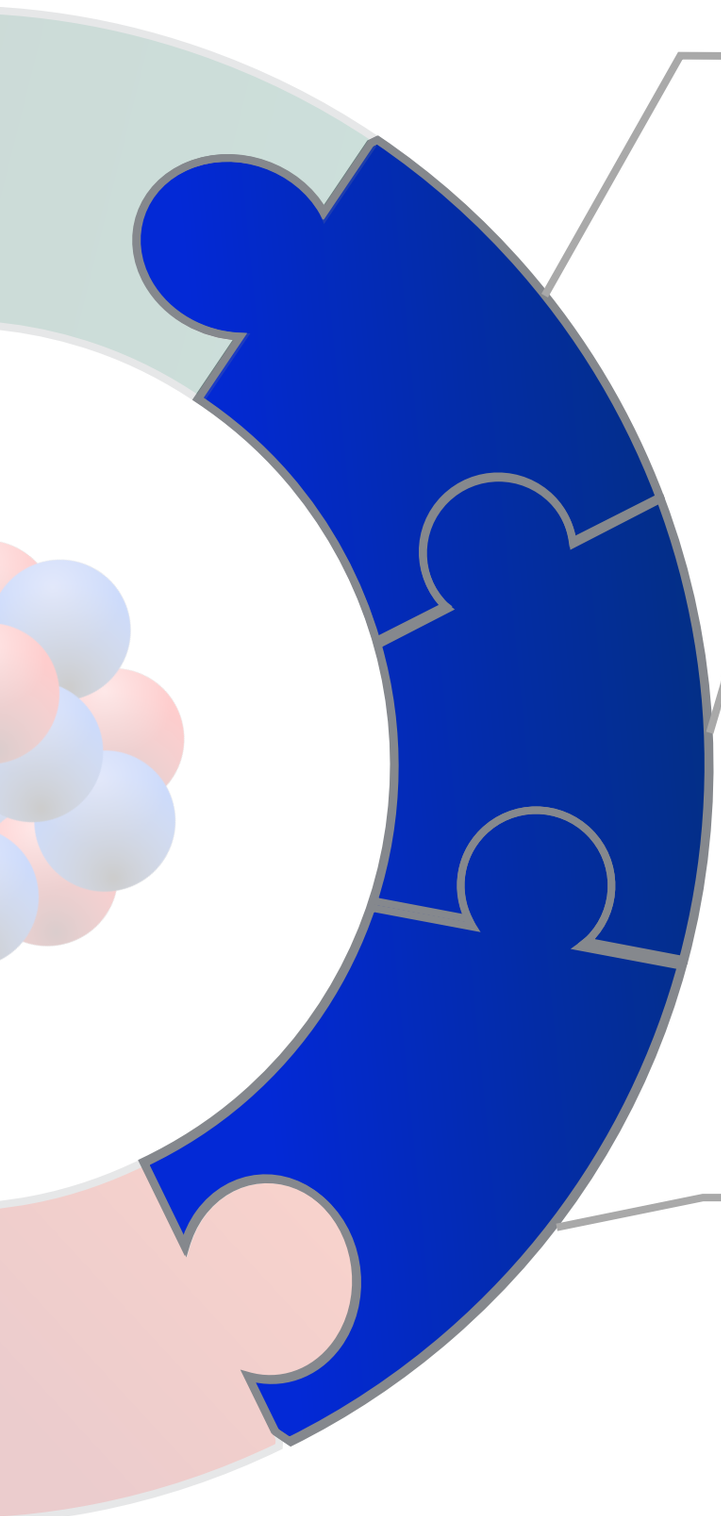


Theory Ingredients



- **Interactions (& Operators) from Chiral EFT**
  - symmetries of low-energy QCD
  - power counting
- **Similarity Renormalization Group**
  - systematically dial resolution scales (cutoffs) of theory
  - trade-off: enhanced convergence & accuracy of many-body methods vs. omitted induced 4N, …, AN forces
- ***Ab Initio* Many-Body Method**
  - systematically improvable towards exact solution

Uncertainty Quantification



- **Interactions (& Operators) from Chiral EFT**
  - symmetries of low-energy QCD
  - power counting
- **Similarity Renormalization Group**
  - systematically dial resolution scales (cutoffs) of theory
  - trade-off: enhanced convergence & accuracy of many-body methods vs. omitted induced 4N, …, AN forces
- ***Ab Initio* Many-Body Method**
  - systematically improvable towards exact solution

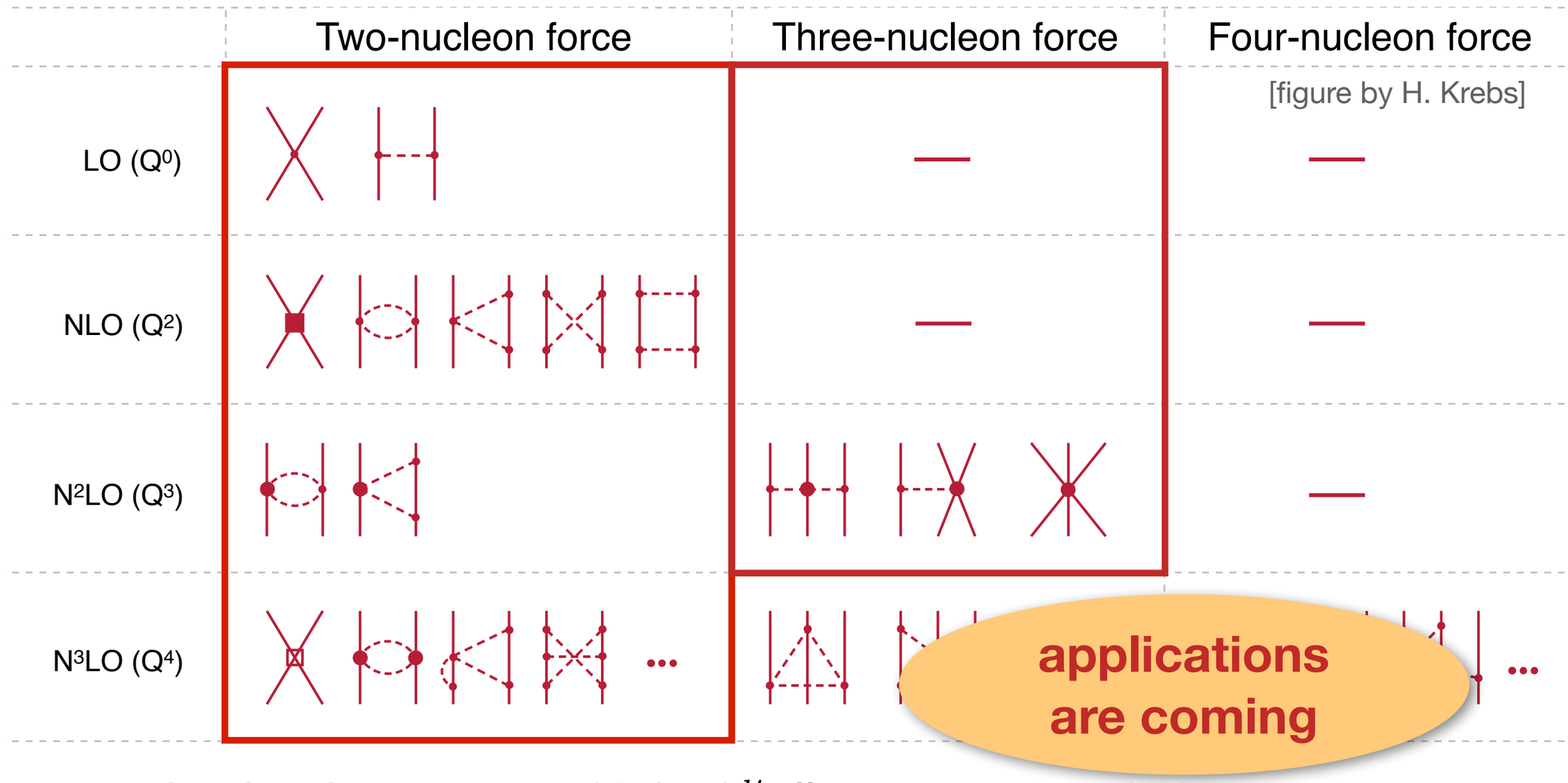
Nuclear Interactions from Chiral Effective Field Theory

Reviews:

R. Machleidt, D. R. Entem, Phys. Rept. **503**, 1 (2011)

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

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 (**electroweak transitions!**)

The Similarity Renormalization Group

Review:

S. Bogner, R. Furnstahl, and A. Schwenk, Prog. Part. Nucl. Phys. **65**, 94 (2010)

E. Anderson, S. Bogner, R. Furnstahl, and R. Perry, Phys. Rev. C **82**, 054001 (2011)
E. Jurgenson, P. Navratil, and R. Furnstahl, Phys. Rev. C **83**, 034301 (2011)
R. Roth, S. Reinhardt, and H. H., Phys. Rev. C **77**, 064003 (2008)
H. H. and R. Roth, Phys. Rev. C **75**, 051001 (2007)

Similarity Renormalization Group

Basic Idea

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

- flow equation for Hamiltonian $H(s) = U(s) H U^\dagger(s)$:

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

- 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

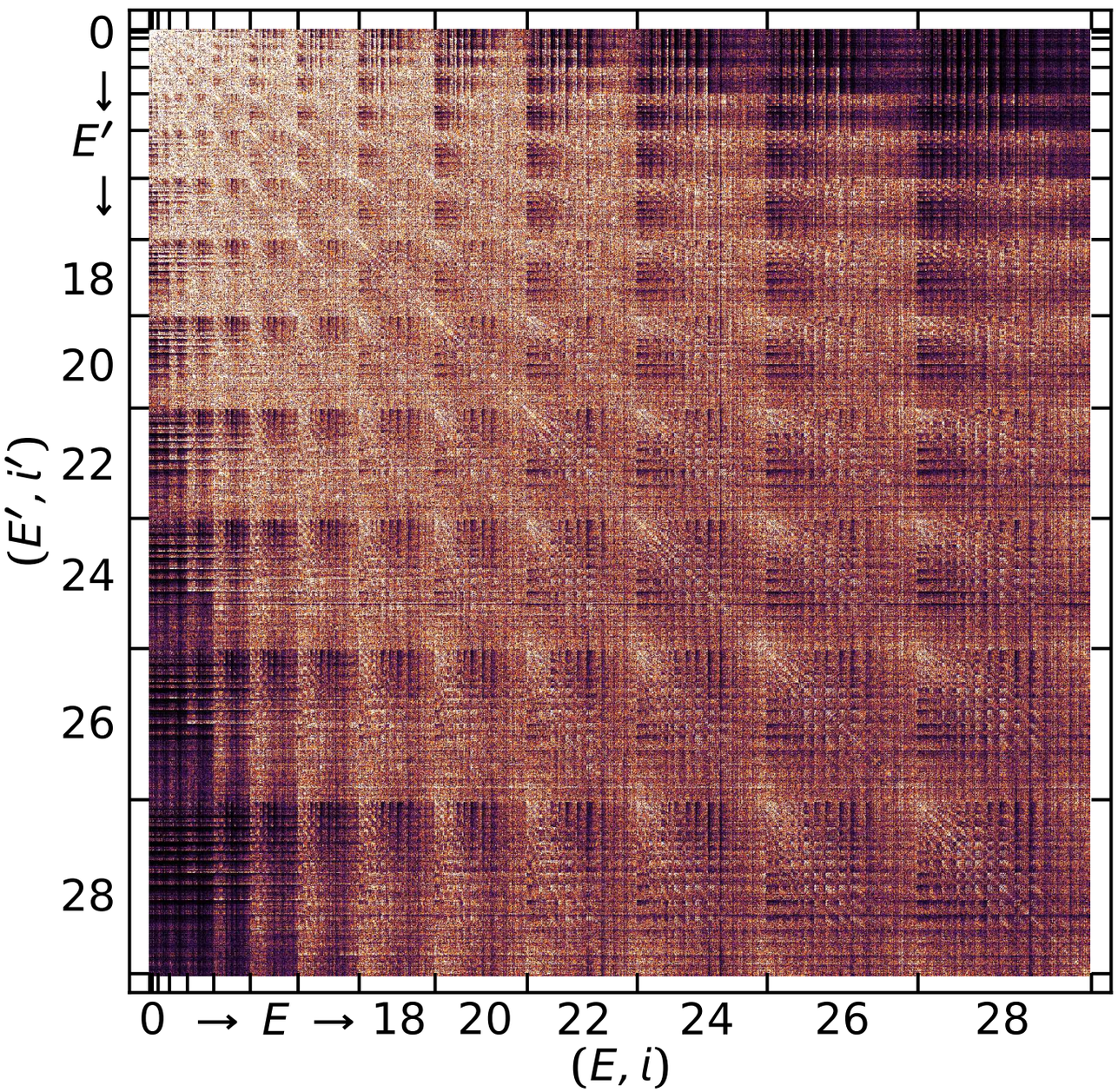
- consistent evolution for all observables of interest

SRG in Three-Body Space

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

3B Jacobi-HO Matrix Elements

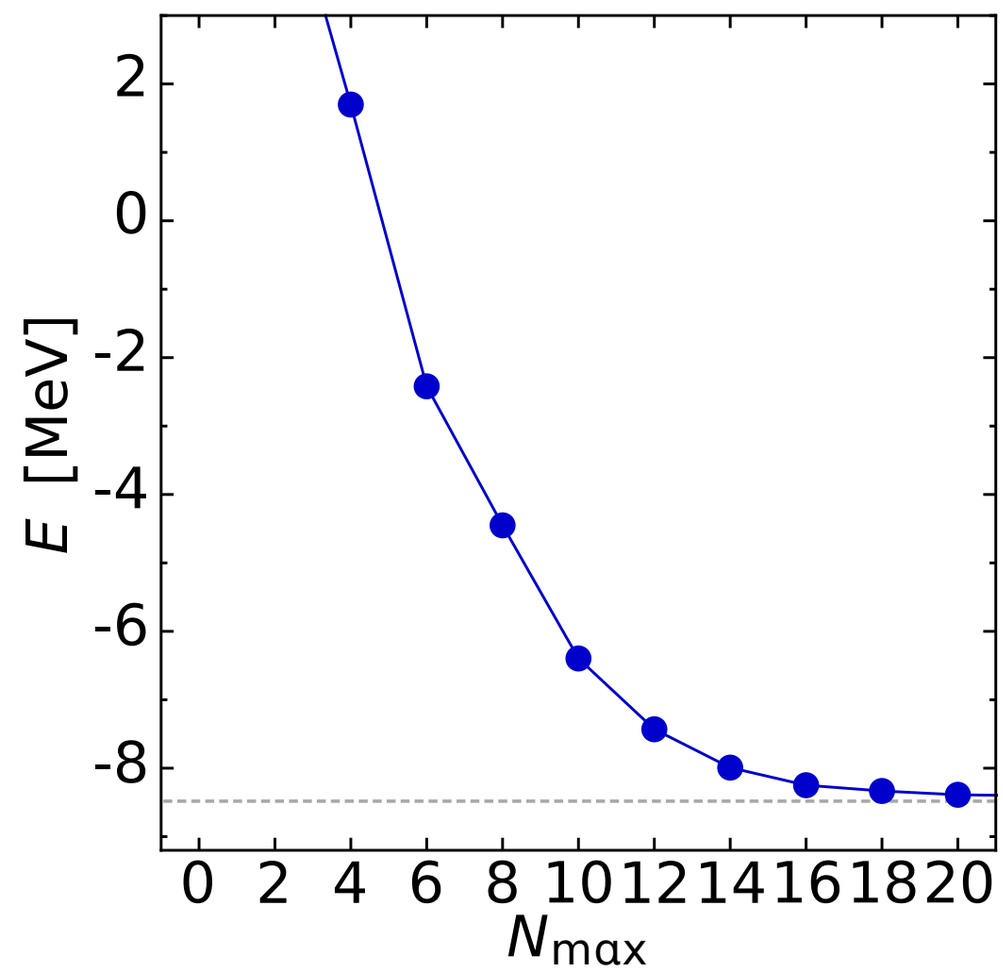
$J^\pi = \frac{1}{2}^+, T = \frac{1}{2}, \hbar\Omega = 28$ MeV



chiral NN + 3N

N³LO + N²LO (³H fit)

³H ground-state (NCSM)

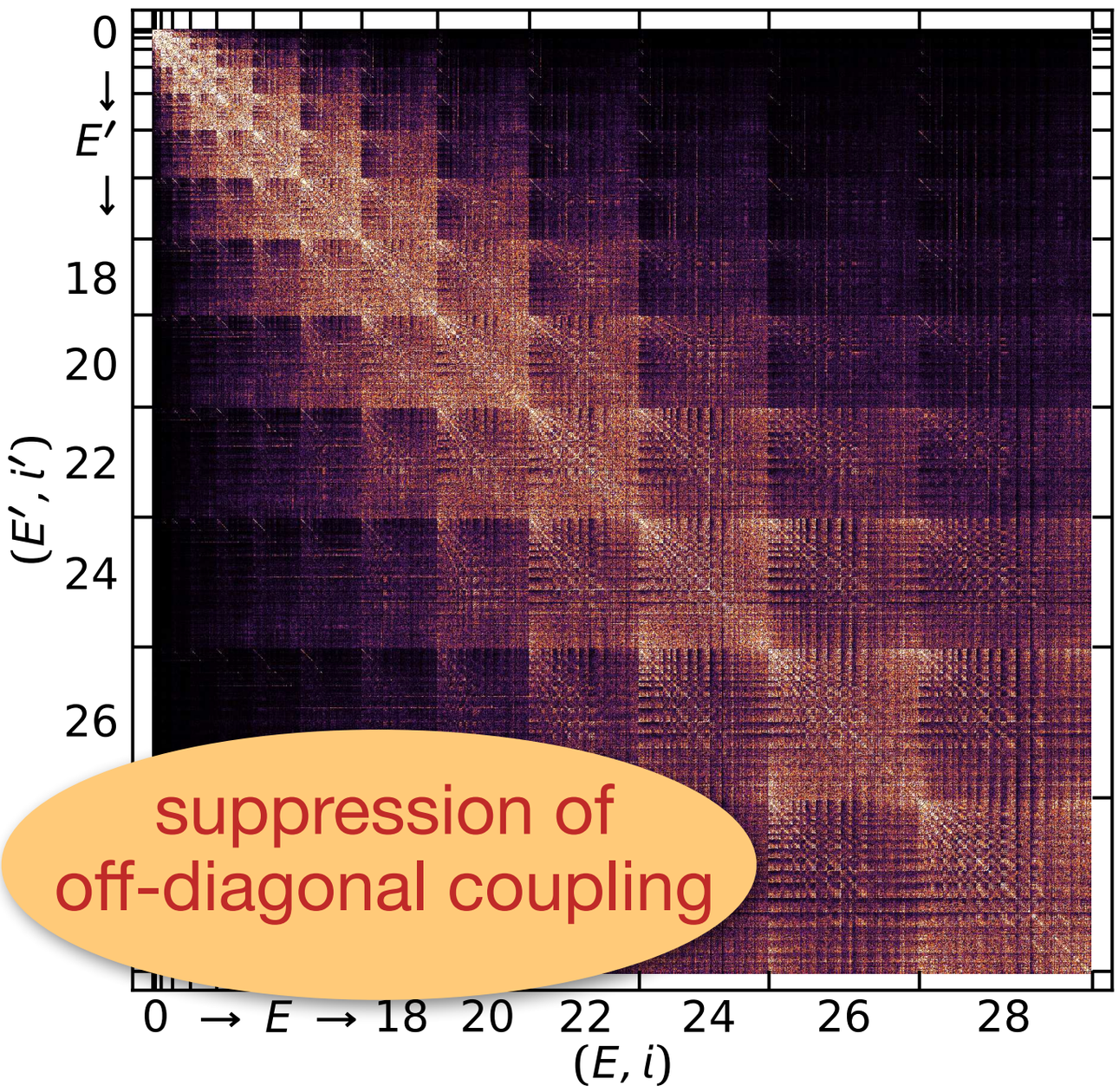


SRG in Three-Body Space

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

3B Jacobi-HO Matrix Elements

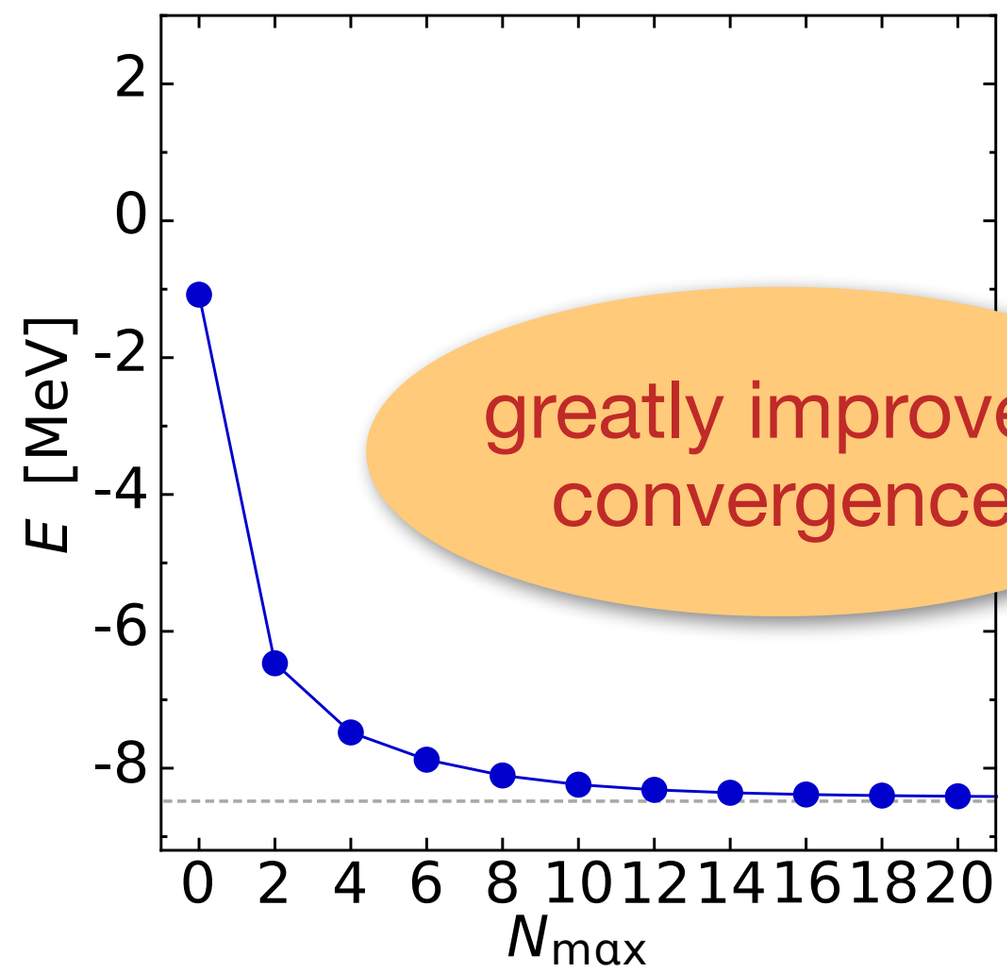
$J^\pi = \frac{1}{2}^+, T = \frac{1}{2}, \hbar\Omega = 28$ MeV



suppression of off-diagonal coupling

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

^{3}H ground-state (NCSM)



greatly improved convergence

Ab Initio Many-Body Methods:

(Multi-Reference) In-Medium SRG

H. H., in preparation

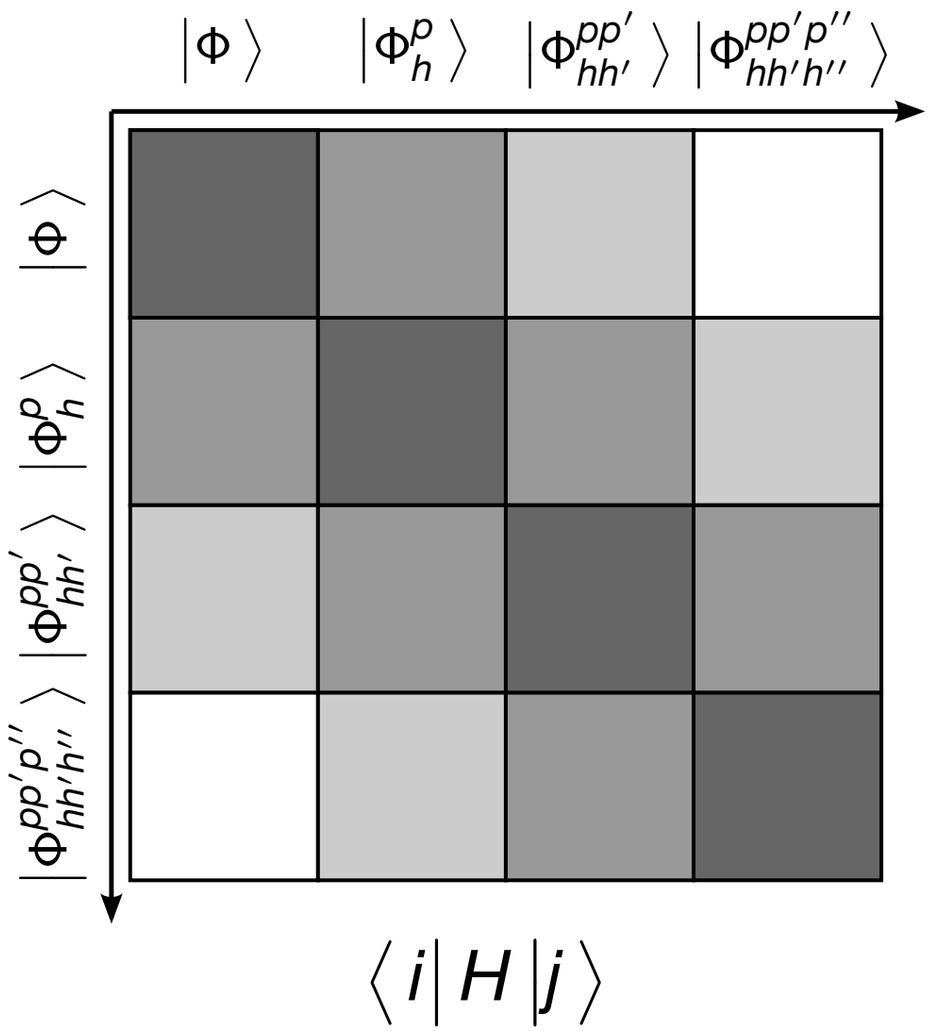
H. H., to appear in Phys. Scripta, arXiv:1607.06882 [nucl-th]

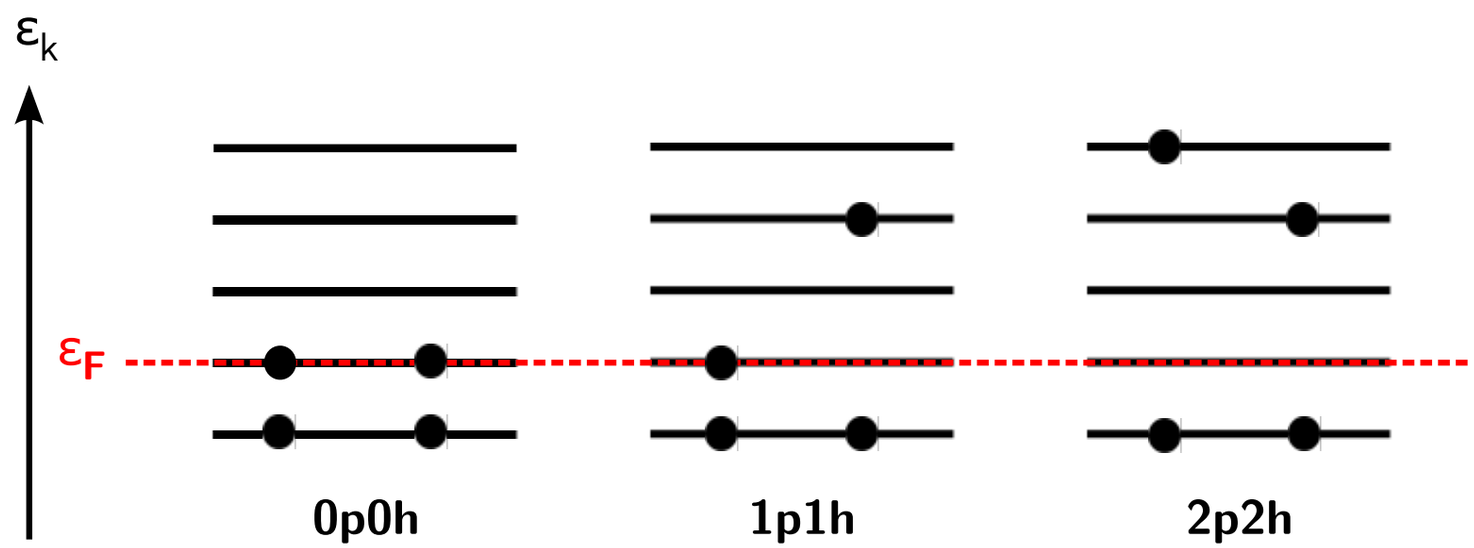
H. H., S. K. Bogner, T. D. Morris, A. Schwenk, and K. Tuskiyama, Phys. Rept. **621**, 165 (2016)

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)

Ground-State Decoupling





excitations relative to reference state: **normal-ordering**

- reference state: **single Slater determinant**

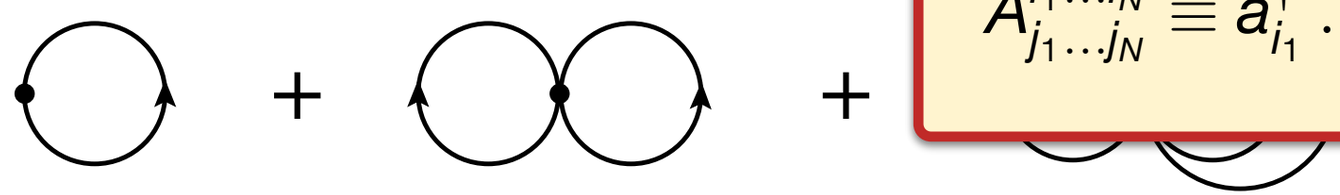
Normal-Ordered Hamiltonian

Normal-Ordered Hamiltonian

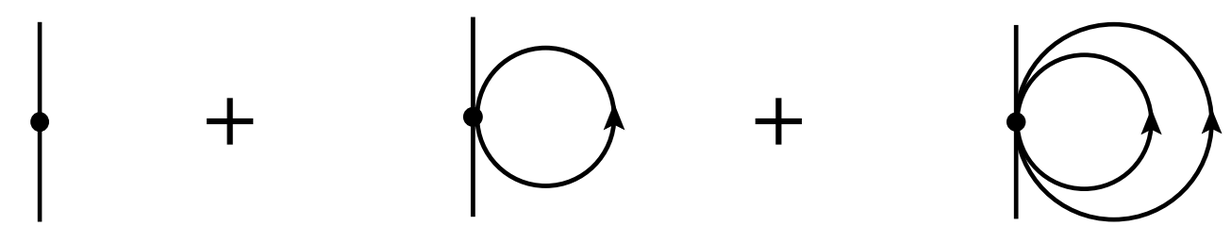
$$H = E_0 + \sum_{kl} f_l^k : A_l^k : + \frac{1}{4} \sum_{klmn} \Gamma_{mn}^{kl} : A_{mn}^{kl} : + \frac{1}{36} \sum_{ijklmn} W_{lmn}^{ijk} : A_{lmn}^{ijk} :$$

$$A_{j_1 \ldots j_N}^{i_1 \ldots i_N} \equiv a_{i_1}^\dagger \ldots a_{i_N}^\dagger a_{j_N} \ldots a_{j_1}$$

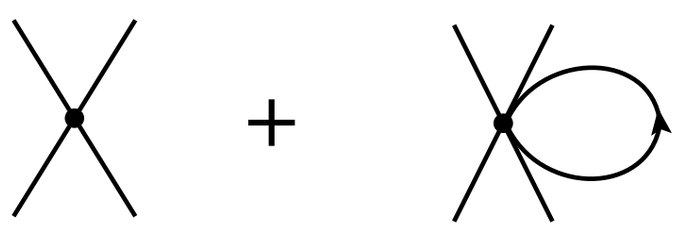
$E_0 =$



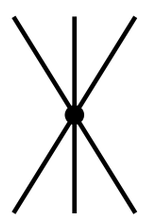
$f =$



$\Gamma =$



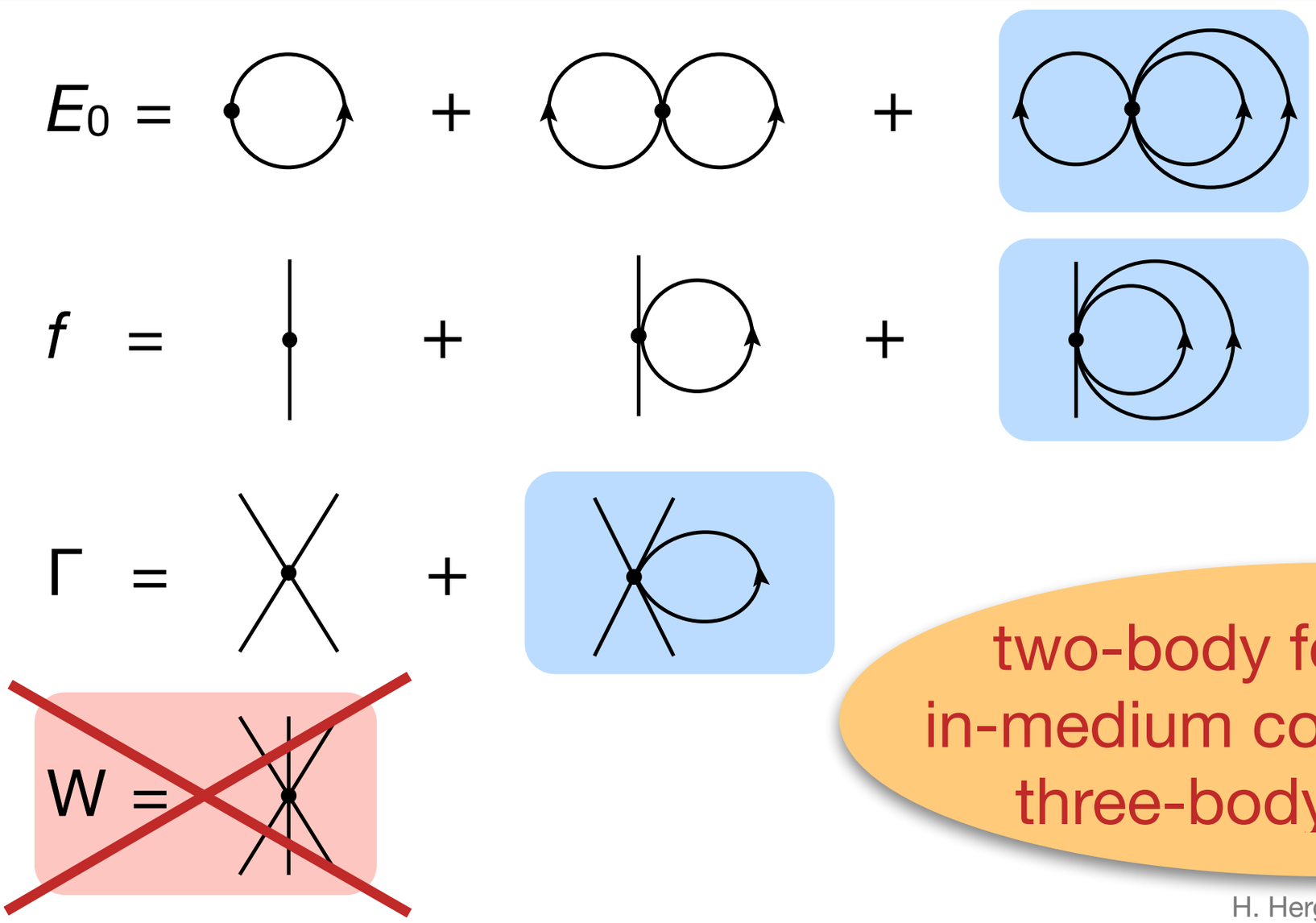
$W =$



Normal-Ordered Hamiltonian

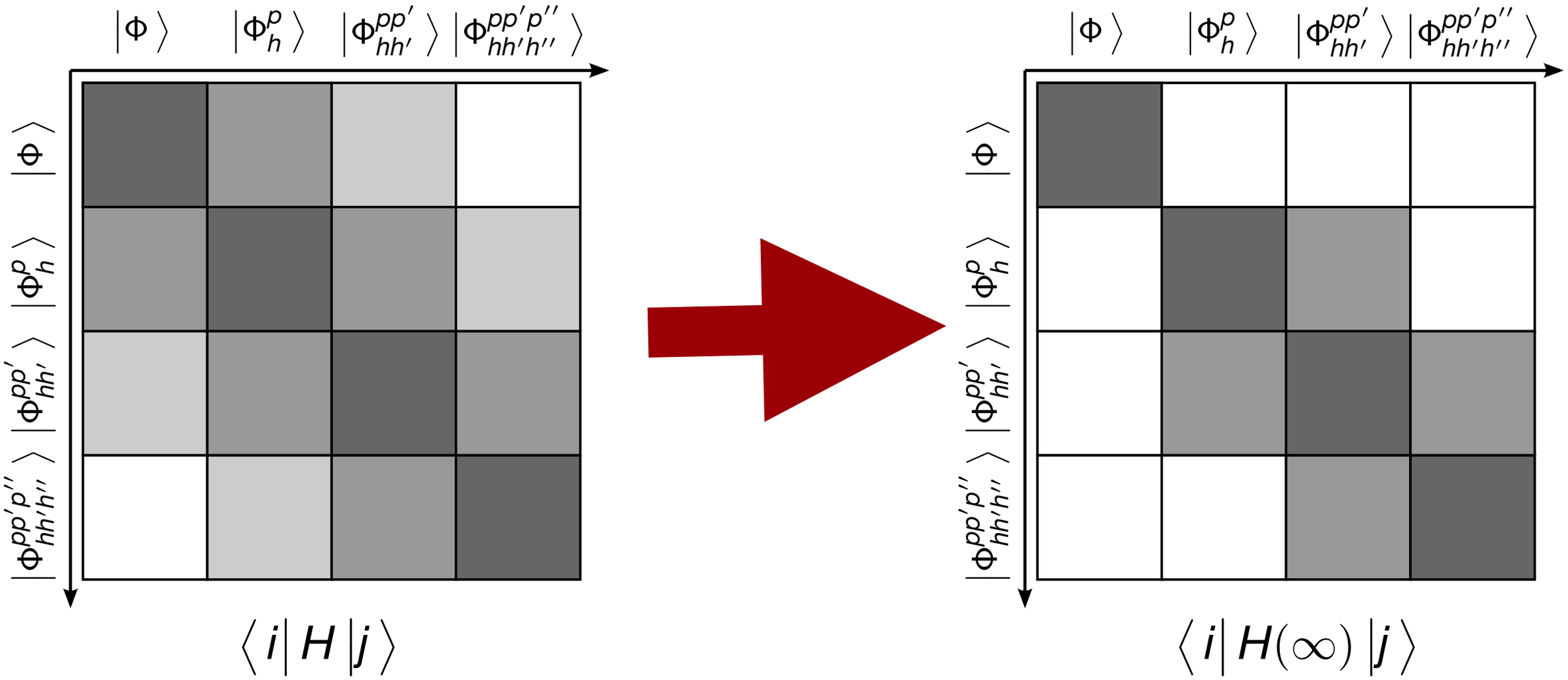
Normal-Ordered Hamiltonian

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



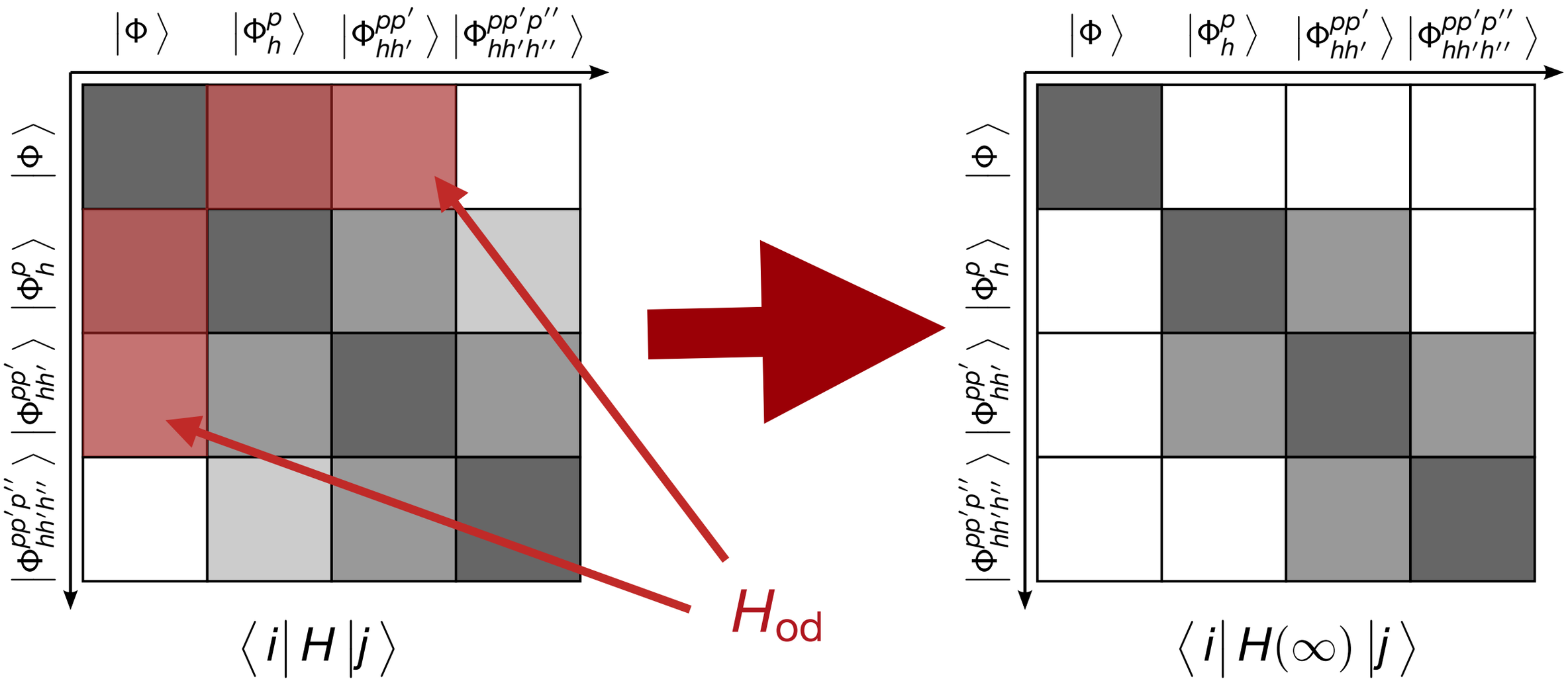
two-body formalism with in-medium contributions from three-body interactions

Decoupling in A-Body Space



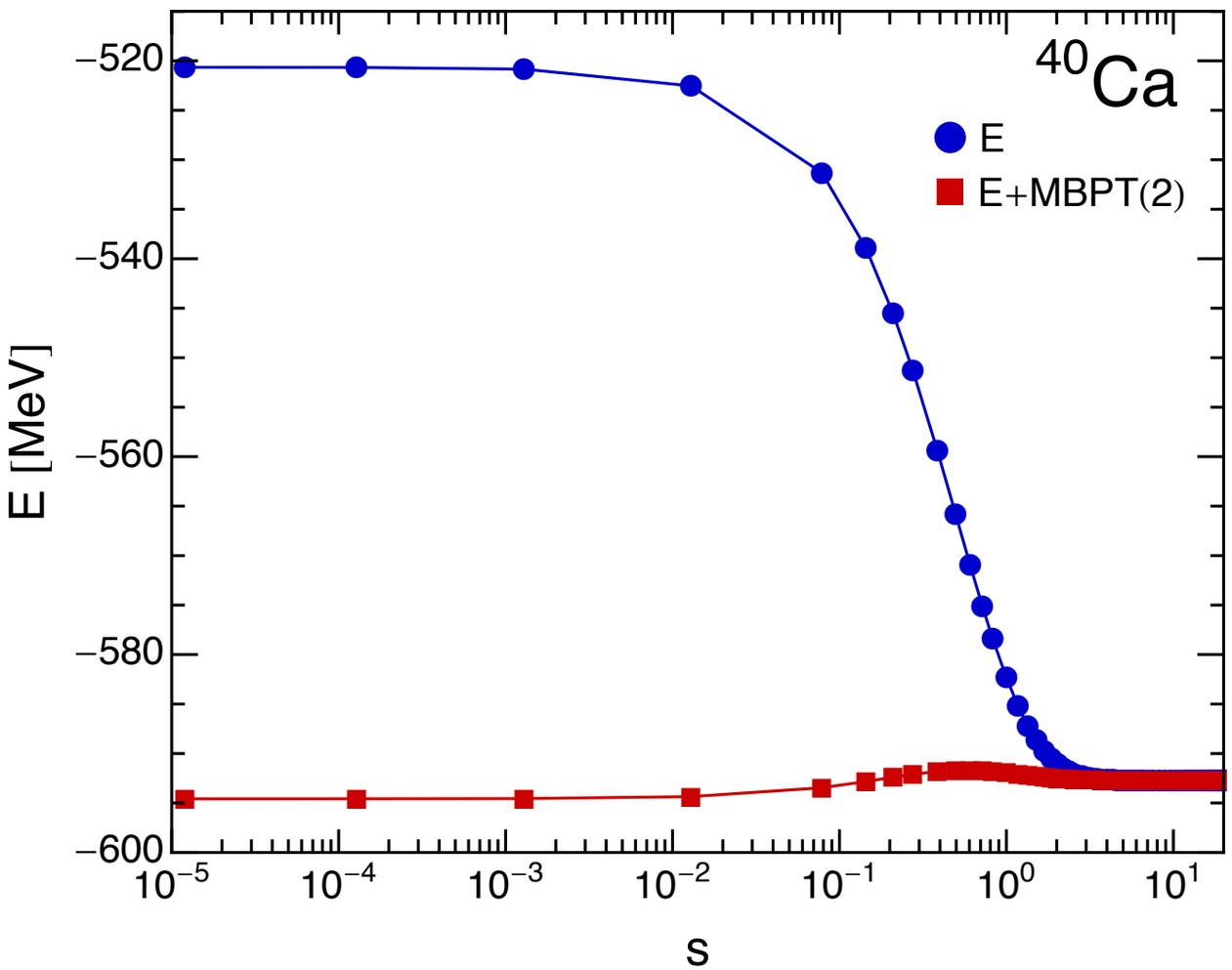
aim: decouple reference state $|\Phi\rangle$
from excitations

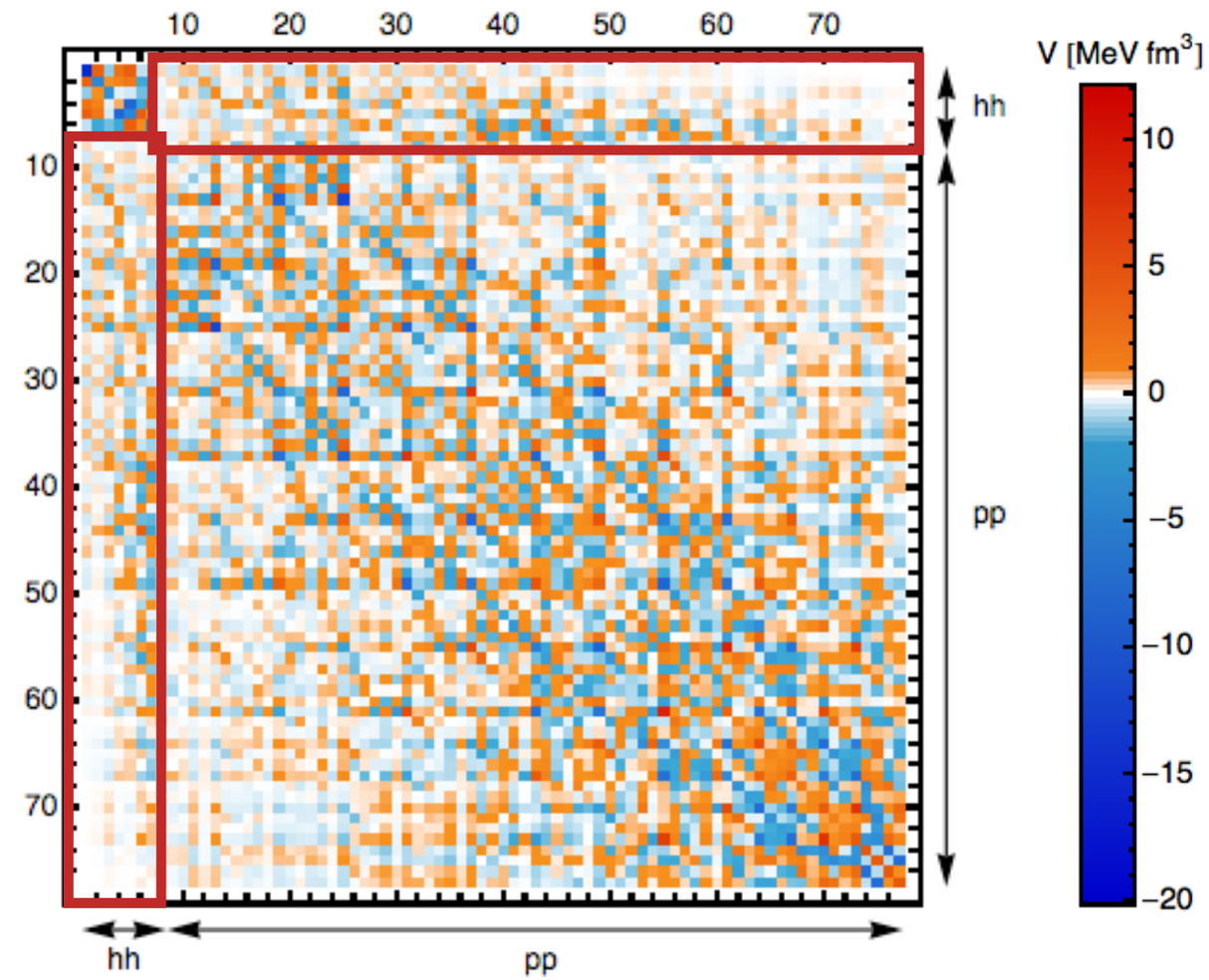
Flow Equation



$$\frac{d}{ds}H(s) = \left[\eta(s), H(s)\right], \quad \text{e.g.,} \quad \eta(s) \equiv \left[H_d(s), H_{od}(s)\right]$$

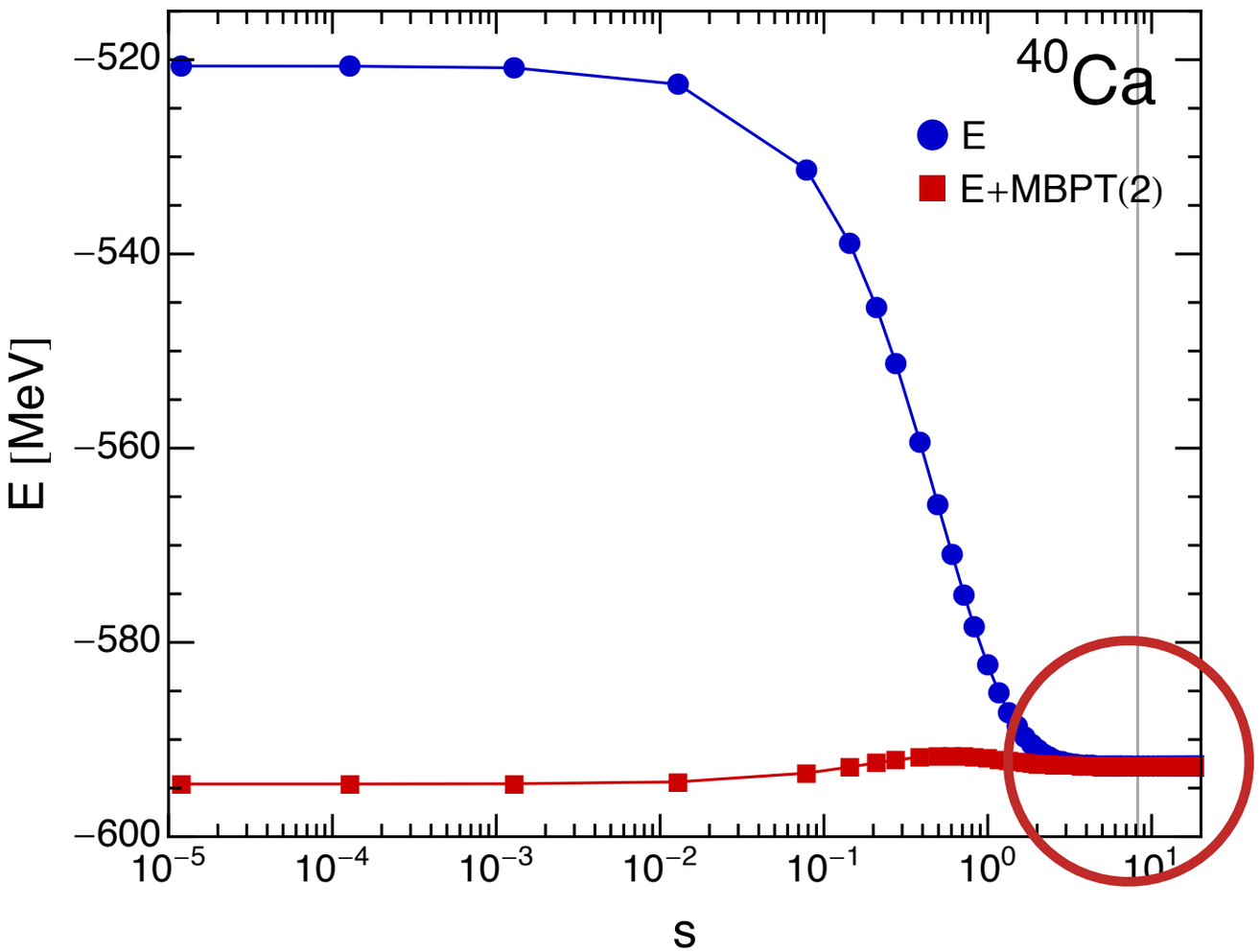
Decoupling

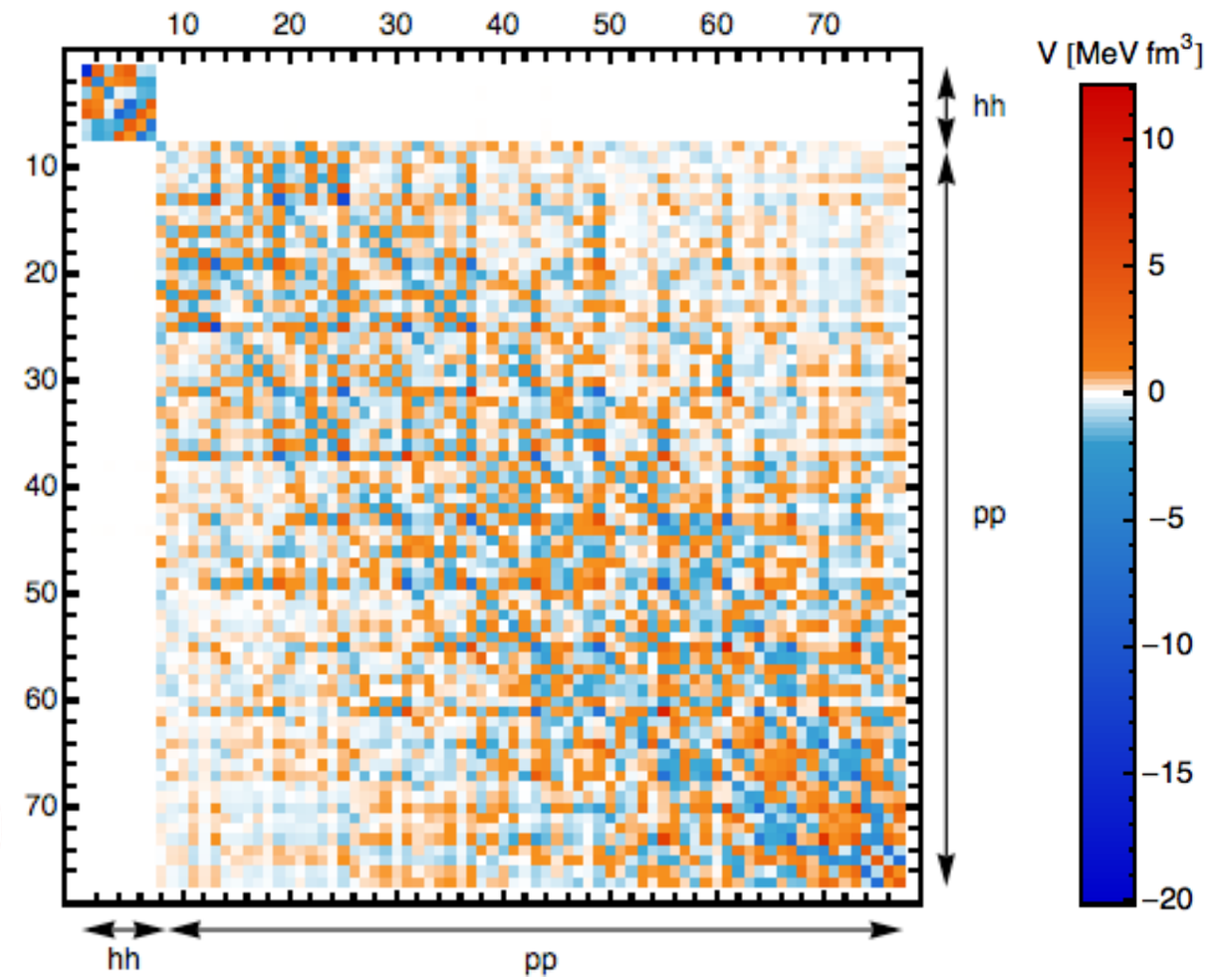




N3LO, $\lambda = 2.0$ fm^{-1}, $e_{\mathrm{Max}} = 8$

Decoupling



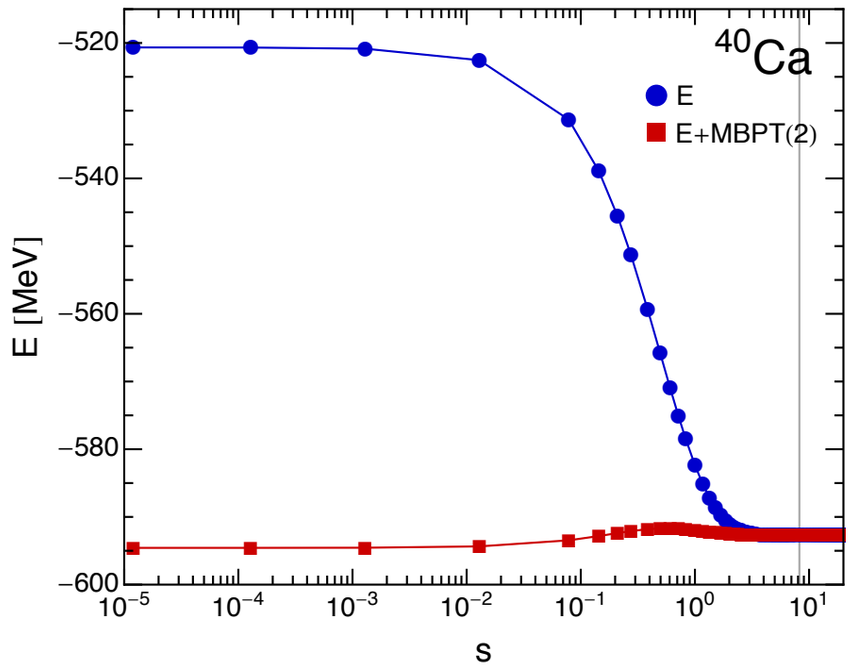


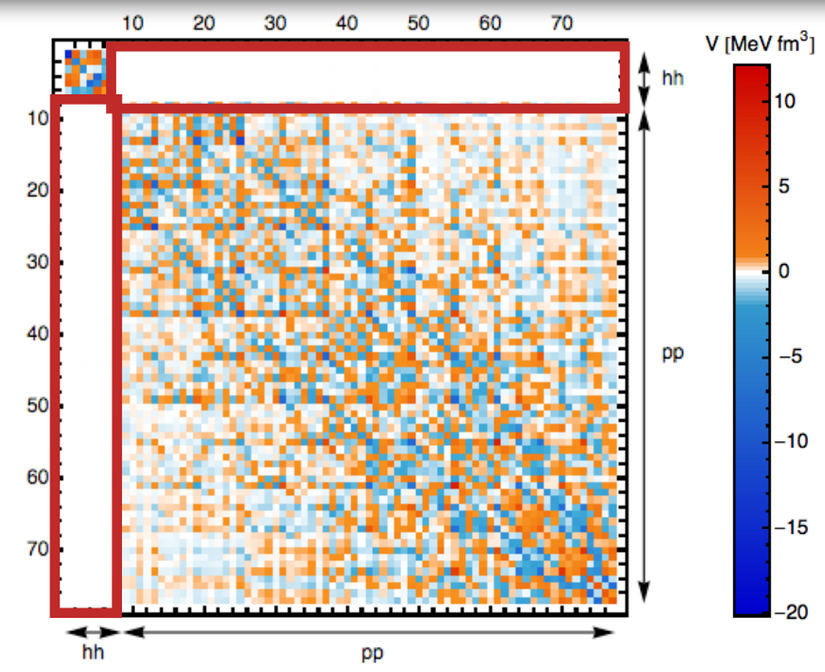
N3LO, $\lambda = 2.0$ fm^{-1}, $e_{\mathrm{Max}} = 8$

non-perturbative resummation of MBPT series (correlations)

off-diagonal couplings are rapidly driven to zero

Decoupling





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

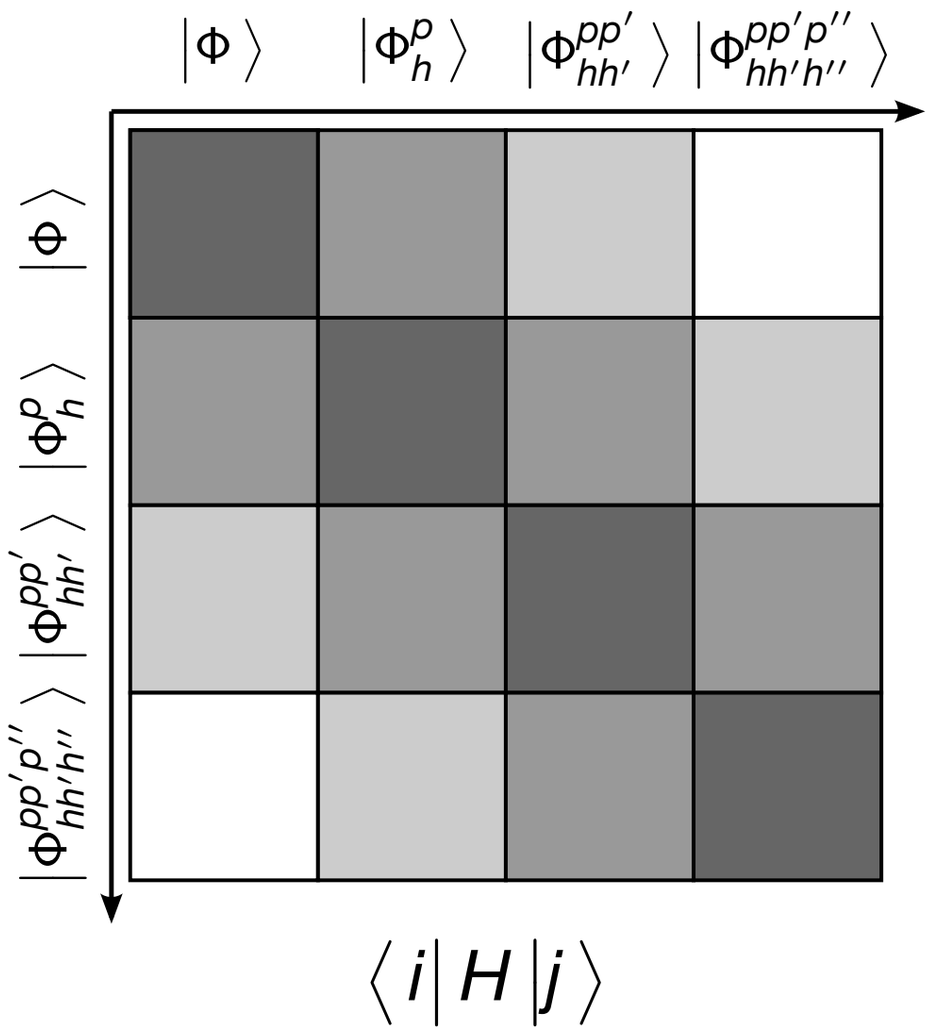
- absorb correlations into **RG-improved Hamiltonian**

$$U(s)HU^{\dagger}(s)U(s)\left|\Psi_n\right\rangle = E_n U(s)\left|\Psi_n\right\rangle$$

- reference state is ansatz for transformed, **less correlated** eigenstate:

$$U(s)\left|\Psi_n\right\rangle \stackrel{!}{=} \left|\Phi\right\rangle$$

Single-Reference Case



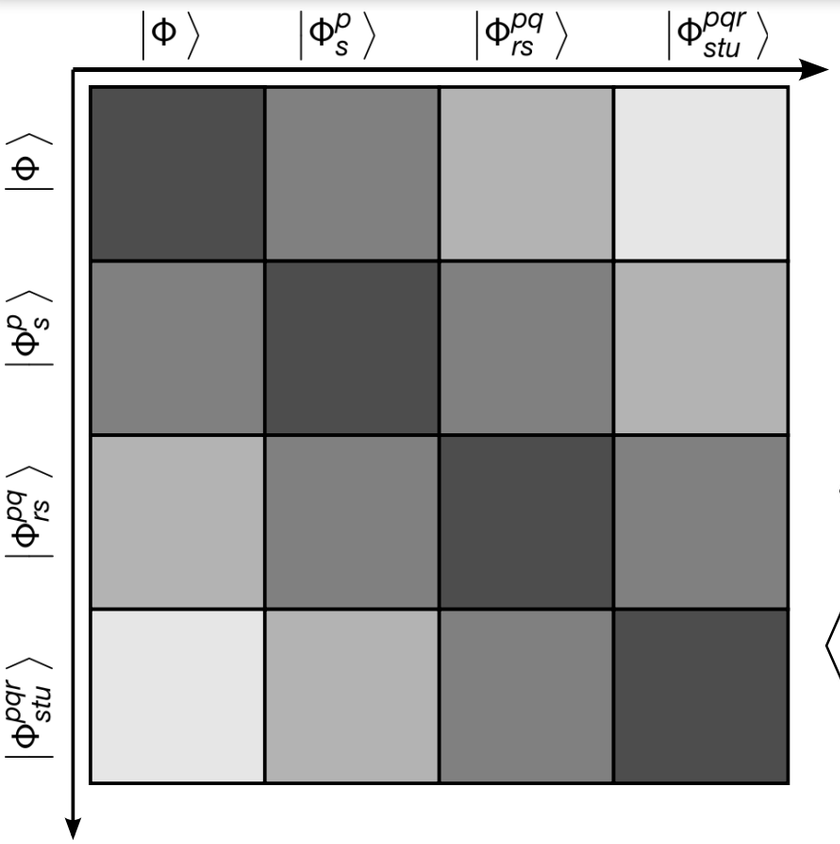
$$A^{i_1\ldots i_N}_{j_1\ldots j_N} \equiv a^\dagger_{i_1}\ldots a^\dagger_{i_N} a_{j_N}\ldots a_{j_1}$$

$$\langle {}^{p}_{h}|H|\Psi\rangle = \sum_{kl} f^k_l \langle\Psi| : A^h_p :: A^k_l : |\Psi\rangle = -n_h\bar{n}_p f^p_h$$

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

- reference state: **Slater determinant**
- normal-ordered operators **depend on occupation numbers (one-body density)**

Multi-Reference Case



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

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

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

- reference state: **arbitrary**
- normal-ordered operators depend on up to **irreducible n-body density matrices** of the reference state

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

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

$$\ldots$$

MR-IM-SRG References States

available

- **number-projected Hartree-Fock Bogoliubov** vacua:

$$\left|\Phi_{ZN}\right\rangle = \frac{1}{(2\pi)^2}\int d\phi_p \int d\phi_n \, e^{i\phi_p(\hat{Z}-Z)} e^{i\phi_n(\hat{N}-N)} \left|\Phi\right\rangle$$

- small-scale (e.g., $0\hbar\Omega$, $2\hbar\Omega$) **No-Core Shell Model**:

$$\left|\Phi\right\rangle = \sum_{N=0}^{N_{\max}} \sum_{i=1}^{\dim(N)} C_i^{(N)} \left|\Phi_i^{(N)}\right\rangle$$

- **Generator Coordinate Method** (w/projections):

$$\left|\Phi\right\rangle = \int dq \, f(q) \, P_{J=0M=0} P_Z P_N \left|q\right\rangle$$

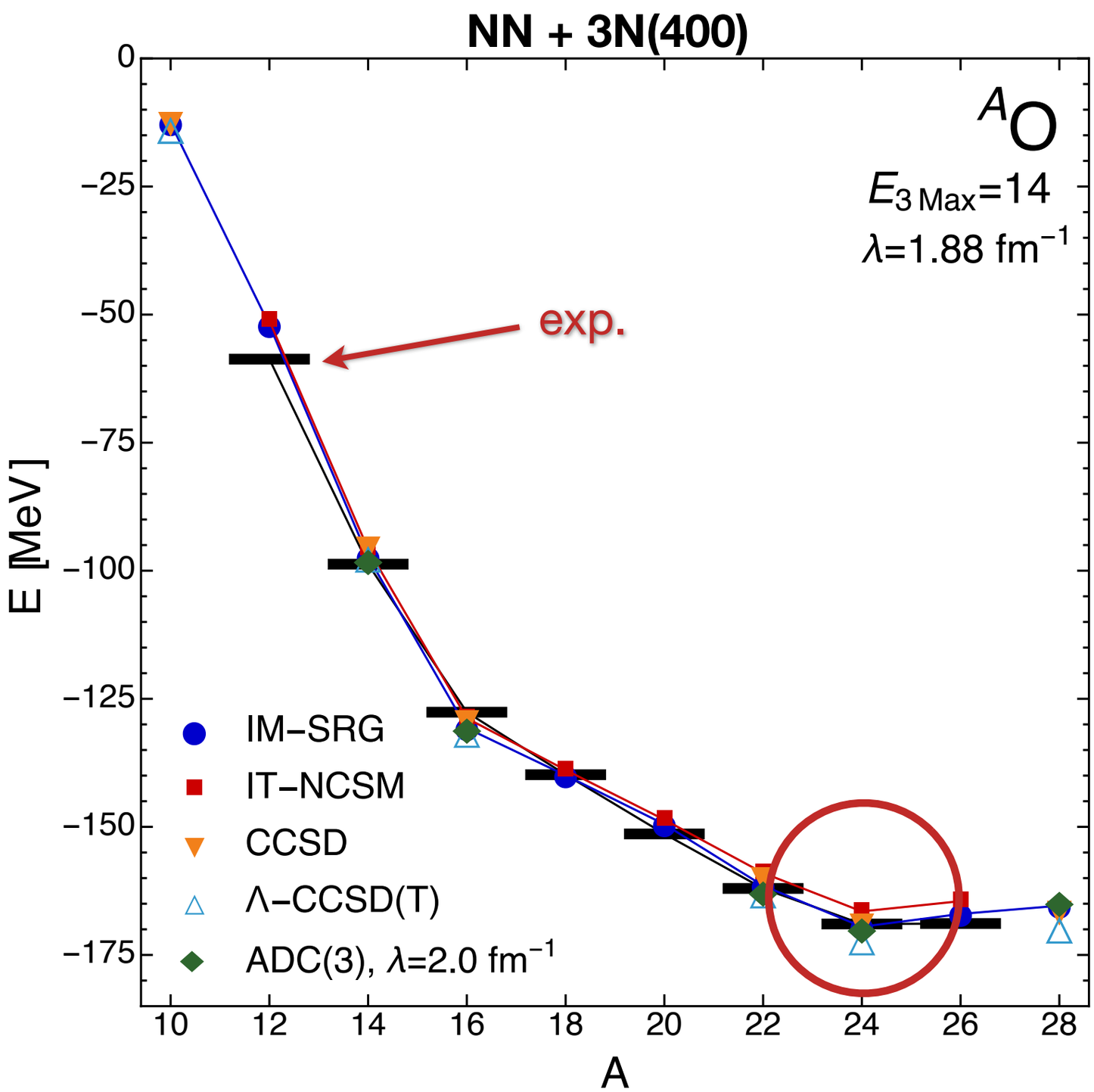
future

- clustered states, Density Matrix Rep
etc.

build static correlations into the reference state

Oxygen Isotopes

*HH et al., PRL **110**, 242501 (2013), ADC(3): A. Cipollone et al., PRL **111**, 242501 (2013)*

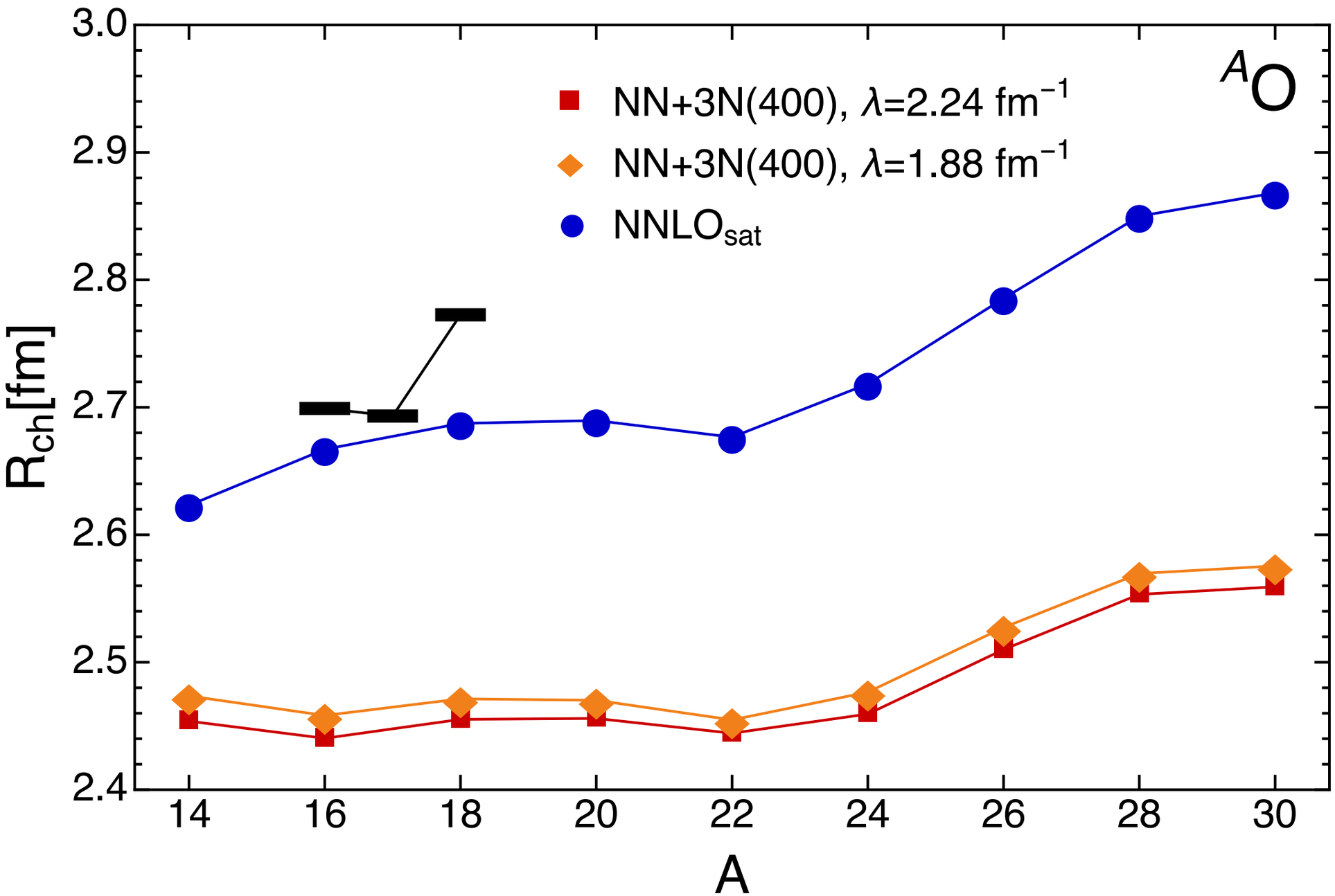


- MR-IM-SRG with particle-number projected HFB reference state
- consistent results from different many-body methods

drip line at ^{24}O

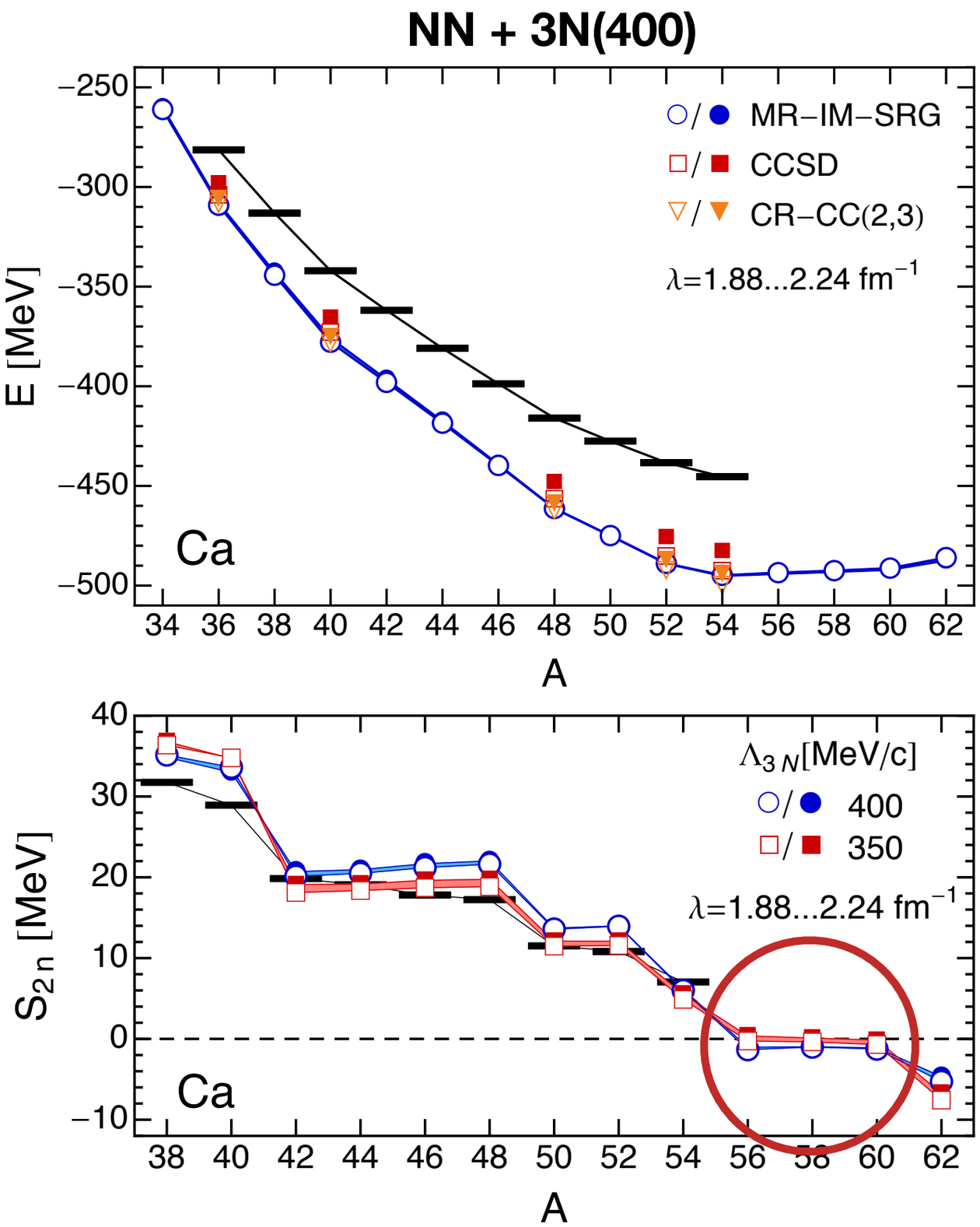
Oxygen Radii

V. Lapoux, V. Somà, C. Barbieri, H. H., J. D. Holt, and S. R. Stroberg, to appear in PRL



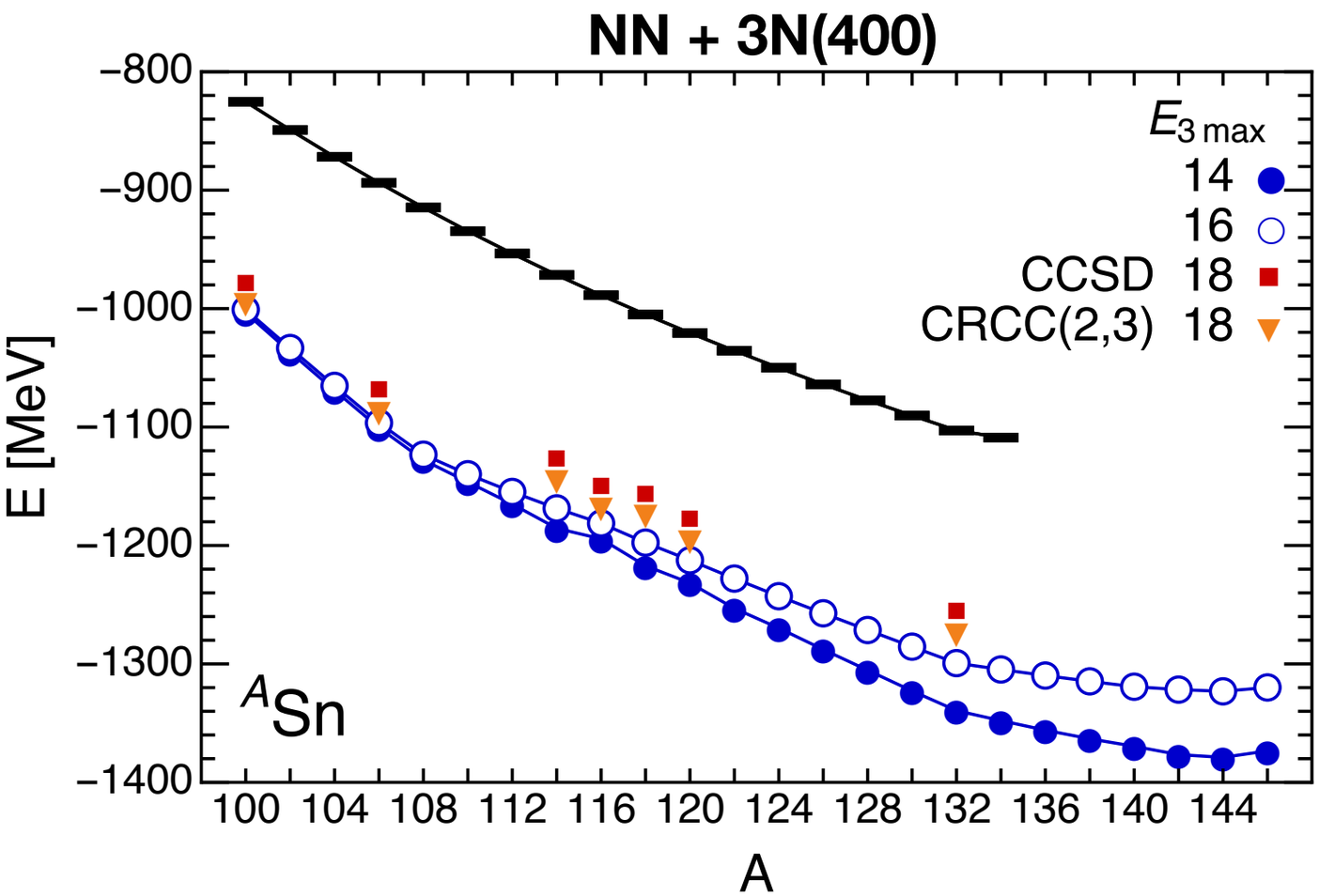
Calcium Isotopes

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



- 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 magic for these NN+3N interactions
- no continuum coupling yet, other S_{2n} uncertainties < 1MeV

The Mass Frontier: Tin



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

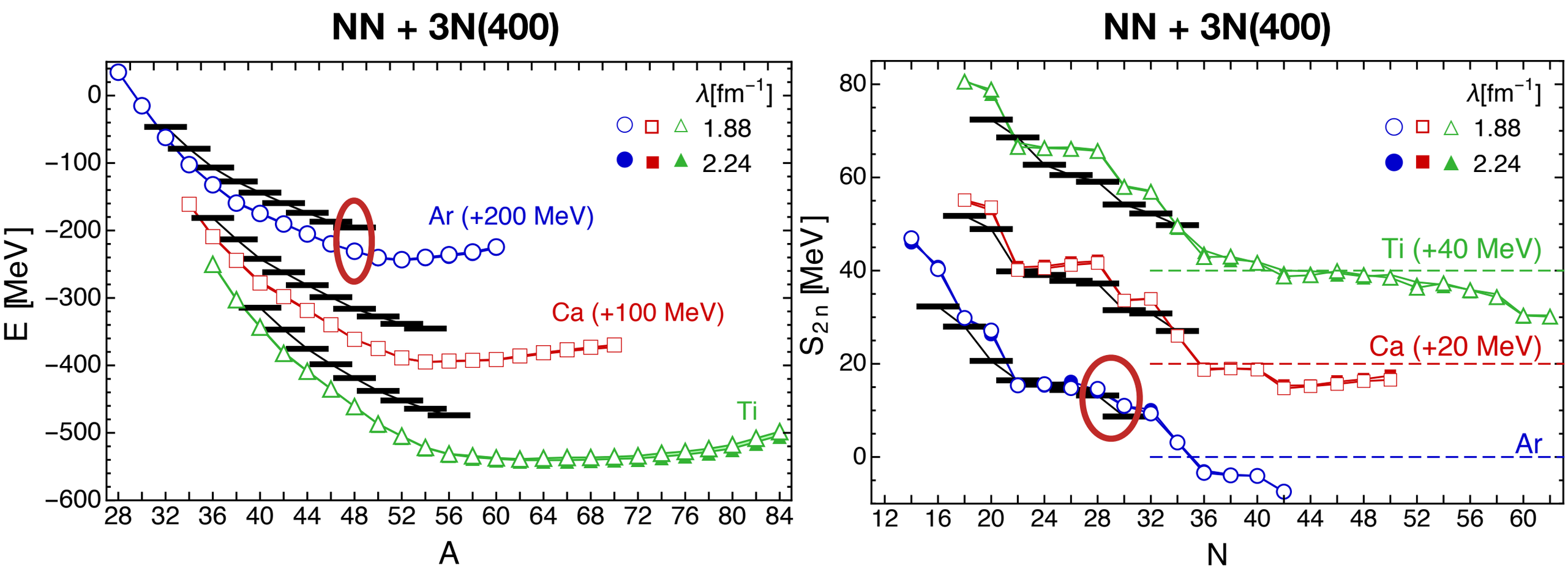
- systematics of overbinding similar to Ca/Ni
- not converged with respect to 3N matrix element truncation:

$$e_1 + e_2 + e_3 \leq E_{3max}$$

($e_{1,2,3}$: SHO energy quantum numbers)

- need technical improvements to go further

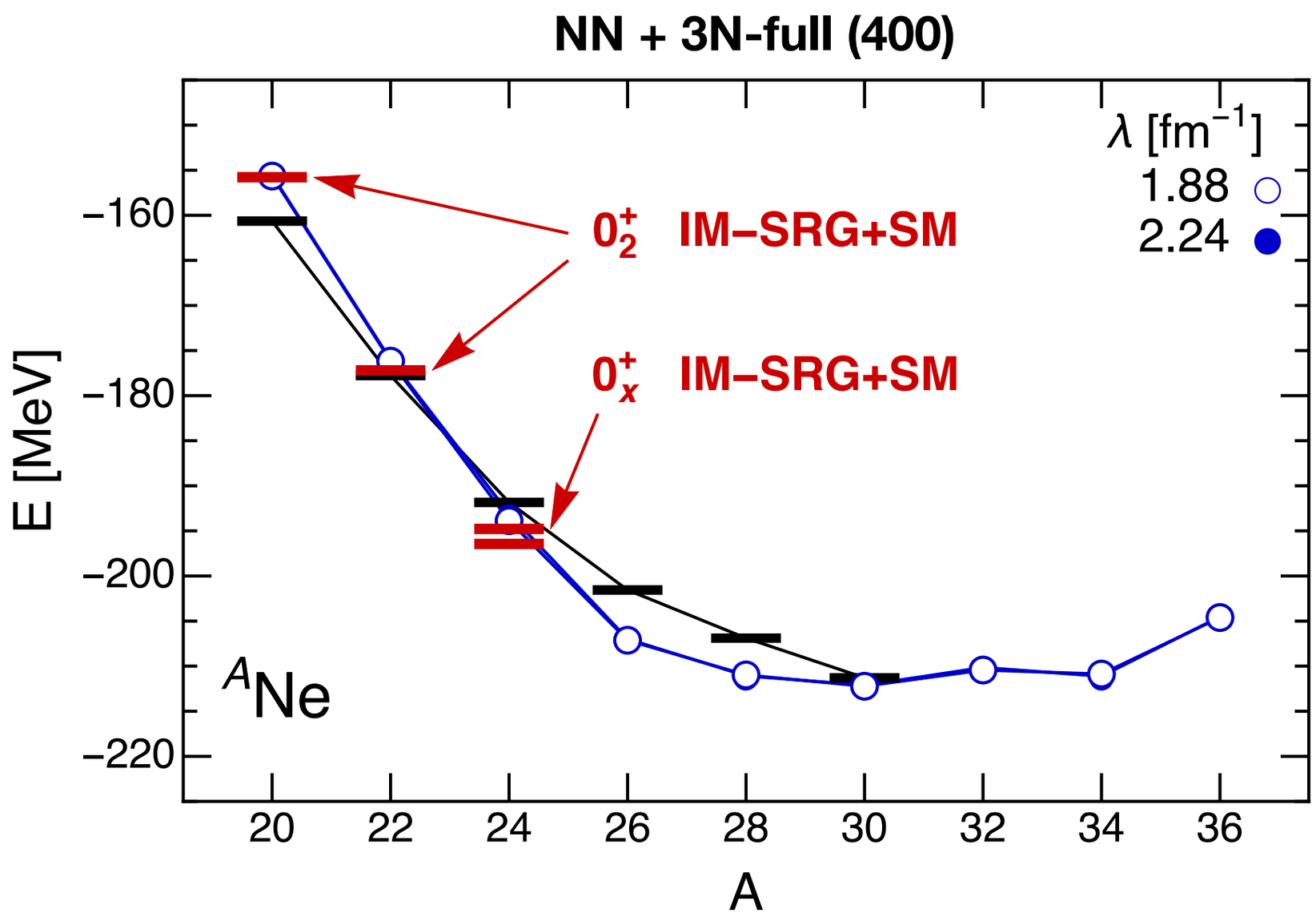
Isotopic Chains Around Ca



- S_{2n} consistent with Gor'kov GF, (weak) shell closure predicted in ^{46}Ar
  (Somà et al., PRC 89, 061301(R), 2014)

- ^{48,49}Ar masses measured at NSCL, ^{46}Ar shell closure found
  (Meisel et al., PRL 114, 022501, 2015)

Neon Isotopes



➡ MR-IM-SRG selects excited 0^+ state
(from intrinsically spherical reference state)

MR-IM-SRG References States

available

- **number-projected Hartree-Fock Bogoliubov** vacua:

$$\left|\Phi_{ZN}\right\rangle = \frac{1}{(2\pi)^2}\int d\phi_p \int d\phi_n \, e^{i\phi_p(\hat{Z}-Z)} e^{i\phi_n(\hat{N}-N)} \left|\Phi\right\rangle$$

- small-scale (e.g., $0\hbar\Omega$, $2\hbar\Omega$) **No-Core Shell Model**:

$$\left|\Phi\right\rangle = \sum_{N=0}^{N_{\max}} \sum_{i=1}^{\dim(N)} C_i^{(N)} \left|\Phi_i^{(N)}\right\rangle$$

- **Generator Coordinate Method** (w/projections):

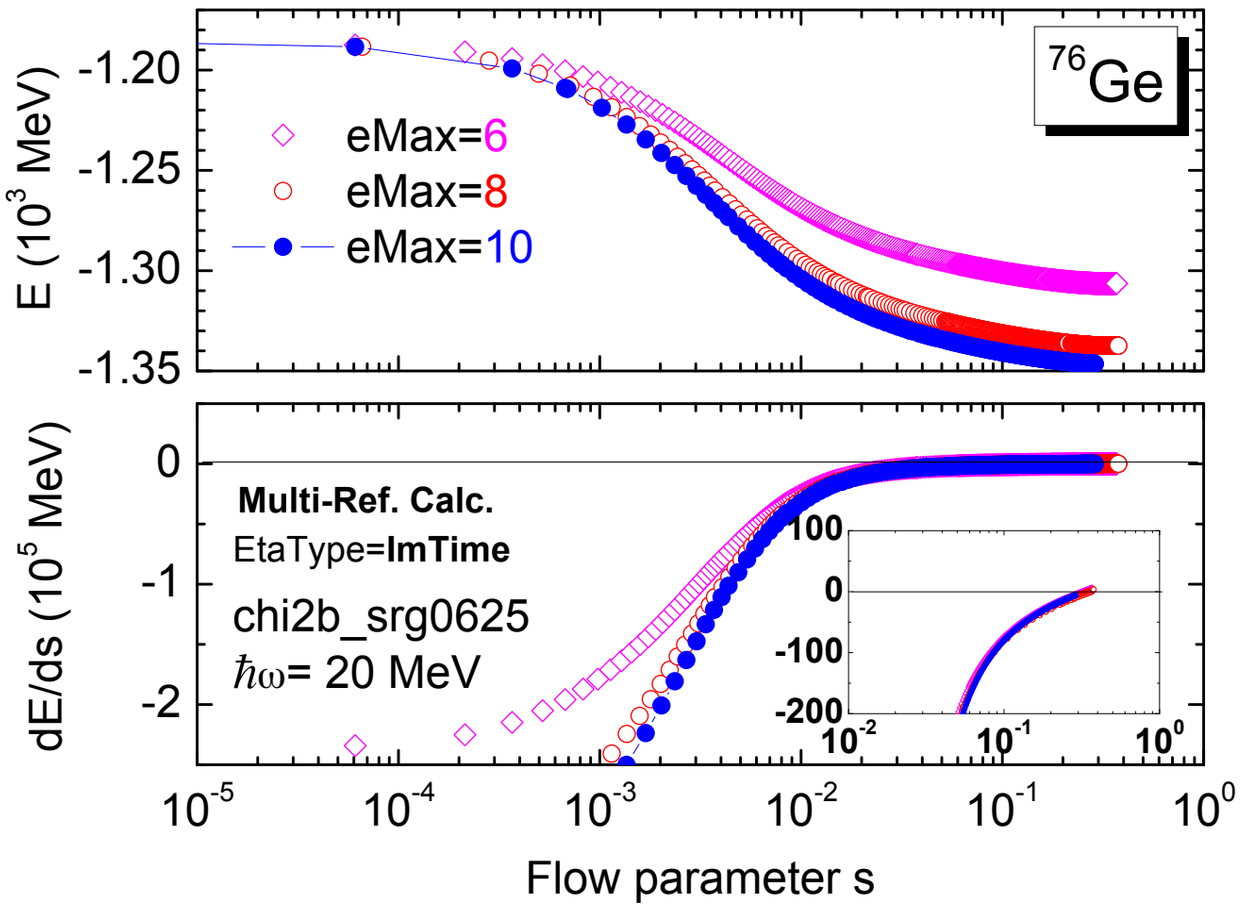
$$\left|\Phi\right\rangle = \int dq \, f(q) \, P_{J=0M=0} P_Z P_N \left|q\right\rangle$$

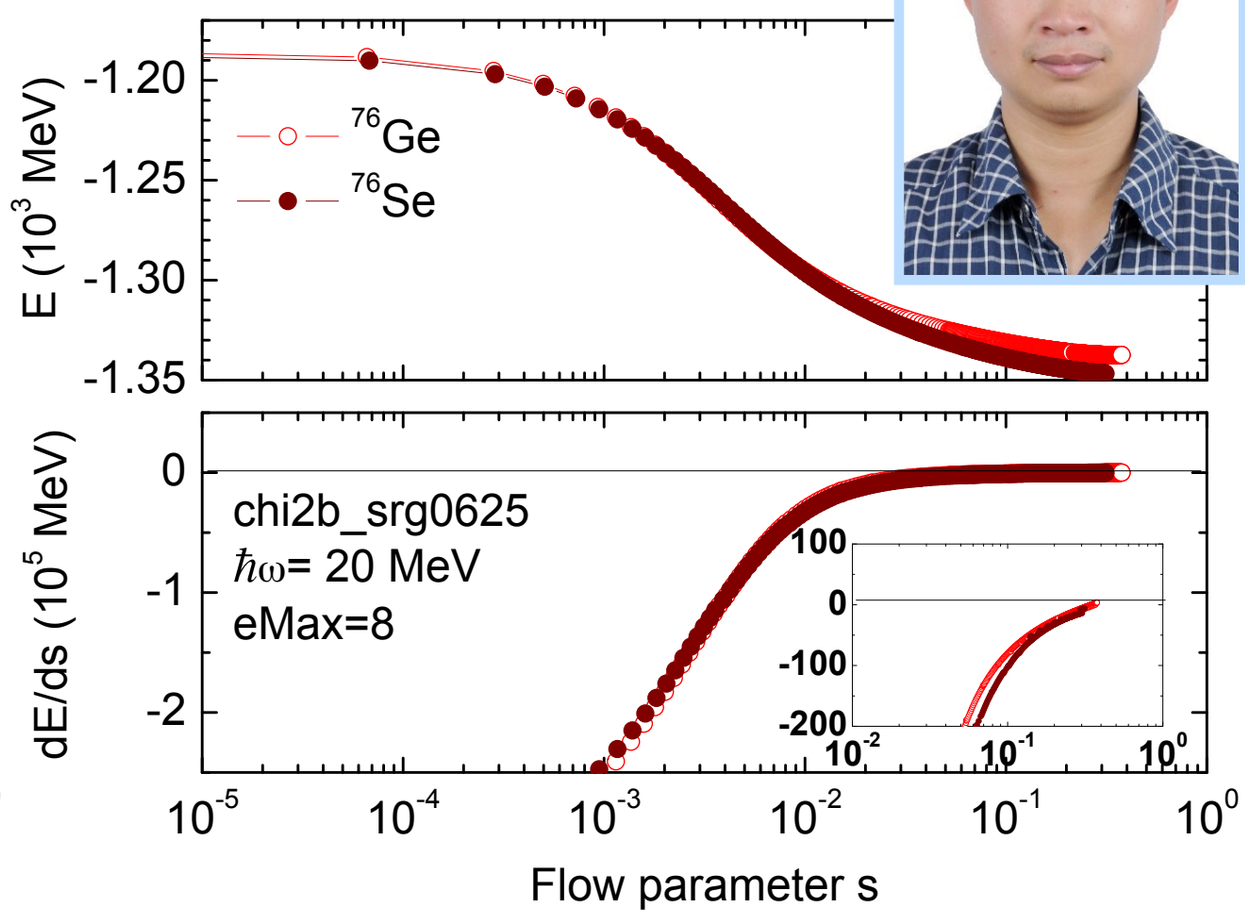
future

- clustered states, Density Matrix Renormalization Group, etc.

$^{76}Ge \longrightarrow {}^{76}Se$

with **J. Yao**, C. Jiao, J. Engel (UNC Chapel Hill)





➡ goal: **direct calculation** of nuclear matrix element for $^{76}Ge \longrightarrow {}^{76}Se$ in MR-IM-SRG/MAG

Ab Initio Many-Body Methods:

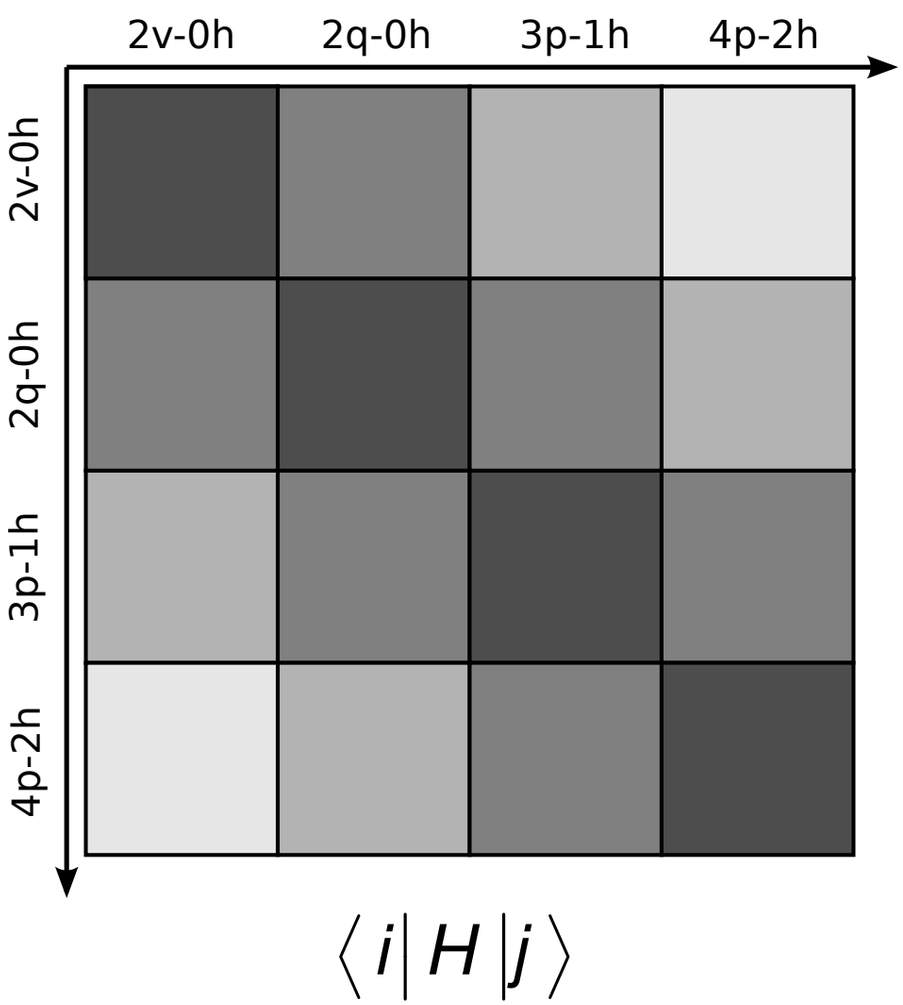
Non-Empirical Shell Model Interactions from the IM-SRG

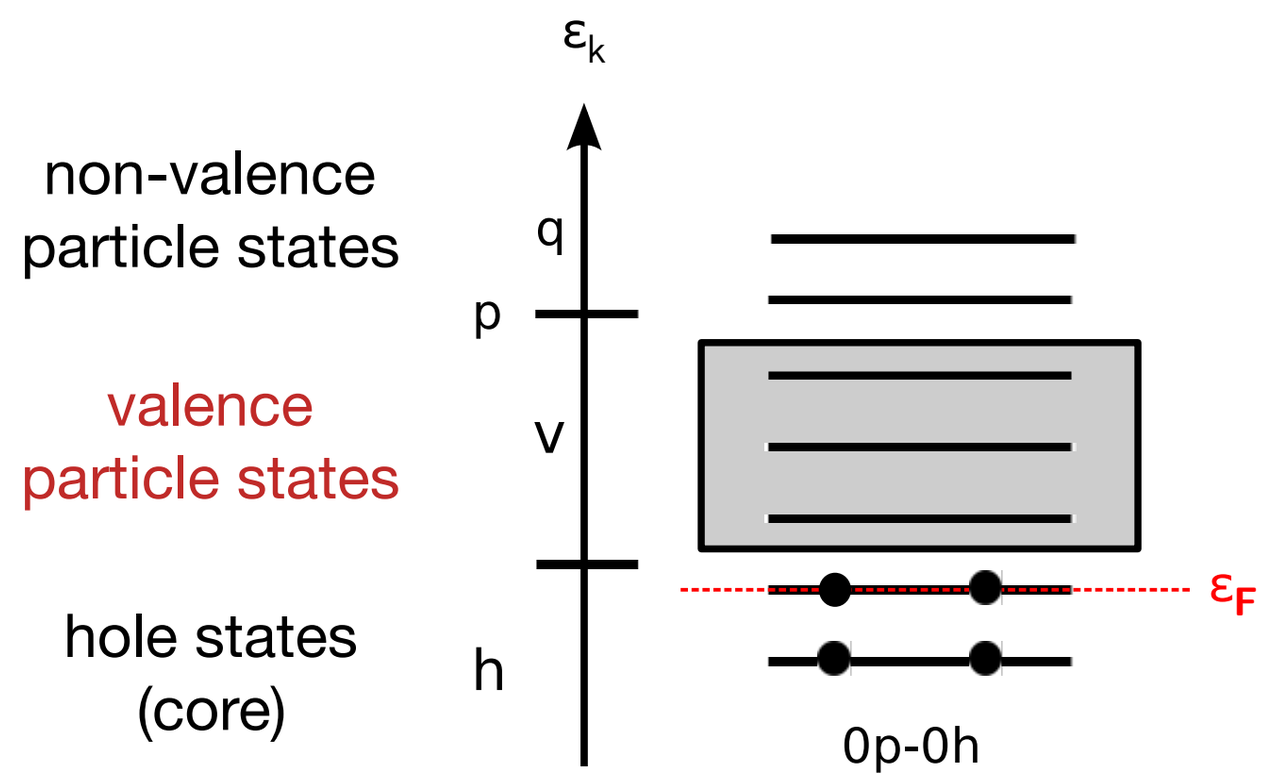
S. R. Stroberg, A. Calci, H. H., J. D. Holt, S. K. Bogner, R. Roth, A. Schwenk, arXiv:1607.03229 [nucl-th]

S. R. Stroberg, H. H., J. D. Holt, S. K. Bogner, A. Schwenk, Phys. Rev. C **93**, 051301(R) (2016)

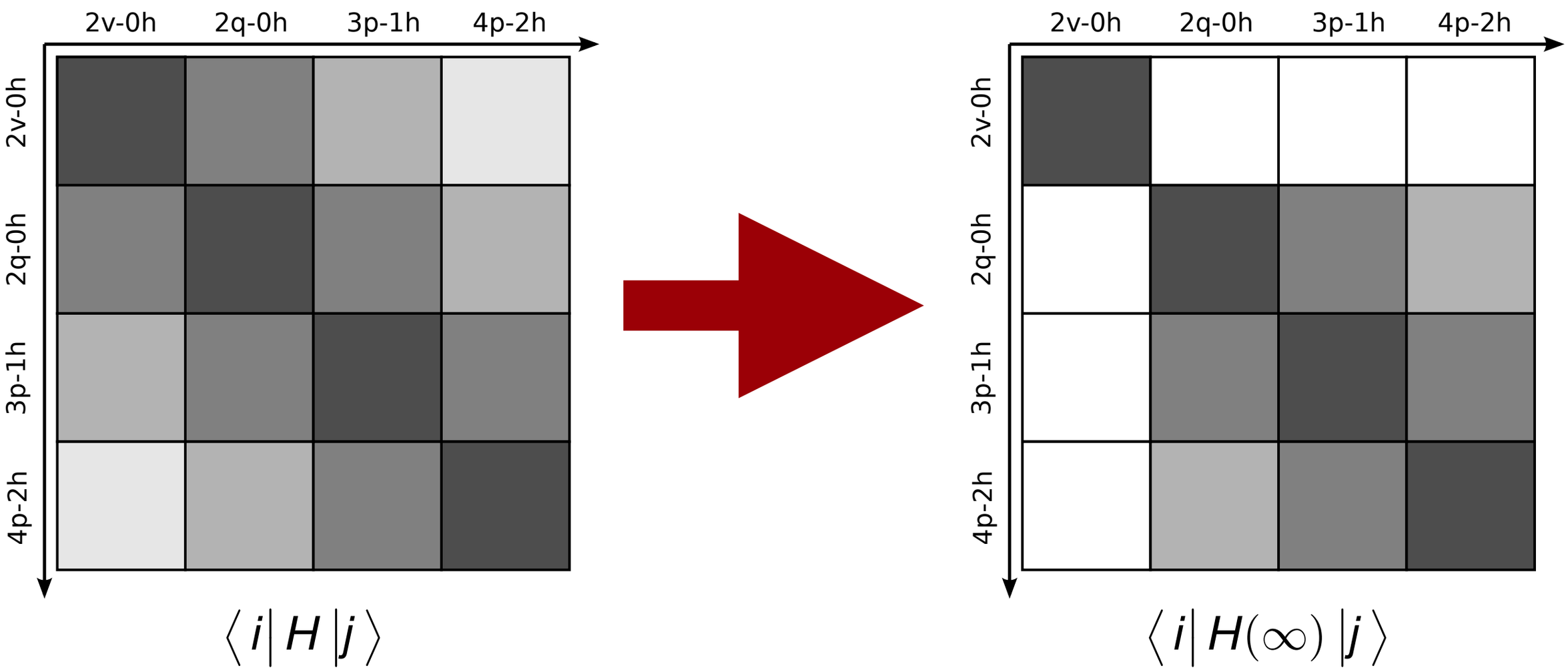
S. K. Bogner, H. H., J. D. Holt, A. Schwenk, S. Binder, A. Calci, J. Langhammer, R. Roth, Phys. Rev. Lett. **113**, 142501 (2014)

Valence Space Decoupling





Valence Space Decoupling

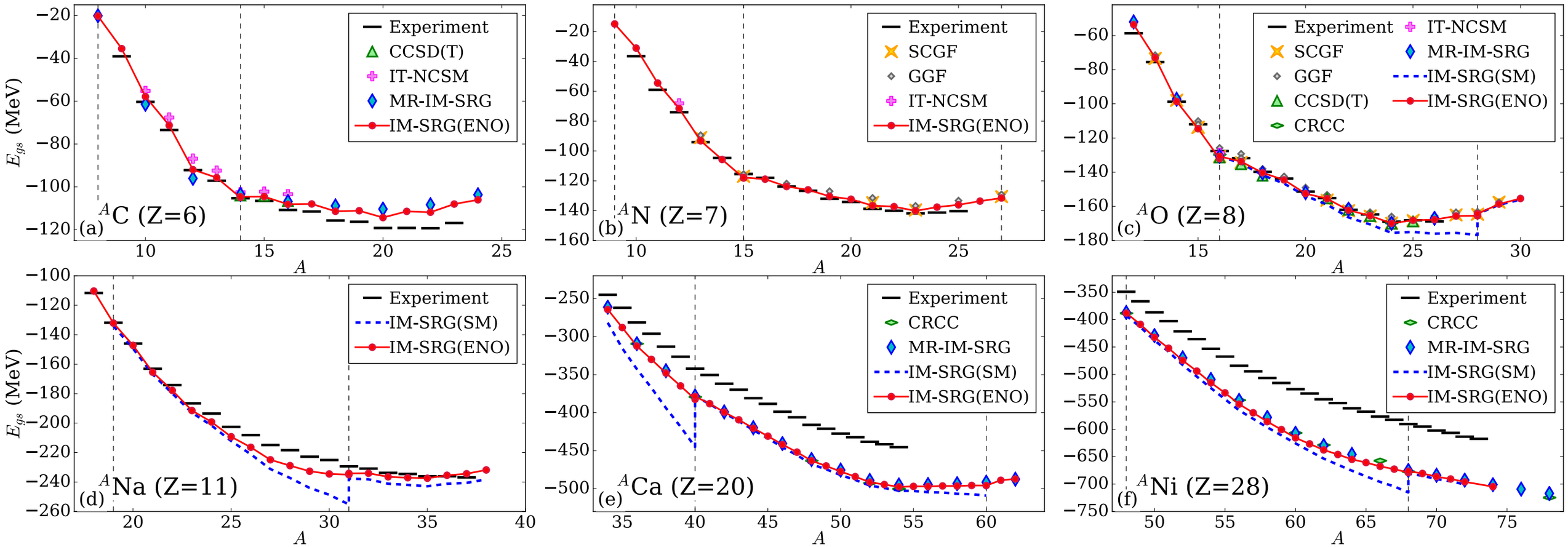


change definition of off-diagonal Hamiltonian:

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

Ground-State Energies

S. R. Stroberg, A. Calci, HH, J. D. Holt, S. K.Bogner, R. Roth, A. Schwenk, arXiv:1607.03229 [nucl-th]

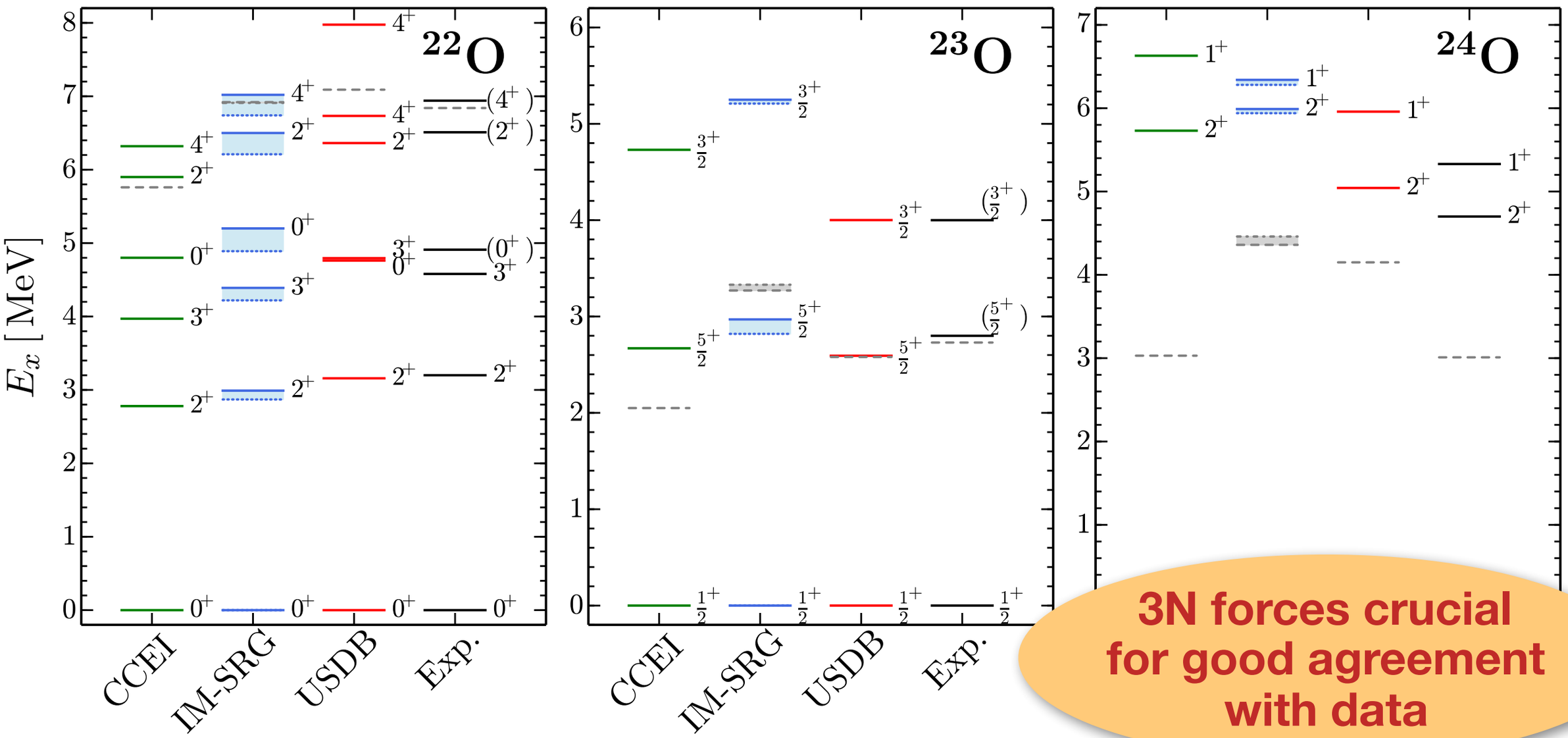


- initial normal ordering and IM-SRG decoupling in the **target nucleus**
- **consistent with (MR-)IM-SRG ground state energies** (and CC, SCGF, …) for the **same Hamiltonian**

Oxygen Spectra

*S. K. Bogner et al., PRL**113**, 142501 (2014); HH, arXiv:1607.06882 [nucl-th]*

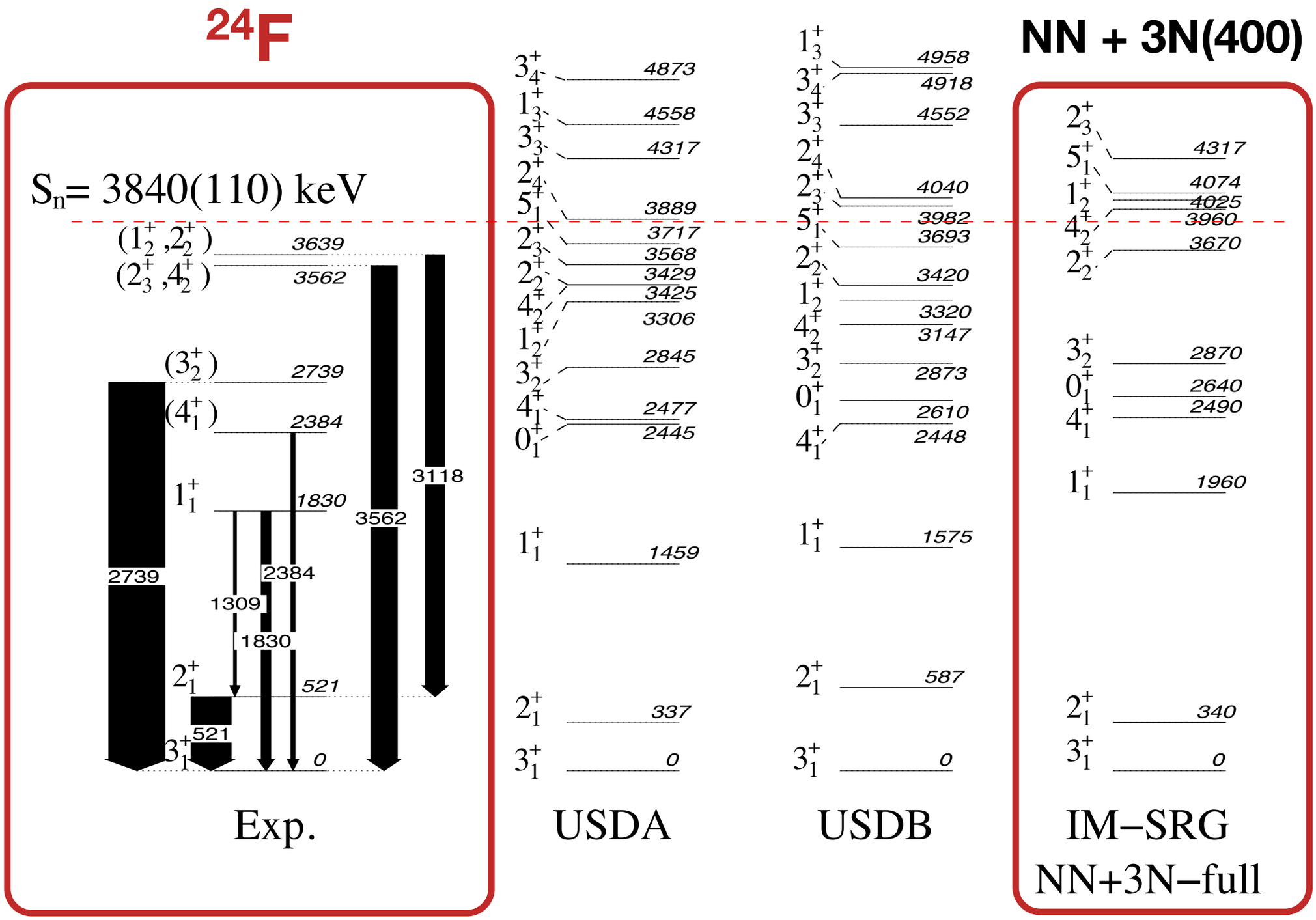
NN + 3N(400)



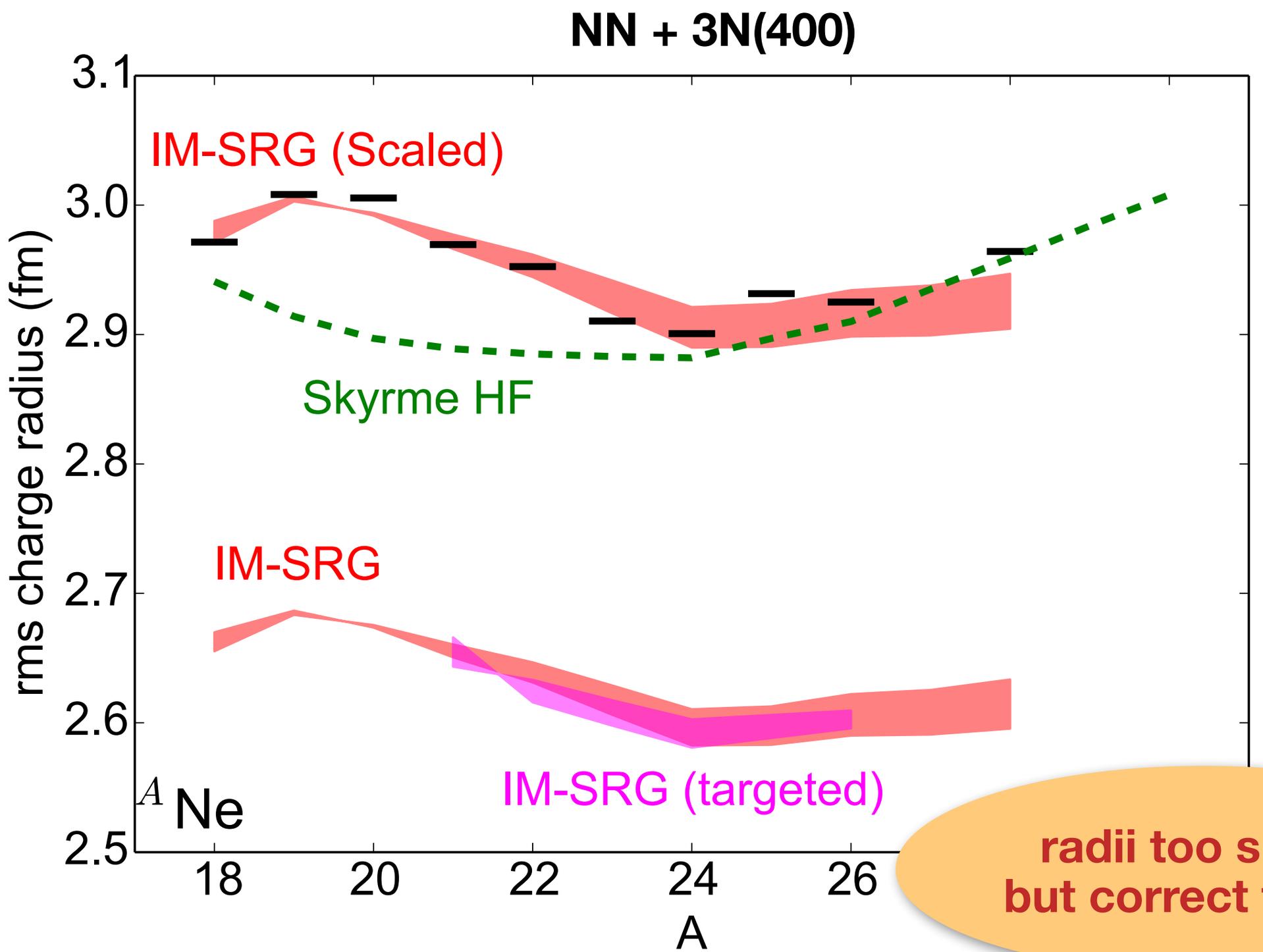
3N forces crucial for good agreement with data

^{24}F Spectrum

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

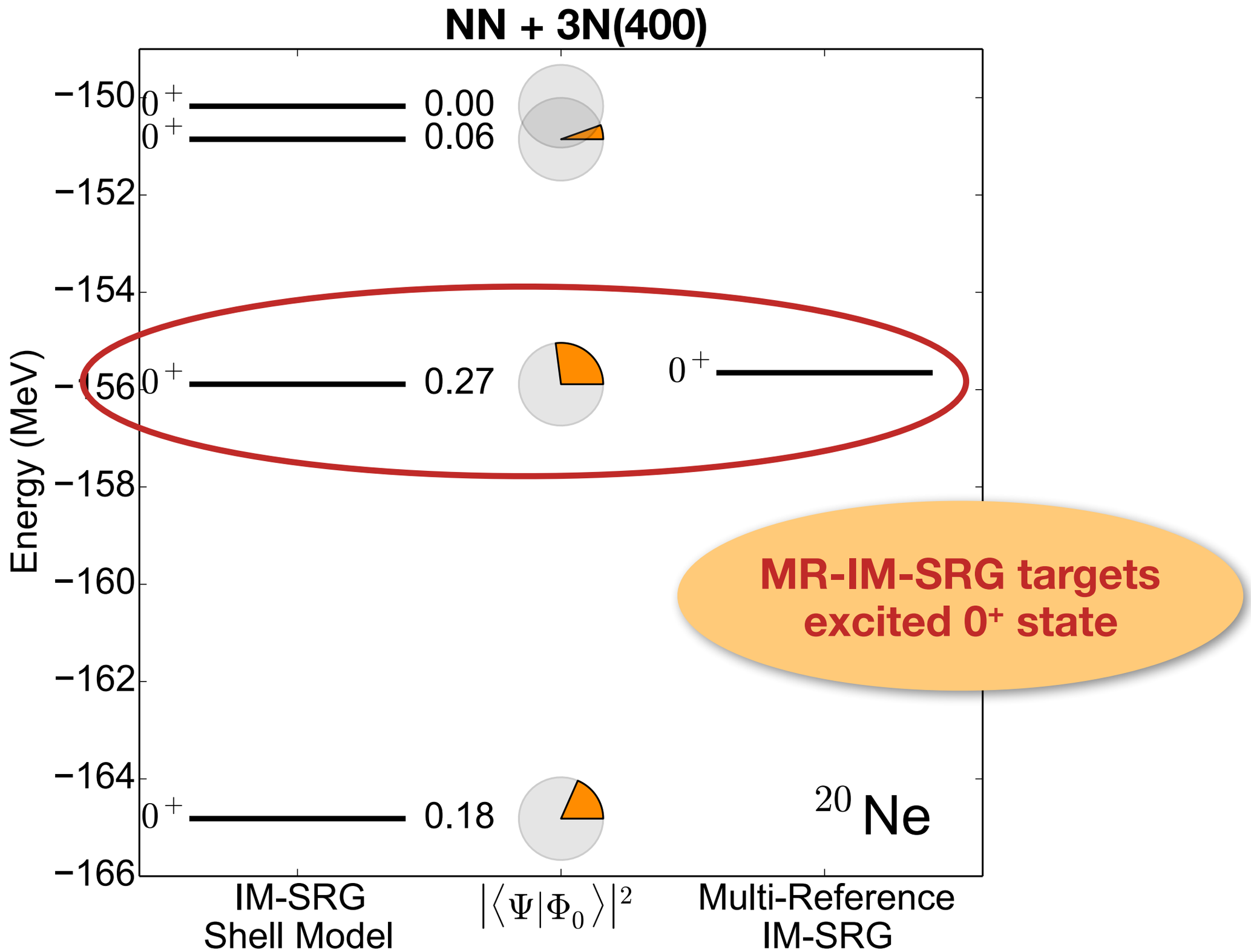


Neon Radii



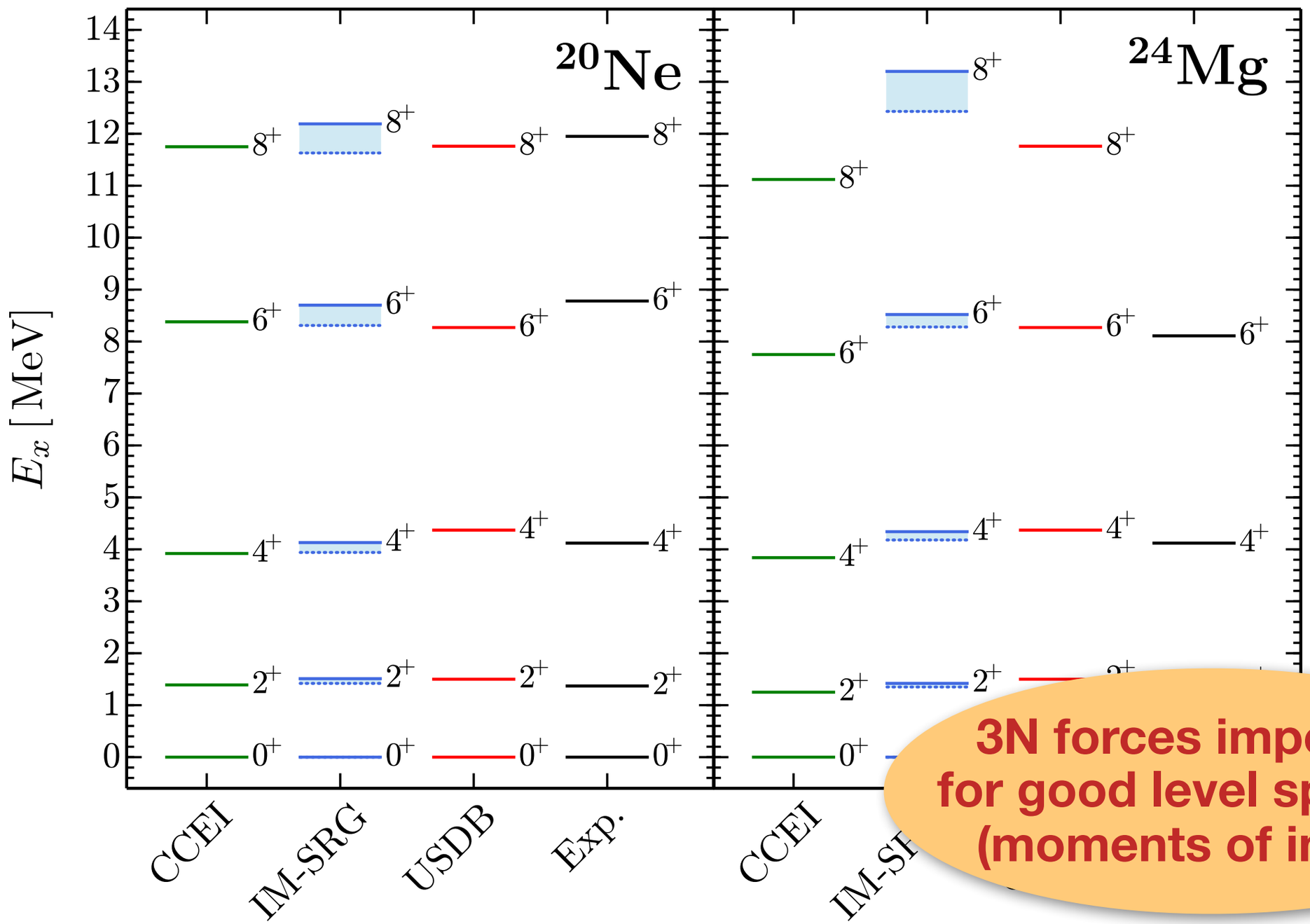
radii too small, but correct trends

Deformation: ^{20}Ne



Rotational Bands

*S. R. Stroberg et al., PRC **93**, 051301(R) (2016); HH, arXiv:1607.06882 [nucl-th]*



3N forces important for good level spacings (moments of inertia)

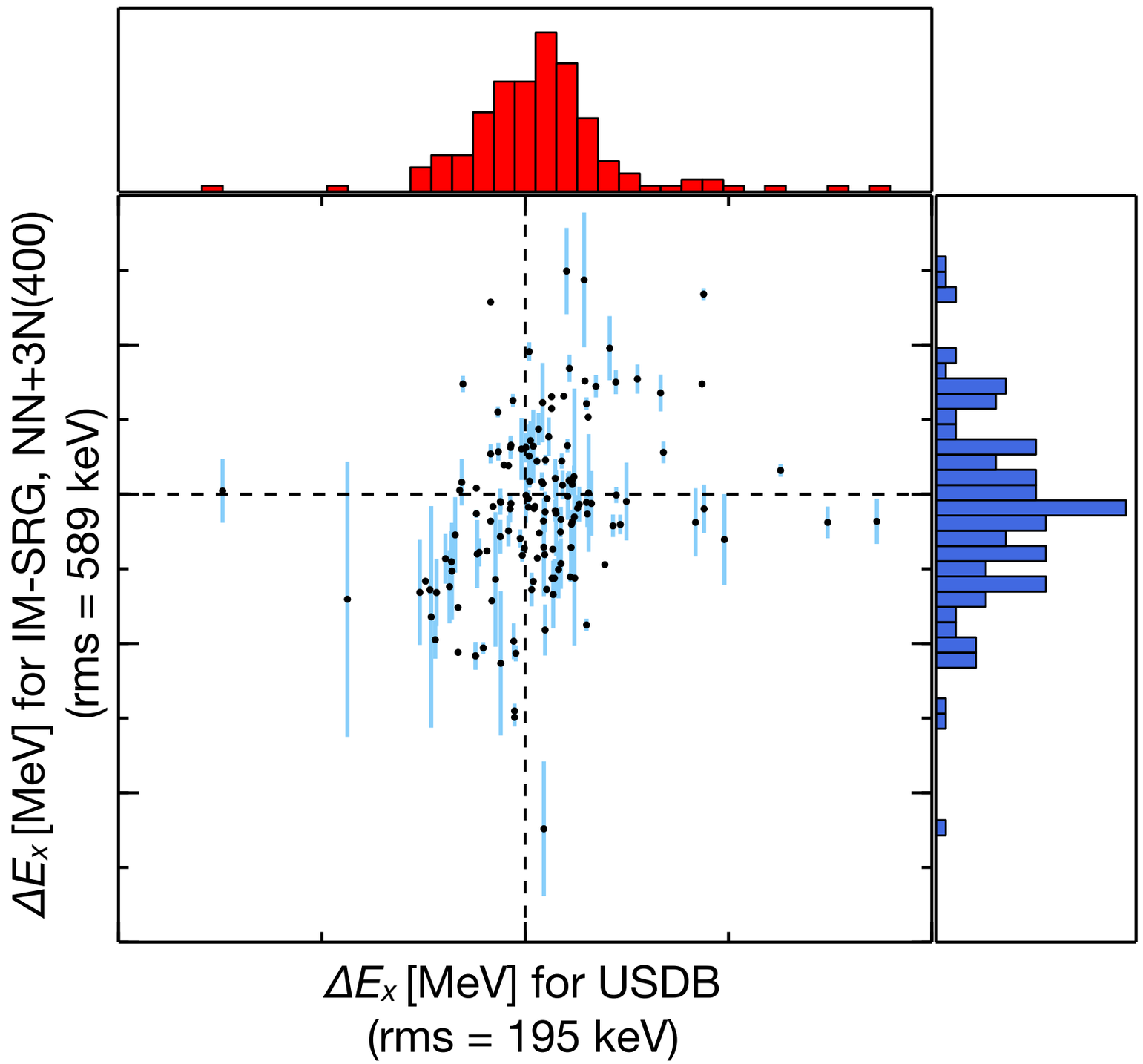
Excited States

144 excited states
in O, F, Ne, Na, Mg

Interaction	RMS [keV]
USD (*)	195
IM-SRG	589
CCEI	582
Kuo-Brown	817
Bonn A (**)	832

(*) phenomenological

(**) G-matrix + phenomenological s.p.e.



Epilogue

Summary

- towards **predictive *ab initio* theory:** interaction, operators, many-body method with systematic uncertainties & convergence to exact result
- **IM-SRG is a novel *ab initio* framework:**
  - **emphasizes RG** aspects of many-body problem
  - **direct calculations** and **RG-improved Hamiltonians**
  - rapidly **growing capabilities**: ground-state energies, spectra, radii, transitions, etc.
- **new generation of chiral NN+3N interactions** is becoming available now ($NNLO_{sat}$, EKM/LENPIC, …), needs to be **confronted with data**

Acknowledgments

S. K. Bogner, M. Hjorth-Jensen, N. M. Parzuchowski, F. Yuan
NSCL/FRIB, Michigan State University

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

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

S. Binder, T. D. Morris
UT Knoxville & Oak Ridge National Laboratory

G. Papadimitriou
Lawrence Livermore National Laboratory

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

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

T. Duguet, V. Somà
CEA Saclay, France

J. Engel, C. Jiao, J. Yao
University of North Carolina - Chapel Hill