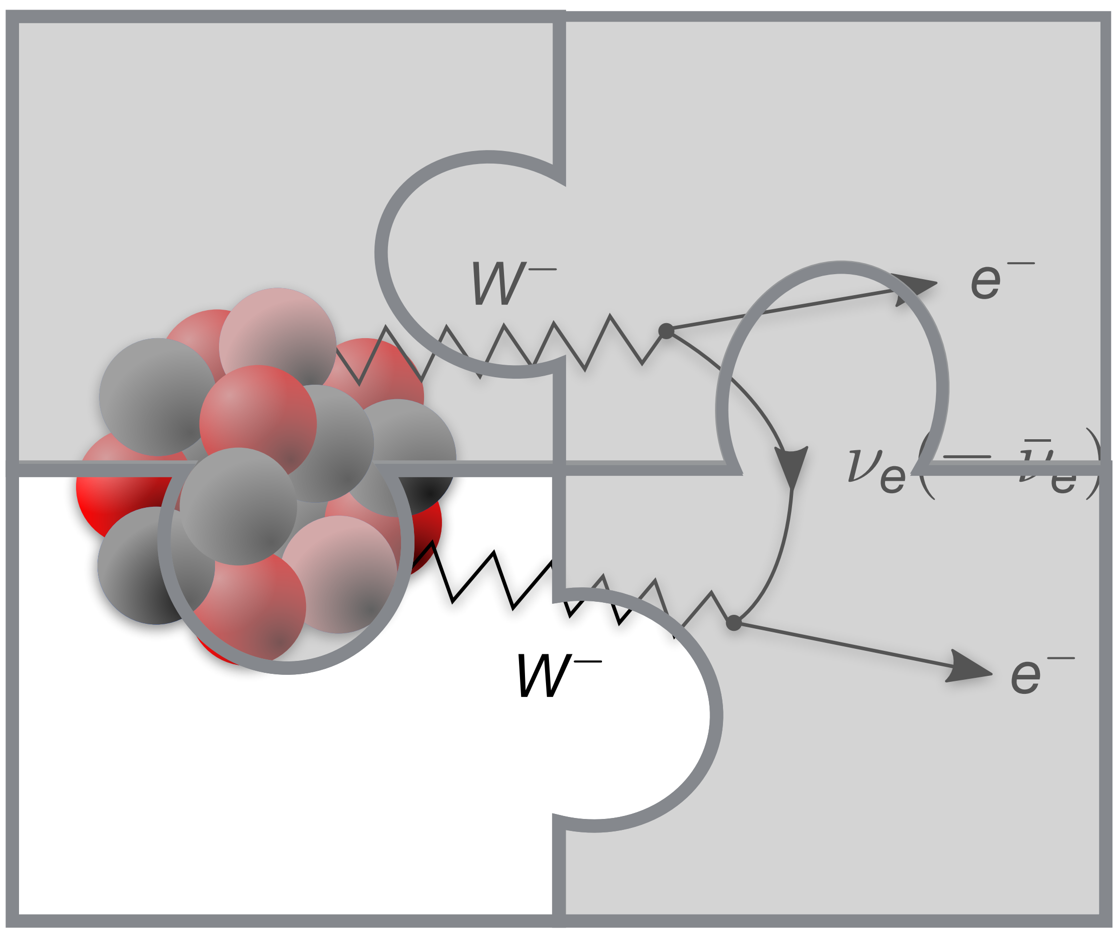
Ab initio Calculation of Nuclear Matrix Elements with IMSRG Methods

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

NSCL FRIB

Neutrinoless Double Beta Decay



- **interactions and transition operators** from Chiral EFT, **including currents**
- tune **resolution scale** of the Hamiltonian / Hilbert space
- **(MR-)IMSRG:** calculate ground (and excited) states or derive Shell Model interaction
- evaluate **1B, 2B** (, 3B,…) **transition operator**

The Similarity Renormalization Group

Review:

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

E. Anderson, S. Bogner, R. Furnstahl, and R. Perry, Phys. Rev. C82 (2011), 054001

E. Jurgenson, P. Navratil, and R. Furnstahl, Phys. Rev. C83 (2011), 034301

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

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

Similarity Renormalization Group

Basic Idea

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

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

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

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

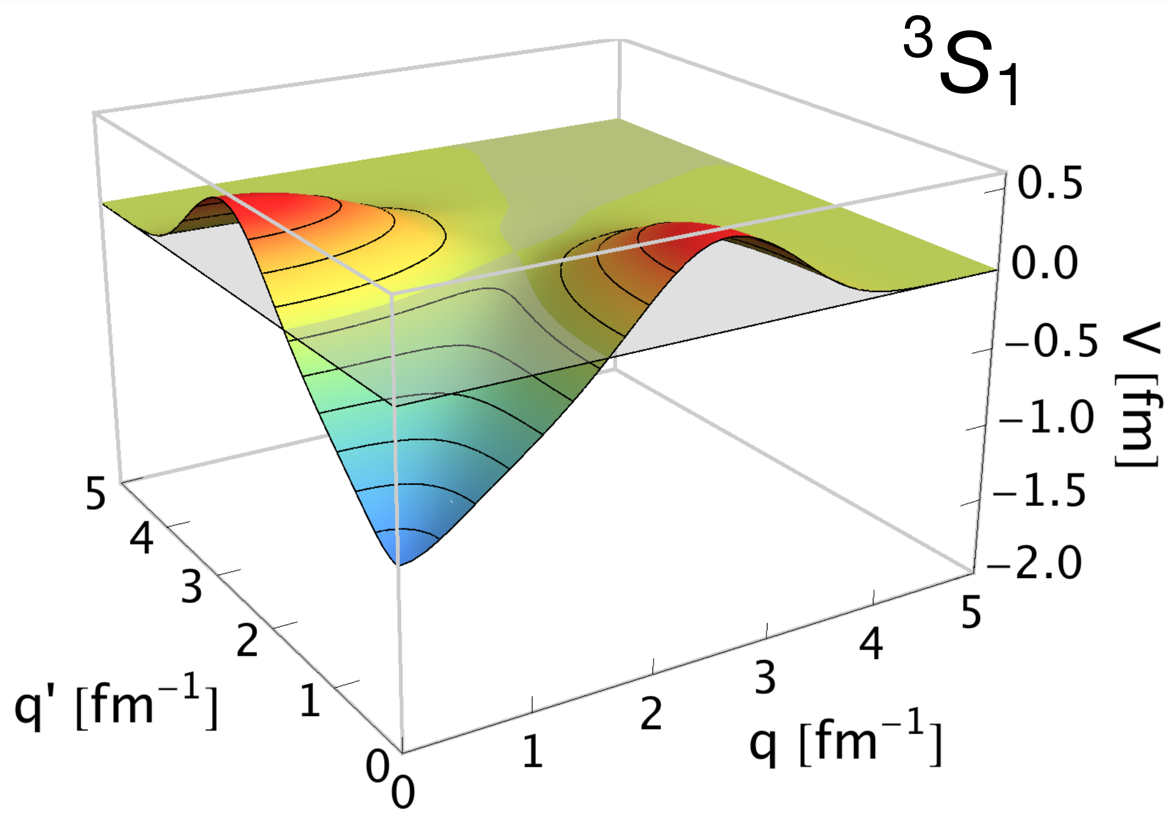
$$\eta(s) = \left[H_d(s), H_{od}(s)\right]$$

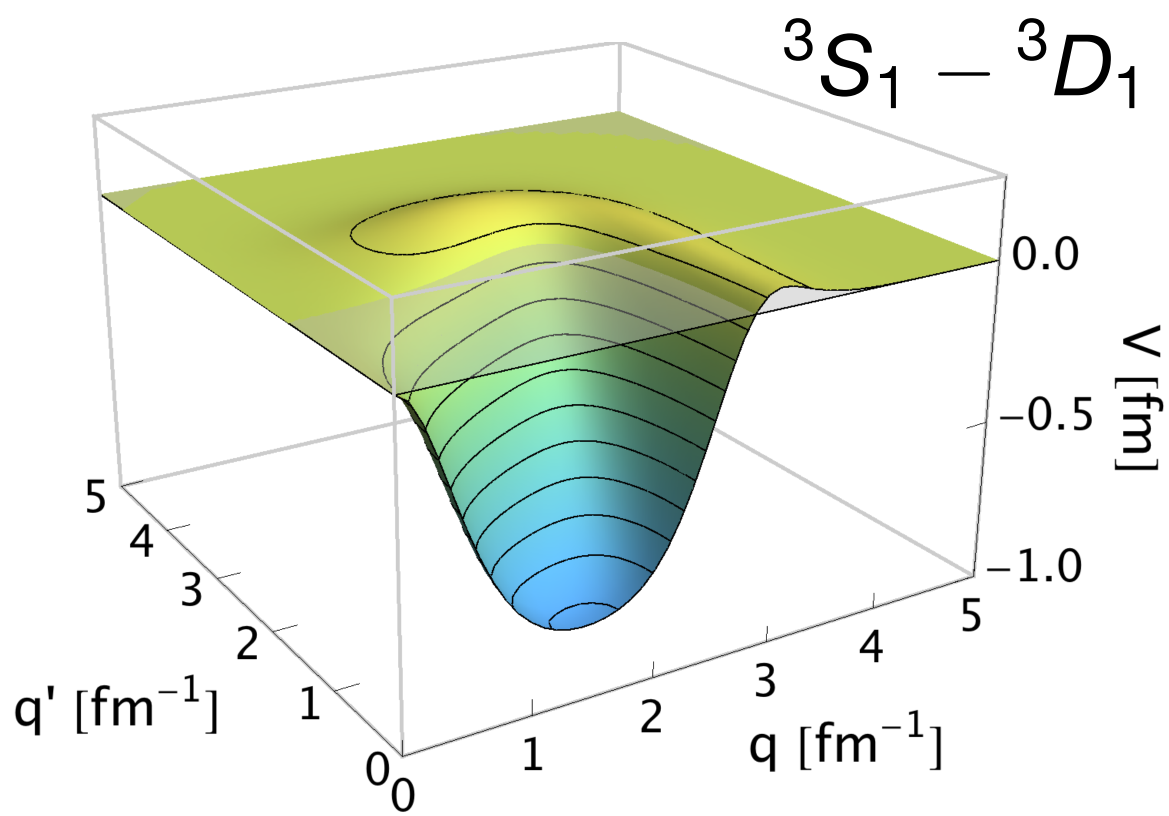
  to suppress (suitably defined) off-diagonal Hamiltonian

- consistent evolution for all observables of interest

SRG in Two-Body Space

momentum space matrix elements





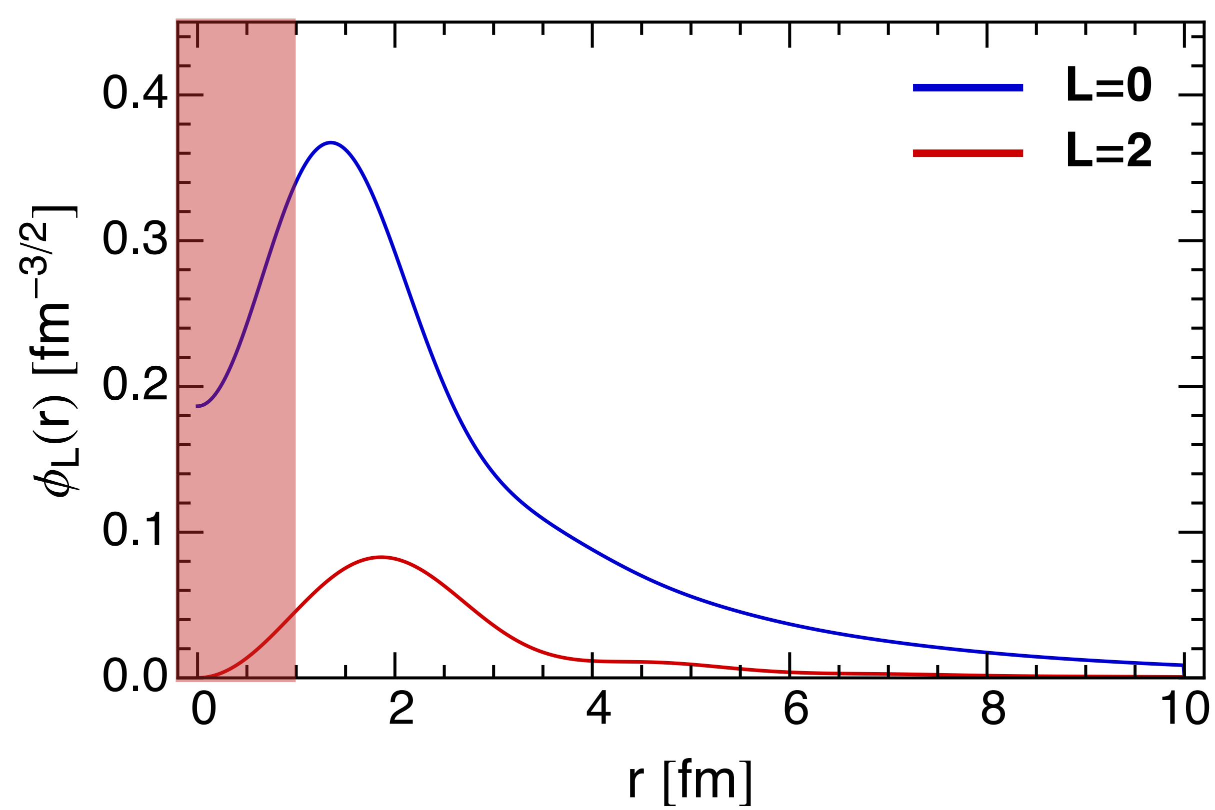
chiral NN

Entem & Machleidt, N3LO

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

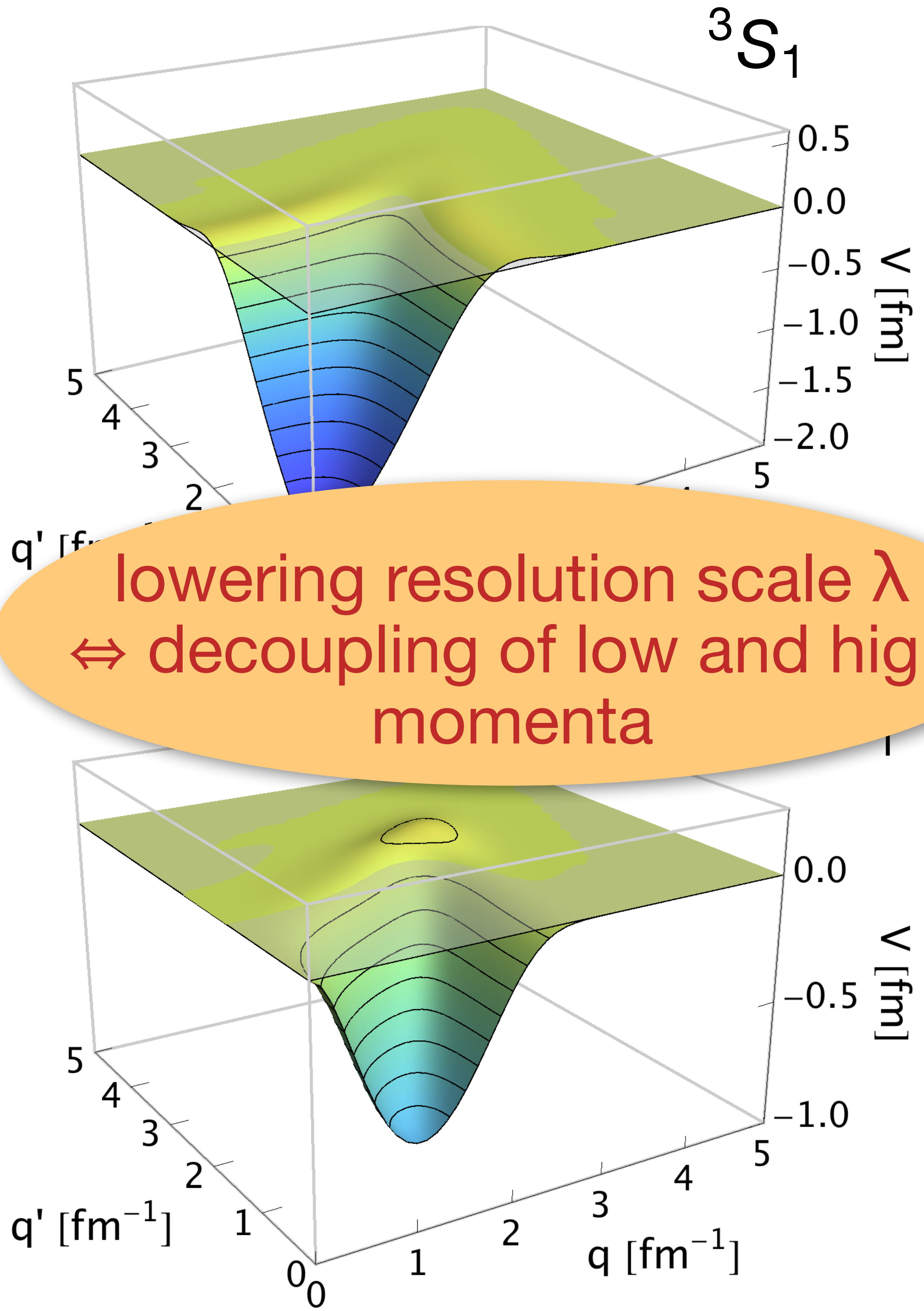
$$\lambda = s^{-1/4}$$

deuteron wave function



SRG in Two-Body Space

momentum space matrix elements



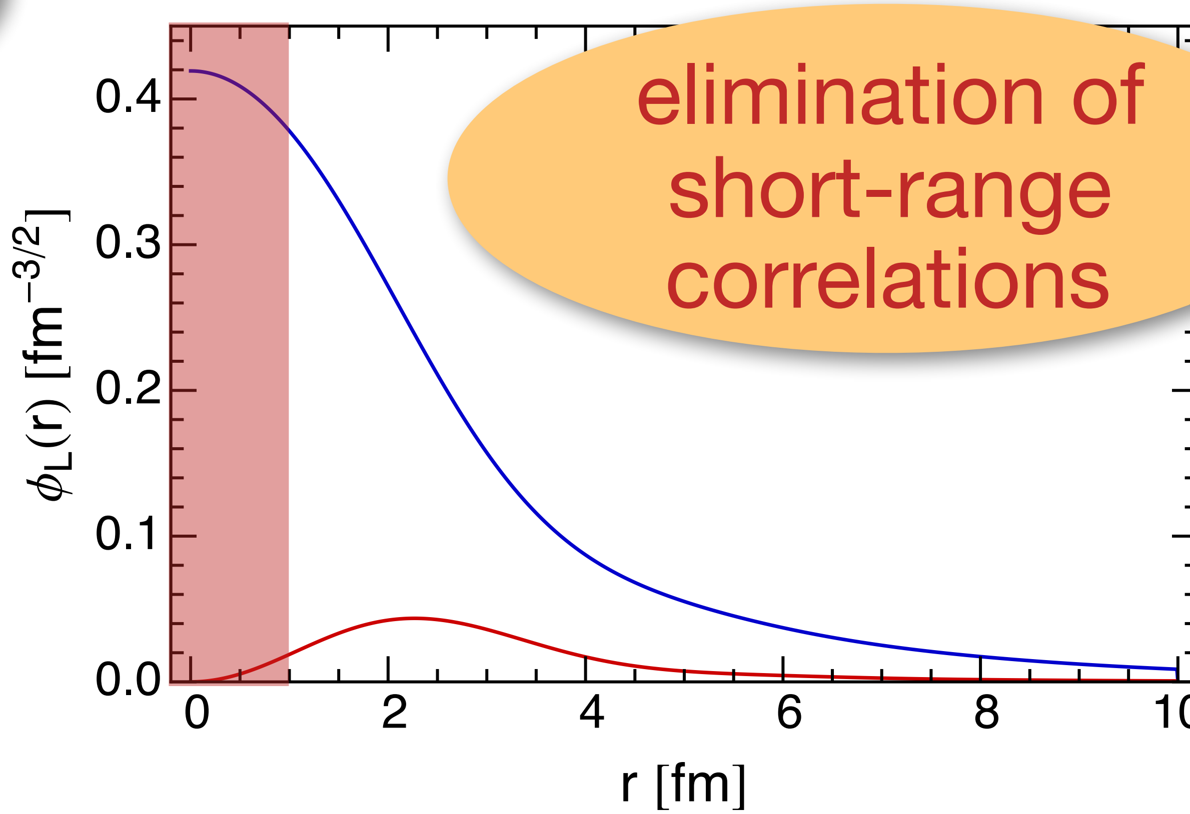
lowering resolution scale λ
⇔ decoupling of low and high momenta

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

(Multi-Reference) In-Medium SRG

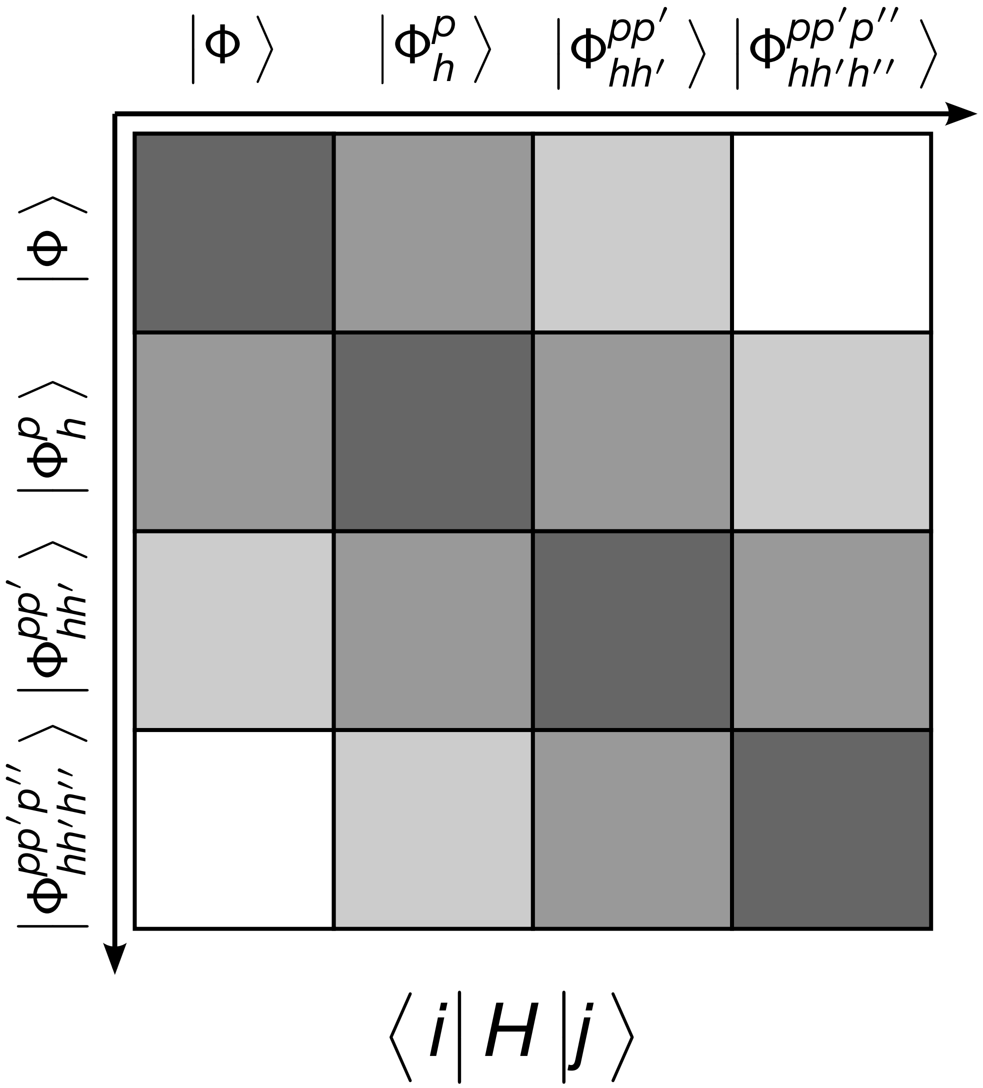
H. H., Phys. Scripta **92**, 023002 (2017)

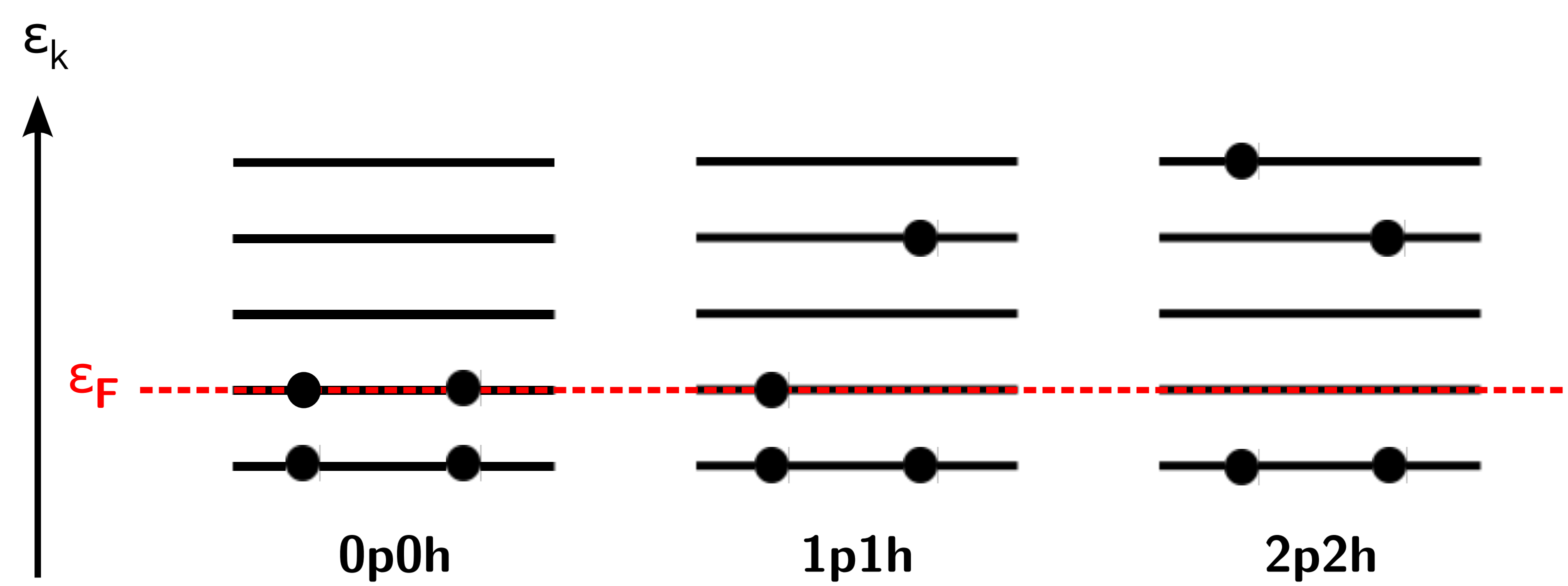
H. H., S. K. Bogner, T. D. Morris, A. Schwenk, and K. Tuskiyama, Phys. Rept. **621**, 165 (2016)

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)

Transforming the Hamiltonian





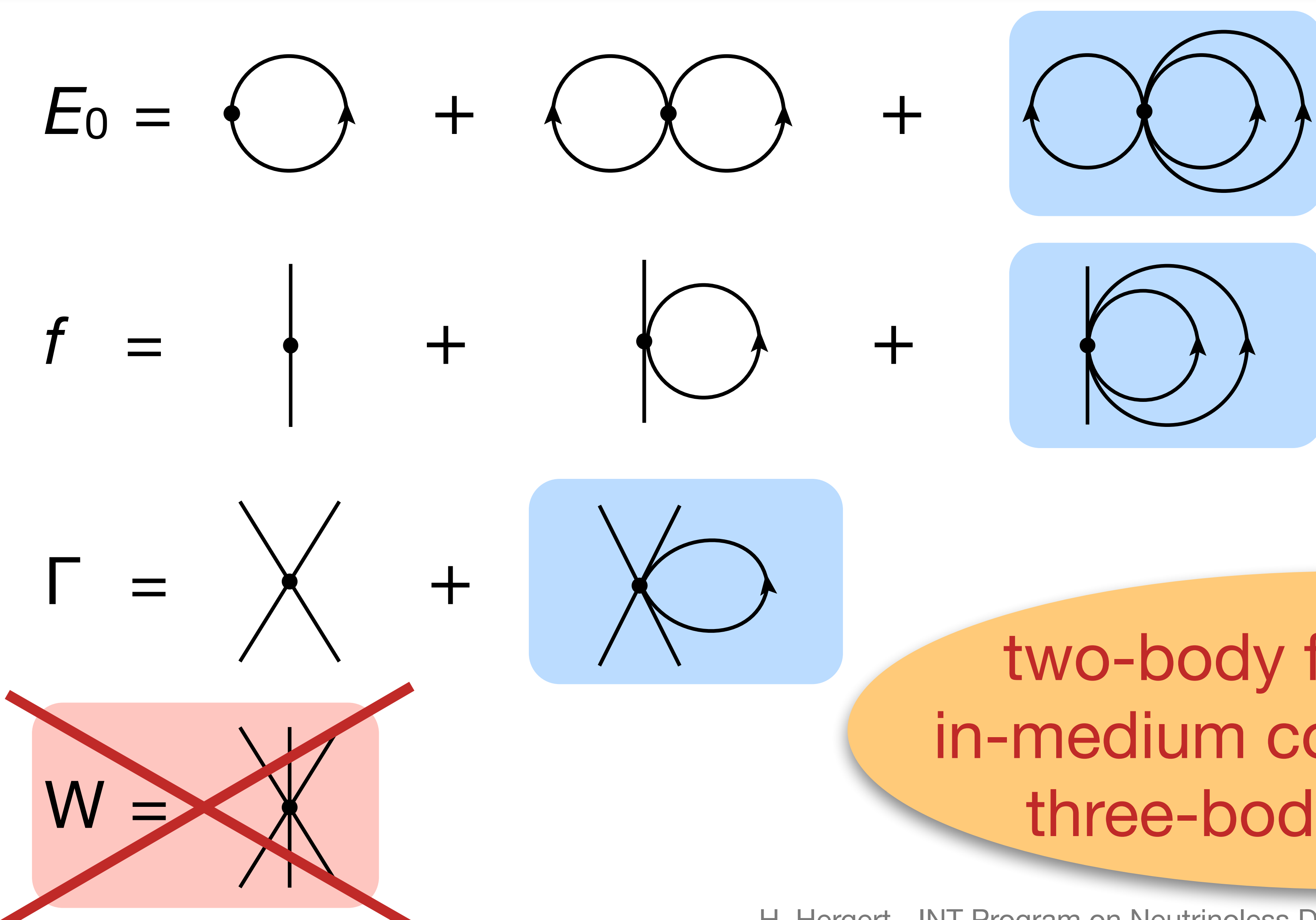
excitations relative to reference state: **normal-ordering**

- reference state: **single Slater determinant**

Normal-Ordered Hamiltonian

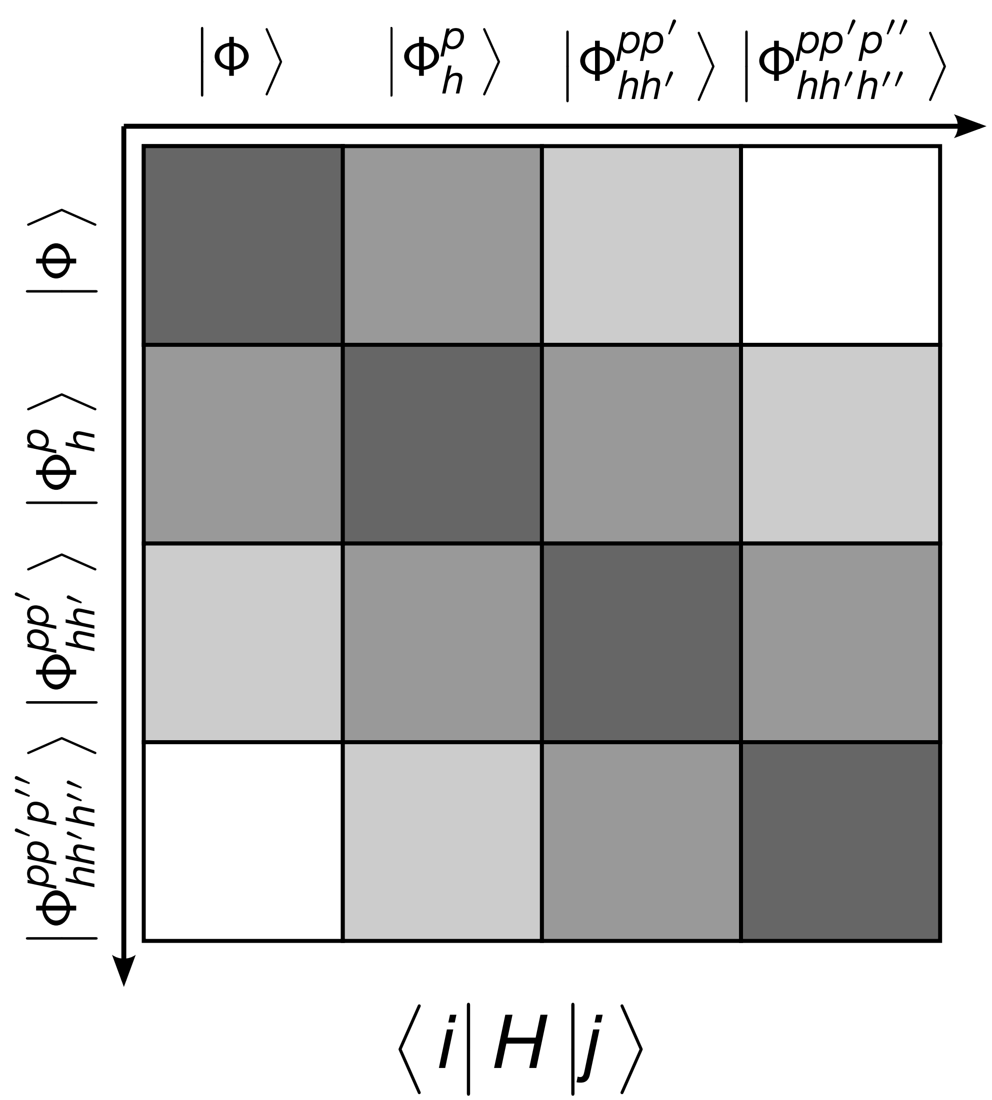
Normal-Ordered Hamiltonian

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



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

Single-Reference Case



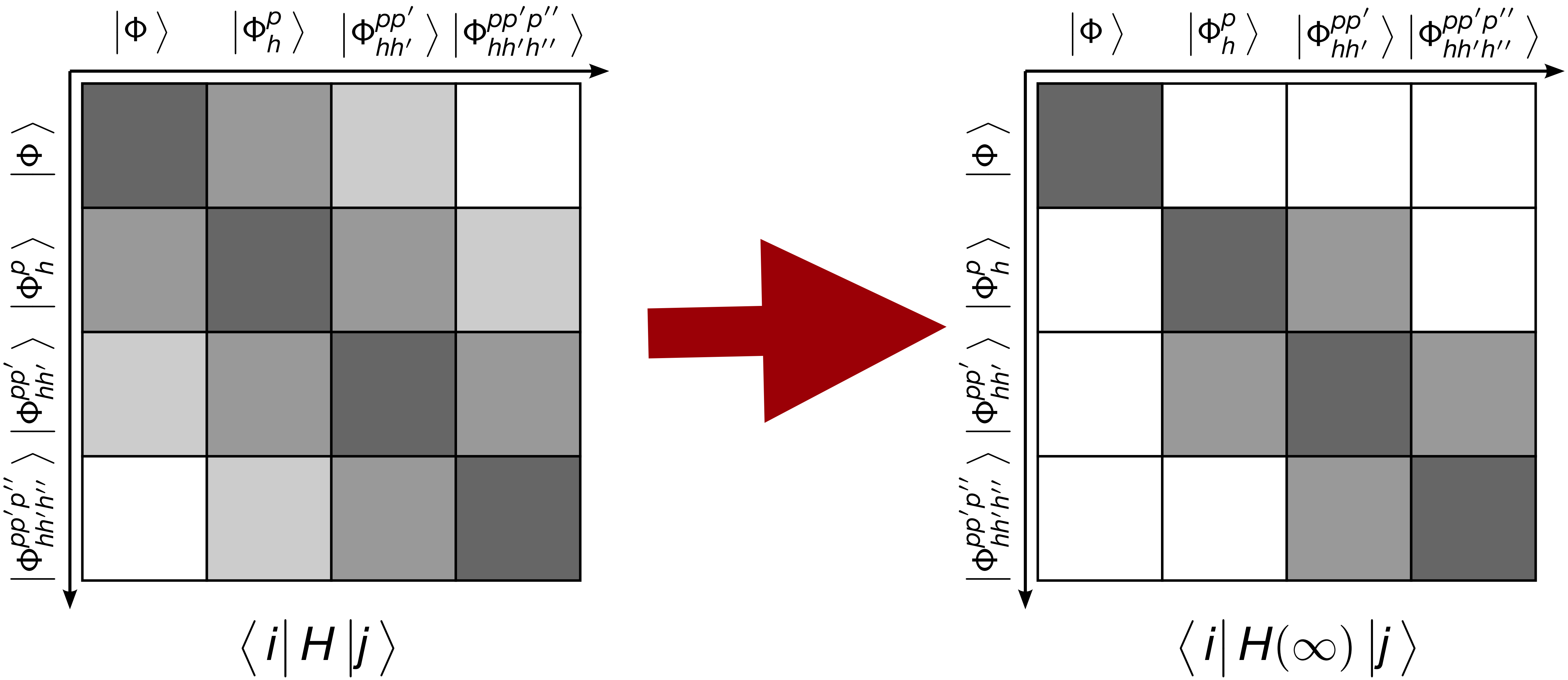
$$A^{i_1\dots i_N}_{j_1\dots j_N} \equiv a^\dagger_{i_1}\dots a^\dagger_{i_N} a_{j_N}\dots a_{j_1}$$

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

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

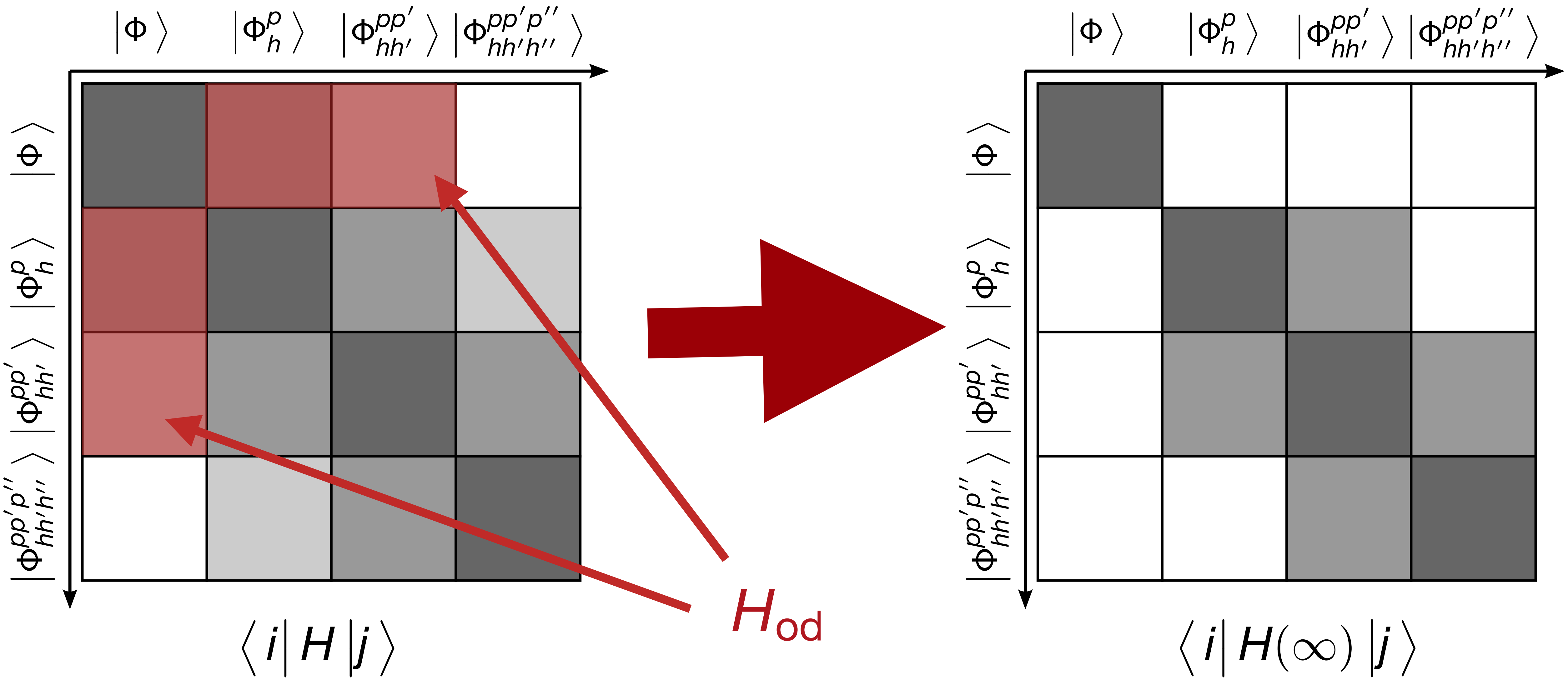
- reference state: **Slater determinant**
- normal-ordered operators **depend on occupation numbers (one-body density)**

Decoupling in A-Body Space



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

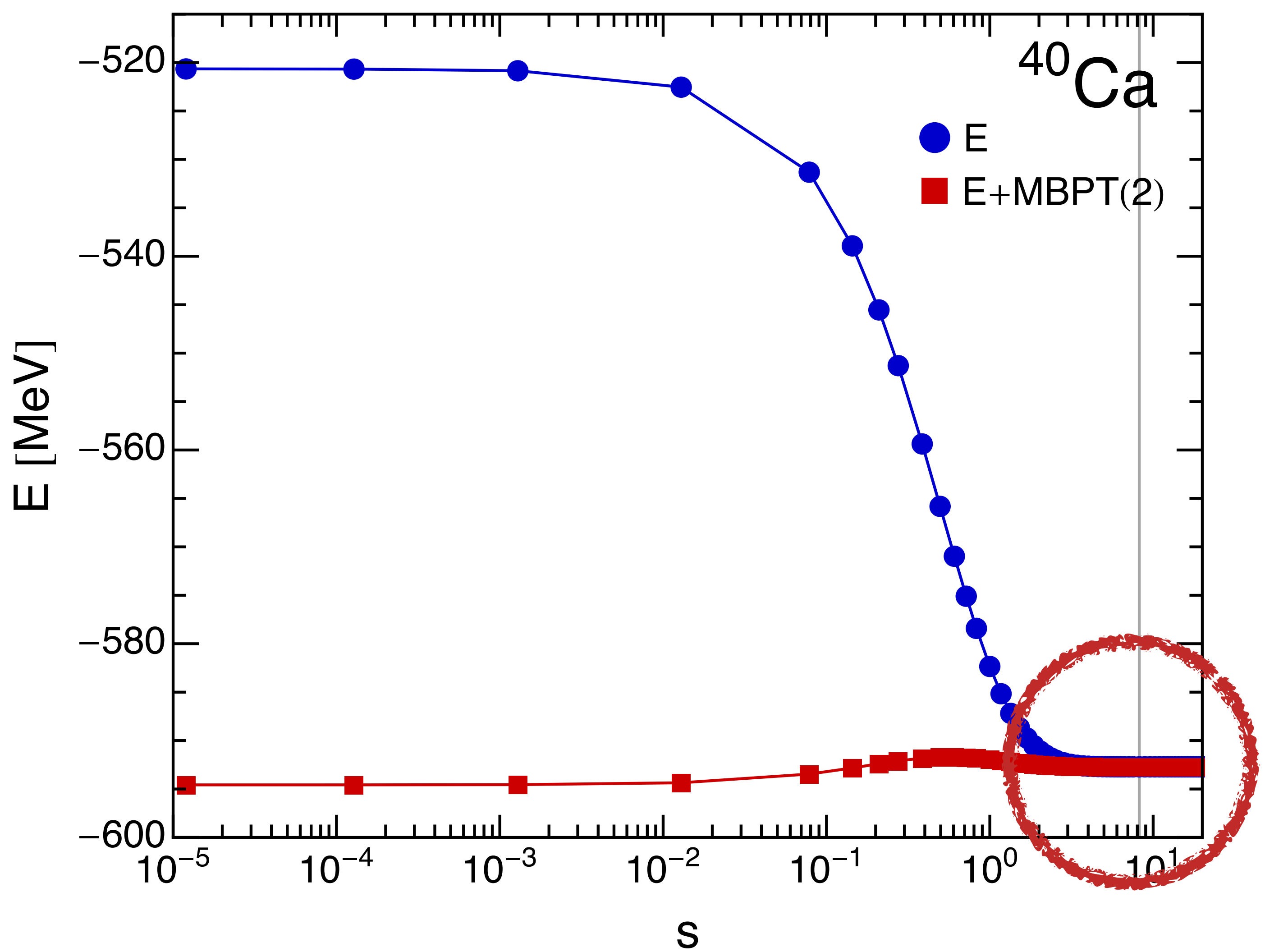
Flow Equation

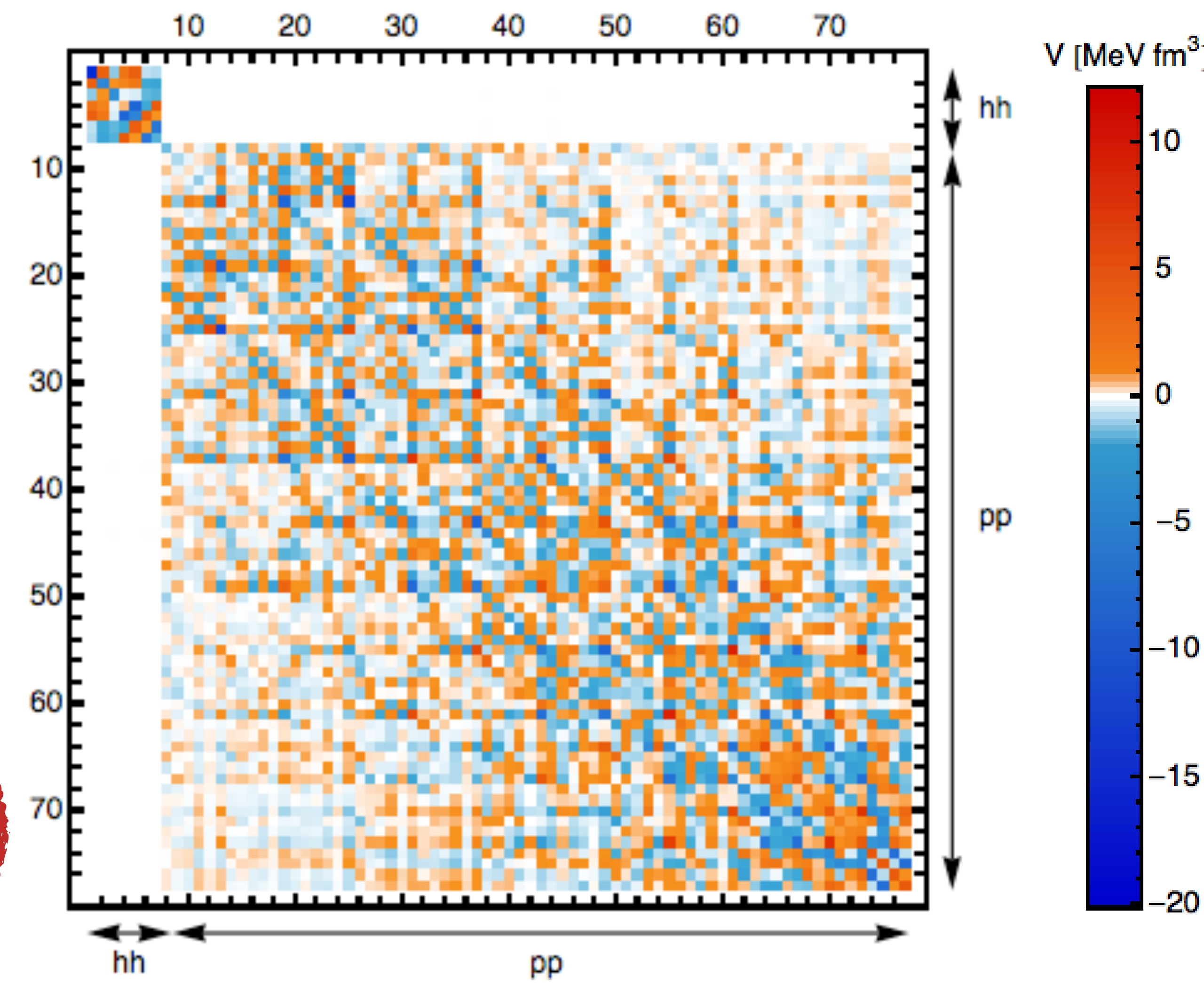


$$\frac{d}{ds}H(s) = [\eta(s), H(s)], \quad \text{e.g}$$

Matrix is never constructed explicitly!

Decoupling



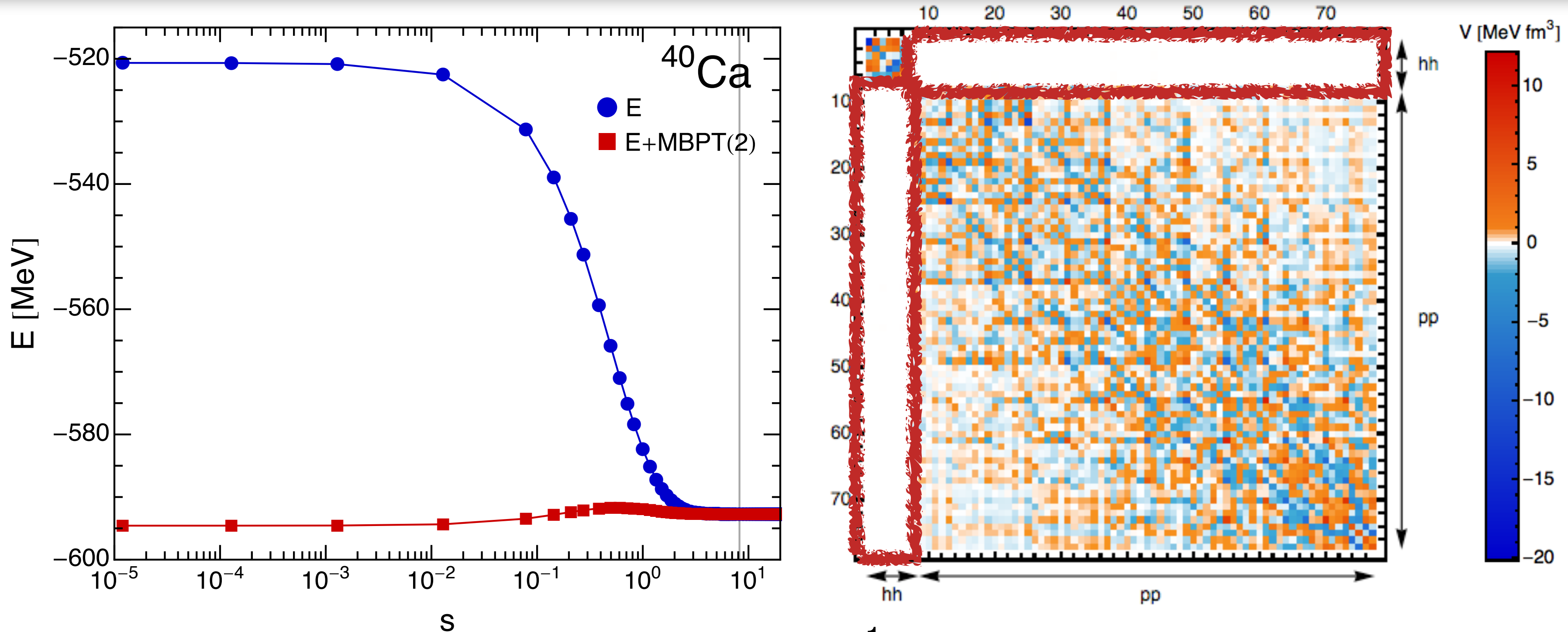


N3LO, $\lambda = 2.0\ \mathrm{fm}^{-1}, e_{\mathrm{Max}} = 8$

non-perturbative resummation of MBPT series (correlations)

off-diagonal couplings are rapidly driven to zero

Decoupling



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

- 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:

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

MR-IMSRG 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):

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

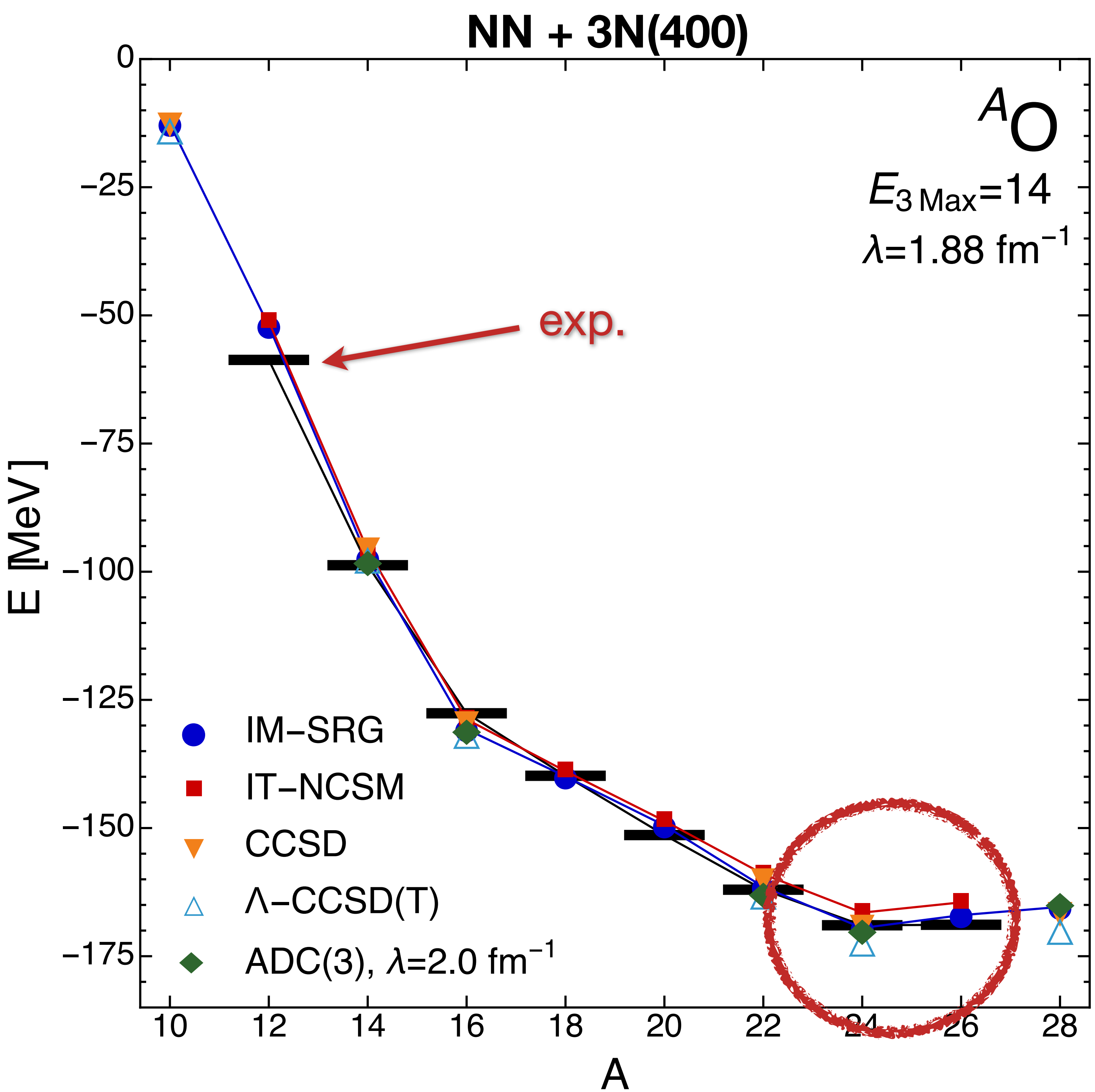
future

- clustered states, Density Matrix Ren… etc.

build static correlations into the reference state

Oxygen Isotopes

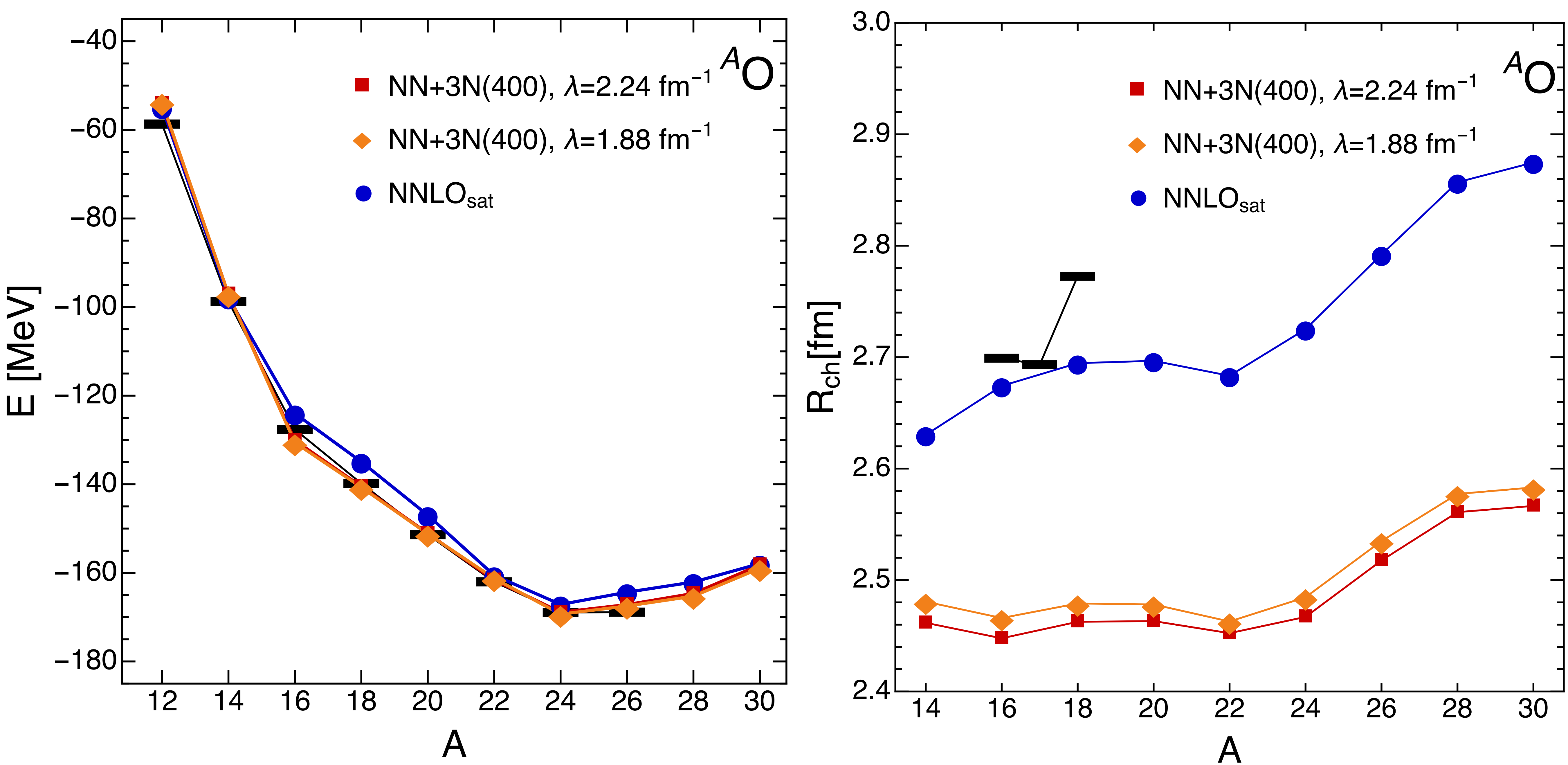
*HH et al., PRL **110**, 242501 (2013), ADC(3): A. Cipollone et al., PRL **111**, 242501 (2013)*



- **MR-IMSRG** with particle-number projected HFB reference state
- **consistency between many-body methods**
- ^{24}O drip line, but ^{25,26}O g.s. resonances too high: continuum and interaction

Oxygen Radii

V. Lapoux, V. Somà, C. Barbieri, HH, J. D. Holt, and S. R. Stroberg, PRL 117, 052501 (2016)



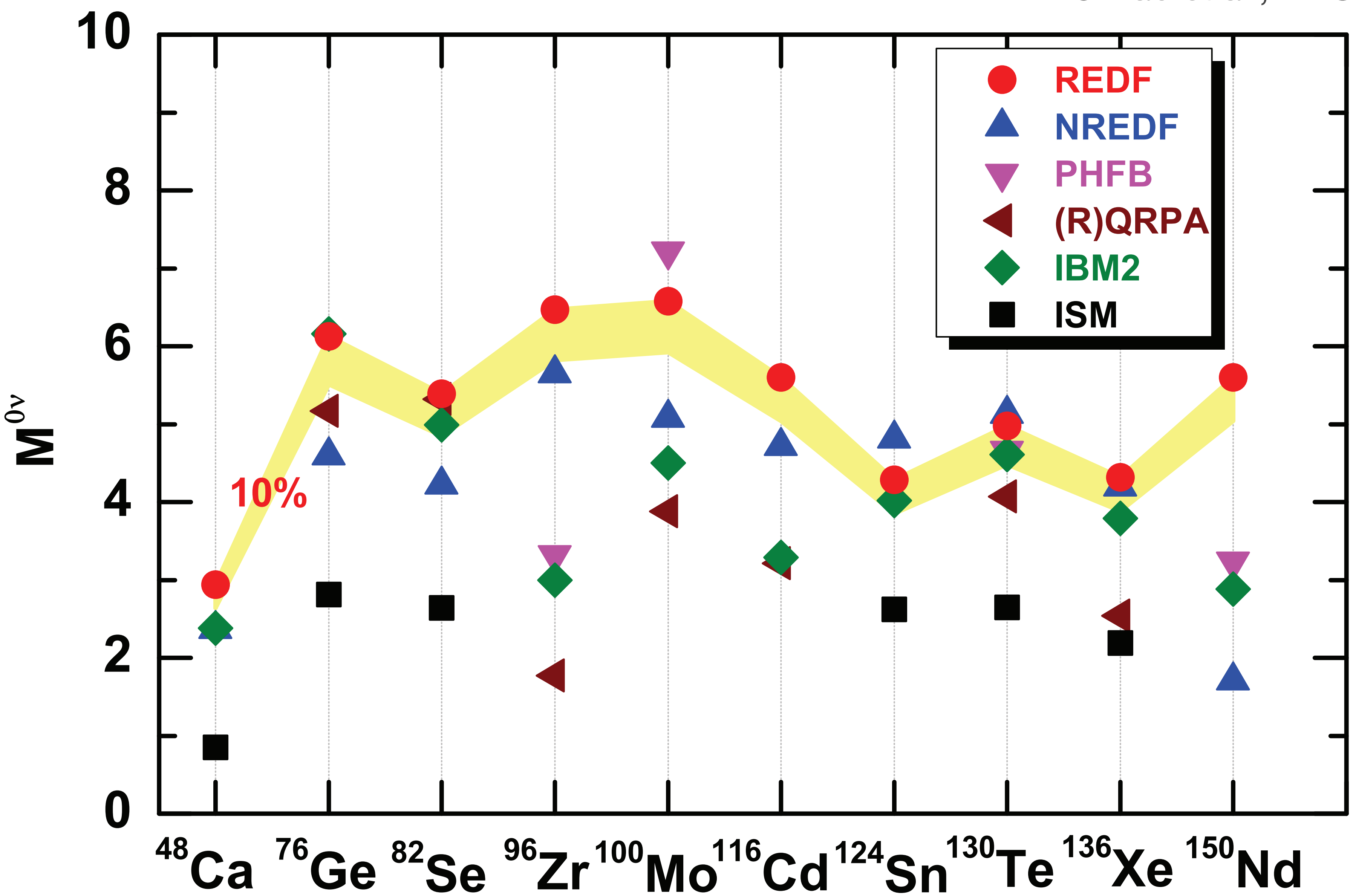
Neutrinoless Double Beta Decay:

Ground-State to Ground-State Decay

with **J. Yao**, J. Engel

Nuclear Matrix Elements

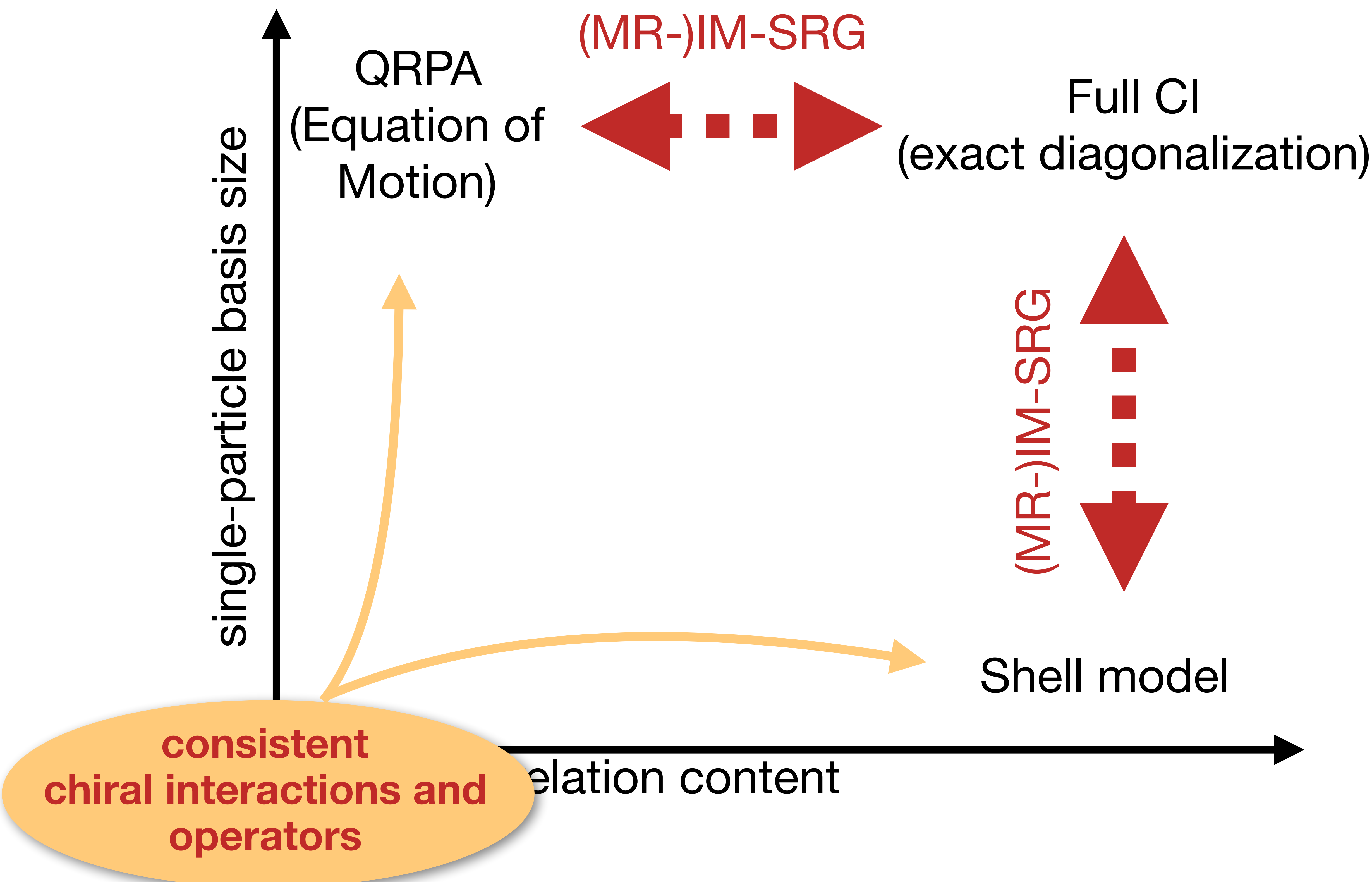
J. Yao et al., PRC **91**, 024316 (2015)



- inputs tailored to specific methods: phenom… EDFs, Shell Model interactions, …
- quenched g_A, "renormalization" of operato…

comparing apples and oranges

Many-Body Approaches



MR-IMSRG 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**:

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

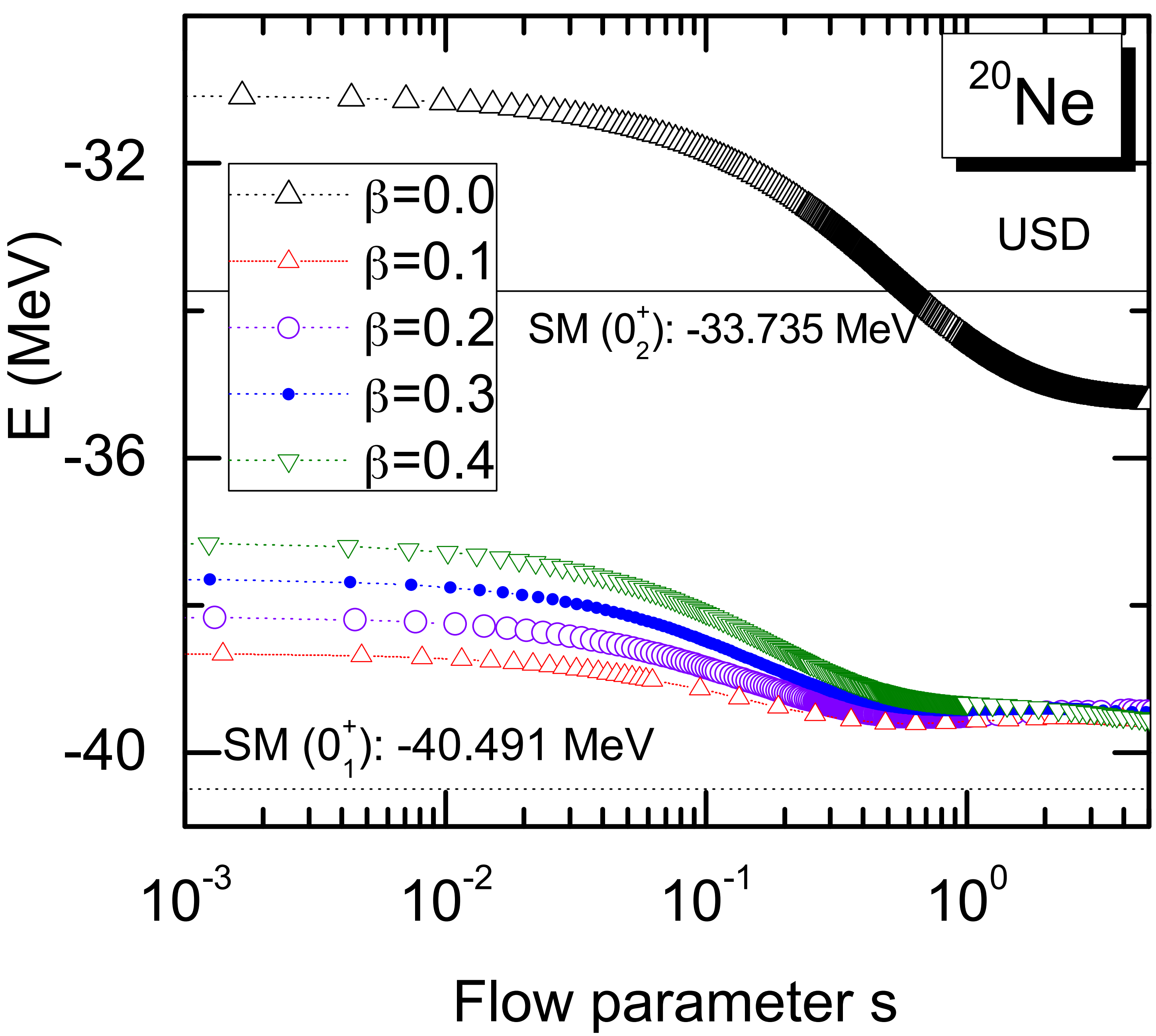
future

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

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

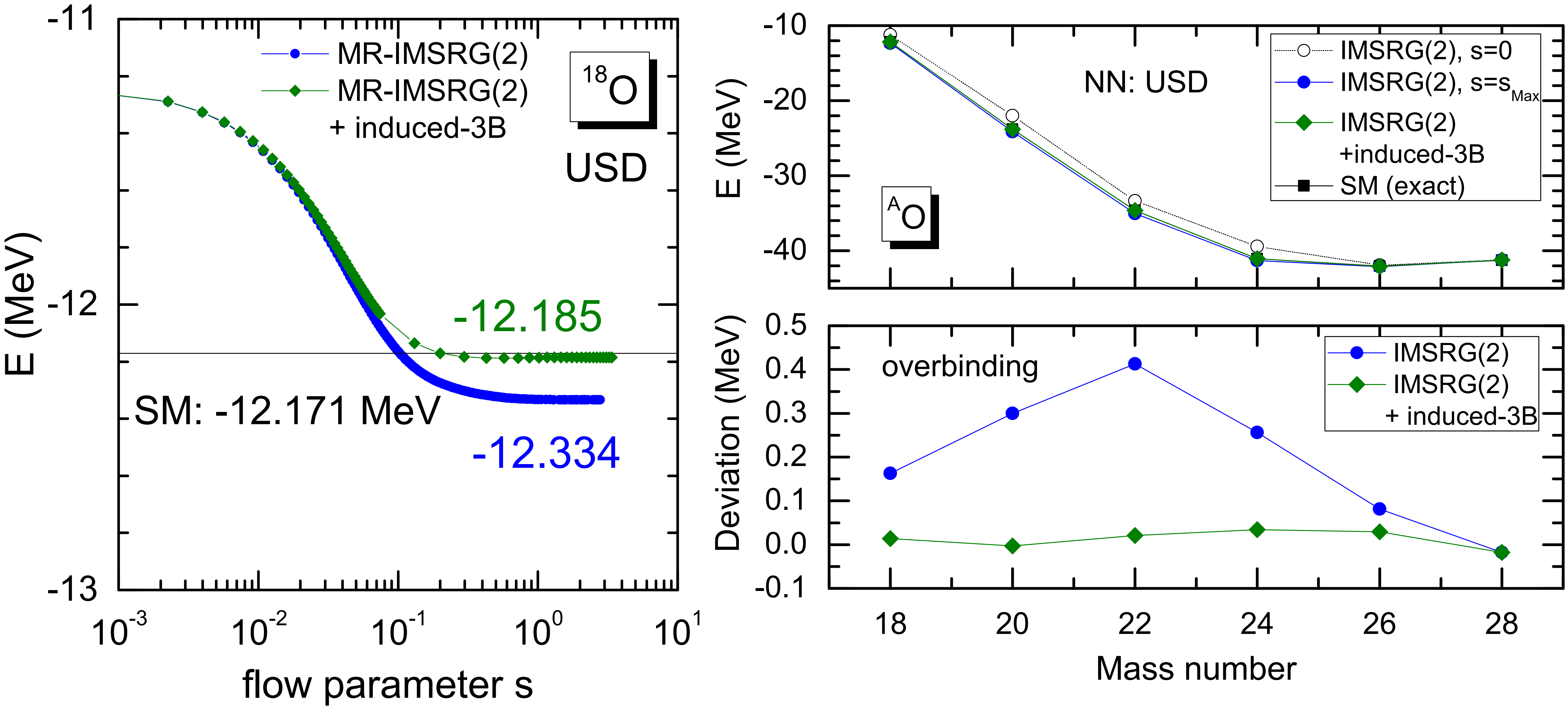
- Density Matrix Renormalization Group, Tensor Network States, …

Example: ^{20}Ne



- reference: particle-number & angular-momentum projected HFB
- **range of deformed reference states flow to the ^{20}Ne ground state**
- deviation from Shell model result: **correlations beyond MR-IMSRG(2)**

Approximate MR-IMSRG(3)



- **approximate MR-IMSRG(3):** induced 3B terms recover bulk of missing correlation energy
- expected to be **reference-state dependent**

Direct DBD Calculation

- **direct** MR-IMSRG (Magnus) calculation of **initial and final states**:

$$\left|\Psi_{I,F}\right\rangle = e^{\overline{\Omega}_{I,F}}\left|\Phi_{I,F}\right\rangle$$

- evaluate NME for transition operator in **closure approximation**:

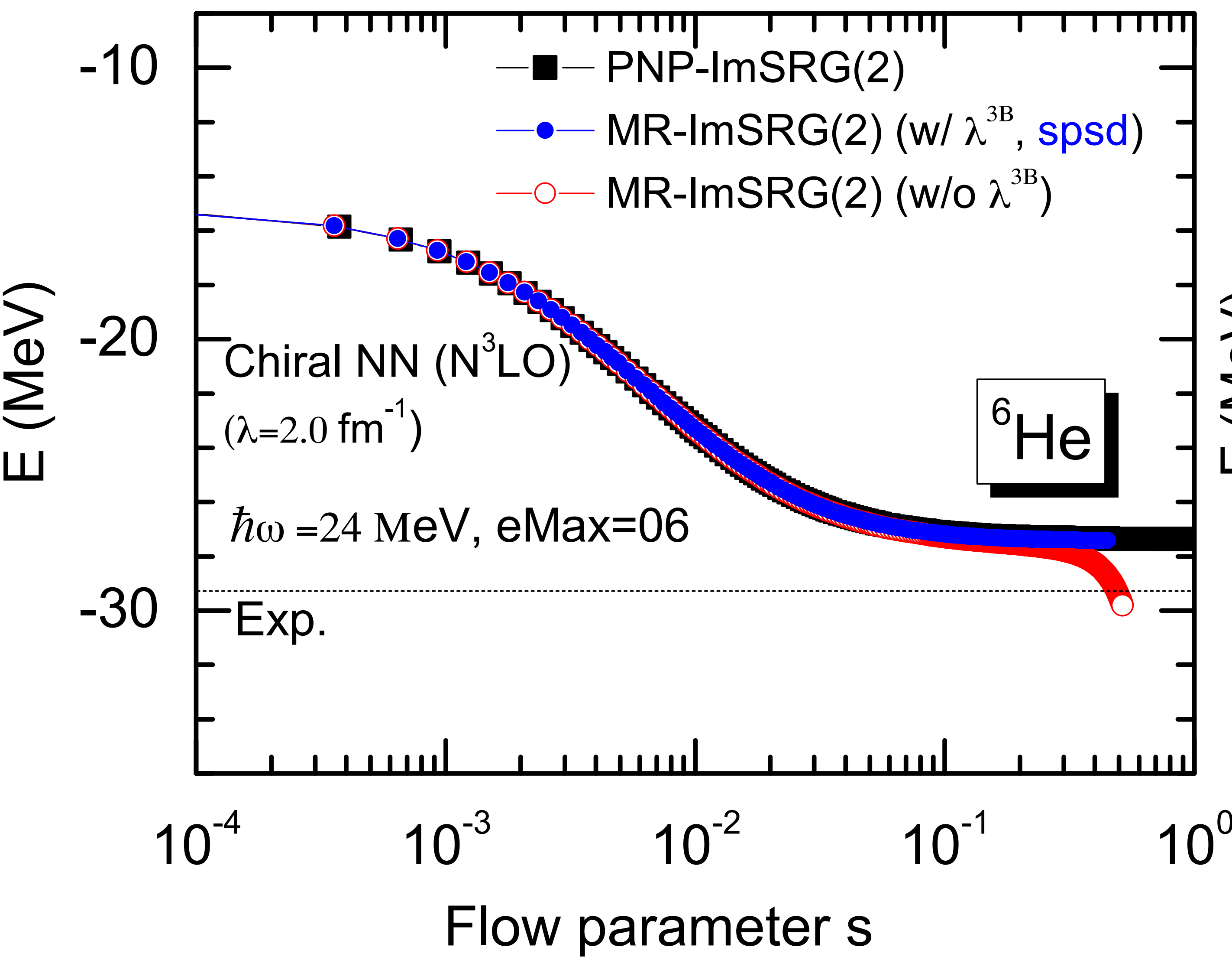
$$M_{0\nu\beta\beta} = \left\langle \Phi_F\right| e^{-\overline{\Omega}_F} O_{0\nu\beta\beta} e^{\overline{\Omega}_I} \left|\Phi_I\right\rangle$$

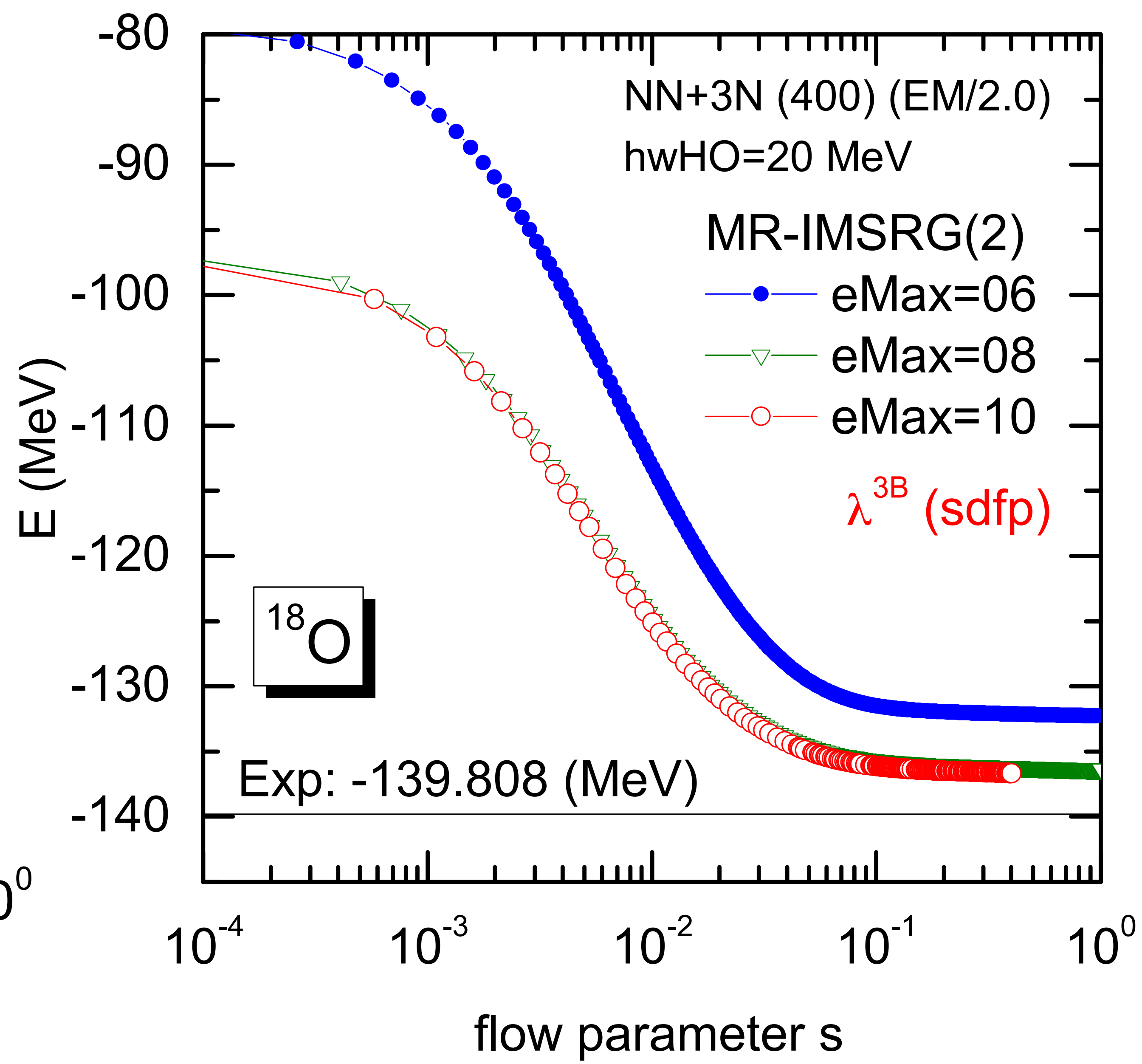
- explore possible expansions and check consistency, e.g.,

$$e^{-\overline{\Omega}_F} = e^{-(\overline{\Omega}_I + \delta\overline{\Omega})} = e^{-\delta\overline{\Omega}} e^{-\overline{\Omega}_I} + \ldots$$

in progress

Isospin Multiplets

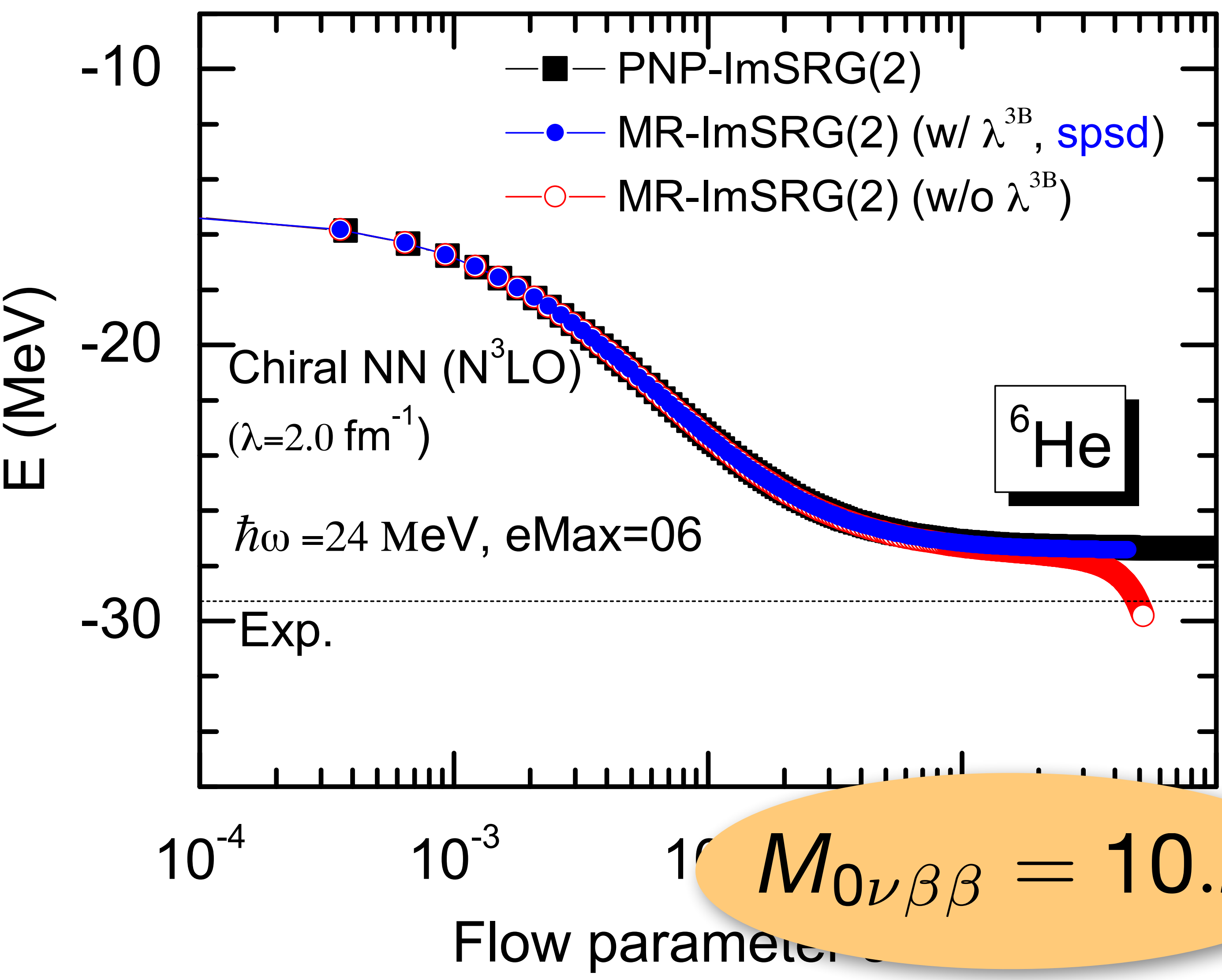




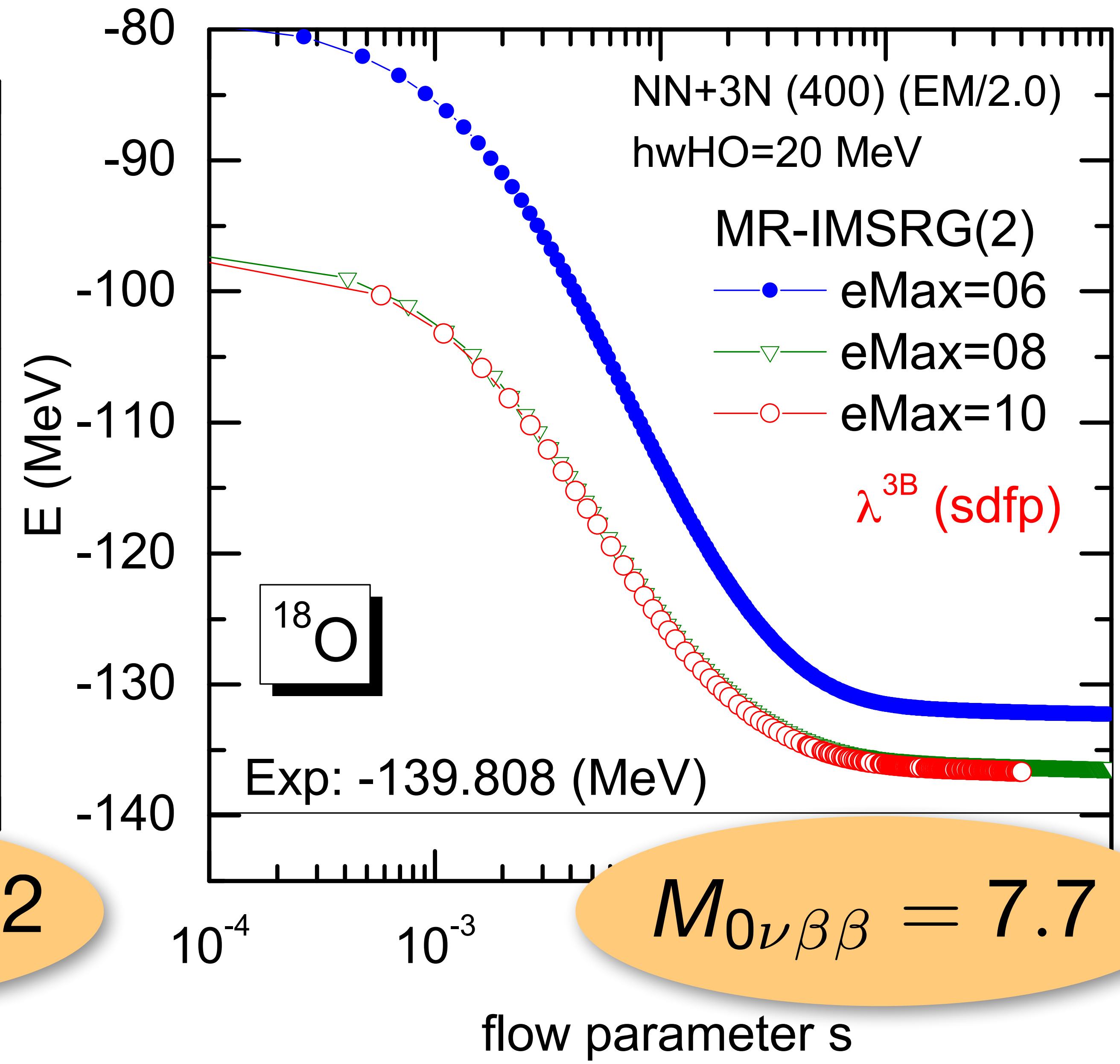
- use **isospin symmetry**:

$$\left\langle T T_z - 2 \right| \left[\overline{O}_{0\nu\beta\beta}\right]^{2-2} \left| T T_z \right\rangle \quad \longleftrightarrow \quad \left\langle T T_z \right| \left[\overline{O}_{0\nu\beta\beta}\right]^{20} \left| T T_z \right\rangle$$

Isospin Multiplets



$M_{0\nu\beta\beta} = 10.2$



$M_{0\nu\beta\beta} = 7.7$

- use **isospin symmetry**:

$$\langle T T_z - 2 | \, [\overline{O}_{0\nu\beta\beta}]^{2-2} \, | T T_z \rangle \quad \longleftrightarrow \quad \langle T T_z | \, [\overline{O}_{0\nu\beta\beta}]^{20} \, | T T_z \rangle$$

Neutrinoless Double Beta Decay:

Explicit Treatment of Excited States

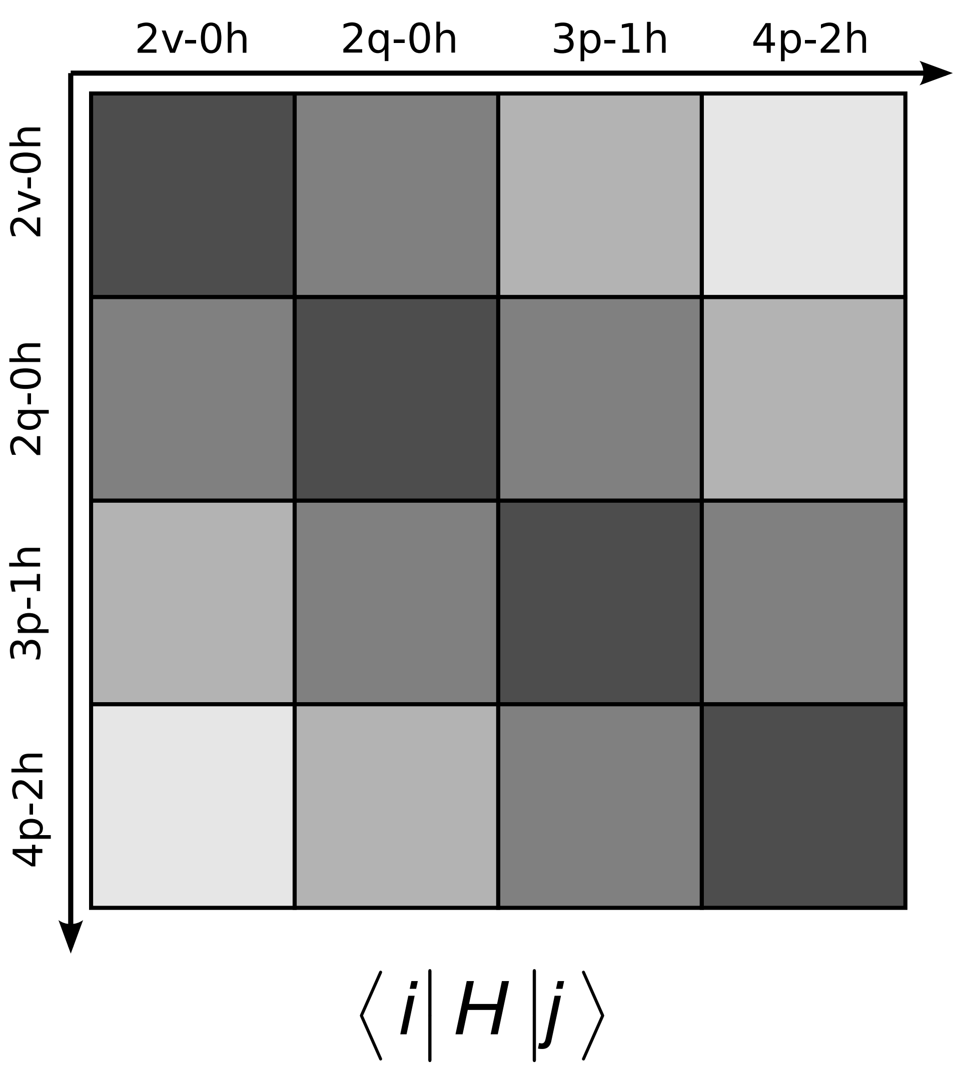
N. M. Parzuchowski, **S. R. Stroberg**, P. Navratil, H. H., S. K. Bogner, arXiv: 1705.05511

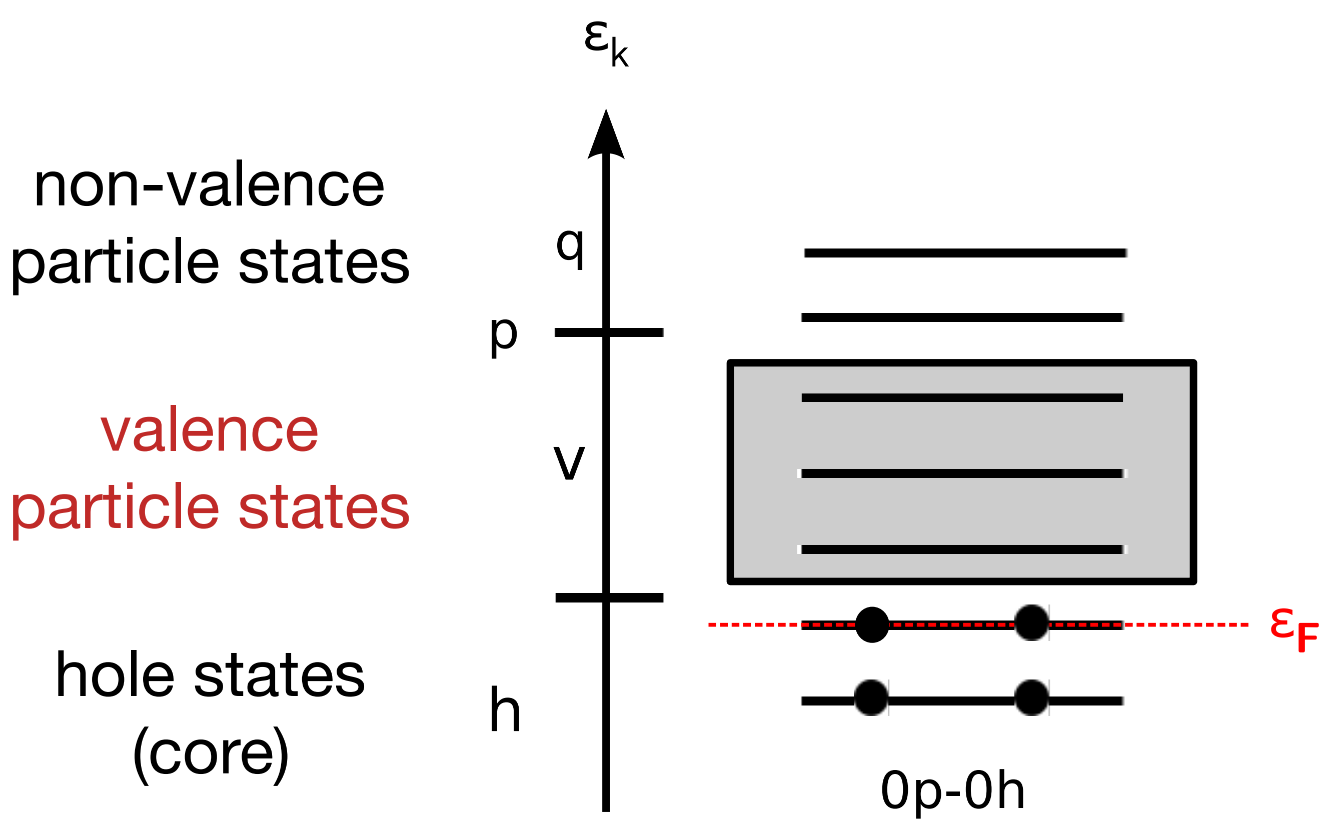
S. R. Stroberg, A. Calci, H. H., J. D. Holt, S. K. Bogner, R. Roth, A. Schwenk, PRL **118**, 032502 (2017)

S. R. Stroberg, H. H., J. D. Holt, S. K. Bogner, A. Schwenk, PRC93, 051301(R) (2016)

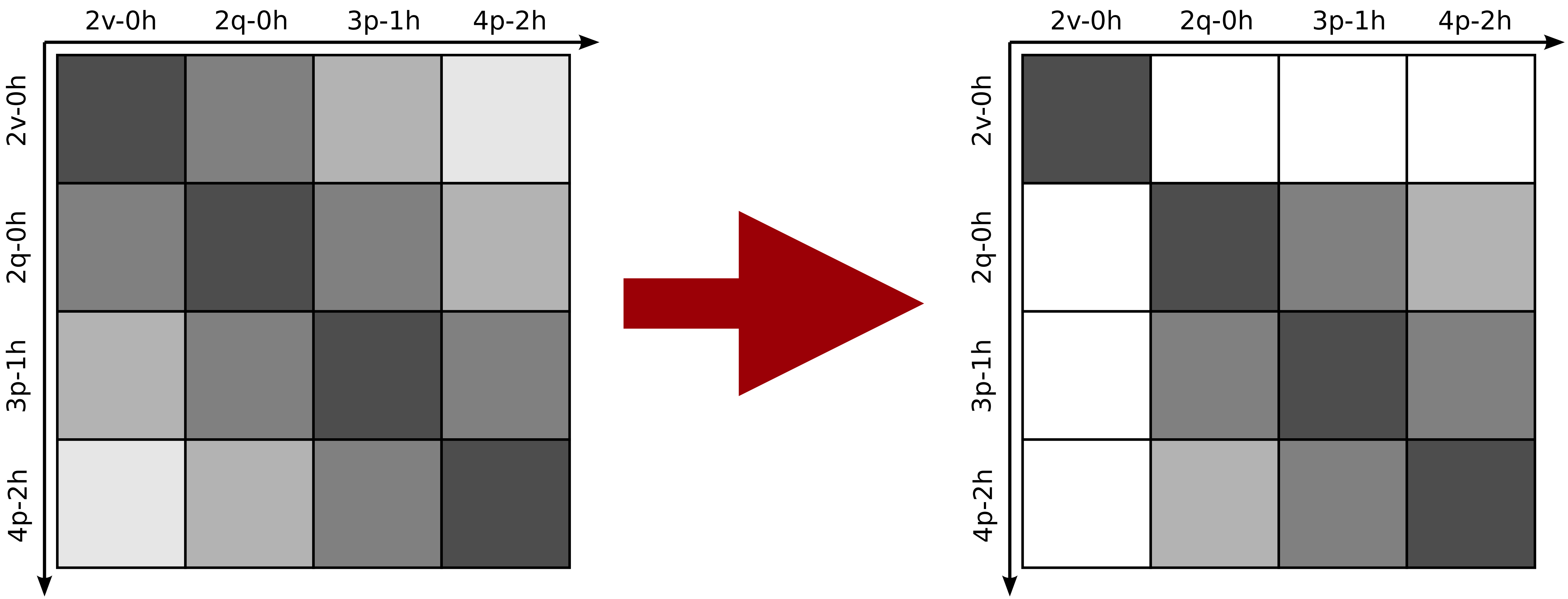
S. K. Bogner, H. H., J. D. Holt, A. Schwenk, S. Binder, A. Calci, J. Langhammer, R. Roth, Phys. Rev. Lett. 113, 142501 (2014)

Valence Space Decoupling





Valence Space Decoupling



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

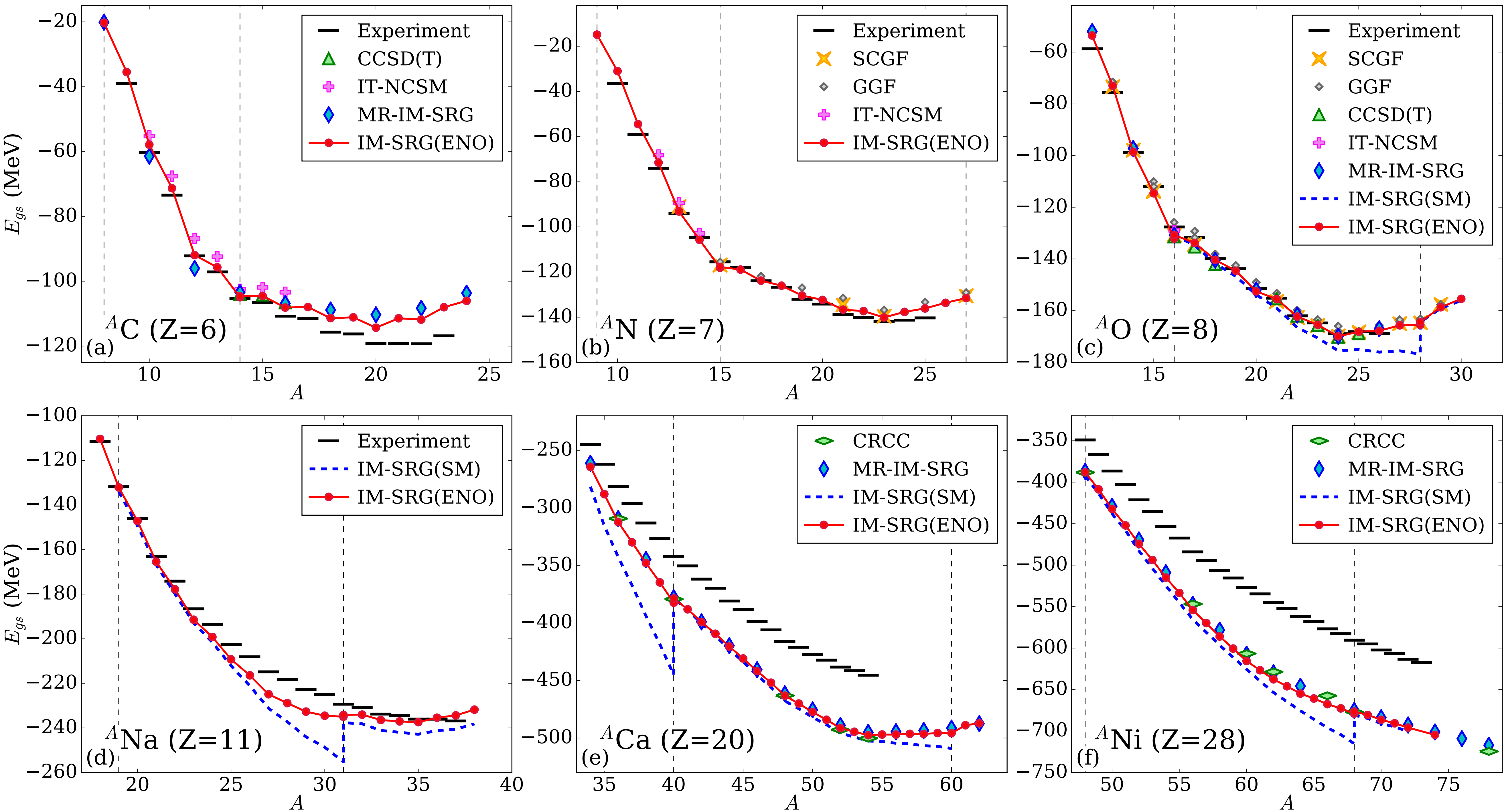
change definition of off-diagonal

$$\left\{ H^{od} \right\} = \{ f^h_{h'}, f^p_{p'}, f^p_h, f^q_v, \Gamma^{pp'}_{hh'}, \Gamma^{pp'}_{hv}, \Gamma_{vv'} \}$$

consistent interaction and DBD operator for Shell Model

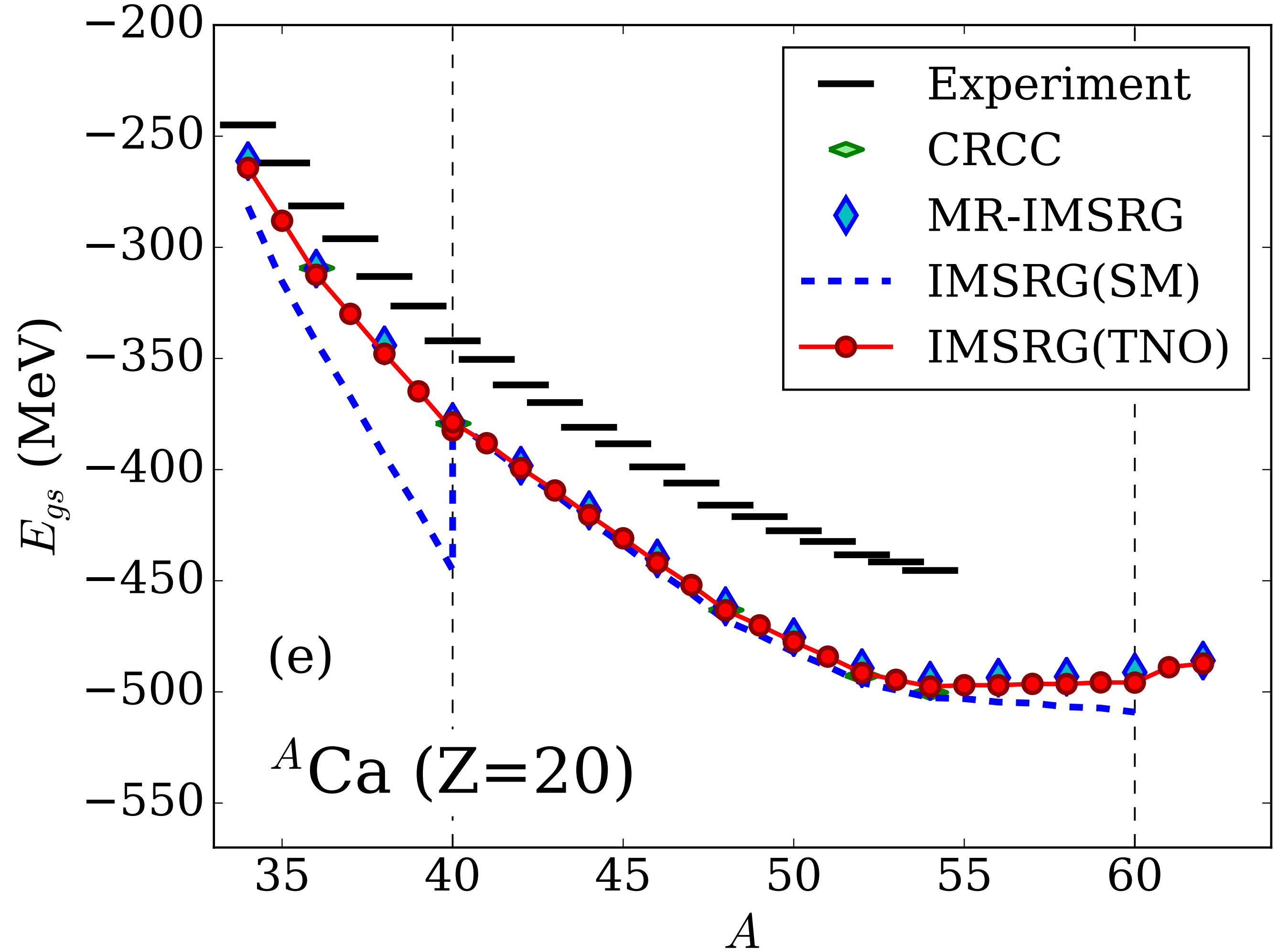
Ground-State Energies

S. R. Stroberg, A. Calci, HH, J. D. Holt, S. K.Bogner, R. Roth, A. Schwenk, PRL **118**, 032502 (2017)



Ground-State Energies

S. R. Stroberg, A. Calci, HH, J. D. Holt, S. K.Bogner, R. Roth, A. Schwenk, PRL **118**, 032502 (2017)

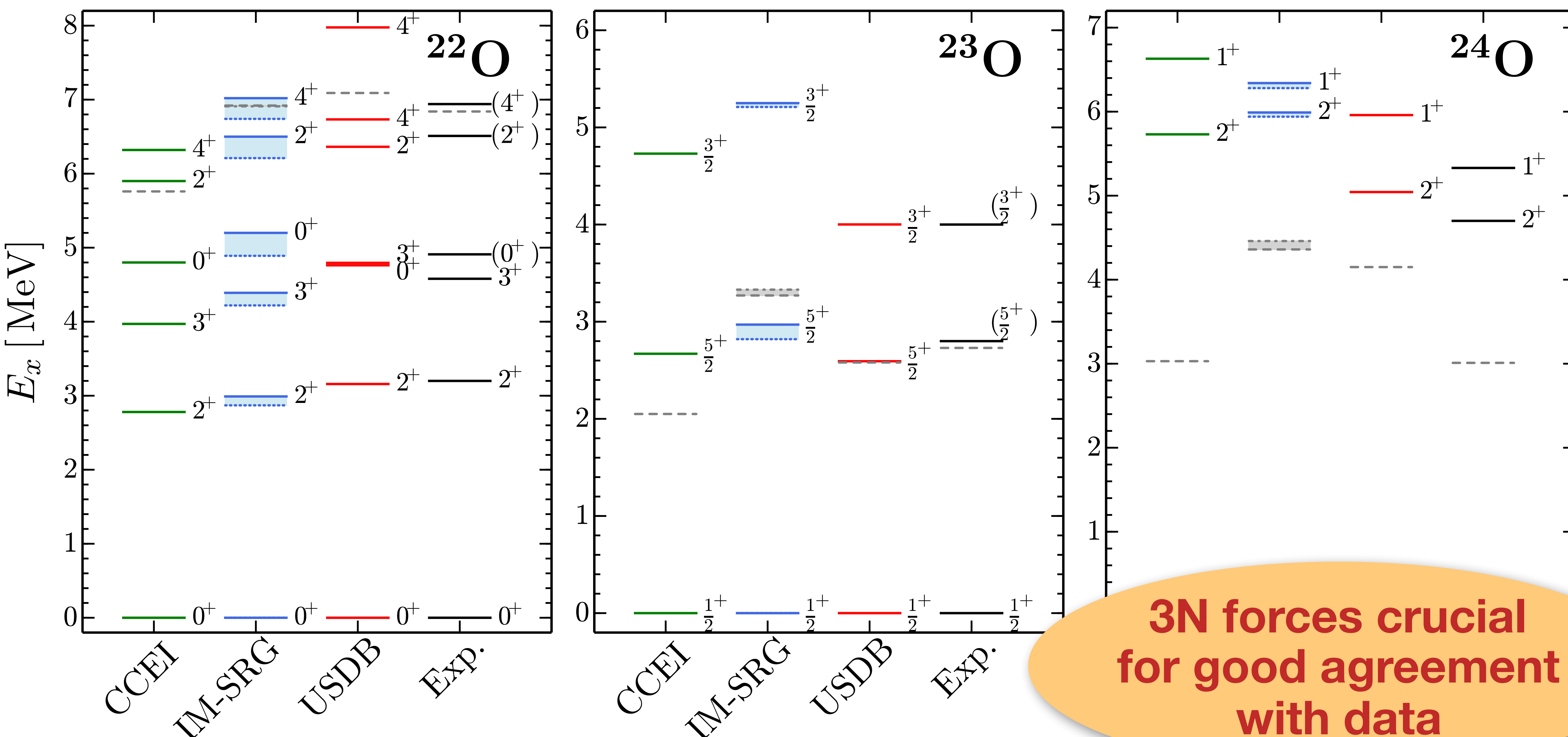


- (initial) normal ordering and IMSRG decoupling in the **target nucleus**
- **consistent with (MR-)IMSRG ground state energies** (and CC, SCGF, …) for the **same Hamiltonian**

Oxygen Spectra

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

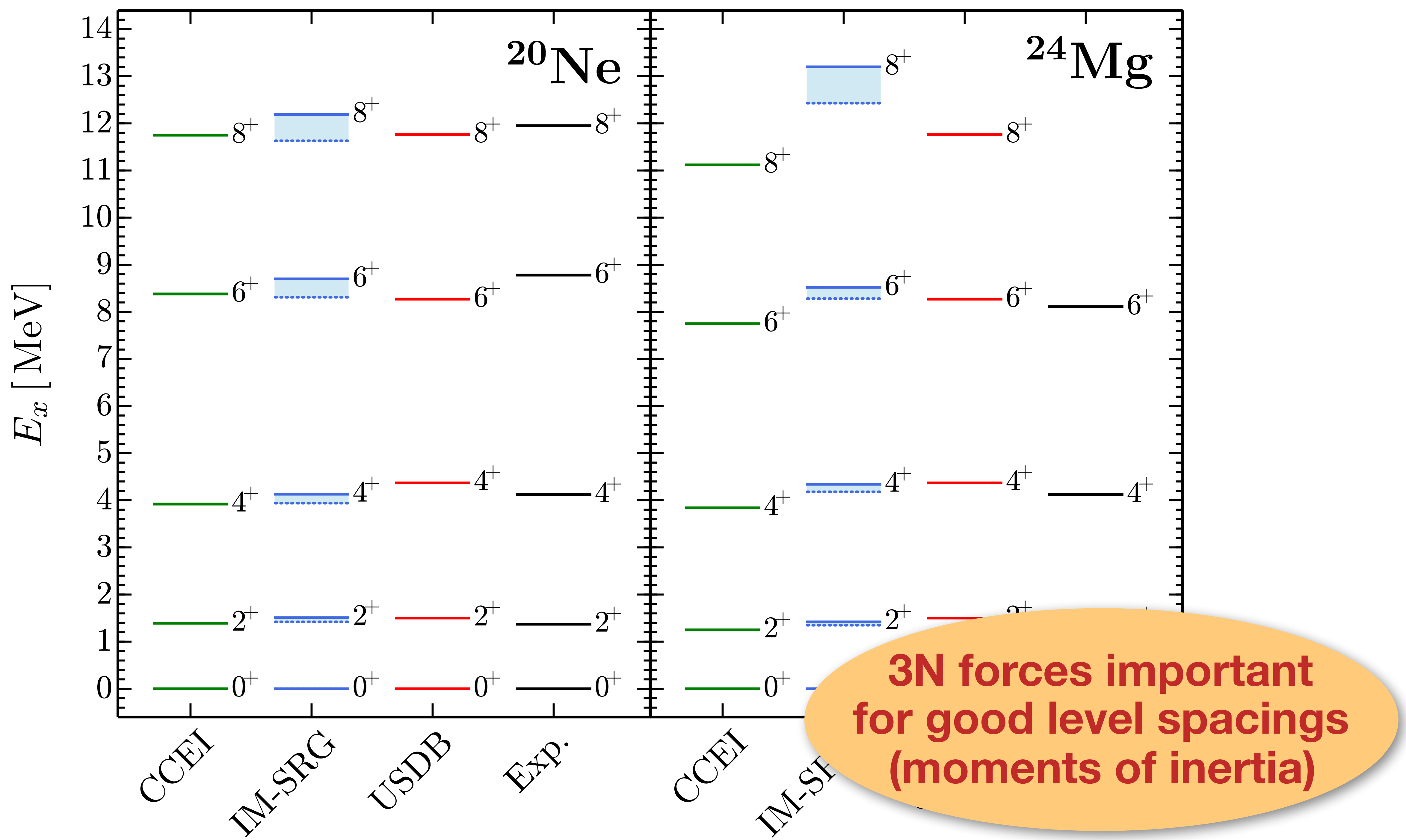
NN + 3N(400)



3N forces crucial for good agreement with data

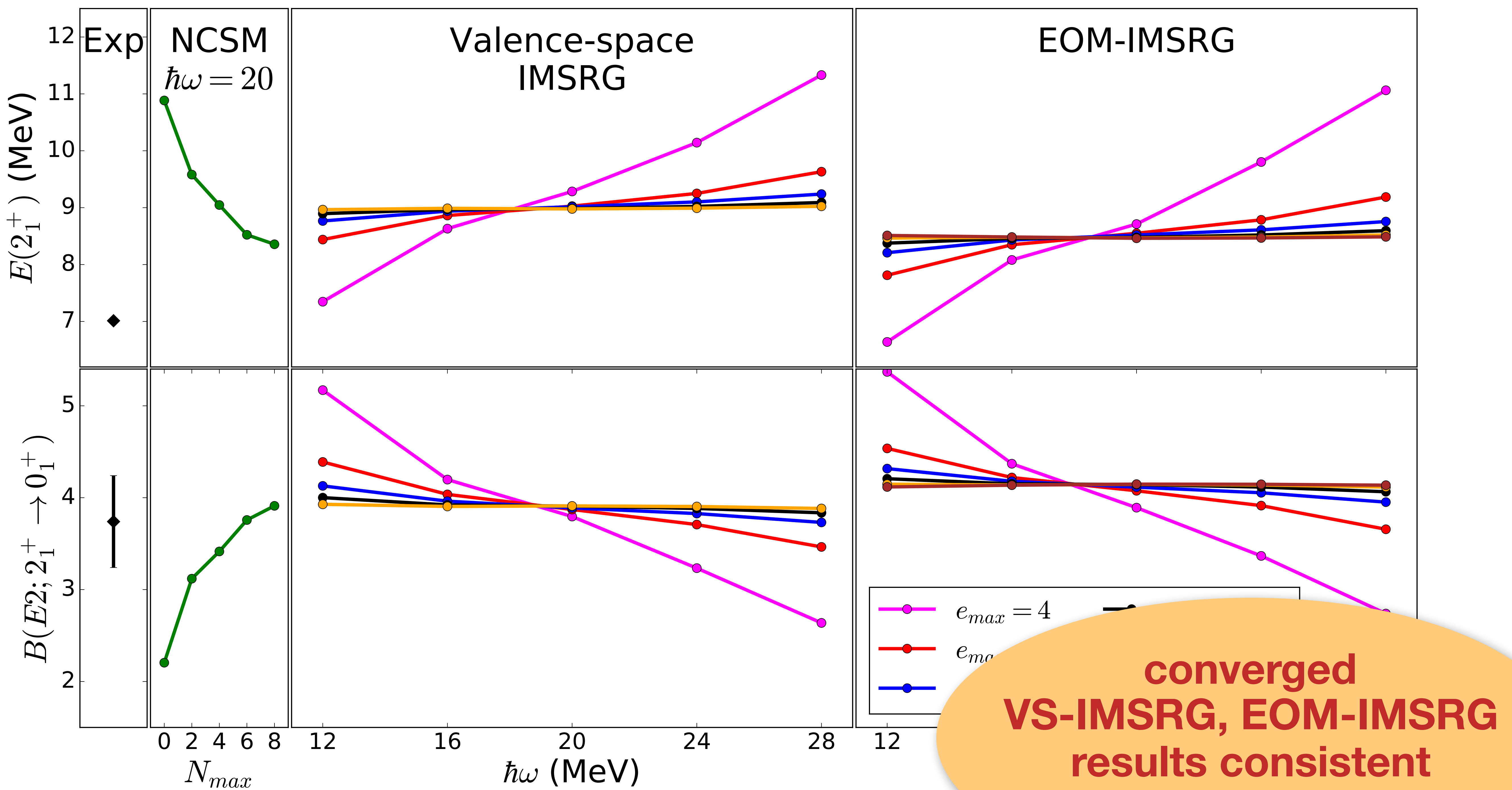
Rotational Bands

S. R. Stroberg et al., PRC **93**, 051301(R) (2016)



E2 Transitions

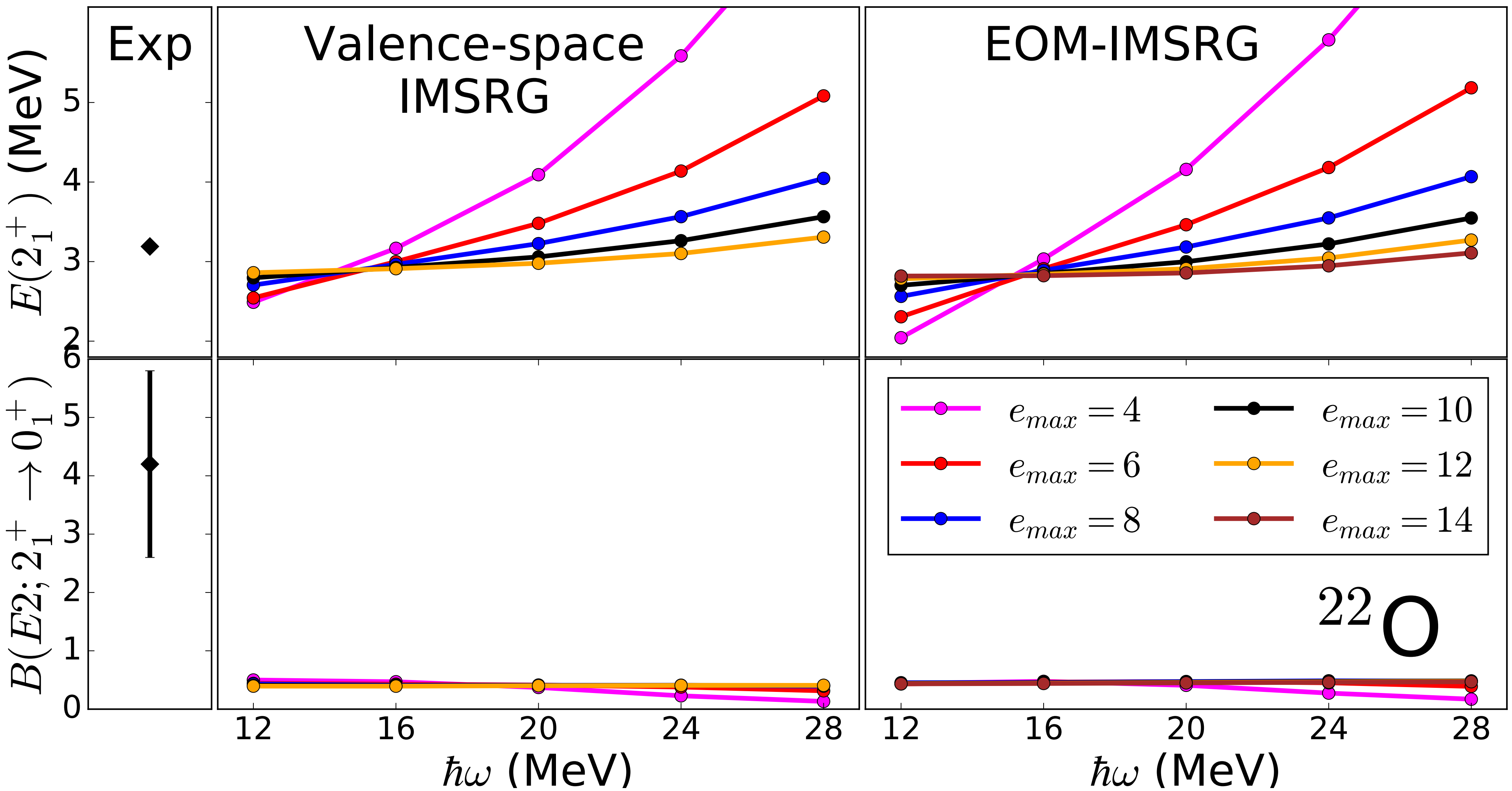
N. M. Parzuchowski, *S. R. Stroberg, P. Navratil, H. H., S. K. Bogner, arXiv: 1705.05511*
EOM-IMSRG: ***N. M. Parzuchowski*** *et al., PRC95, 044304*



converged VS-IMSRG, EOM-IMSRG results consistent with NCSM

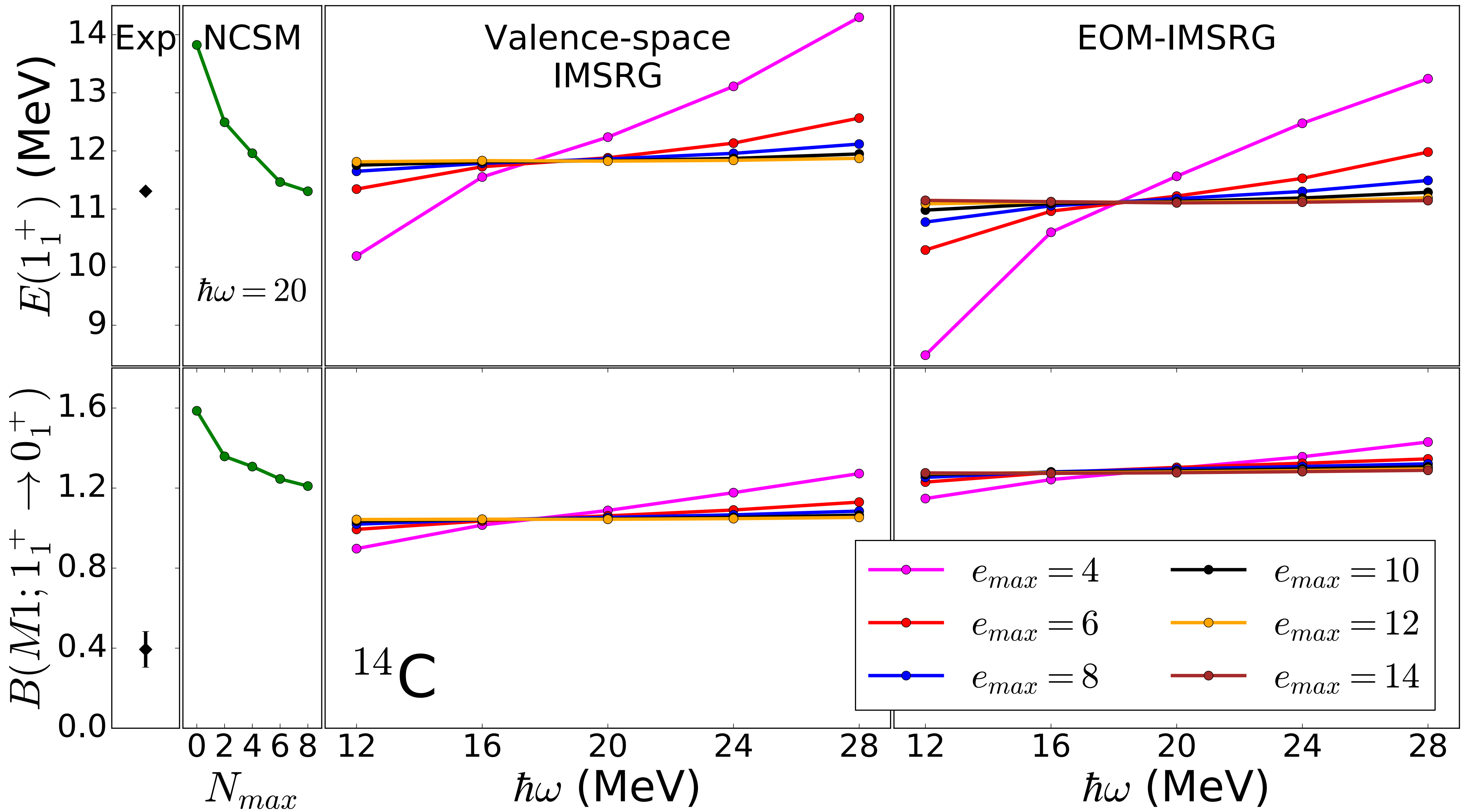
E2 Transitions

N. M. Parzuchowski, S. R. Stroberg, P. Navratil, H. H., S. K. Bogner, arXiv: 1705.05511



- non-zero B(E2) from Shell model: **VS-IMSRG induces effective neutron charge**
- **B(E2) much too small:** effect of intermediate 3p3h, … states that are truncated in IMSRG evolution?

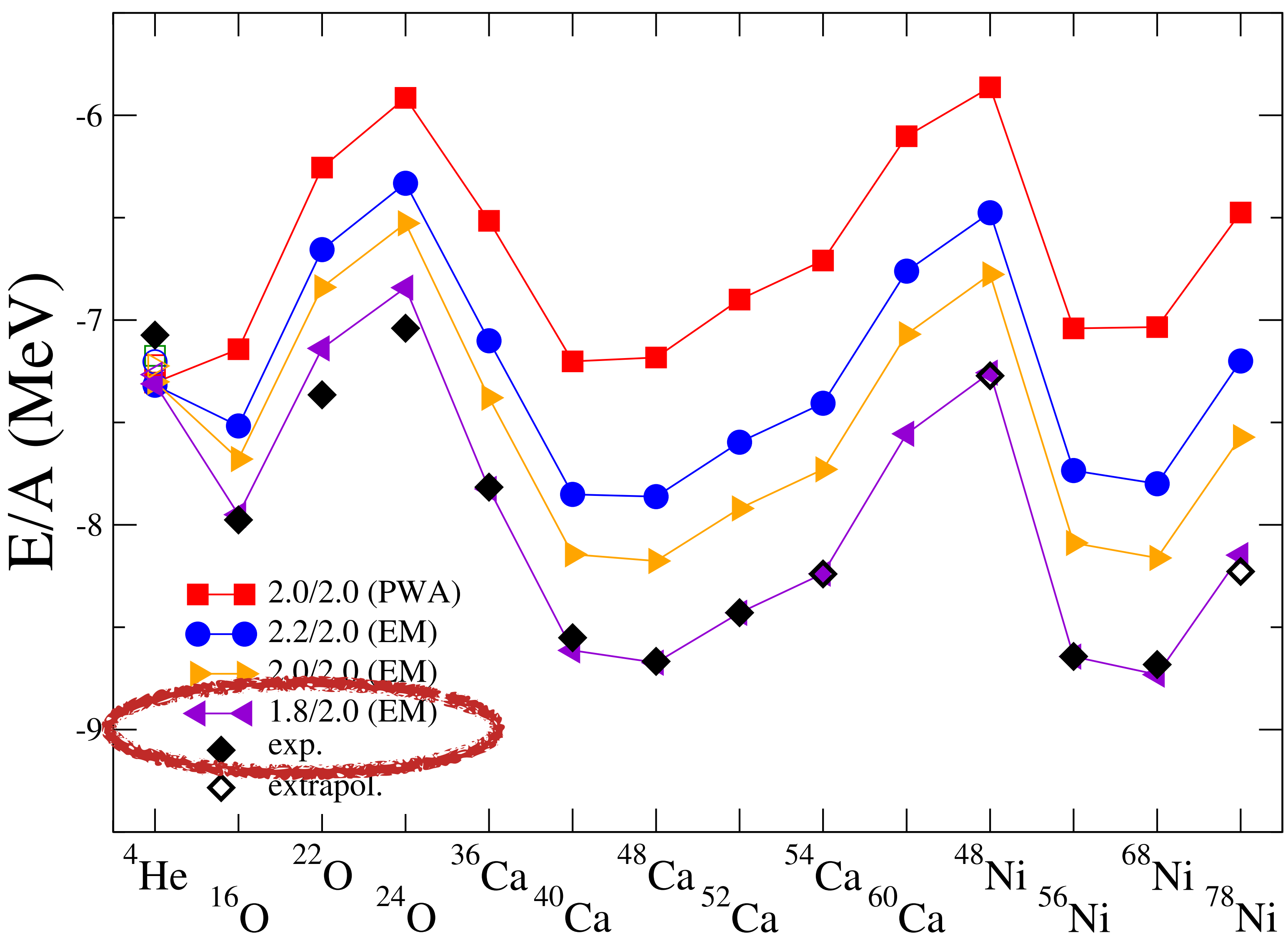
M1 Transitions

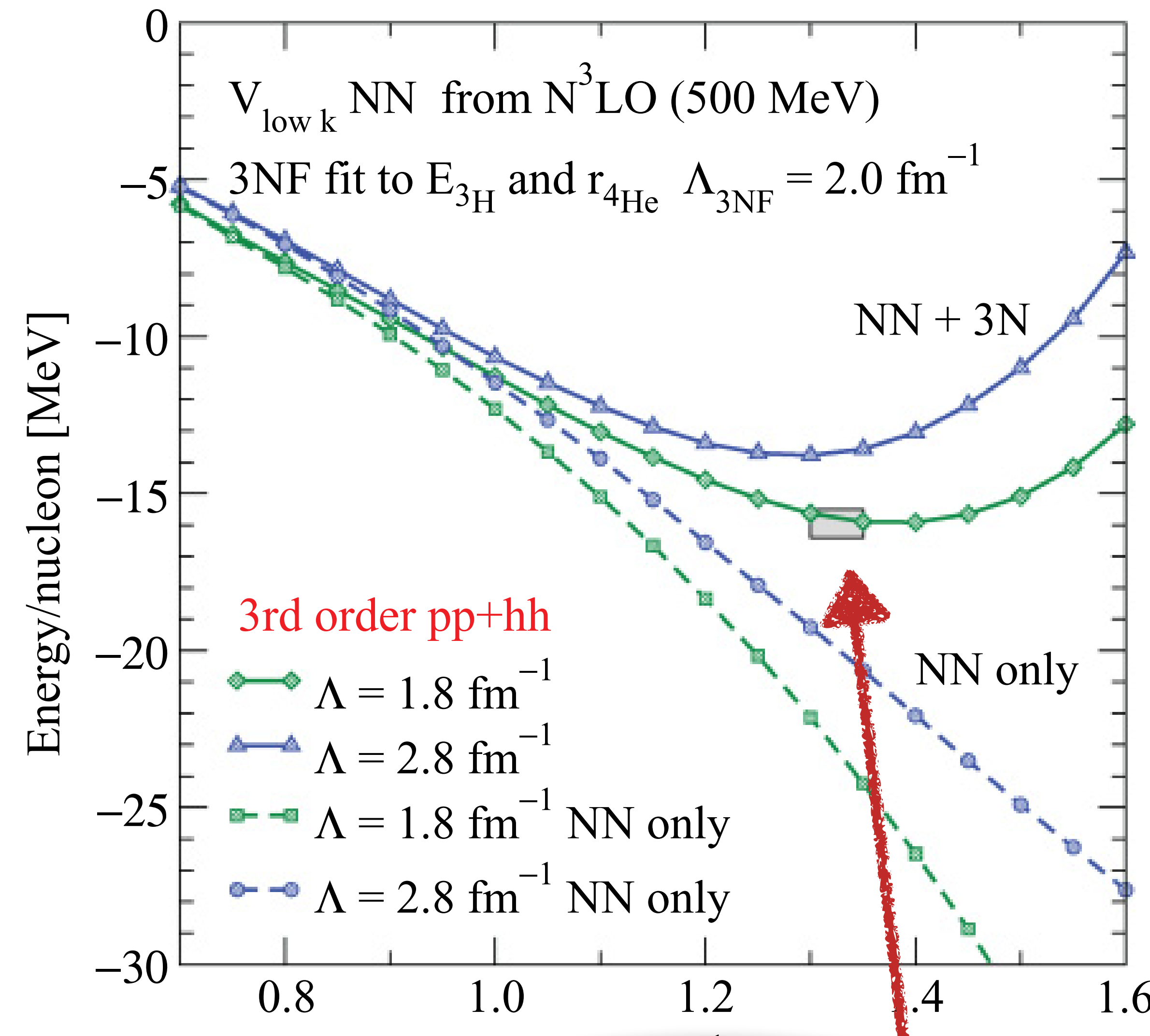


- M1 transitions **consistent** between methods, but **generally too large** - need to include currents

Improving the Interactions

J. Simonis, S. R. Stroberg et al., arXiv:1704.02915; also used in G. Hagen et al., PRL117, 172501 (2016)





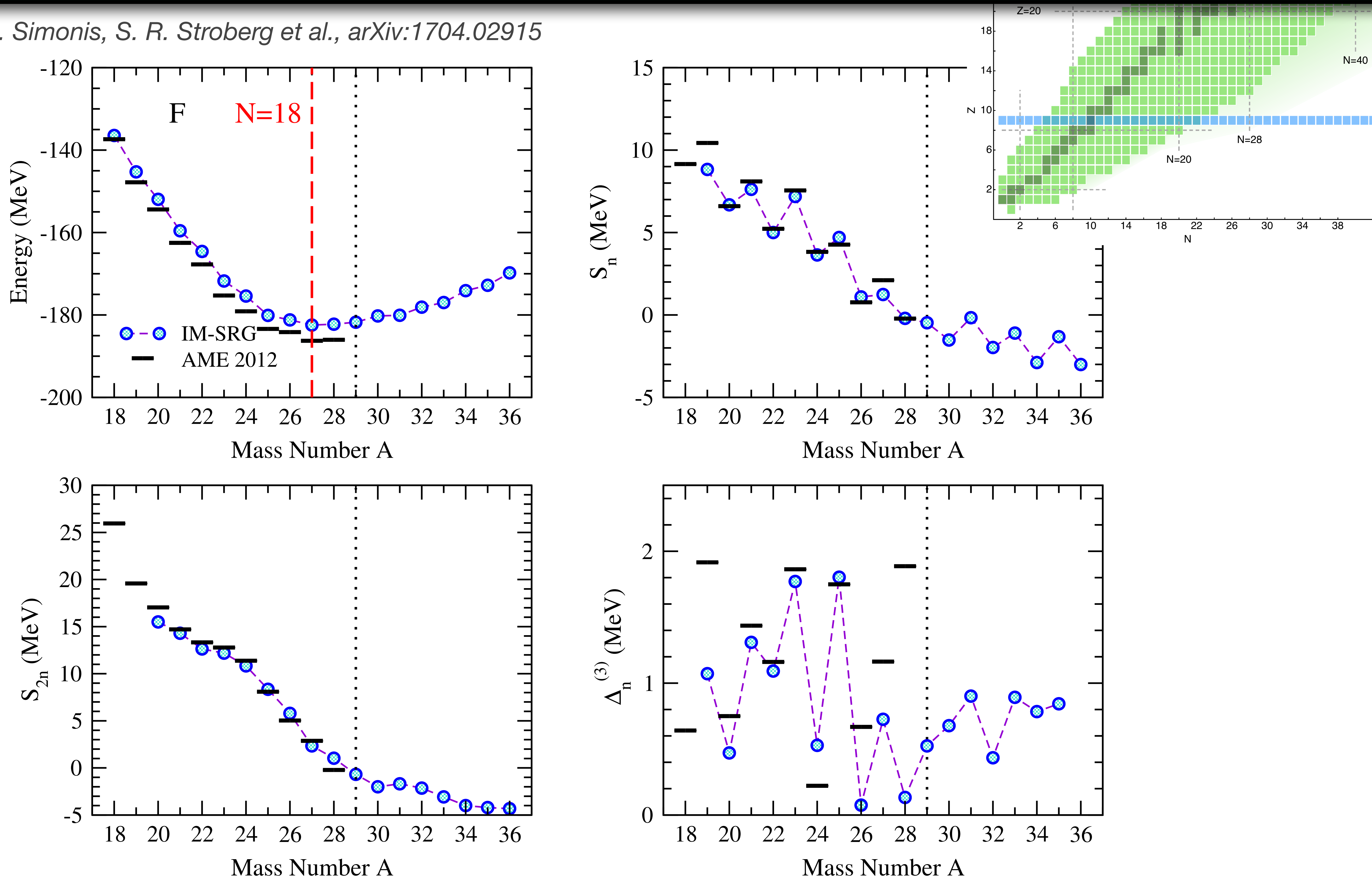
3N LECs fit to ^{3}H binding, ^{4}He charge radius

“hybrid” chiral NN+3N intera[ctions]

Hebeler et al., PRC83, 031301

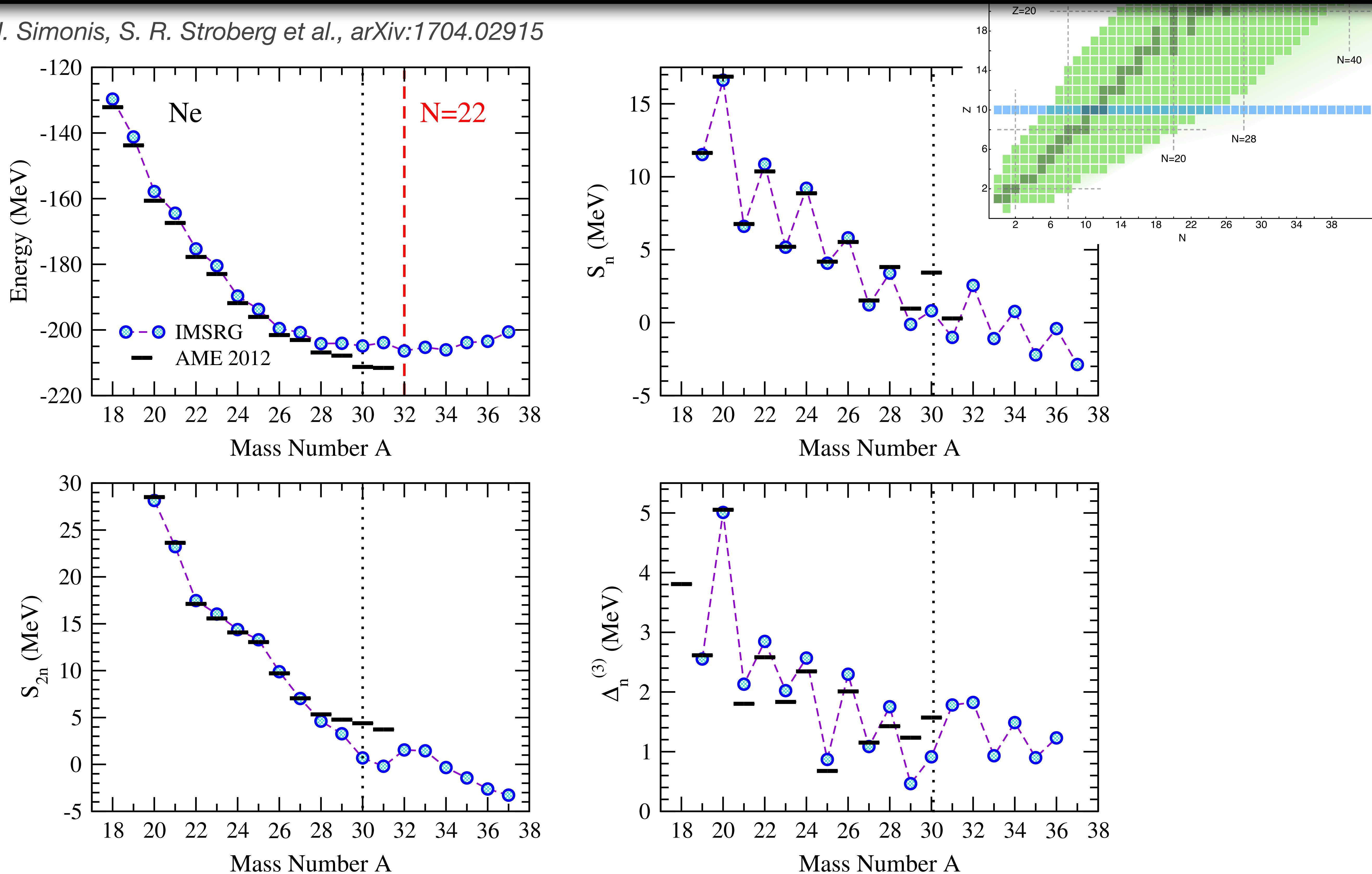
The EM 1.8/2.0 Interaction

J. Simonis, S. R. Stroberg et al., arXiv:1704.02915



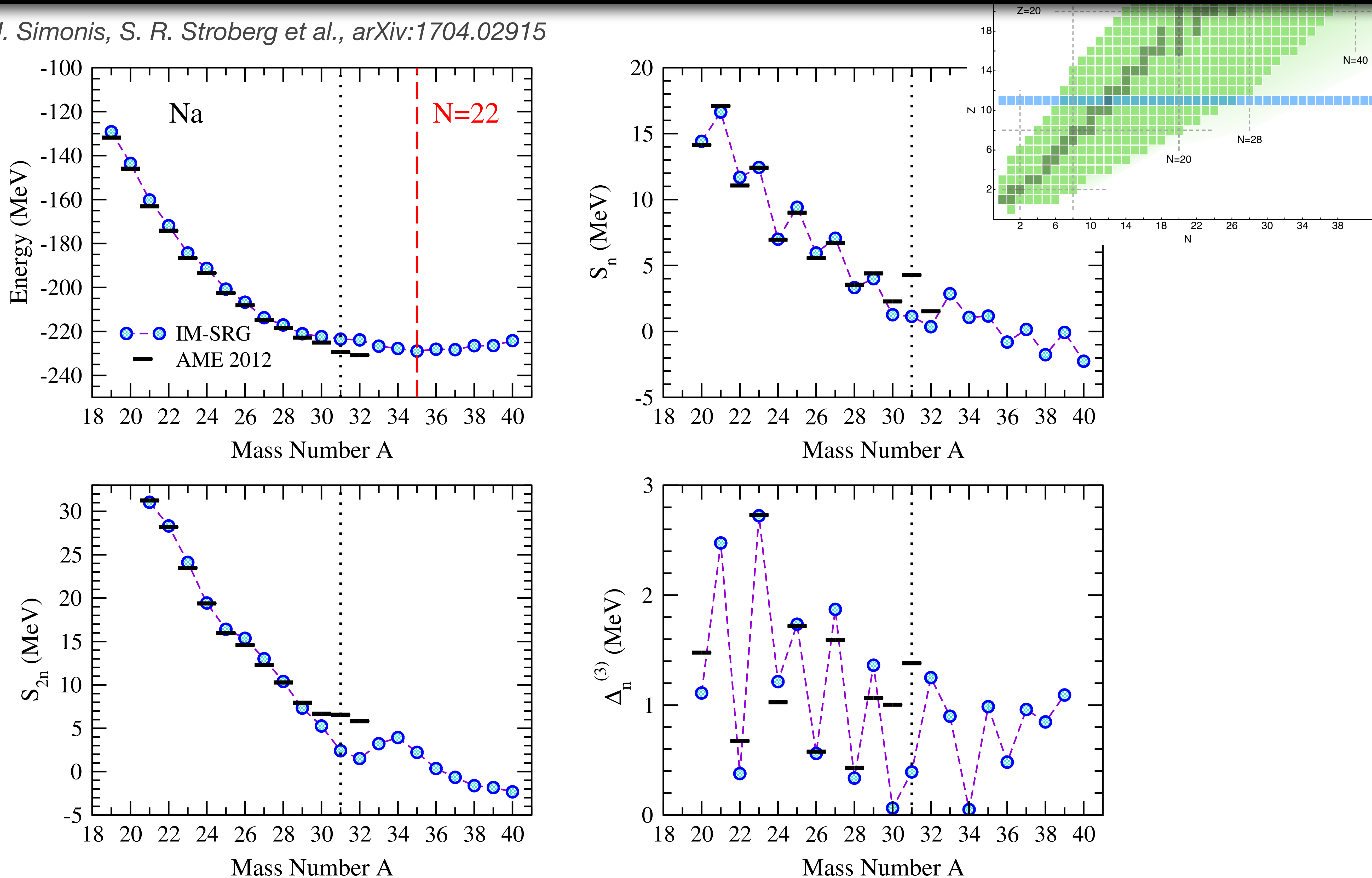
The EM 1.8/2.0 Interaction

J. Simonis, S. R. Stroberg et al., arXiv:1704.02915



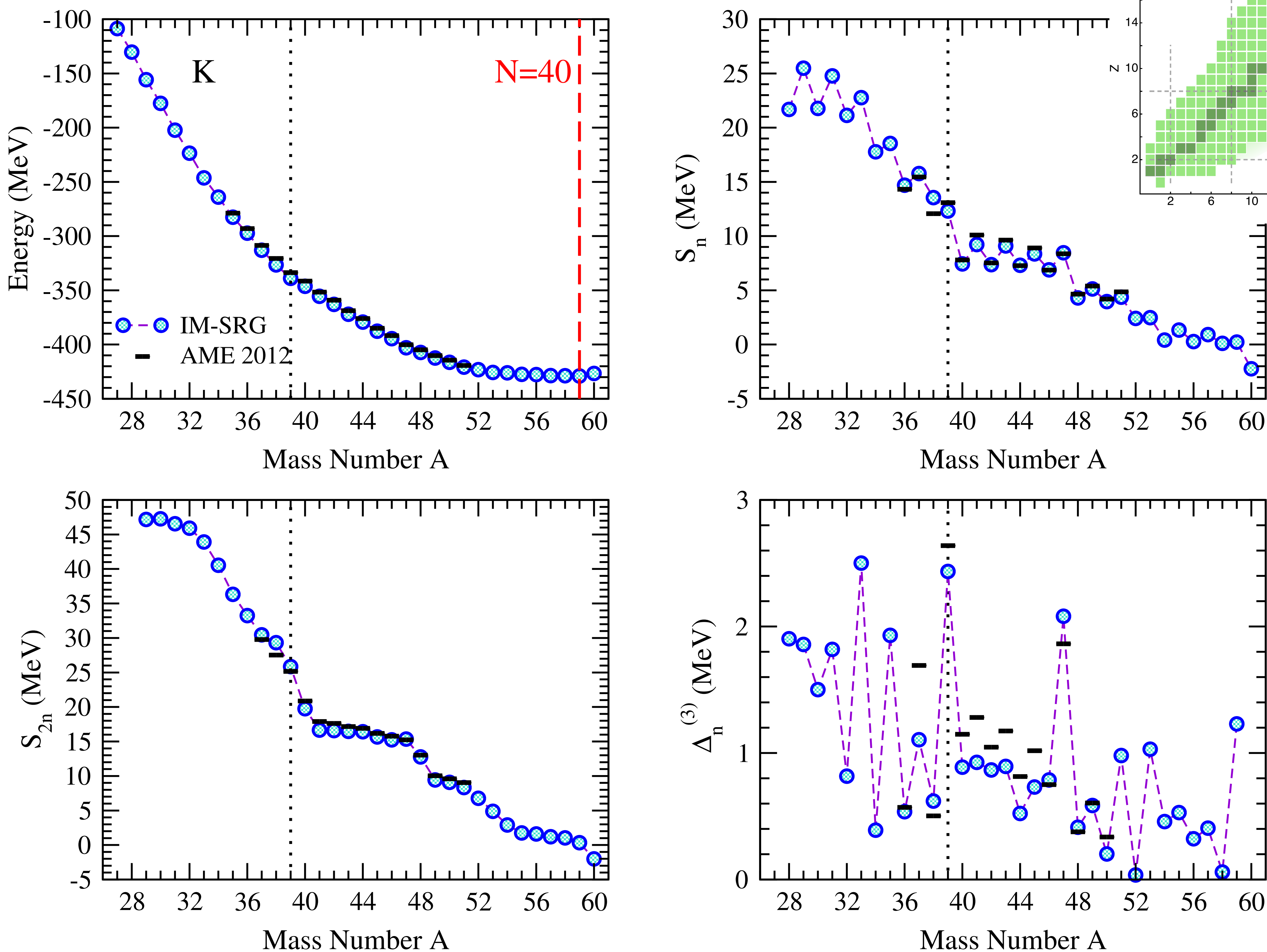
The EM 1.8/2.0 Interaction

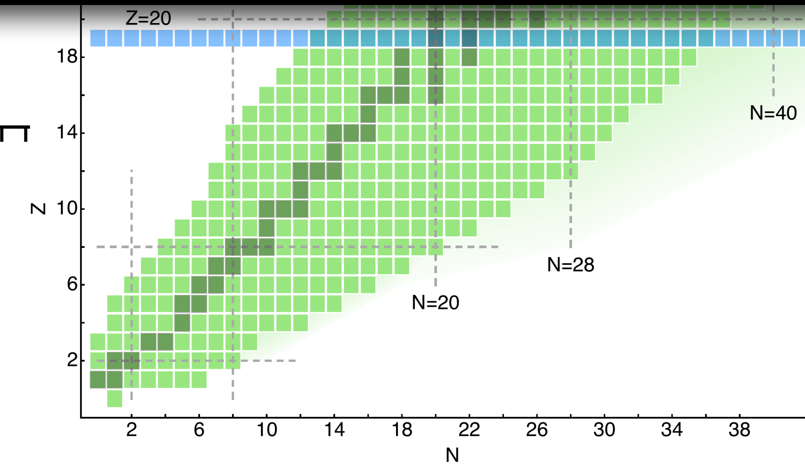
J. Simonis, S. R. Stroberg et al., arXiv:1704.02915



The EM 1.8/2.0 Interaction

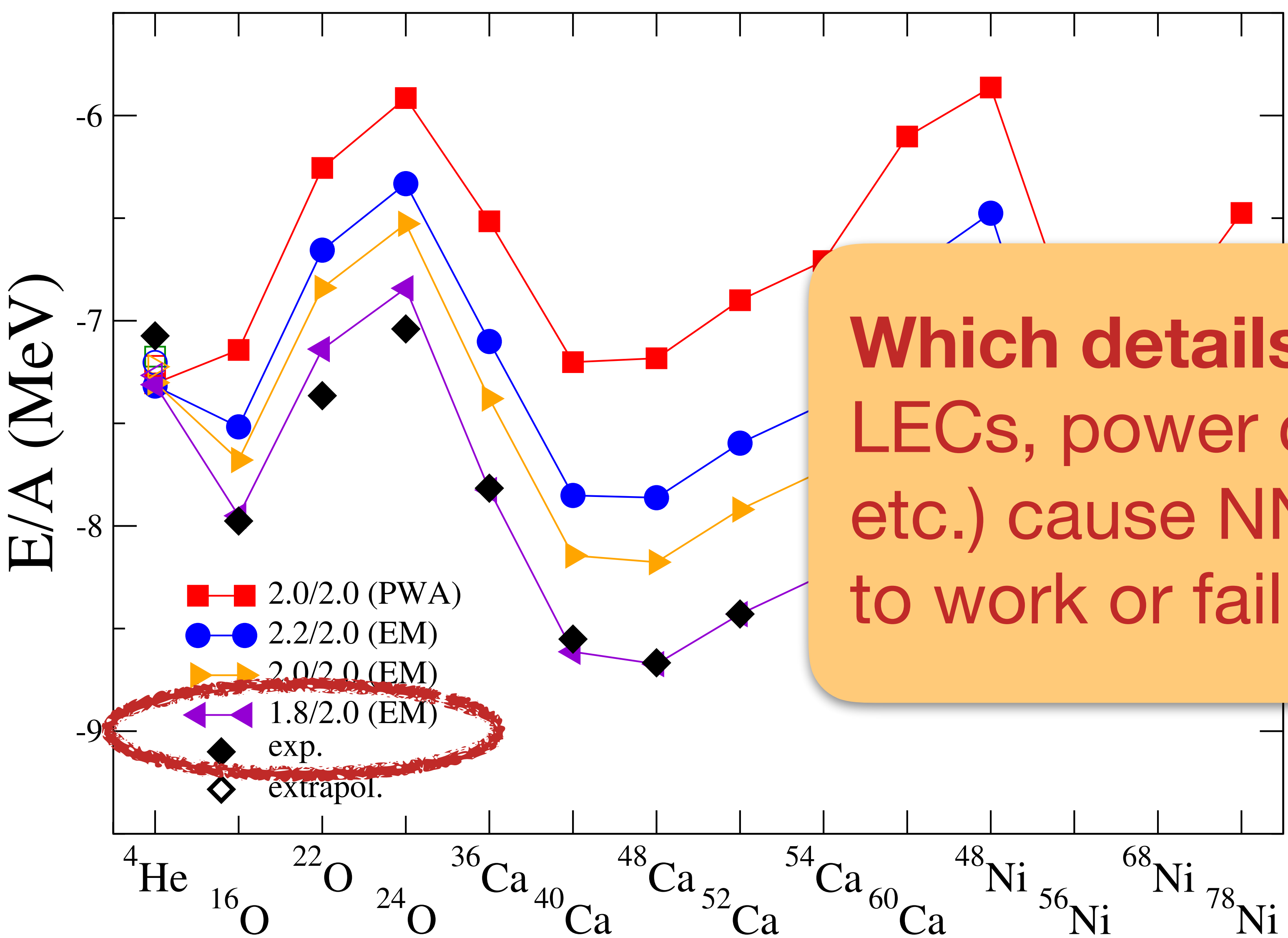
J. Simonis, S. R. Stroberg et al., arXiv:1704.02915

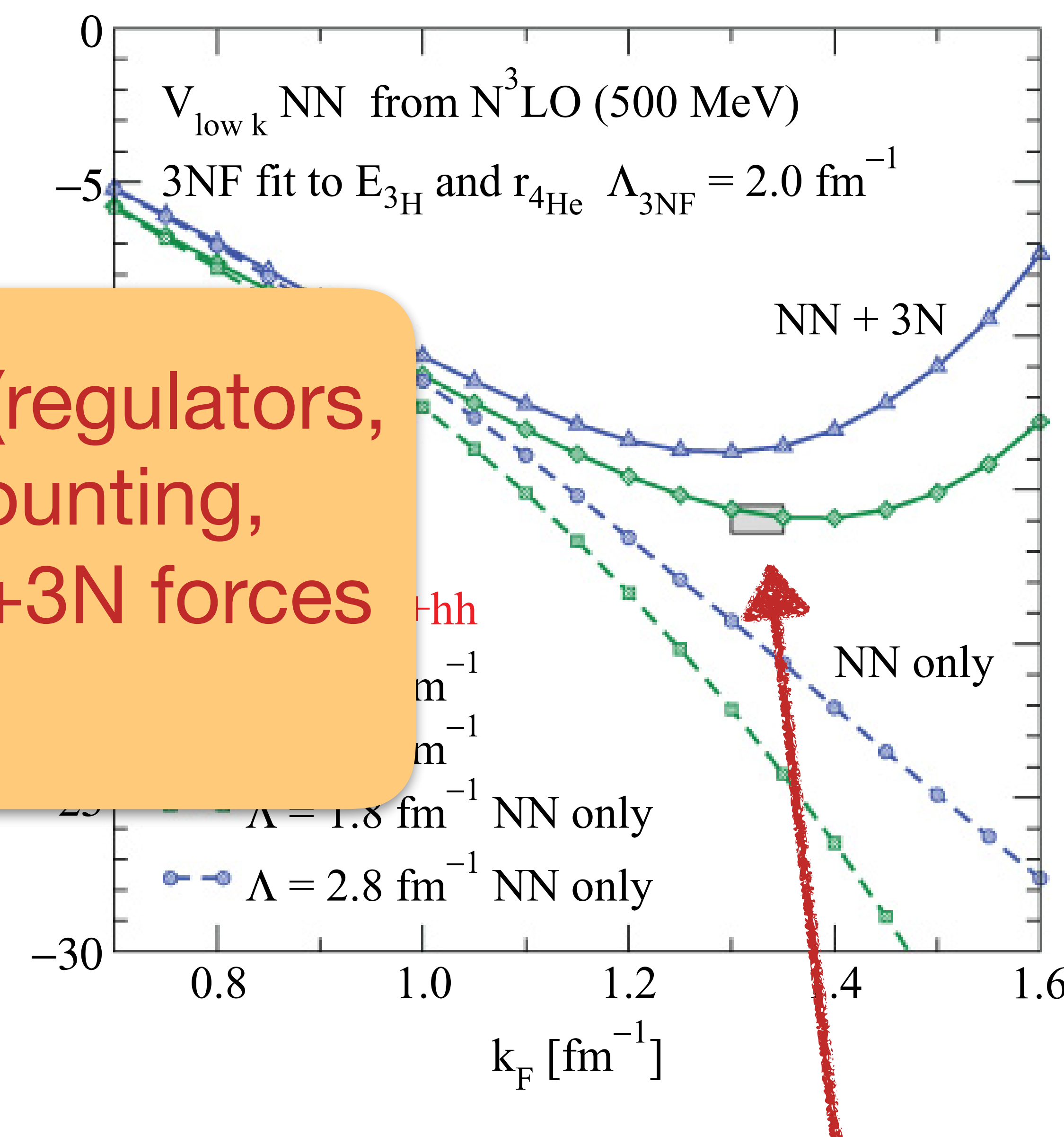




Improving the Interactions

J. Simonis et al., arXiv:1704.02915; also used in G. Hagen et al., PRL117, 172501 (2016)





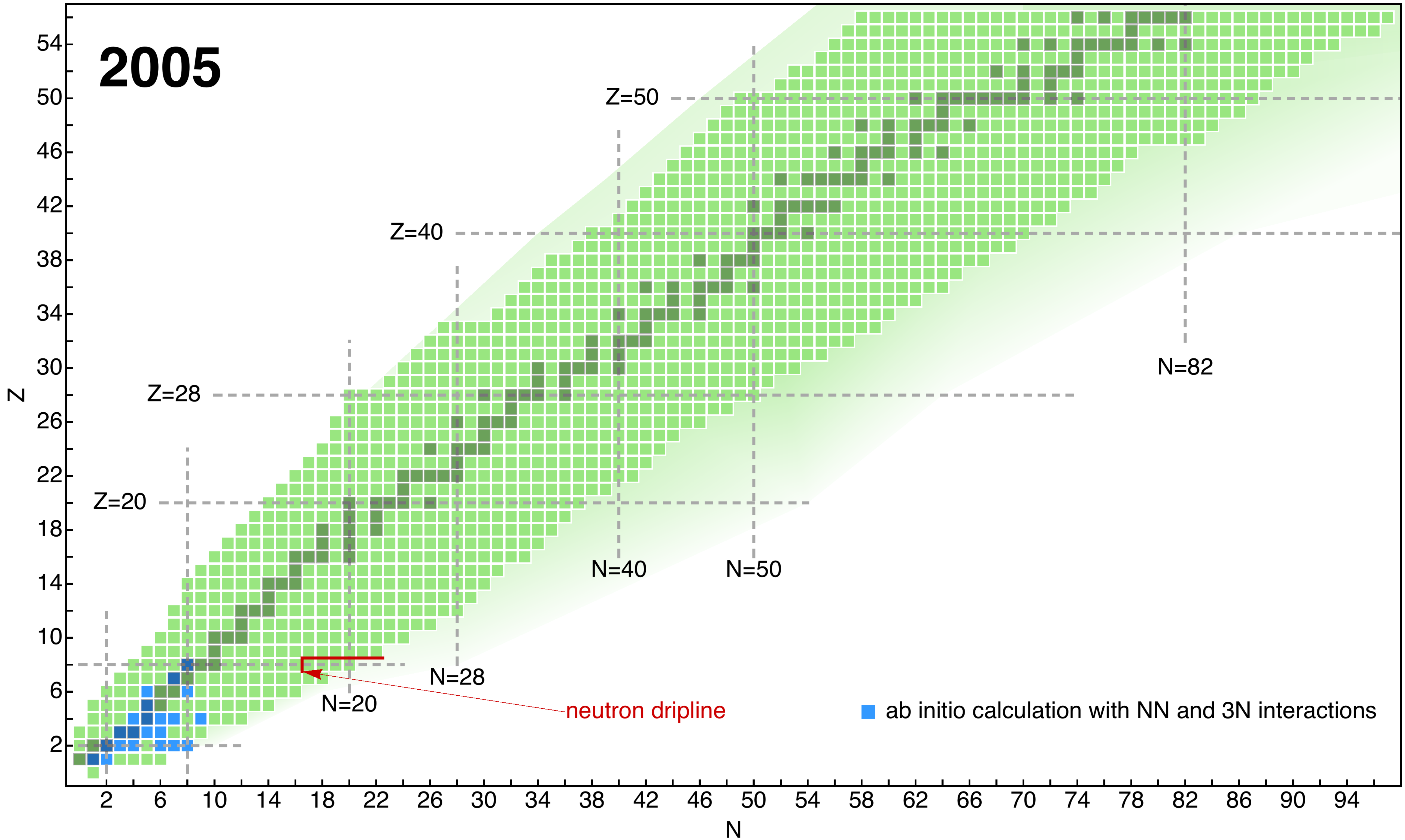
Which details (regulators, LECs, power counting, etc.) cause NN+3N forces to work or fail ?

"hybrid" chiral NN+3N interaction

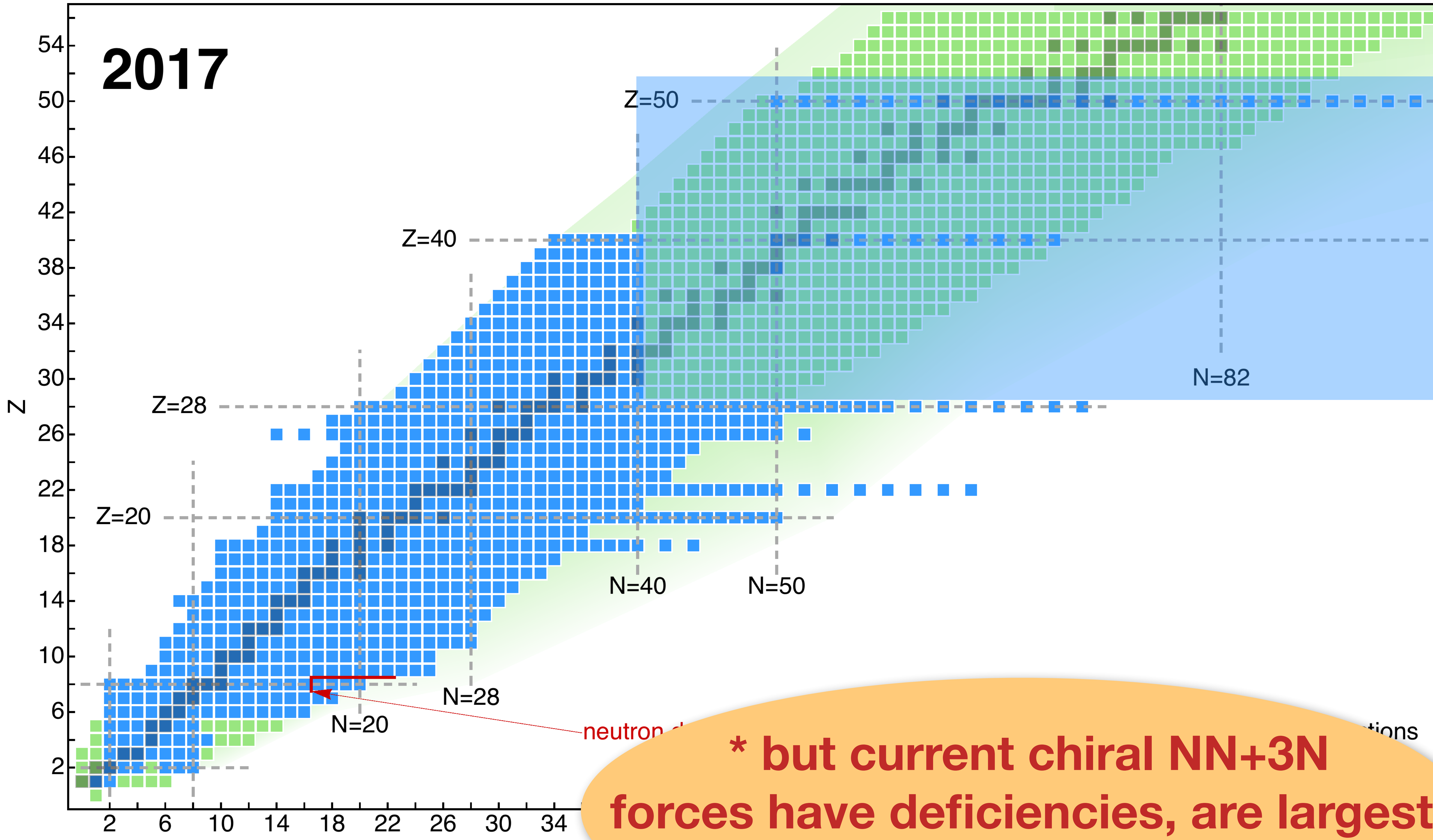
Hebeler et al., PRC83, 031301

Epilogue

Progress in *Ab Initio* Calculations



Progress in *Ab Initio* Calculations



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

Summary

- towards ***ab initio* NMEs:** interaction, operators, many-body method with **systematic uncertainties** & convergence to exact result
- rapidly **growing capabilities**: g.s. energies, spectra, radii, transitions, …

➡ **ingredients for NME calculation, plus validation through other observables**

- uncertainty presently dominated by
  - **deficiencies** in current chiral Hamiltonians
  - **missing collectivity** in description of (certain) transitions

Acknowledgments

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

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

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

T. D. Morris
UT Knoxville & Oak Ridge National Laboratory

R. J. Furnstahl, N. M. Parzuchowski
The Ohio State University

T. Duguet, V. Somà
CEA Saclay, France

C. Barbieri
U. Surrey, UK

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

NUCLEI
Nuclear Computational Low-Energy Initiative

Ohio Supercomputer Center

ICER