Nuclear Shapes from the In-Medium Similarity Renormalization Group

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Facility for Rare Isotope Beams
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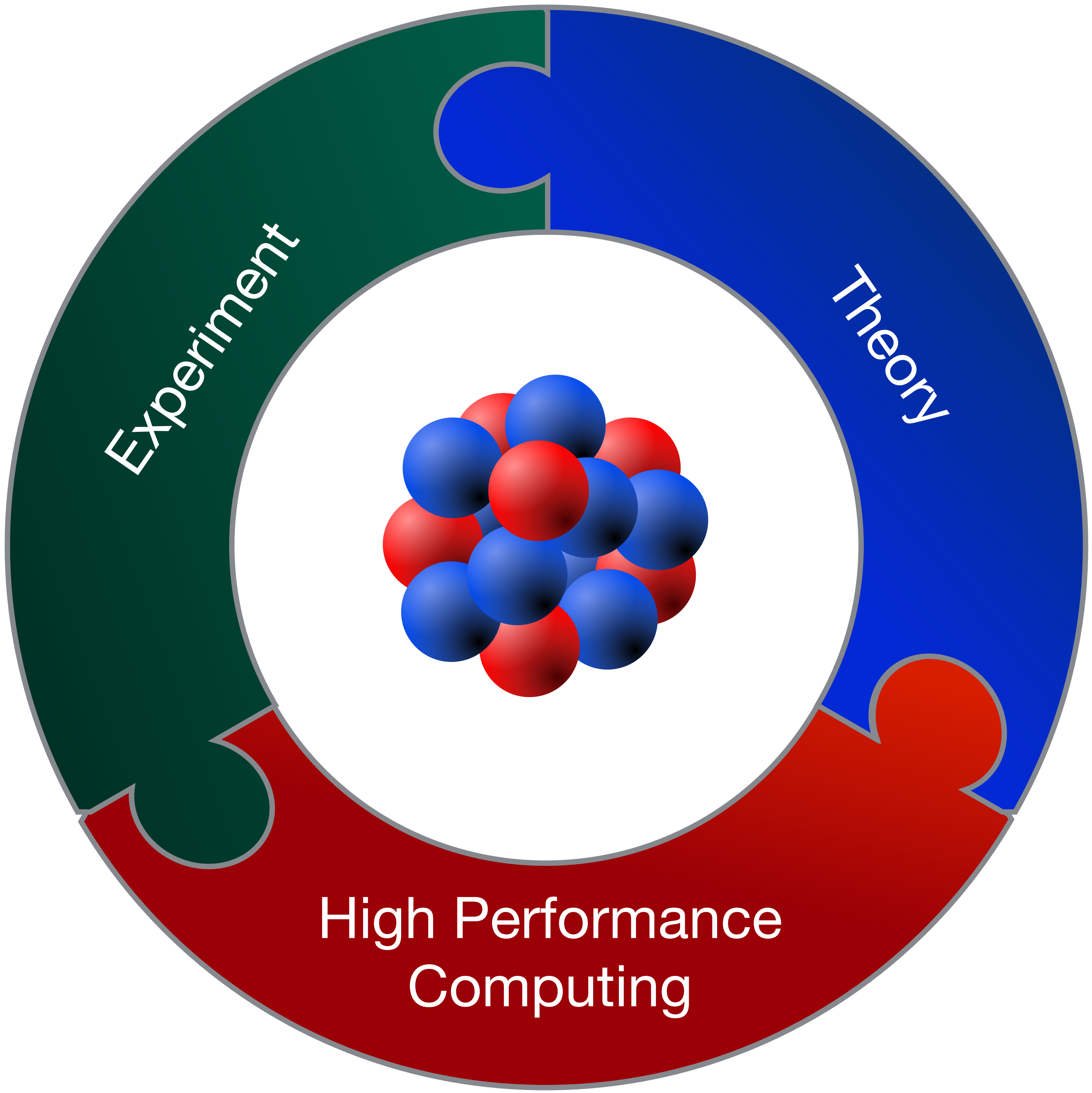
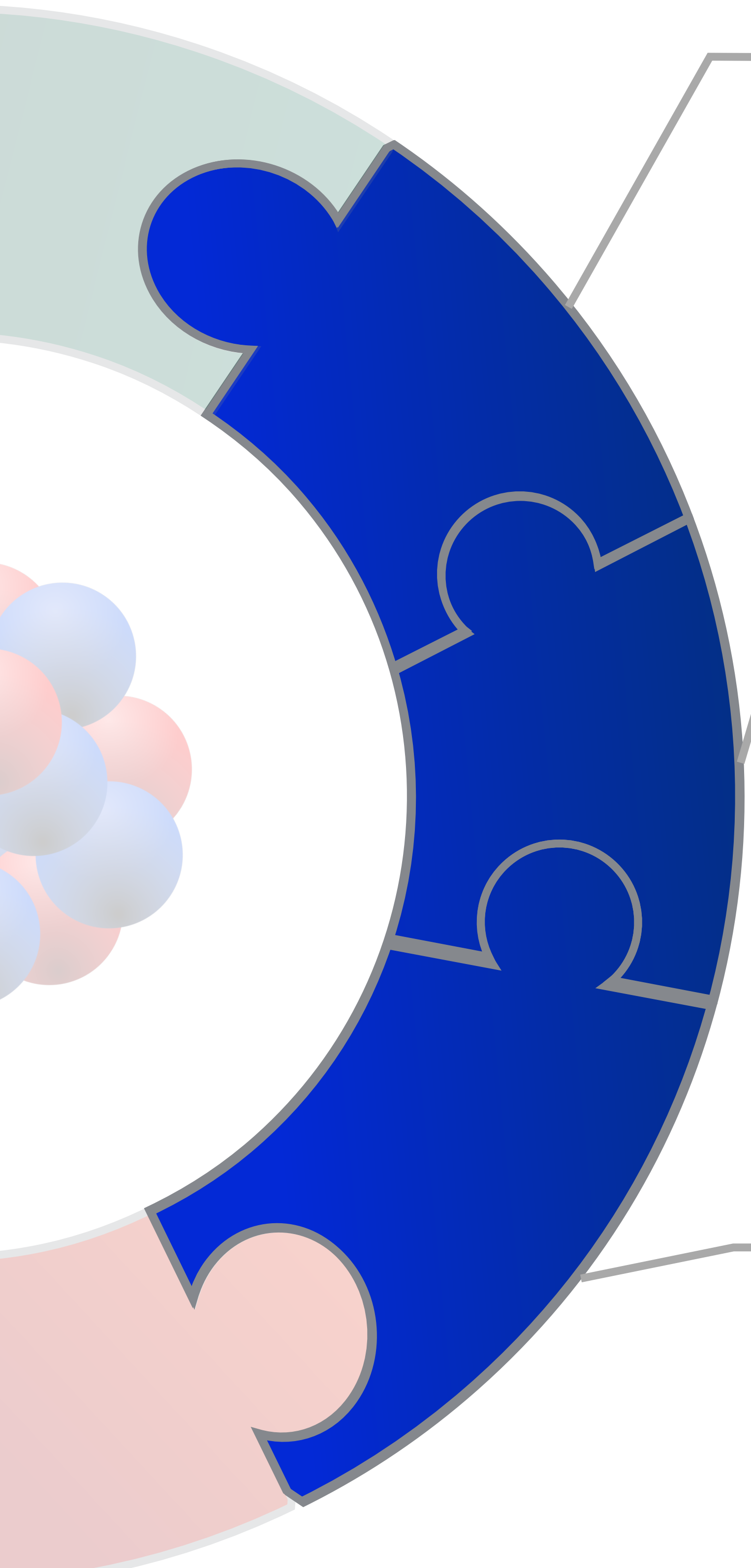
The Nuclear Many-Body Problem

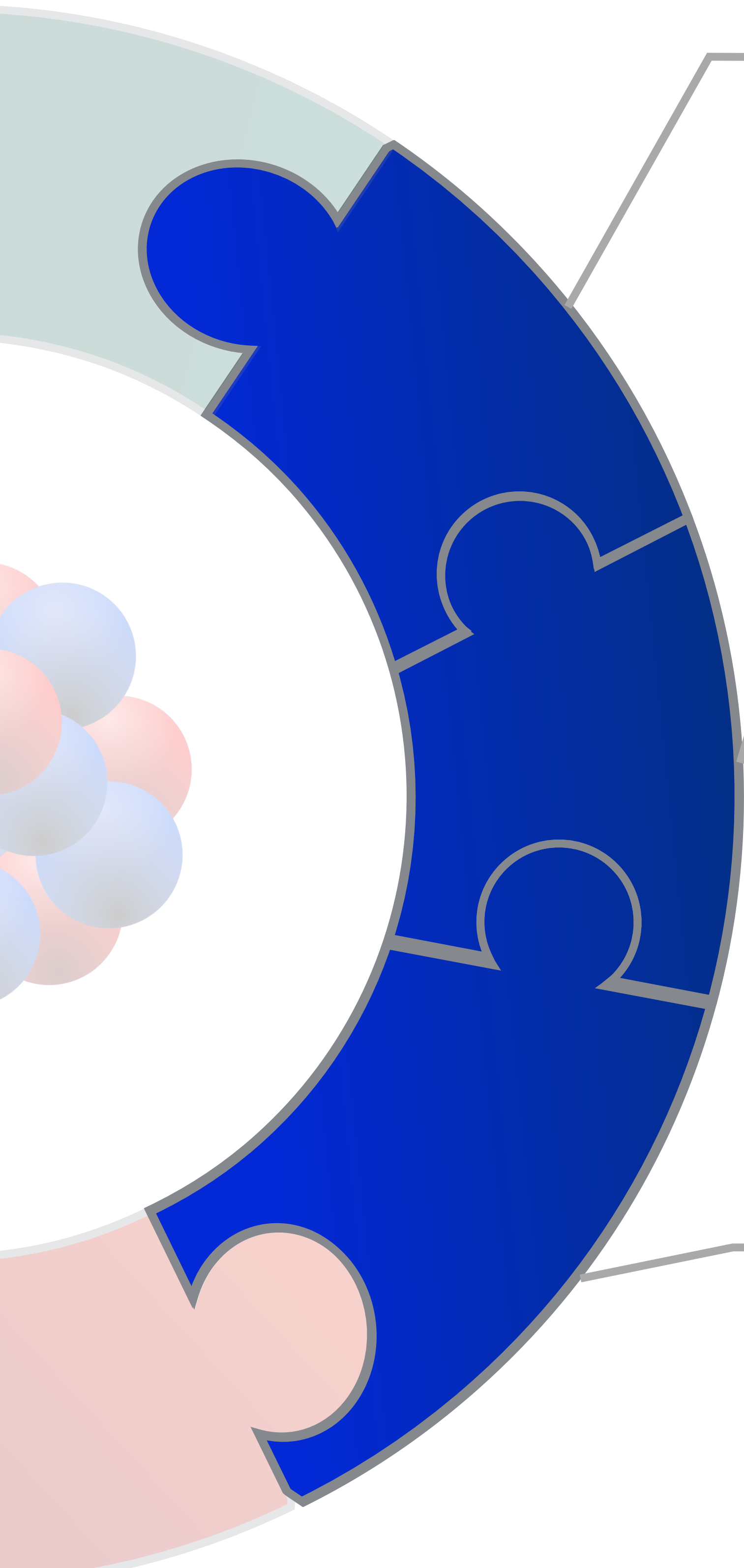


Towards Predictive Theory



- **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 (+ LEC uncertainty)
- **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

Ab Initio Many-Body Methods: (Multi-Reference) In-Medium Similarity Renormalization Group

H. H., in preparation

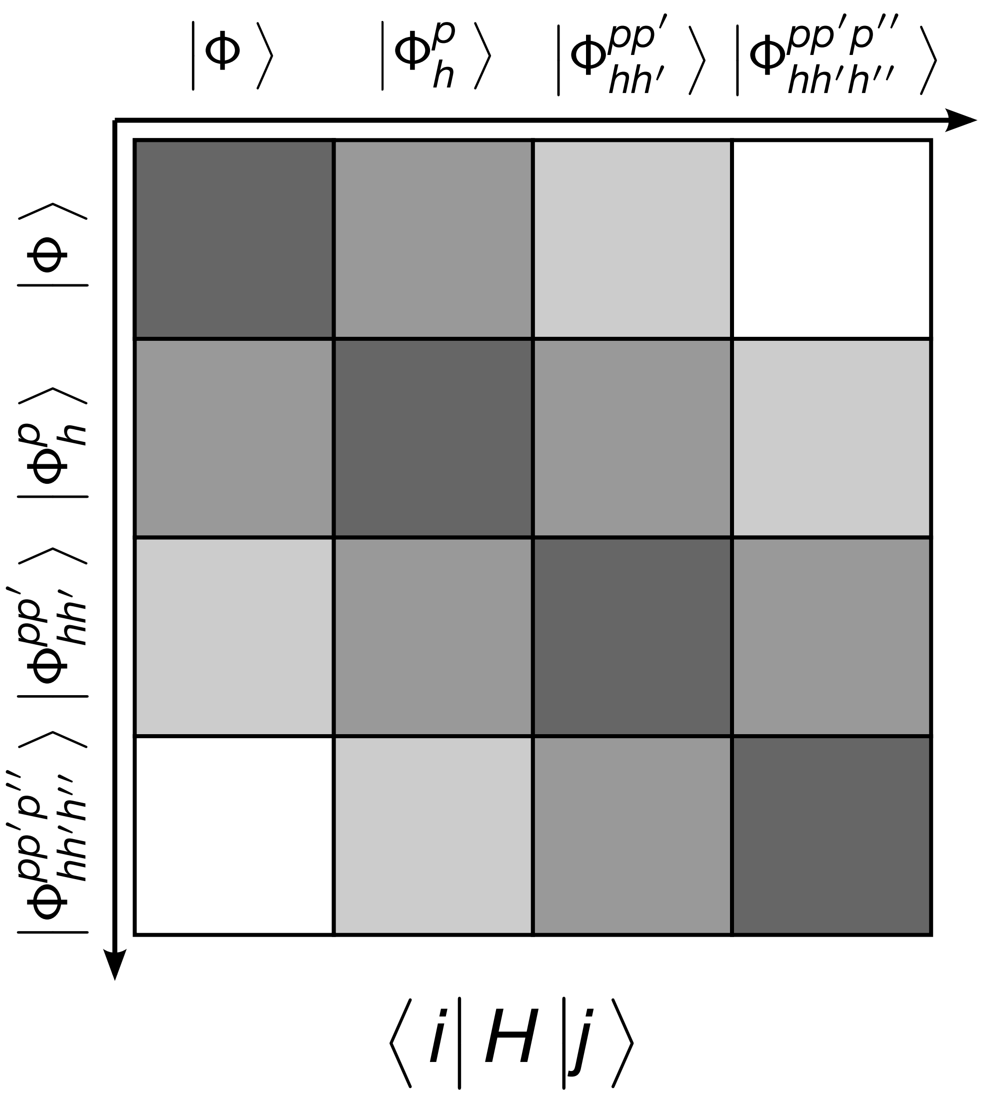
H. H., Phys. Scripta, Phys. Scripta 92, 023002 (2017)

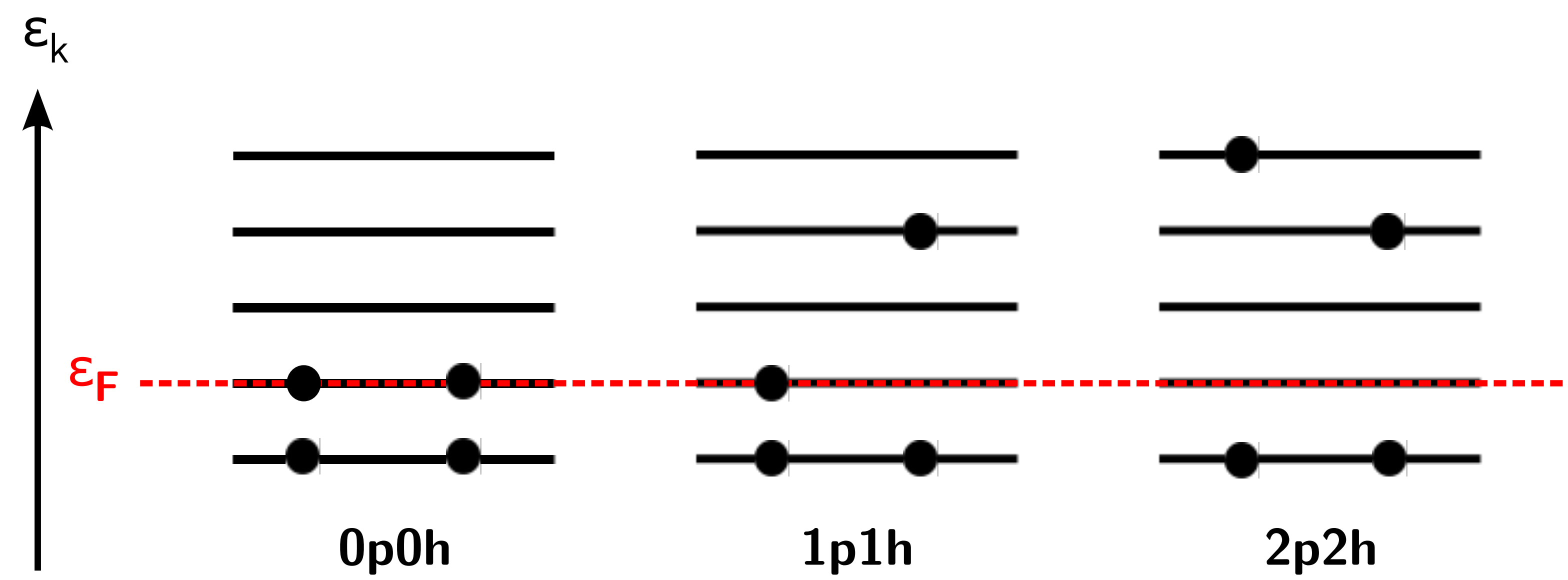
H. H., S. K. Bogner, T. D. Morris, A. Schwenk, and K. Tuskiyama, Phys. Rept. **621**, 165 (2016)

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





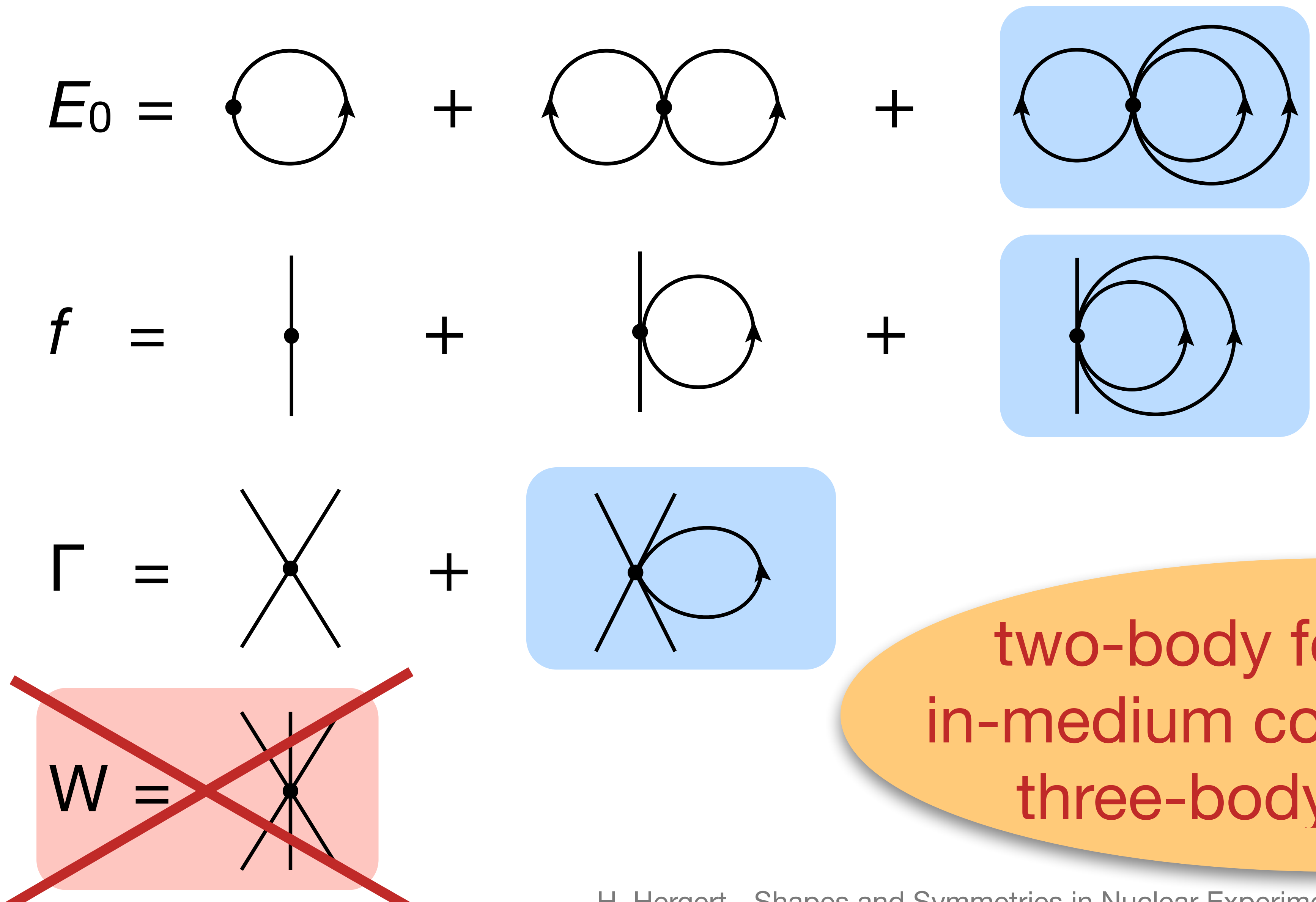
- reference state: **single Slater determinant**

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

Normal-Ordered Hamiltonian

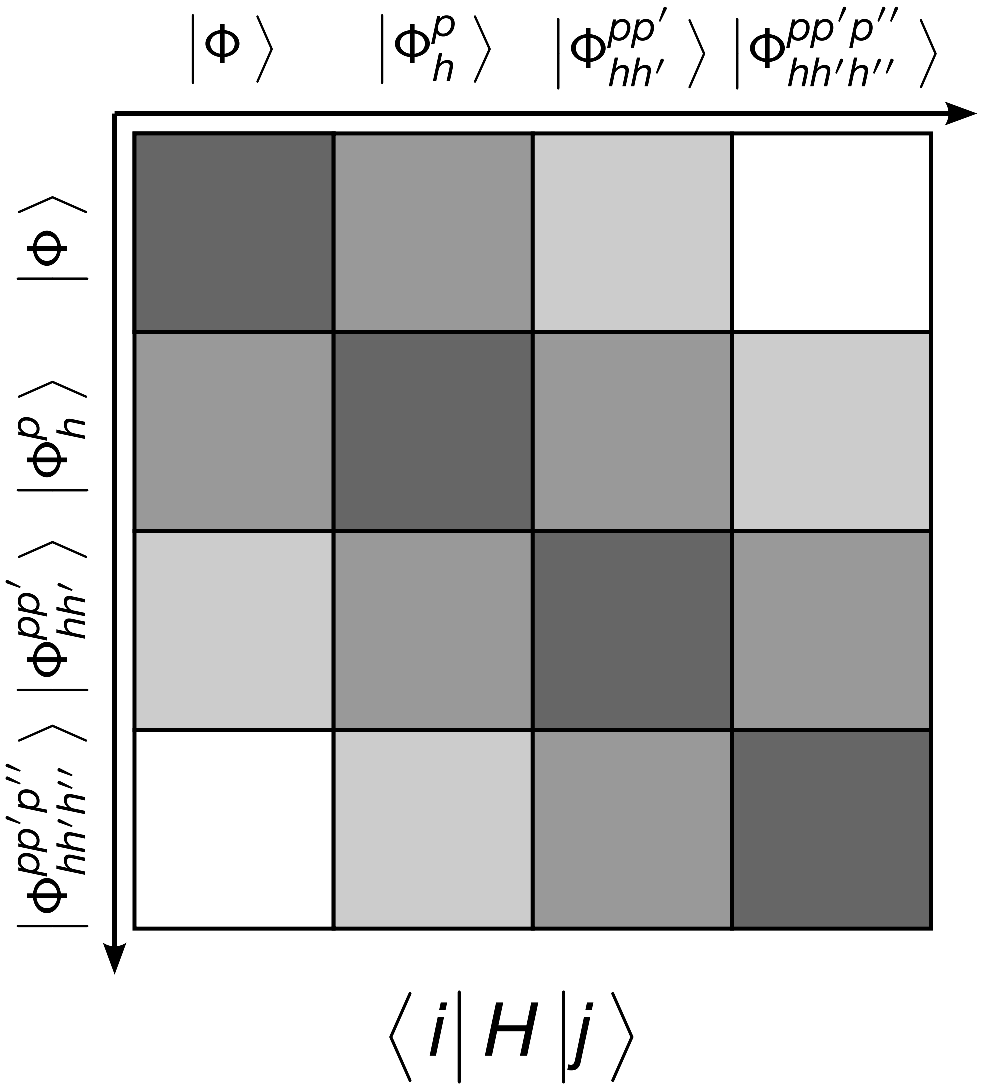
Normal-Ordered Hamiltonian

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



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

Single-Reference Case



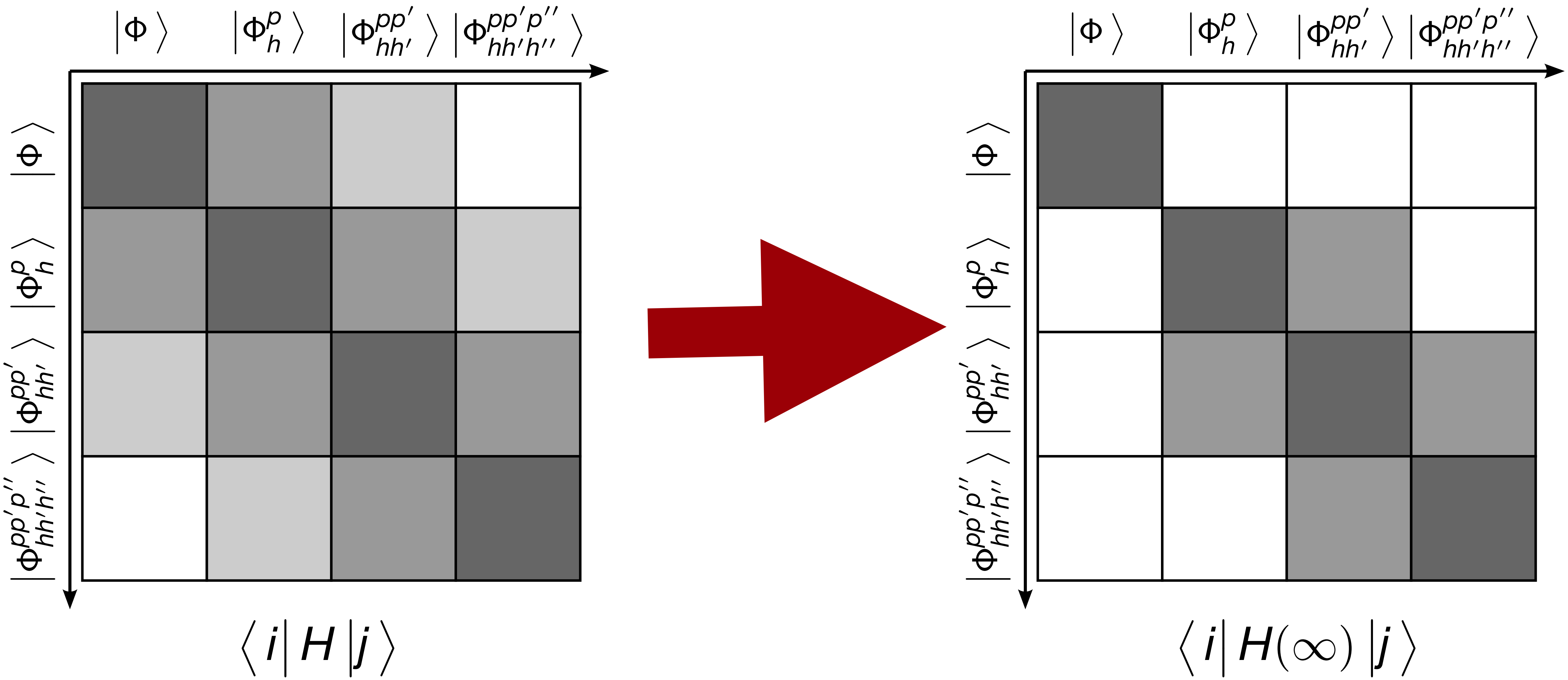
$$A^{i_1\dots i_N}_{j_1\dots j_N} \equiv a^{\dagger}_{i_1}\dots a^{\dagger}_{i_N} a_{j_N}\dots a_{j_1}$$

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

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

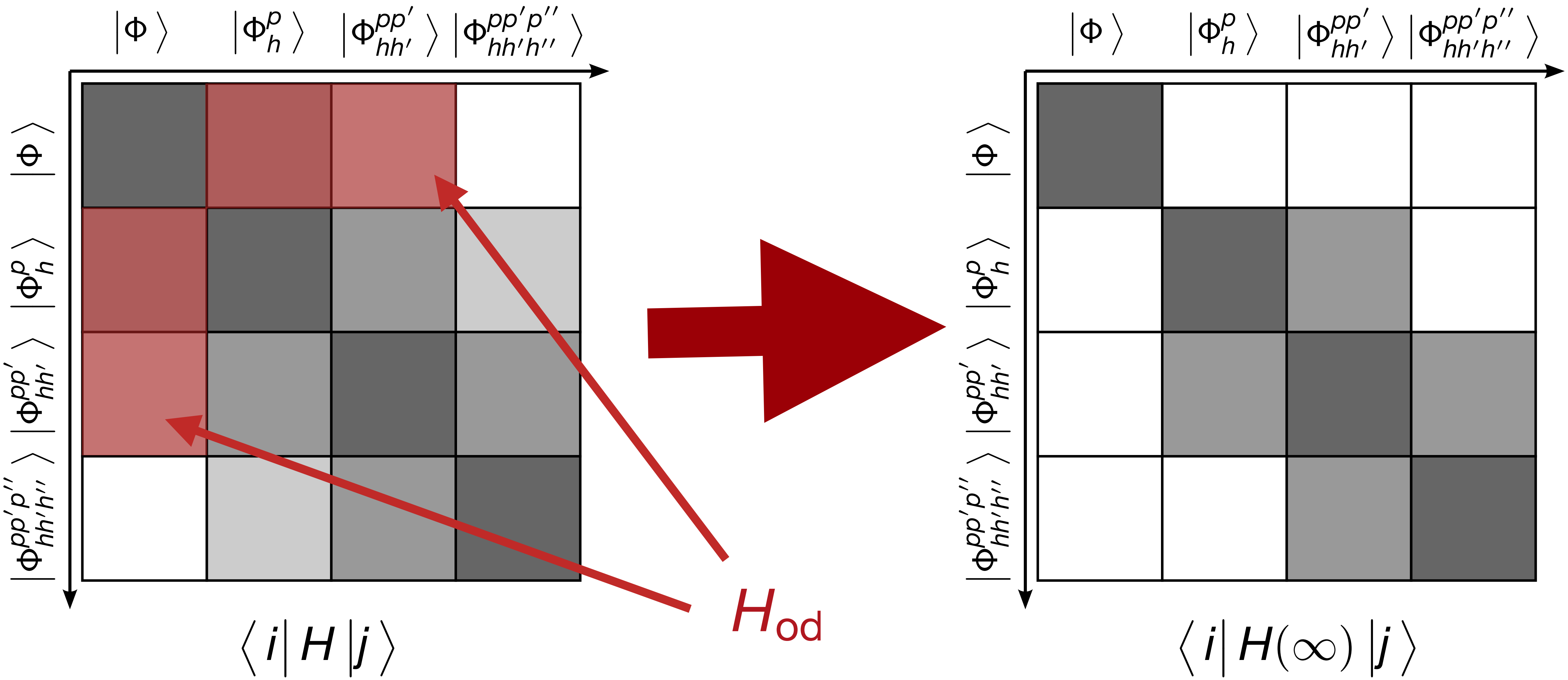
- reference state: **Slater determinant**
- normal-ordered operators **depend on occupation numbers (one-body density)**

Decoupling in A-Body Space



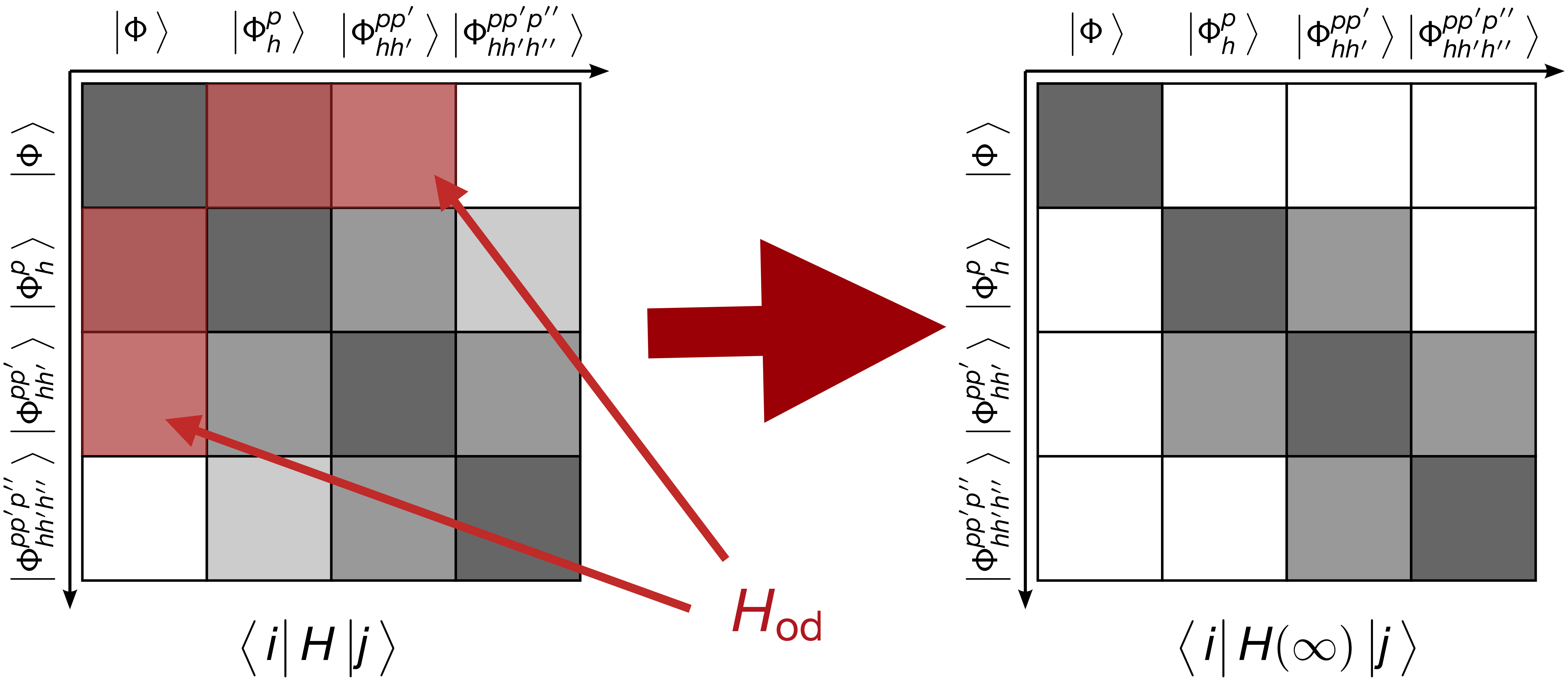
aim: decouple reference state $|\Phi\rangle$ from excitations

Flow Equation



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

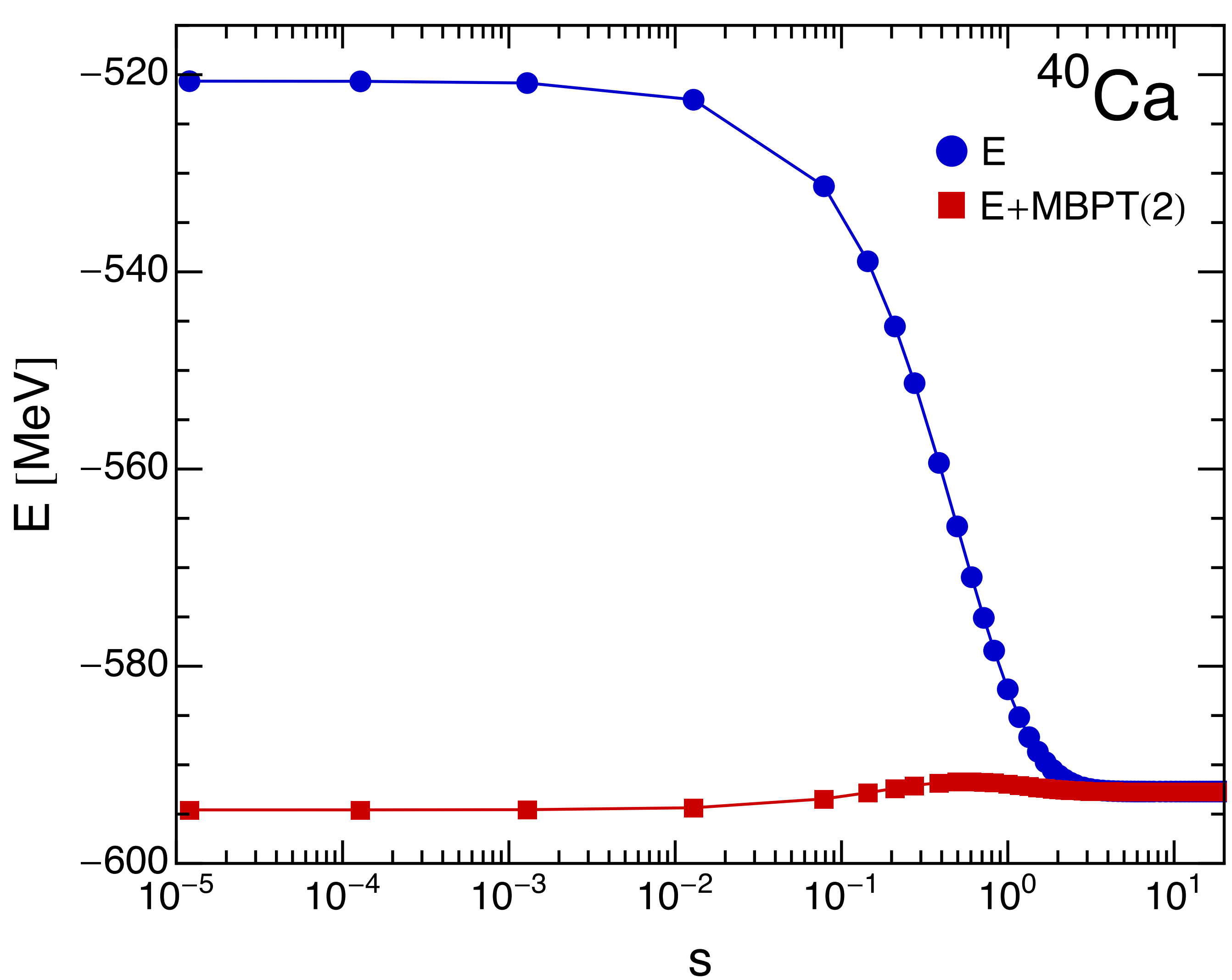
Flow Equation

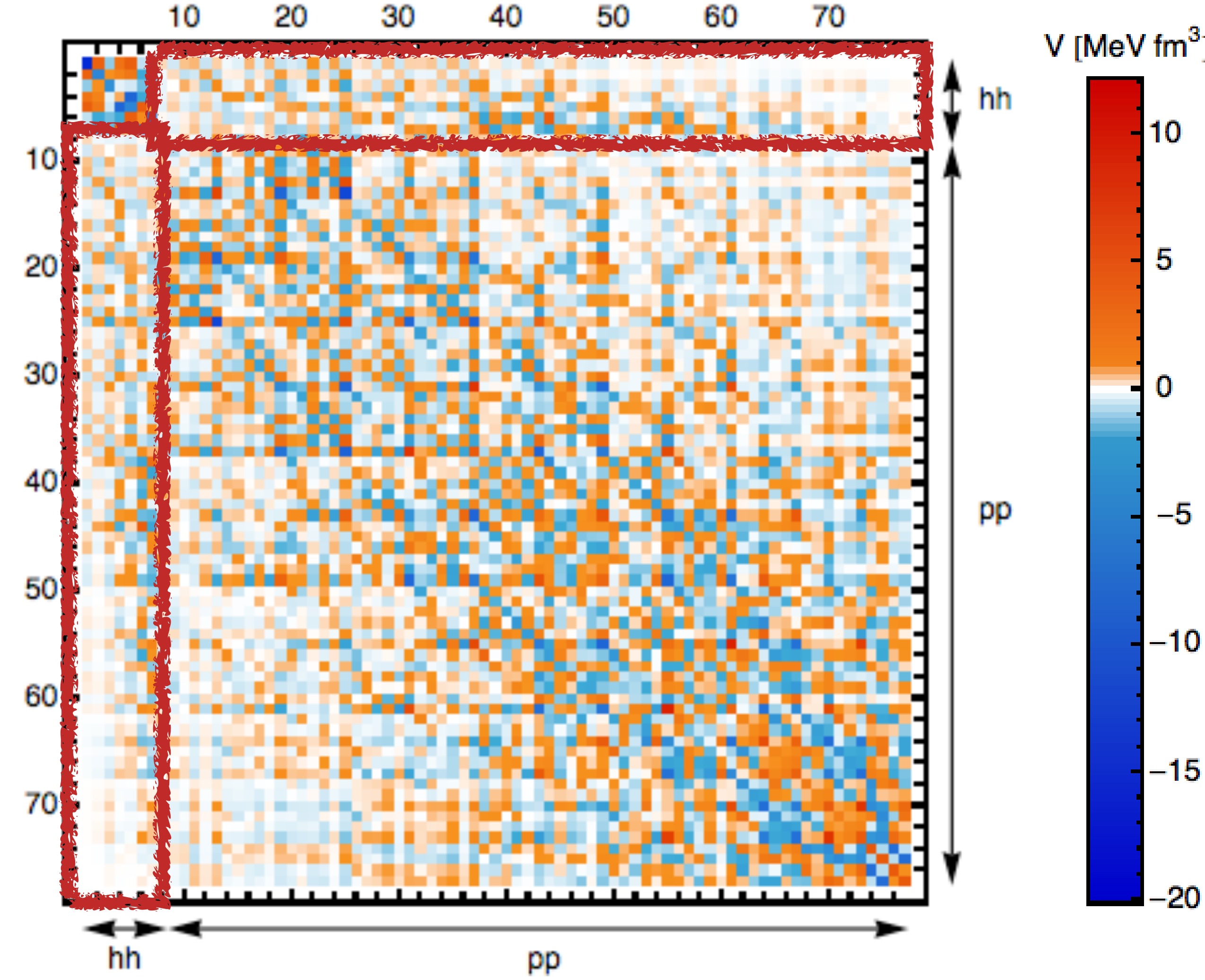


$$\frac{d}{ds}H(s) = \left[\eta(s), H(s)\right], \quad \text{e.g.}$$

Matrix is never constructed explicitly!

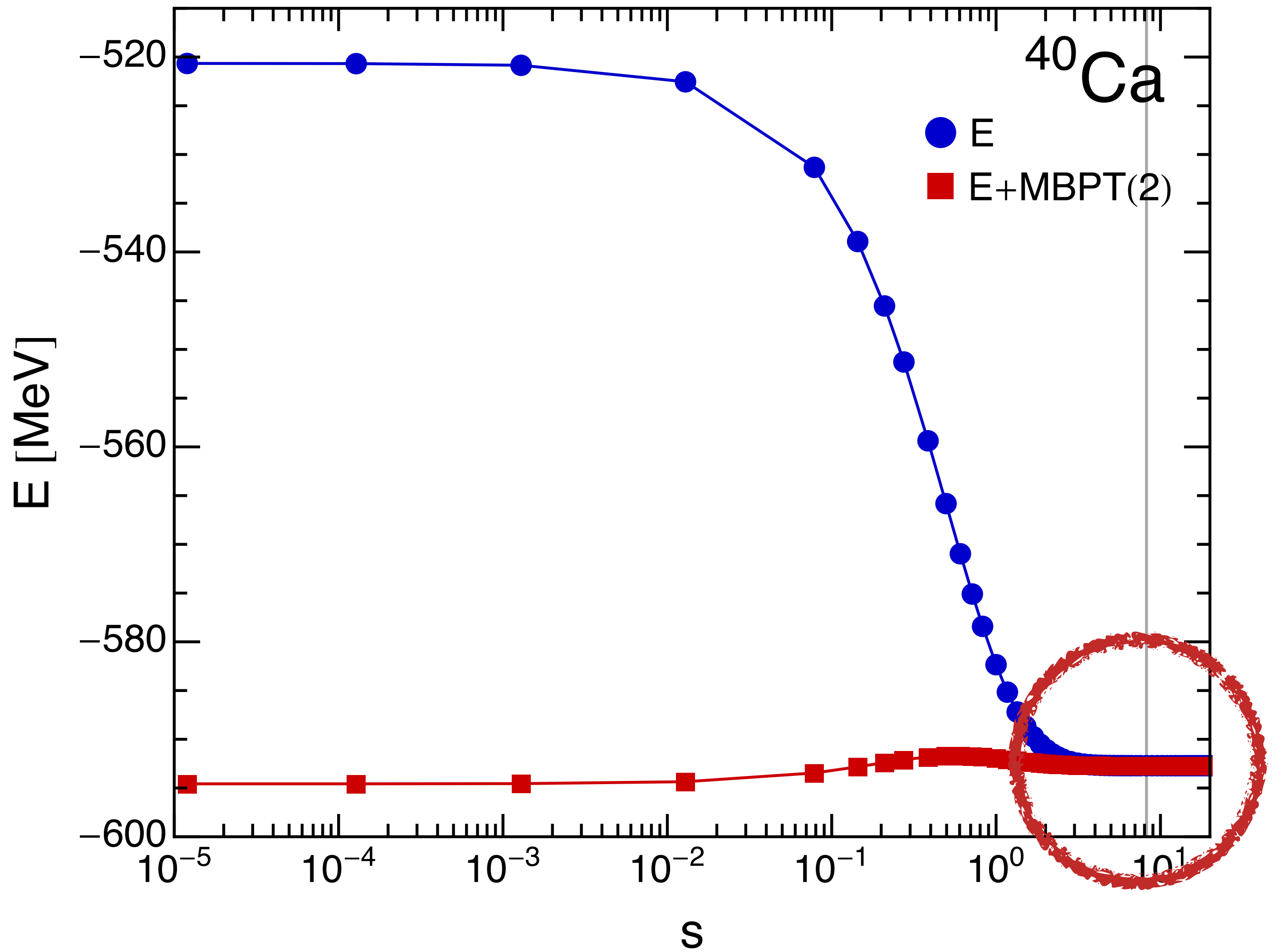
Decoupling

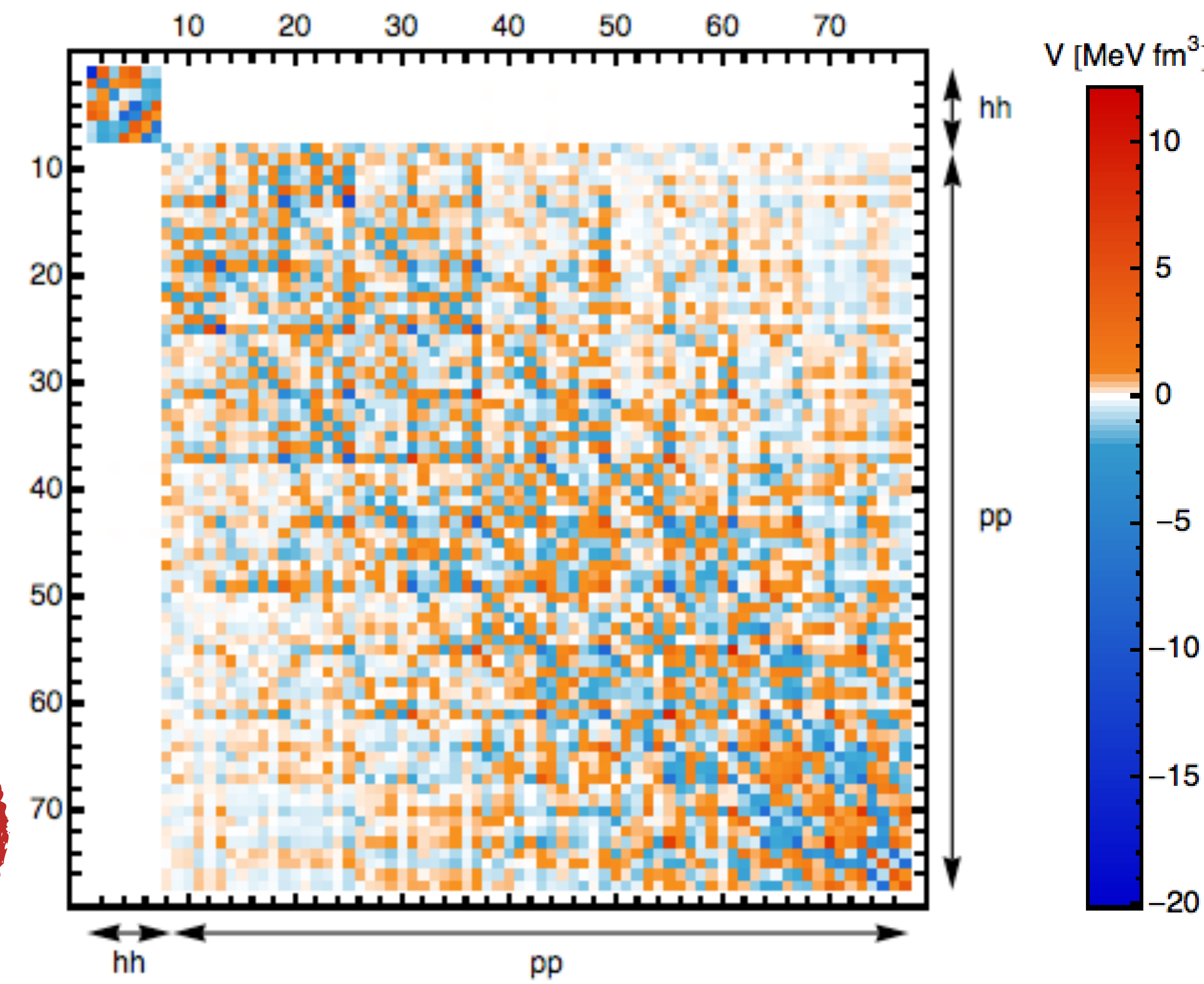




N3LO, $\lambda = 2.0\ \mathrm{fm}^{-1}, e_{\mathrm{Max}} = 8$

Decoupling



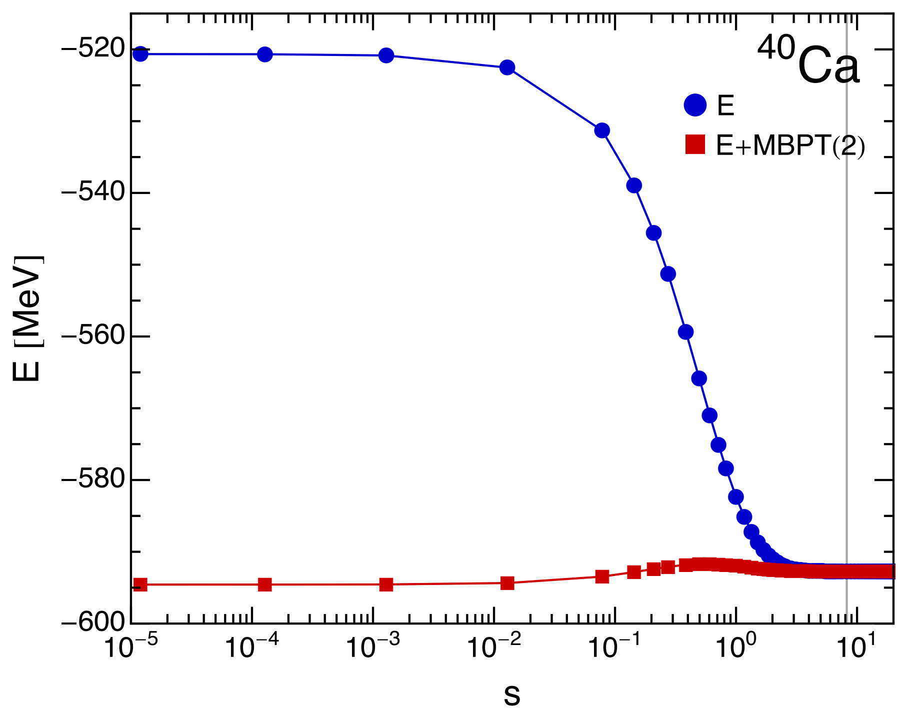


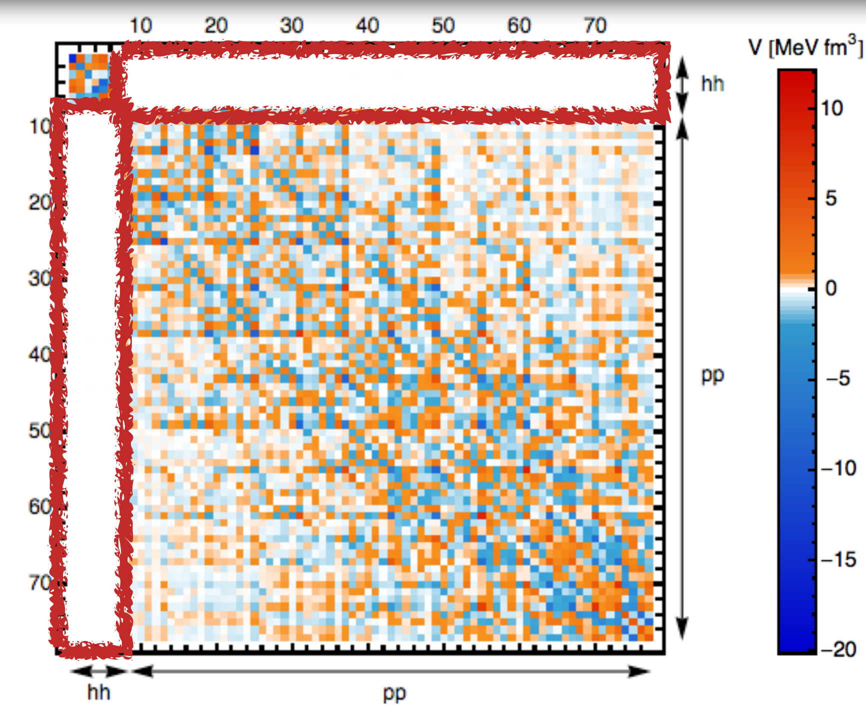
N3LO, $\lambda = 2.0\ \text{fm}^{-1}, e_{\text{Max}} = 8$

non-perturbative resummation of MBPT series (correlations)

off-diagonal couplings are rapidly driven to zero

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:

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

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 Renormalization Group, etc.

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- **Generator Coordinate Method** (w/projection)

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

future

- clustered states, Density Matrix Renormalization Group etc.

build *static* correlations into the reference state

use generalized normal ordering with 2B,… densities

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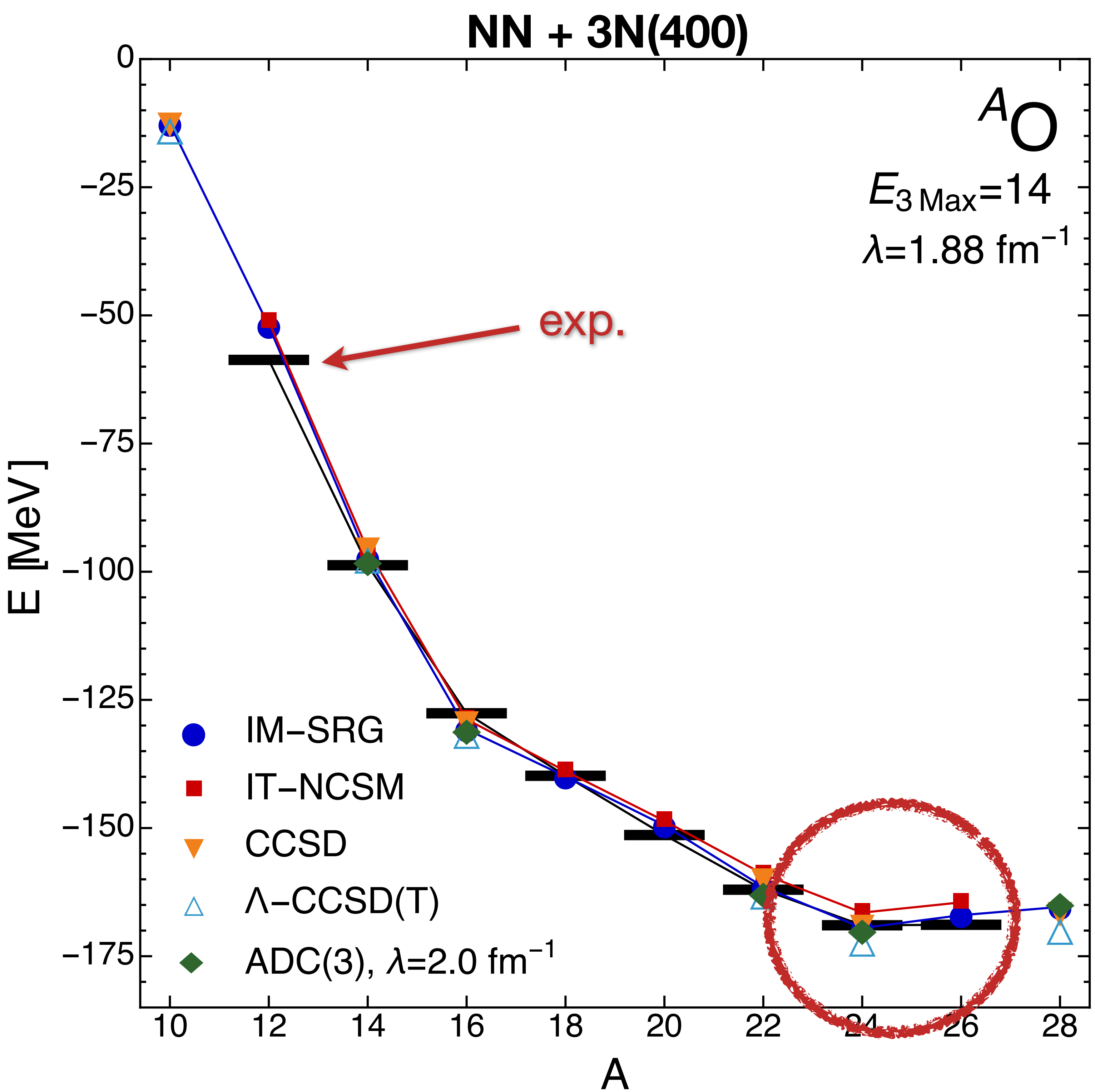
future

- clustered states, Density Matrix Renormalization Group, etc.

Oxygen Isotopes

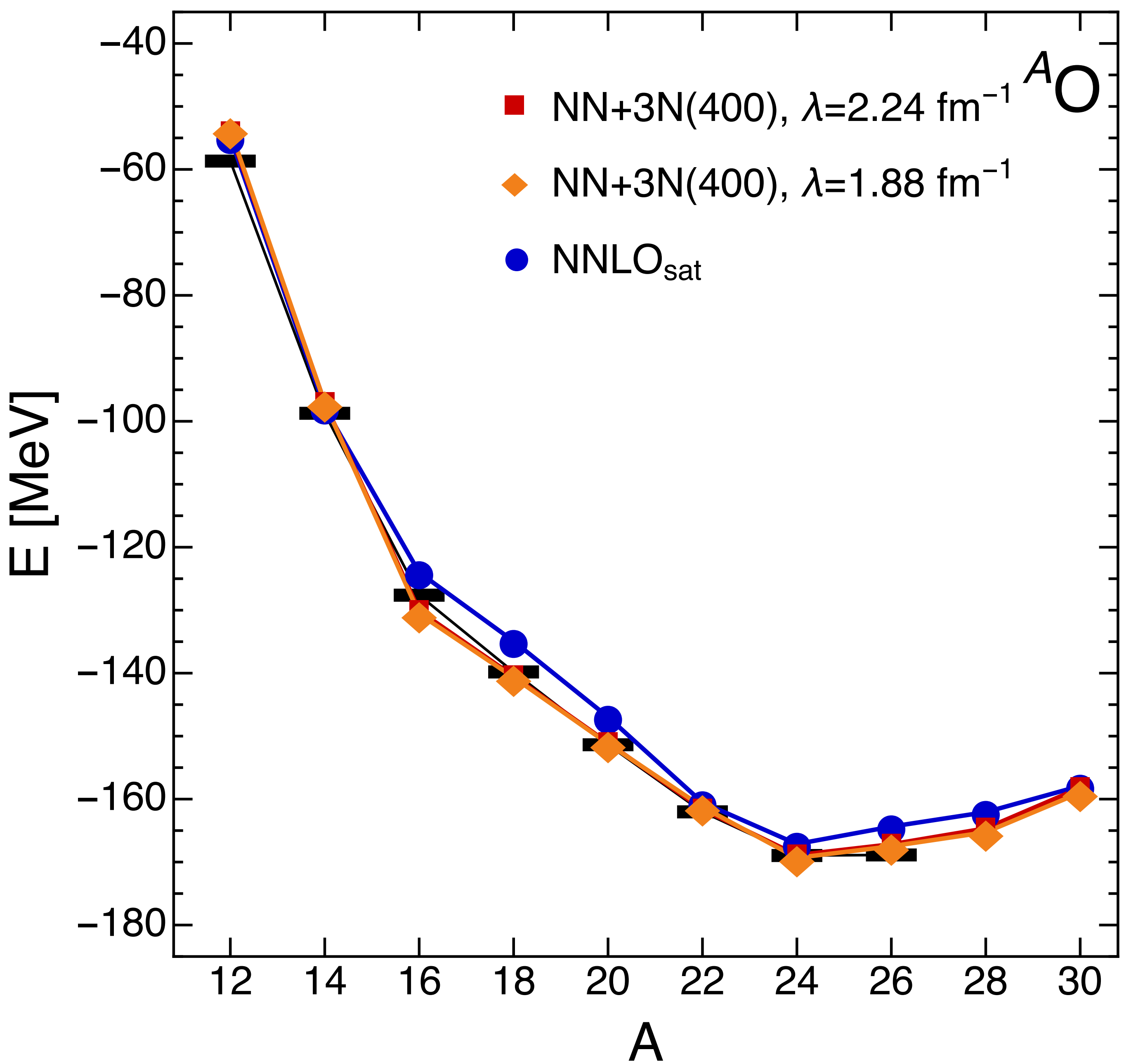
*HH et al., PRL **110**, 242501 (2013), ADC(3): A. Cipollone et al., PRL **111**, 242501 (2013)*

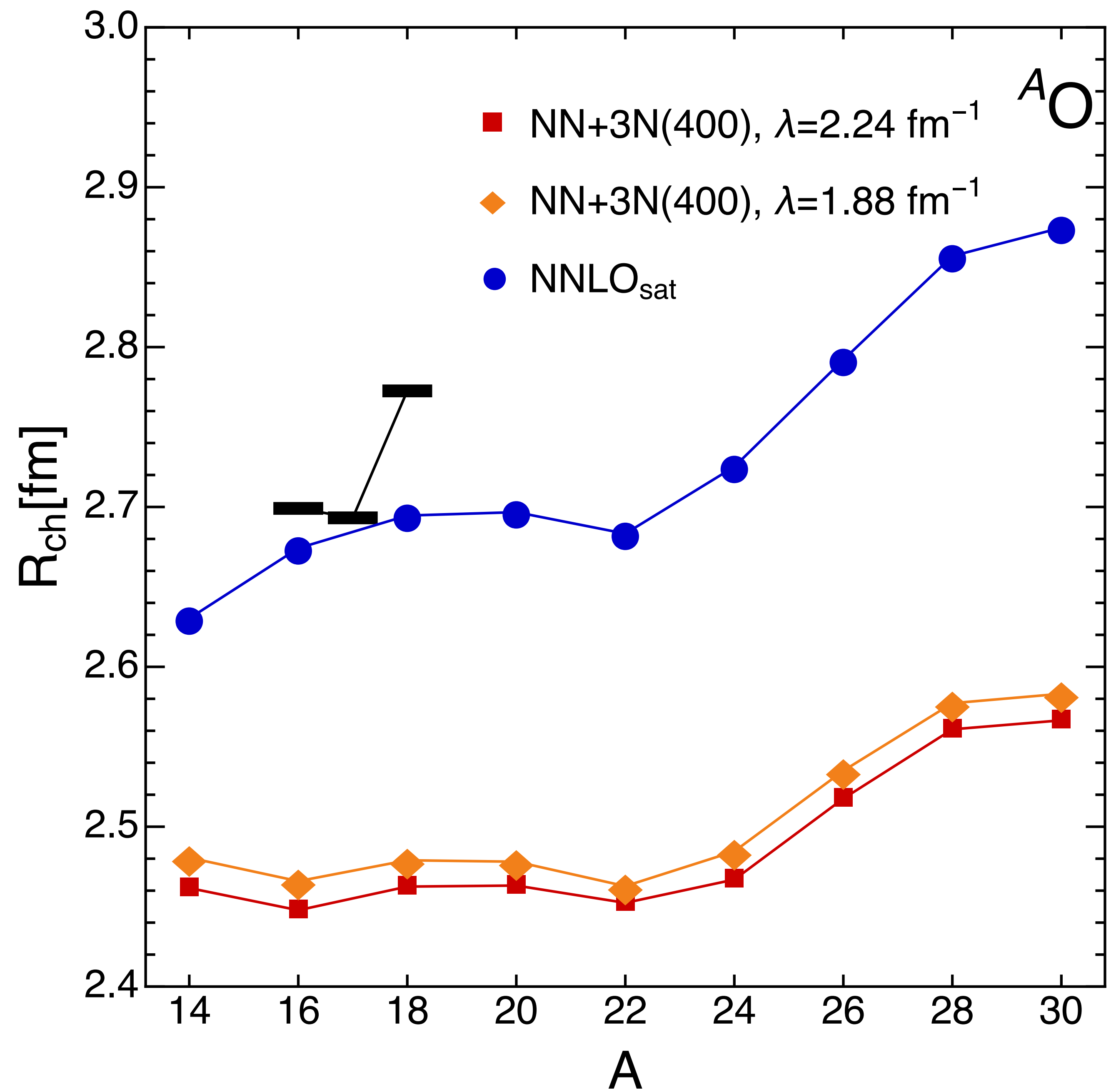


- **consistency between many-body methods**
- ^{24}O drip line, but ^{25,26}O g.s. resonances too high: continuum and interaction

Oxygen Radii

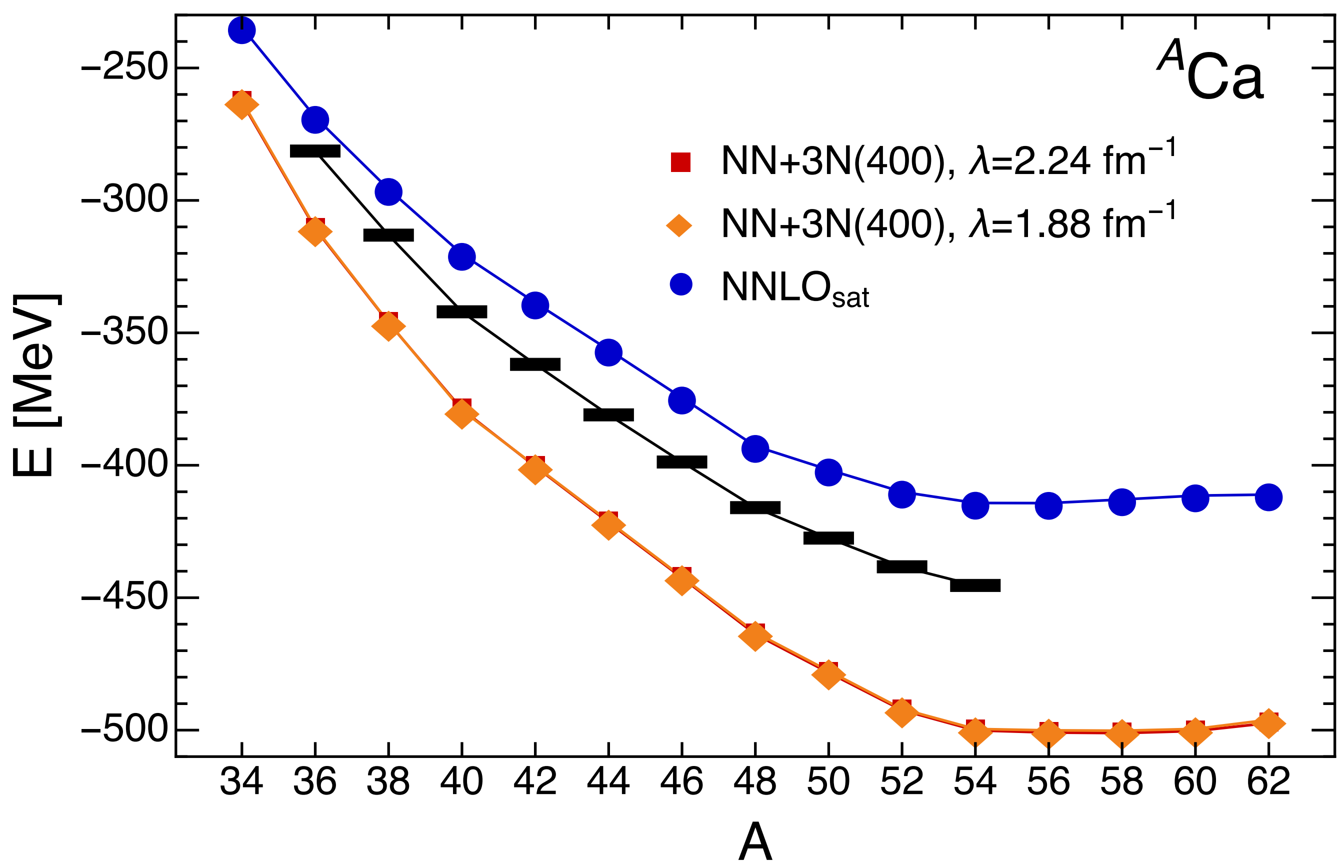
V. Lapoux, V. Somà, C. Barbieri, HH, J. D. Holt, and S. R. Stroberg, PRL 117, 052501 (2016)

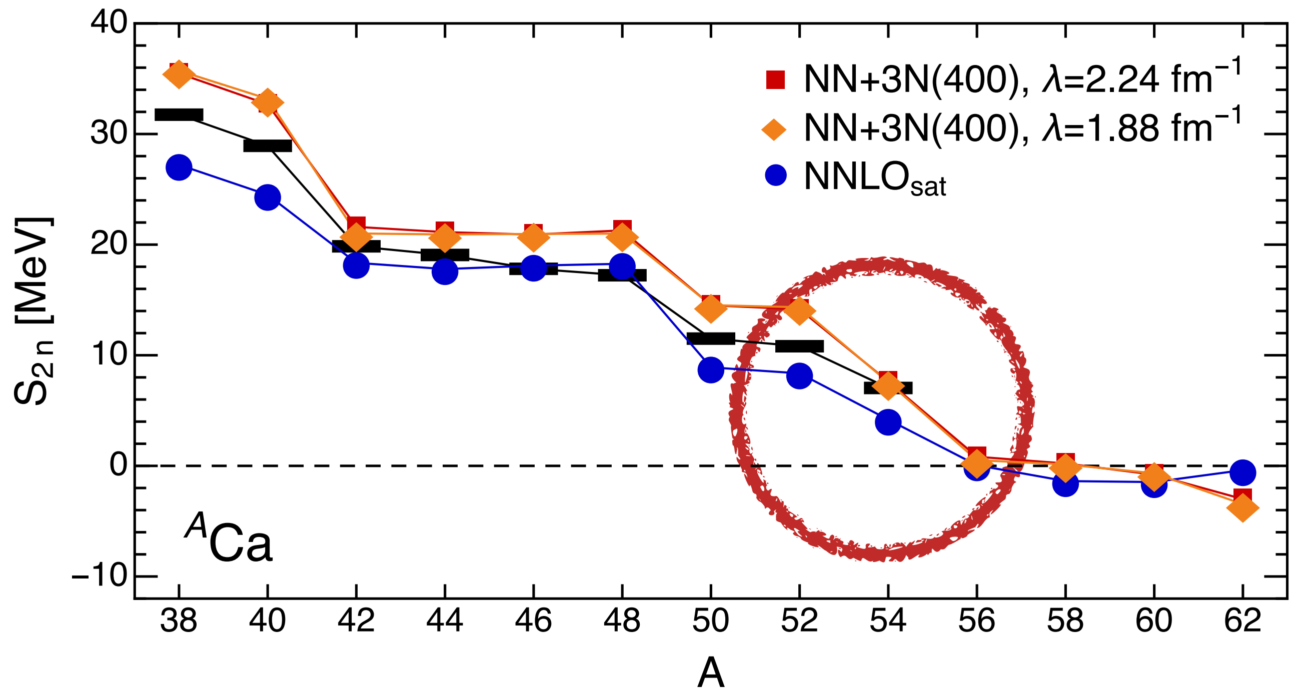




Calcium Isotopes

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

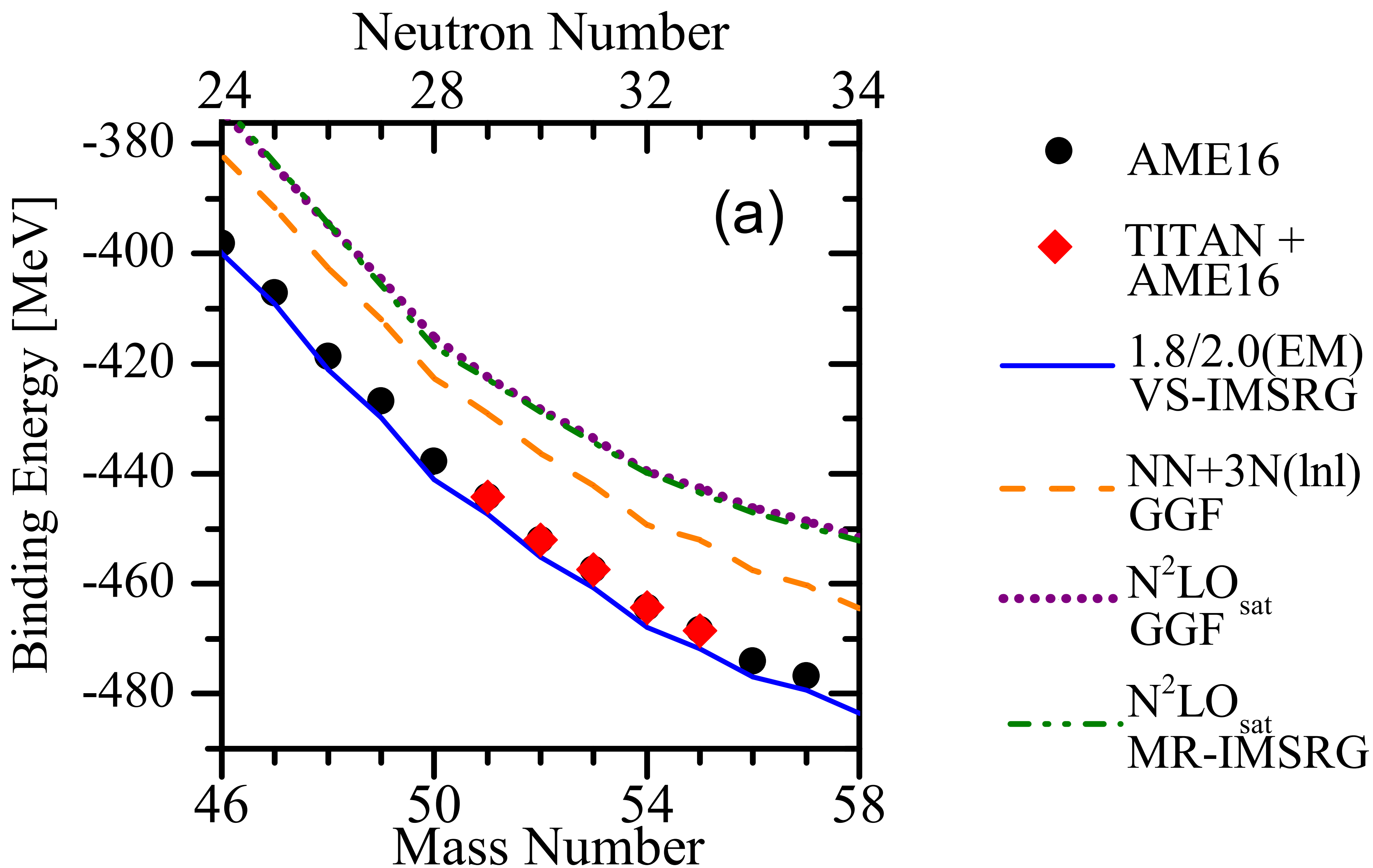




- differential observables (S_{2n}, spectra,...) filter out interaction components that cause over- or underbinding
- predict flat trends for g.s. energies/S_{2n} beyond ^{54}Ca
- ^{52}Ca, ^{54}Ca magic ?
- no continuum coupling included here (stay tuned)

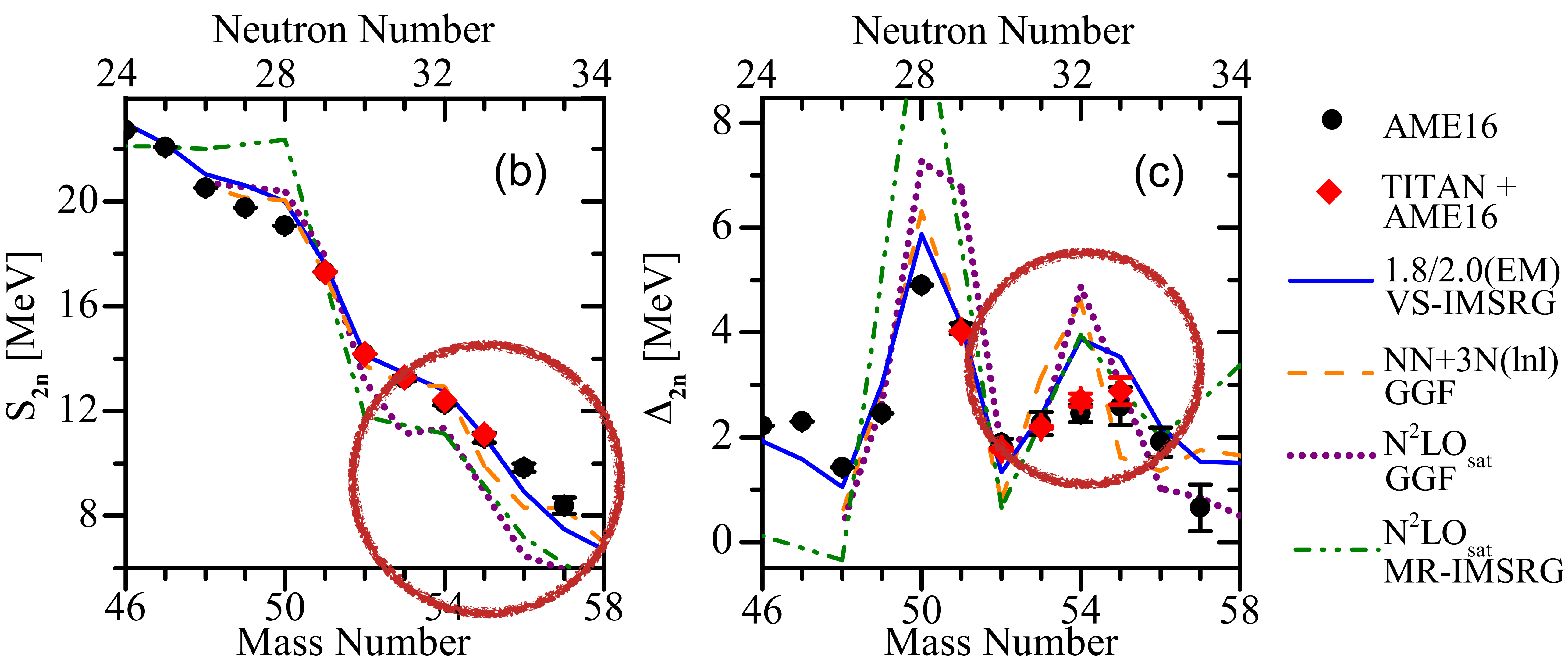
Titanium Isotopes

E. Leistenschneider et al., arXiv:1710.08537



Titanium Isotopes

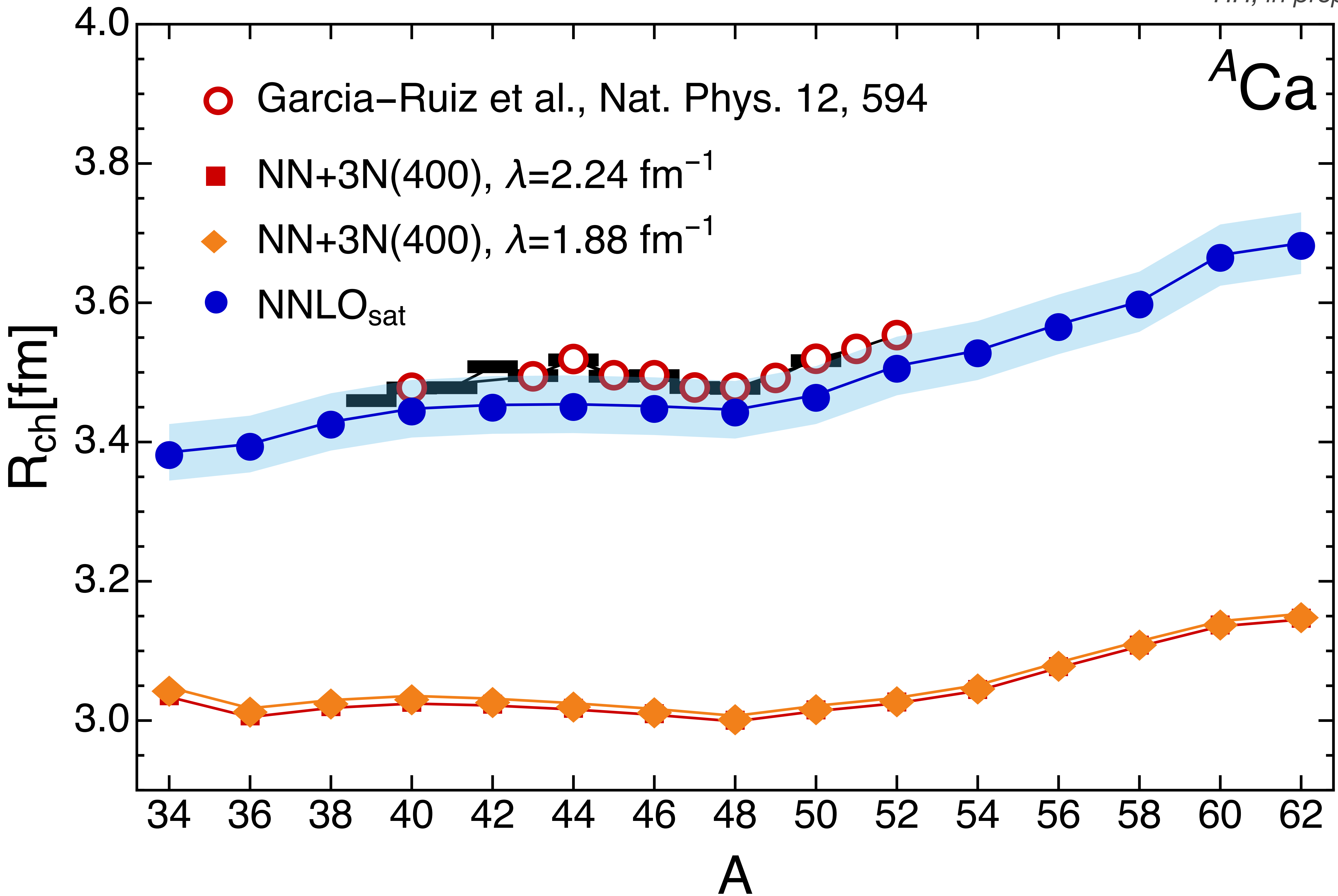
E. Leistenschneider et al., arXiv:1710.08537



N=32 sub-shell **closure too pronounced**: combined effect of **method & interaction** !

Calcium Isotopes

HH, in preparation



Calcium Isotopes

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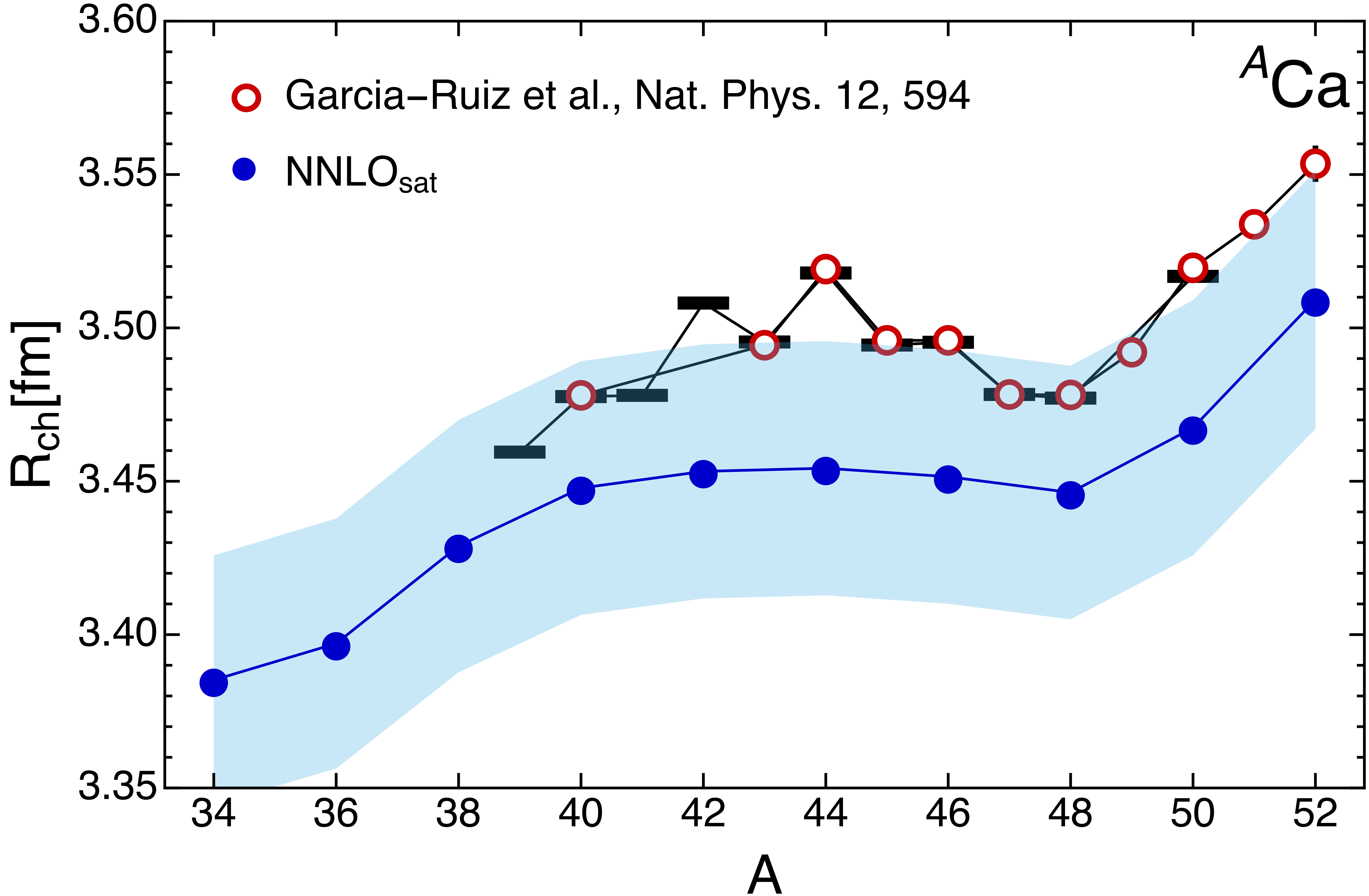

MR-IMSRG References States

available

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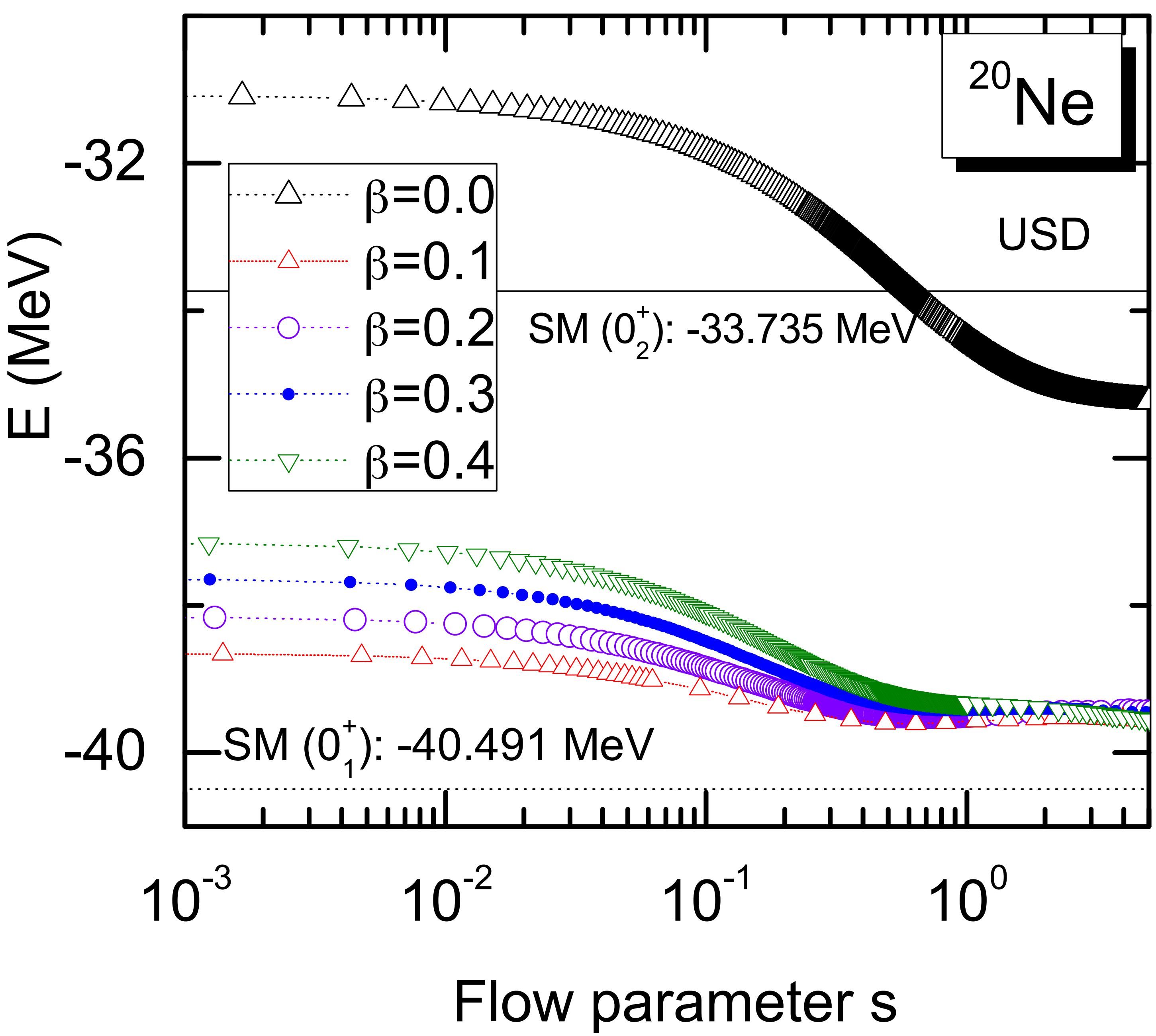
future

- clustered states, Density Matrix Renormalization Group, etc.

Example: ^{20}Ne

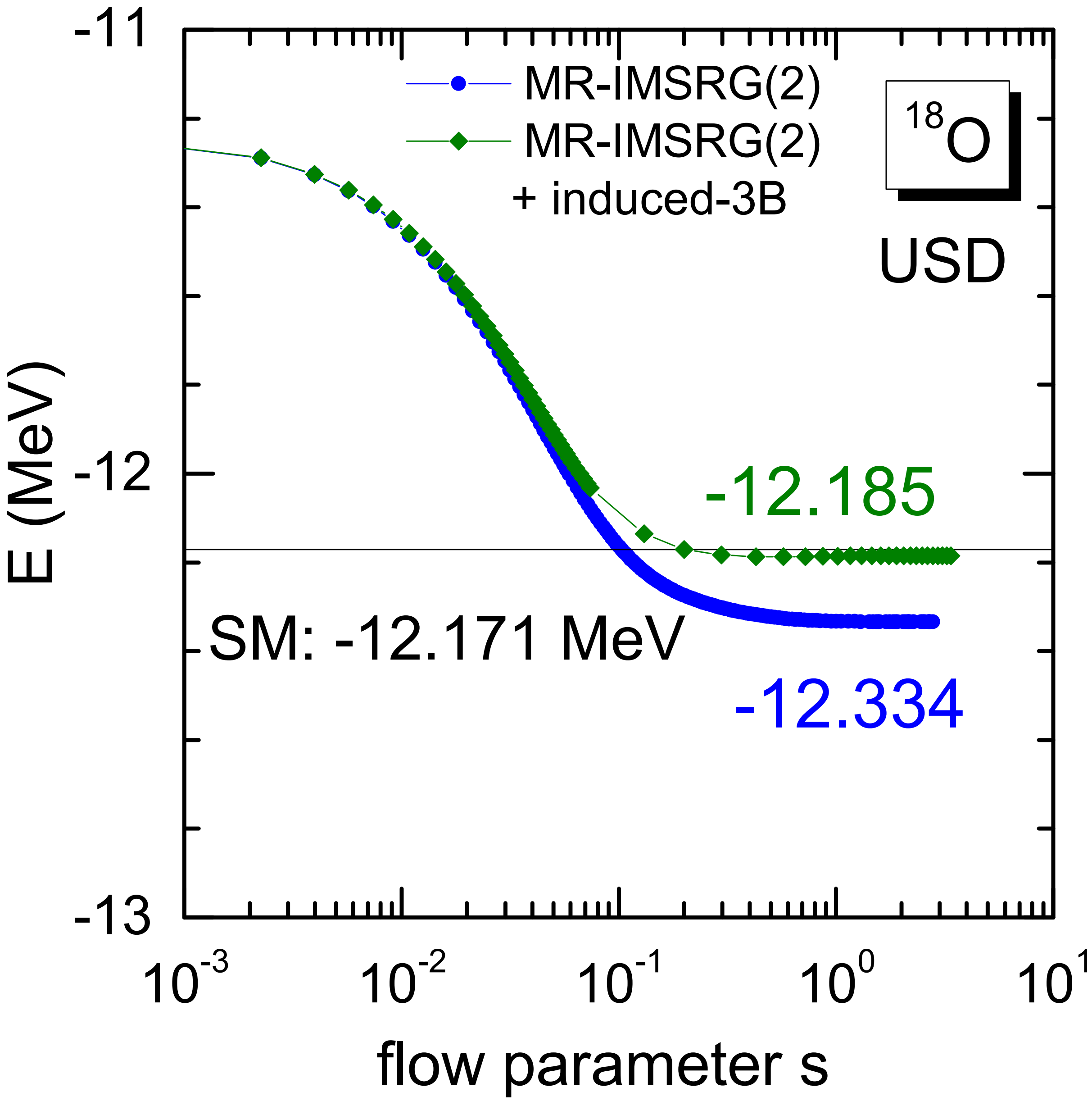
J. Yao, T. D. Morris, HH, J. Engel, in prep.

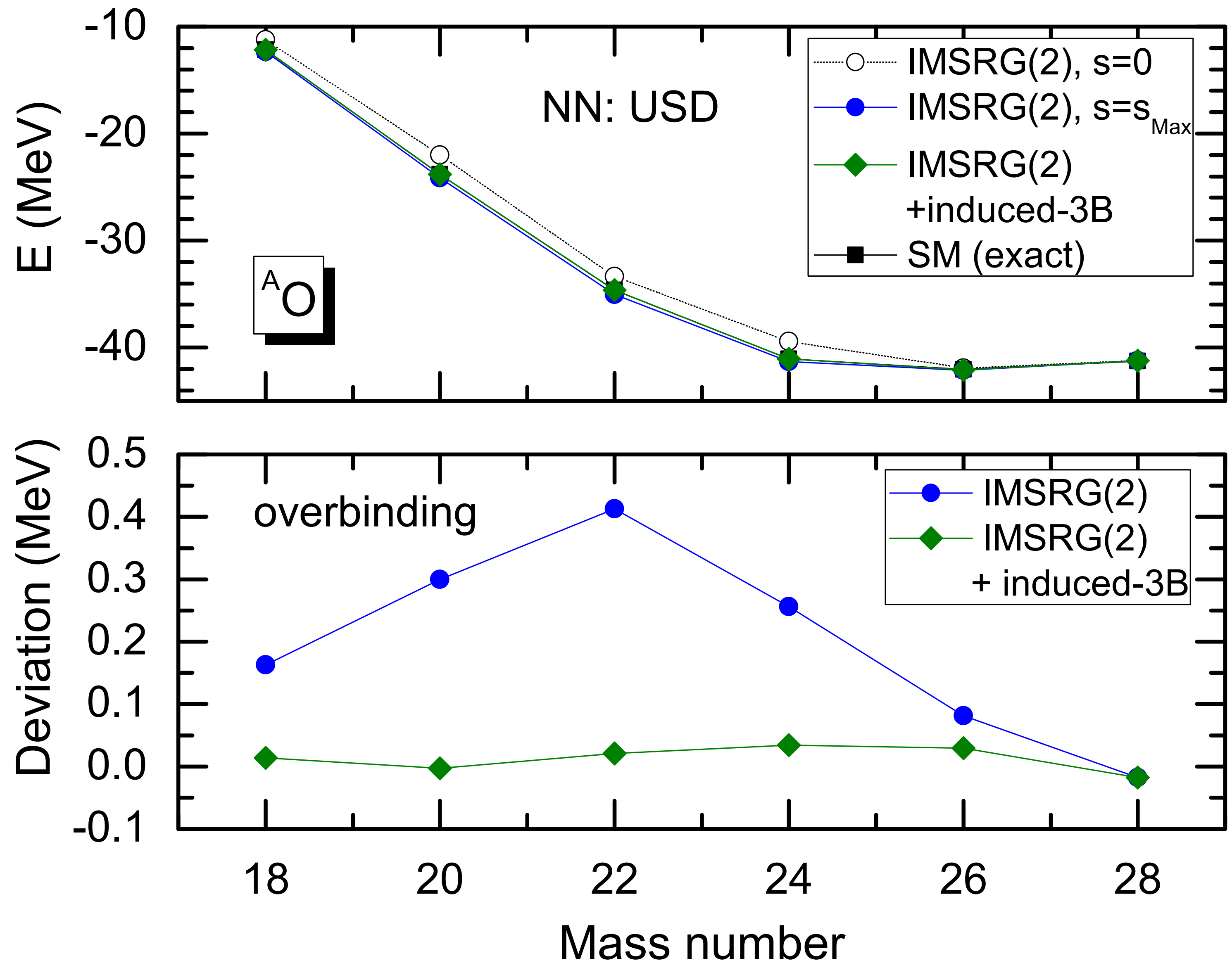


- reference: particle-number & angular-momentum projected HFB
- **range of deformed reference states flow to the ^{20}Ne ground state**
- deviation from Shell model result: **correlations beyond MR-IMSRG(2)**

Approximate MR-IMSRG(3)

J. Yao, T. D. Morris, HH, J. Engel, in prep.





- **approximate MR-IMSRG(3):** induced 3B terms recover bulk of missing correlation energy

- size will be **reference-state dependent**

Ab Initio Many-Body Methods:

Non-Empirical Shell Model Interactions from the IMSRG

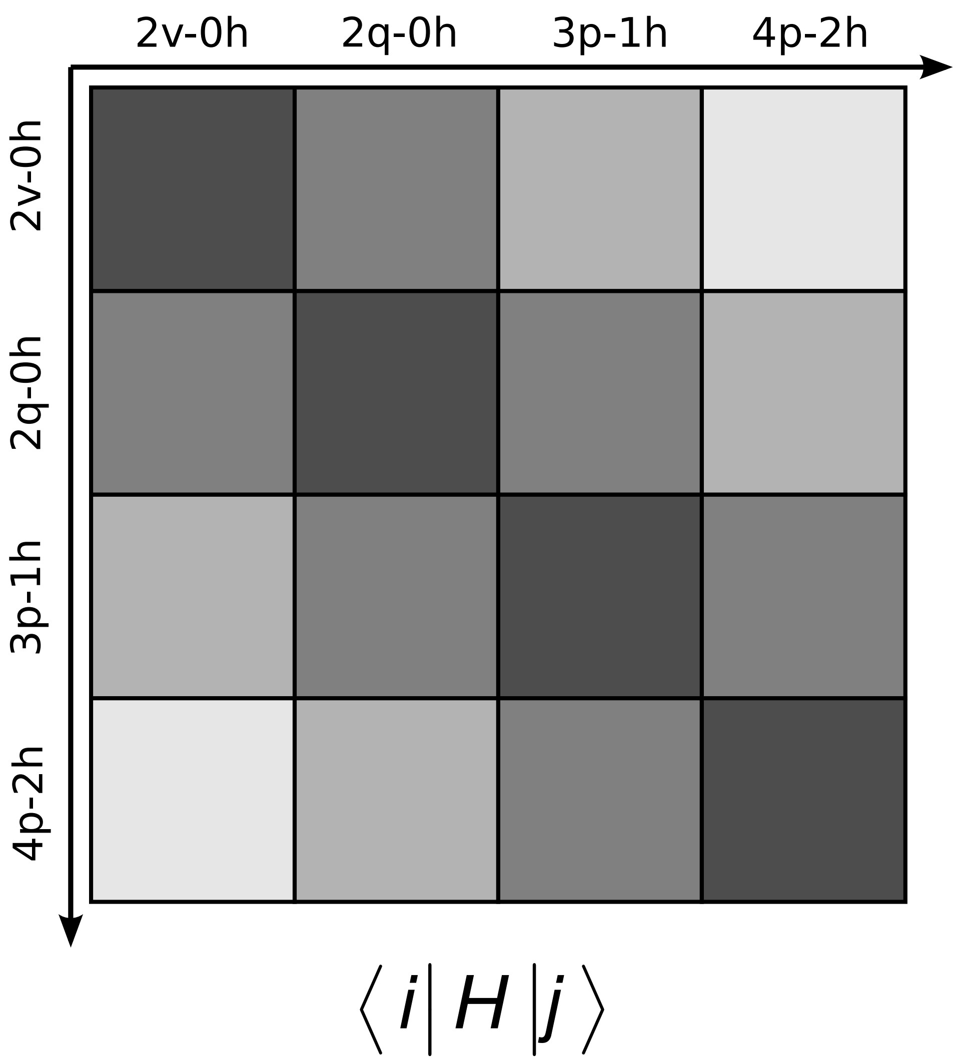
N. M. Parzuchowski, **S. R. Stroberg,** P. Navratil, H. H., S. K. Bogner, Phys. Rev. C **96**, 034324 (2017)

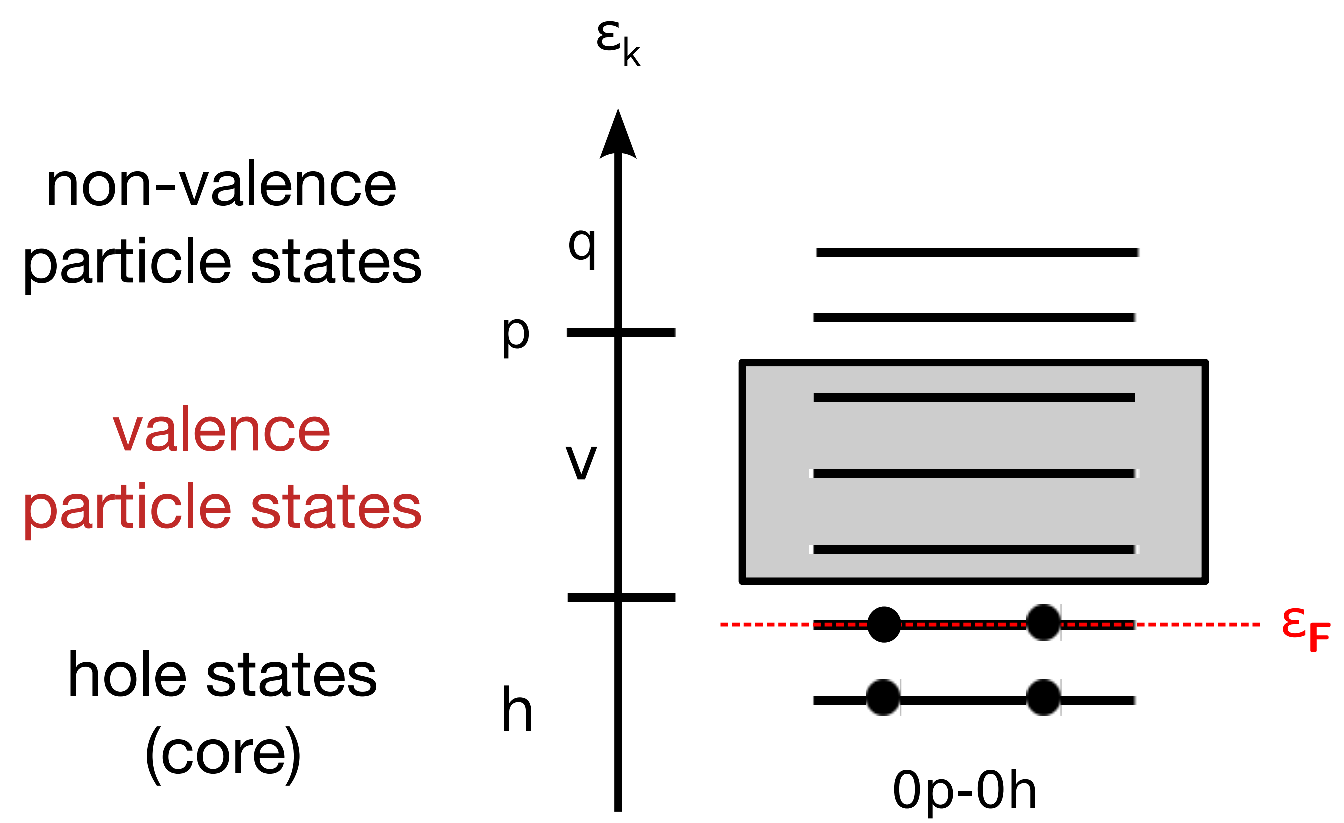
S. R. Stroberg, A. Calci, H. H., J. D. Holt, S. K. Bogner, R. Roth, A. Schwenk, PRL **118**, 032502 (2017)

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





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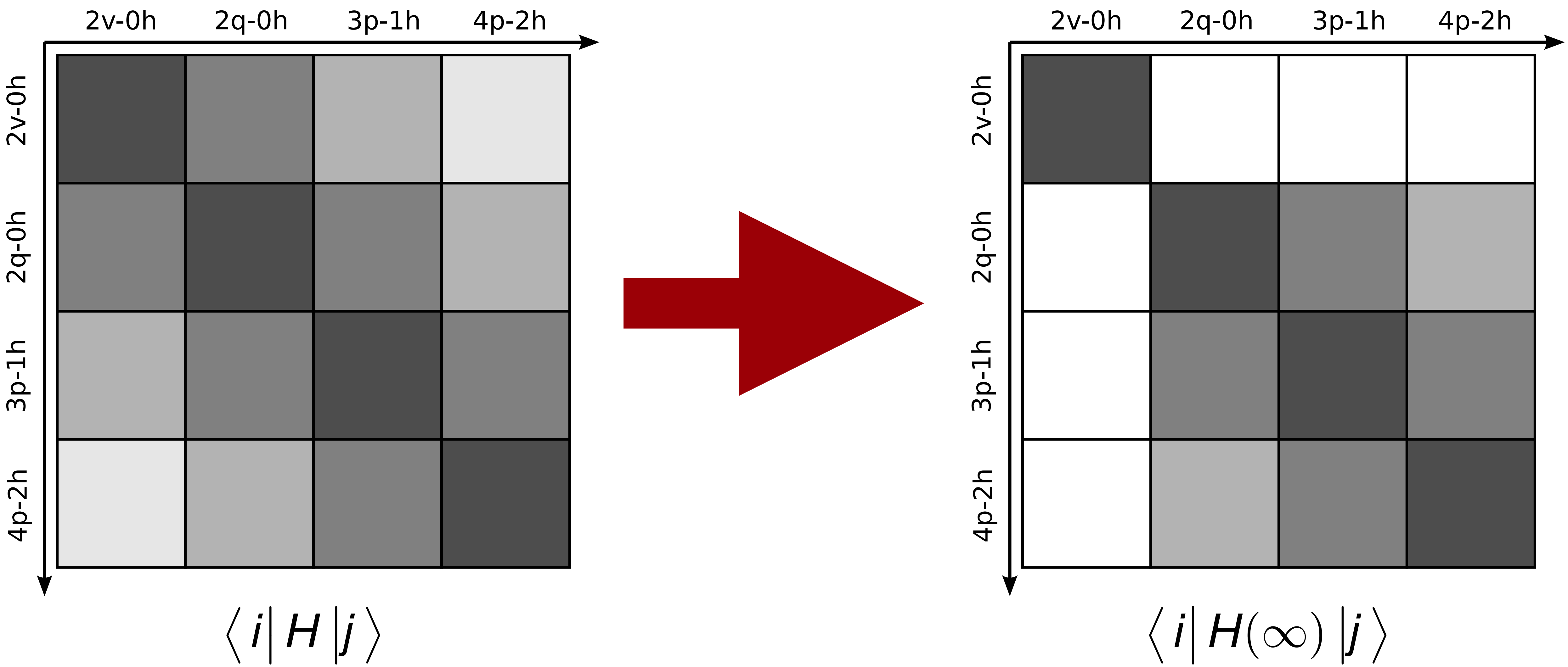
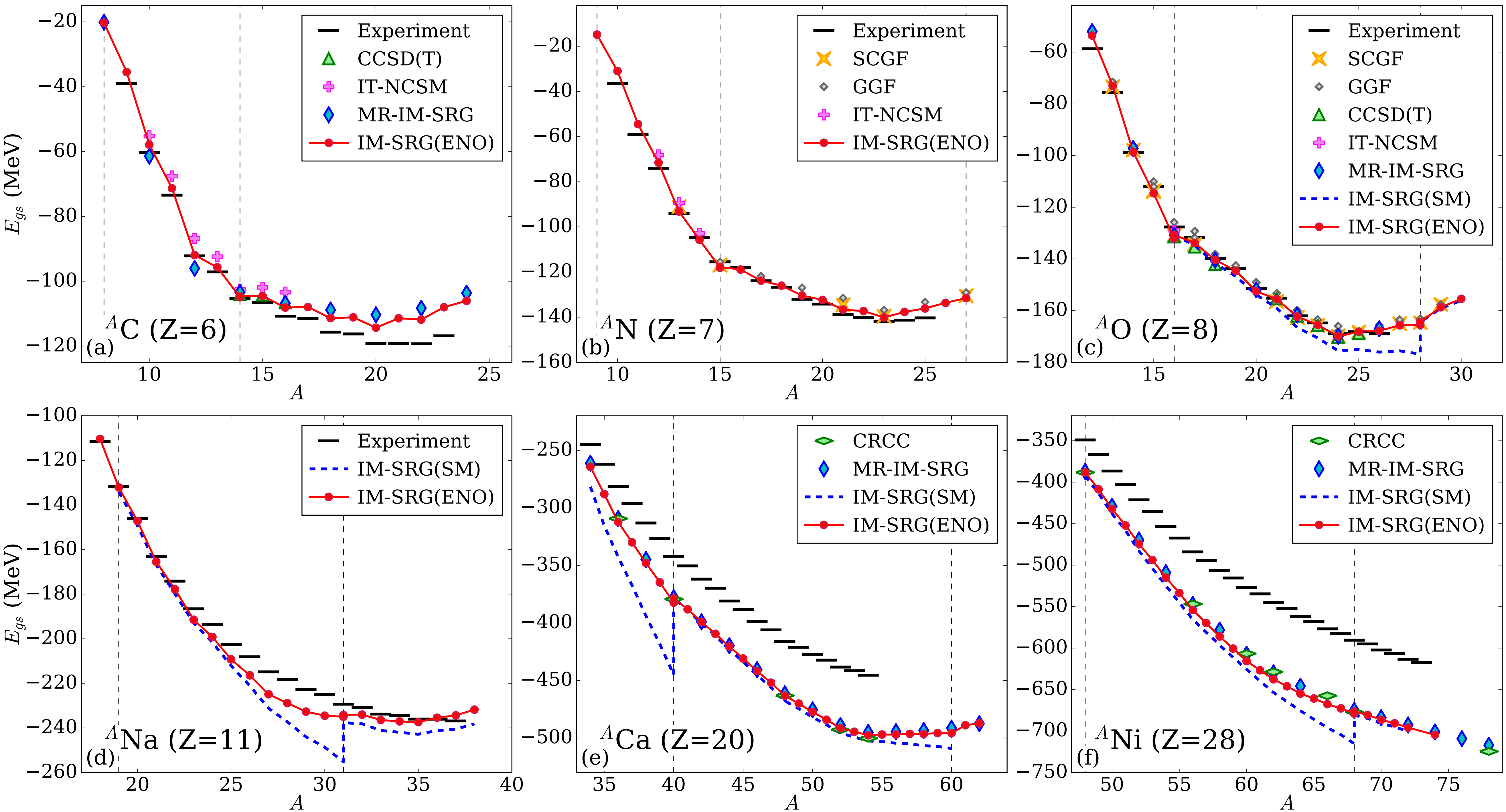


change definition of off-diagonal Hamiltonian:

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

Ground-State Energies

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



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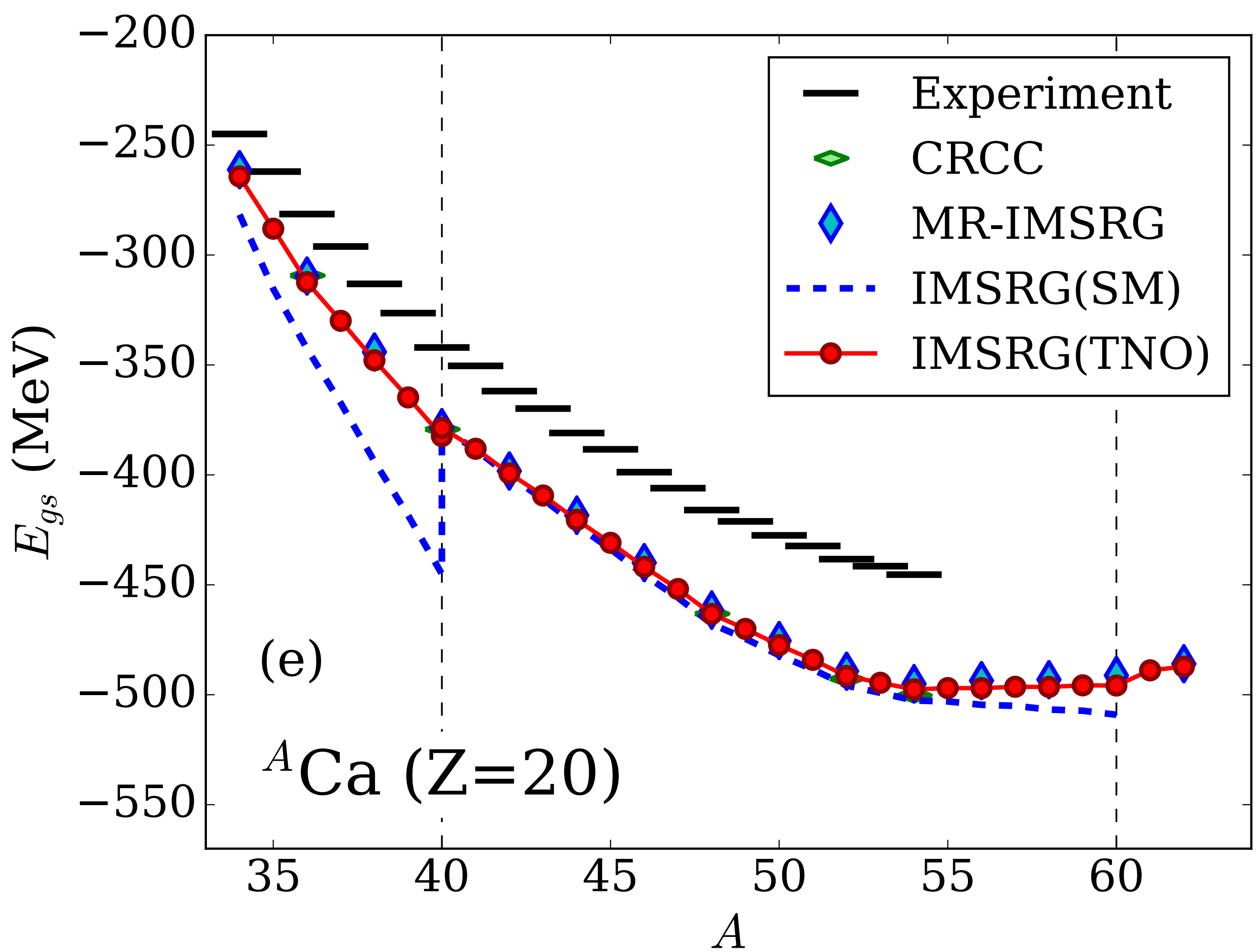
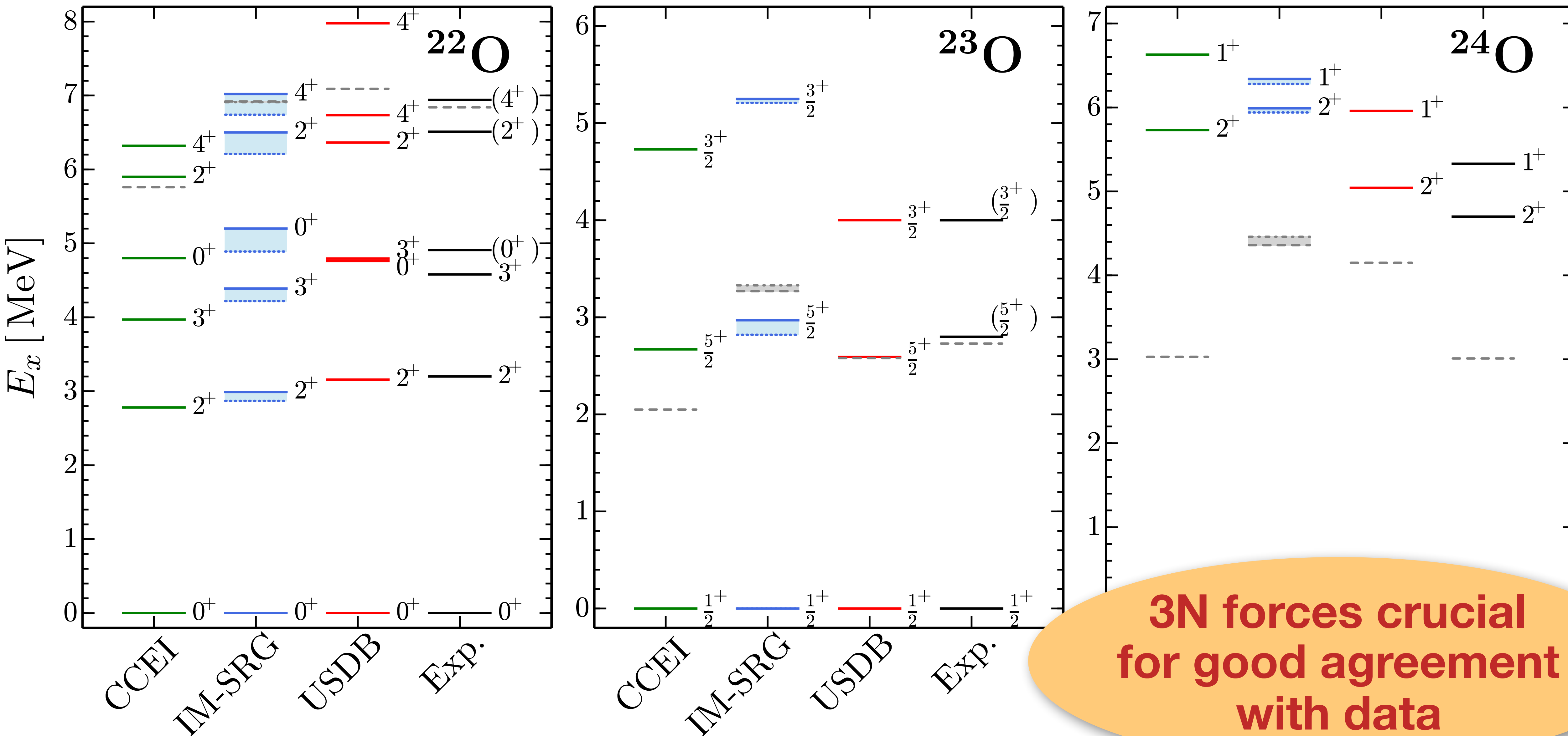


- (initial) normal ordering and IMSRG decoupling in the **target nucleus**
- **consistent with (MR-)IMSRG ground state energies** (and CC, SCGF, …) for the **same Hamiltonian**

Oxygen Spectra

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

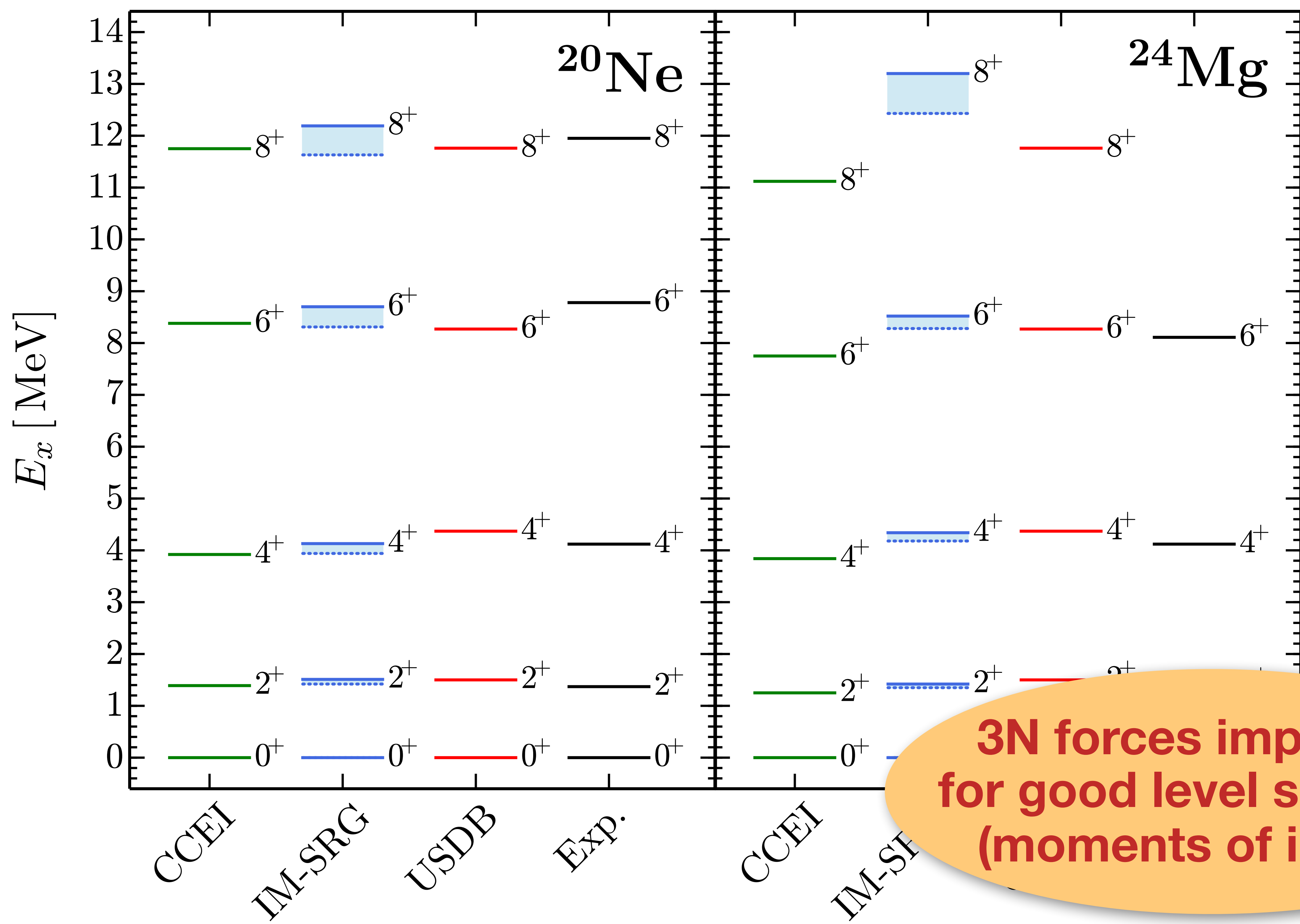
NN + 3N(400)



3N forces crucial for good agreement with data

Rotational Bands

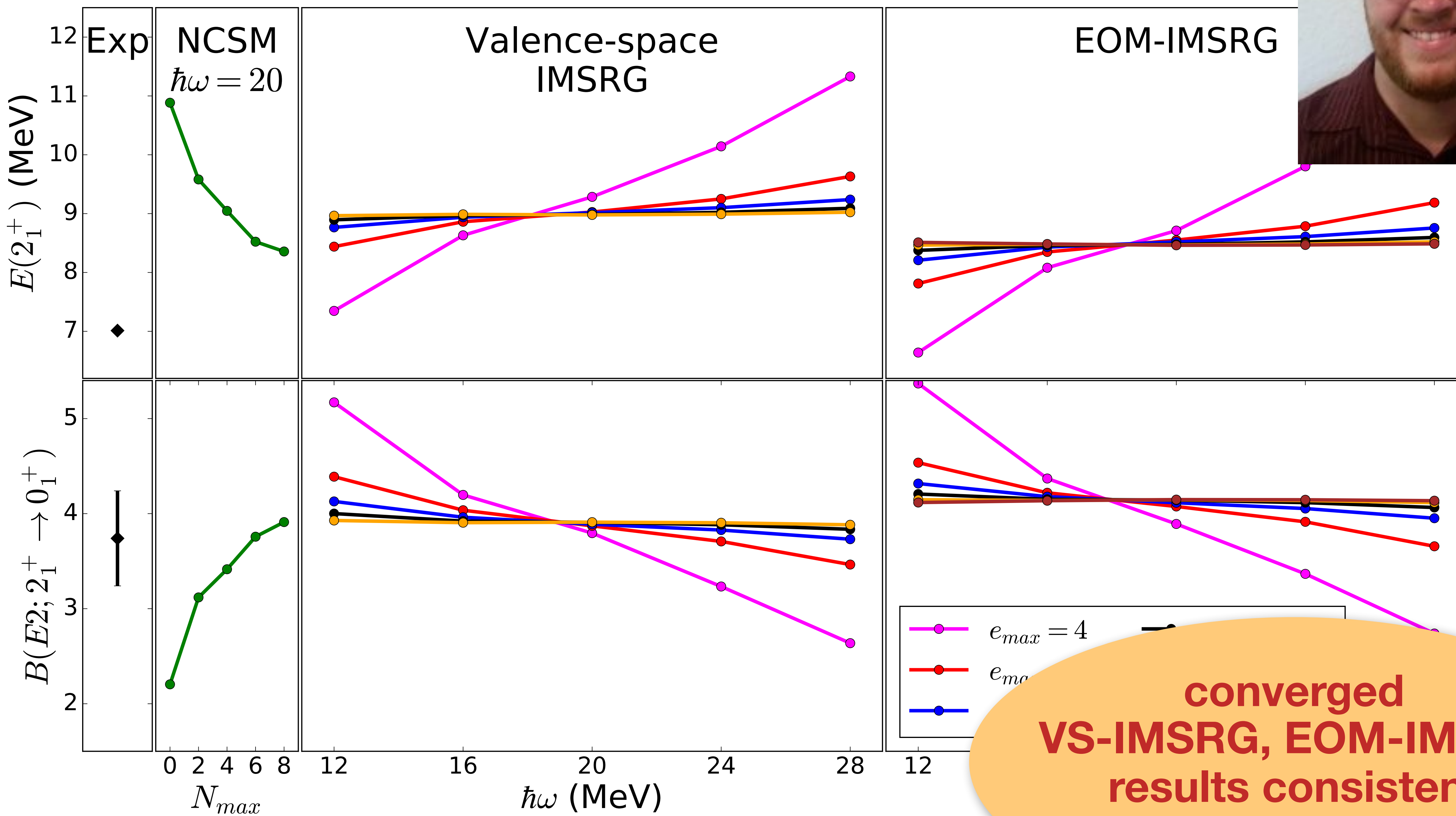
*S. R. Stroberg et al., PRC **93**, 051301(R) (2016)*



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

Transitions

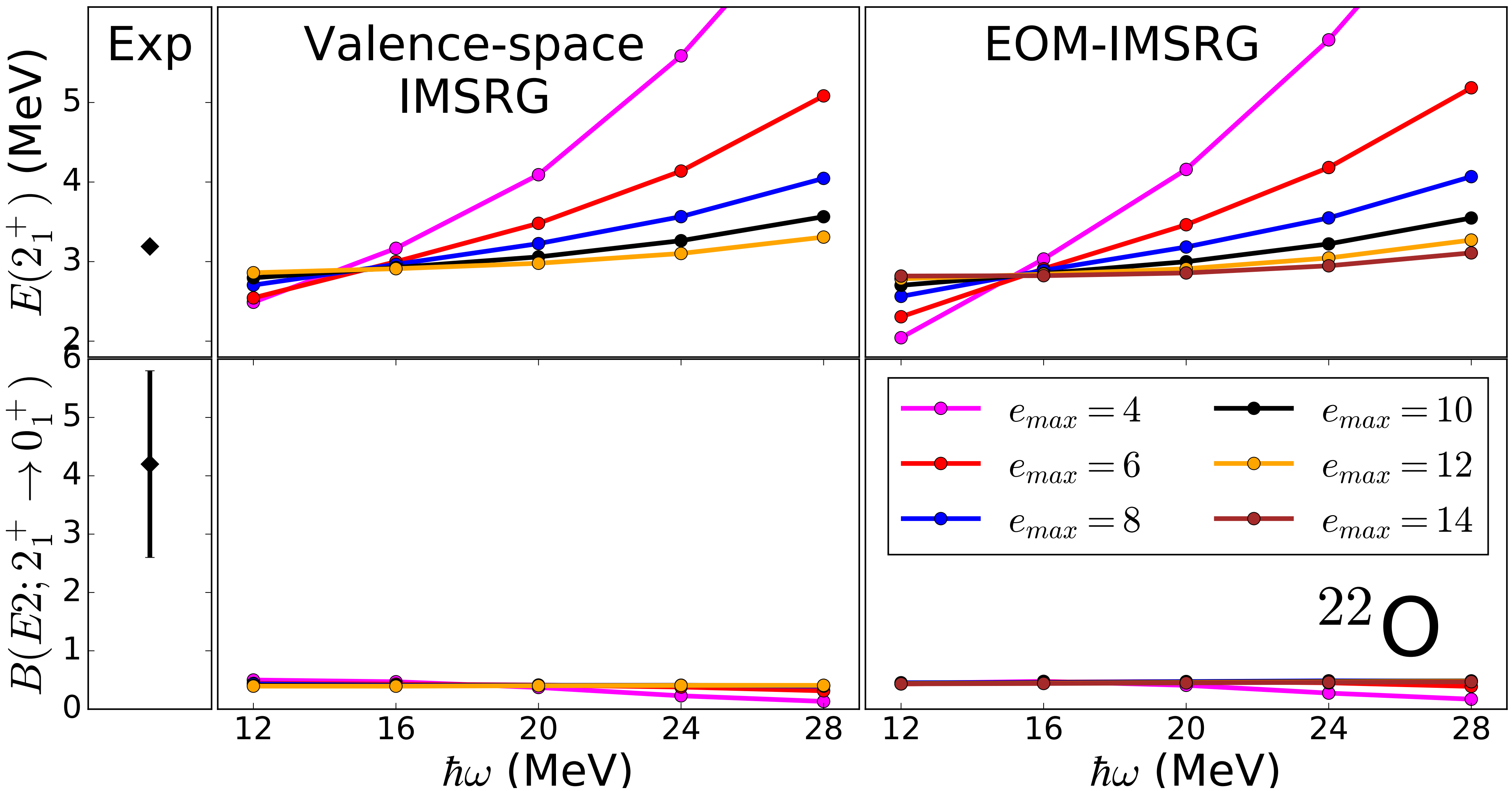
N. M. Parzuchowski, S. R. Stroberg et al., to be submitted;
EOM-IMSRG: N. M. Parzuchowski et al., PRC95, 044304



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

Transitions

N. M. Parzuchowski, S. R. Stroberg et al., PRC; EOM-IMSRG: N. M. Parzuchowski et al., PRC95, 044304



- 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?

Epilogue

The Shape of Things to Come

- the goal: **predictive *ab initio* theory** with systematic uncertainties & convergence to exact result
- rapidly **growing capabilities**: ground-state energies, spectra, radii, transitions, etc.
- **challenges and opportunities:**
    - **coherent** uncertainty quantification & propagation
    - improved **inputs**
    - treatment of **collective** correlations (**theory & computation**)
    - **meaning- and impactful confrontation with experiment**

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J. D. Holt, P. Navrátil
TRIUMF, Canada

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C. Barbieri
U. Surrey, UK

NERSC

NSF

NUCLEI
Nuclear Computational Low-Energy Initiative

Ohio Supercomputer Center

ICER