Weak Transitions in the IMSRG Framework

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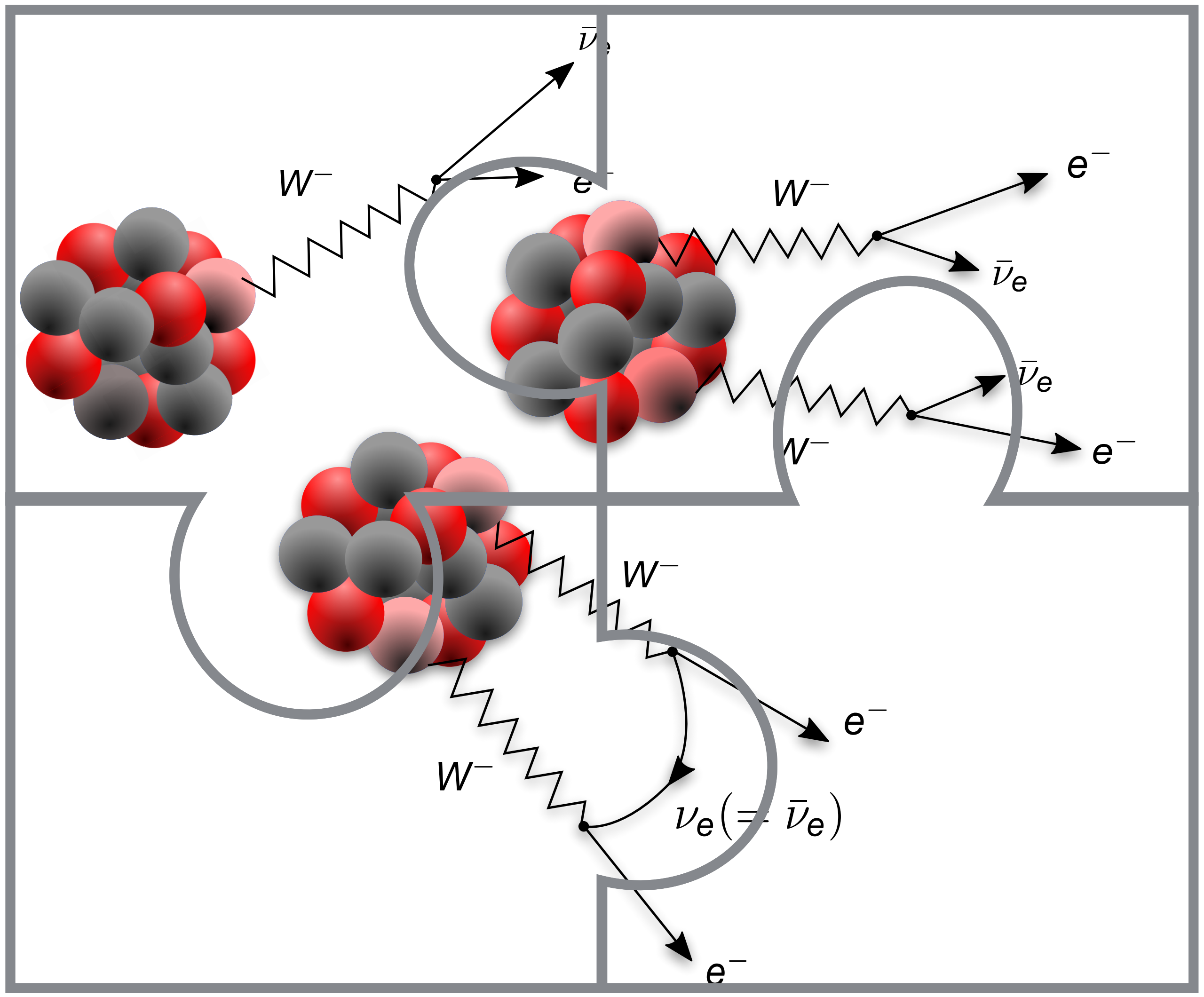
Weak Transitions



- **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**

(Multi-Reference) In-Medium SRG

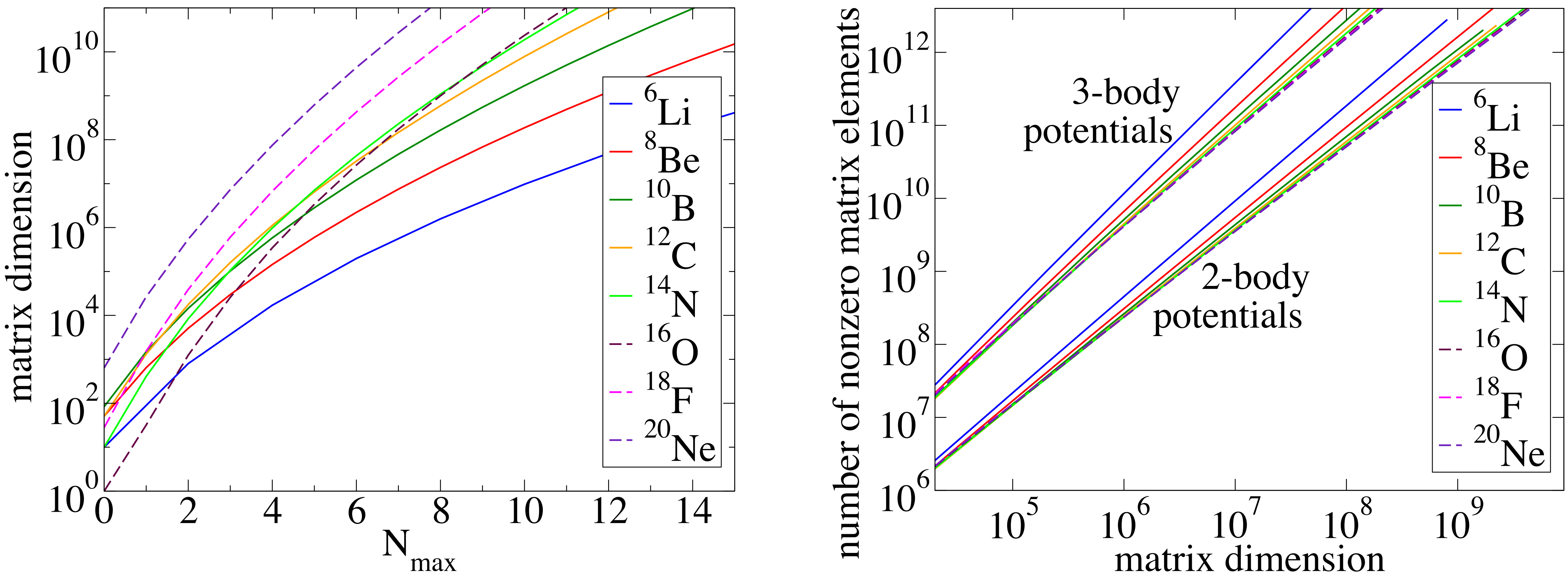
H. H., Phys. Scripta **92**, 023002 (2017)

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)

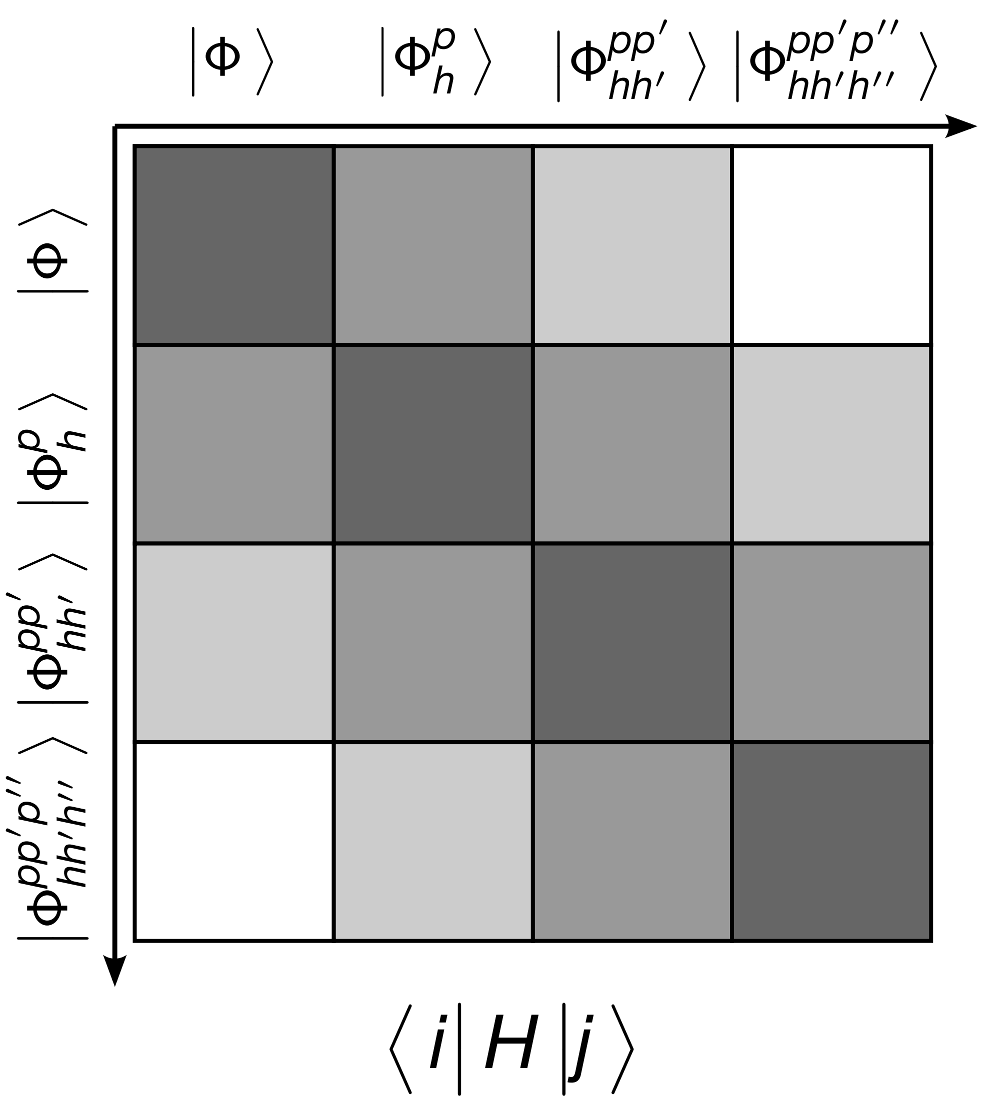
Large-Scale Diagonalization

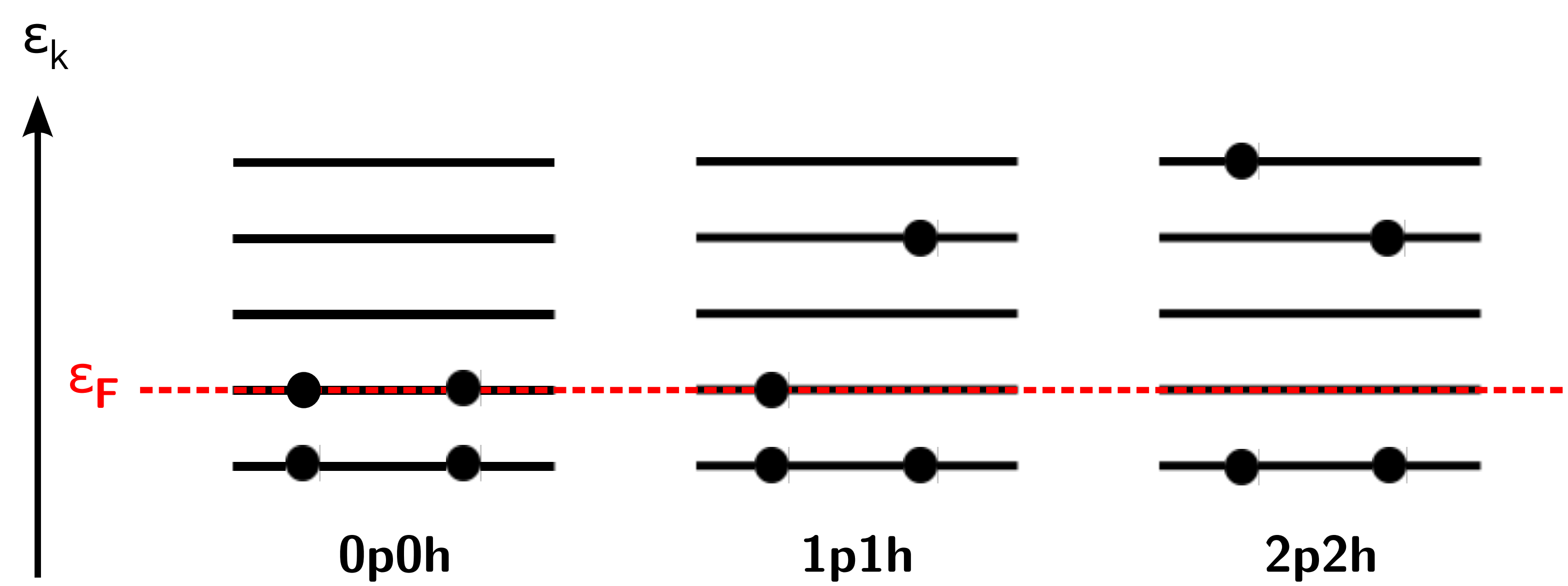


from: C. Yang, H. M. Aktulga, P. Maris, E. Ng, J. Vary, Proceedings of NTSE-2013

- basis-size "explosion": **factorial growth**
- **importance truncation** etc. cannot fully compensate this growth as A increases

Transforming the Hamiltonian





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

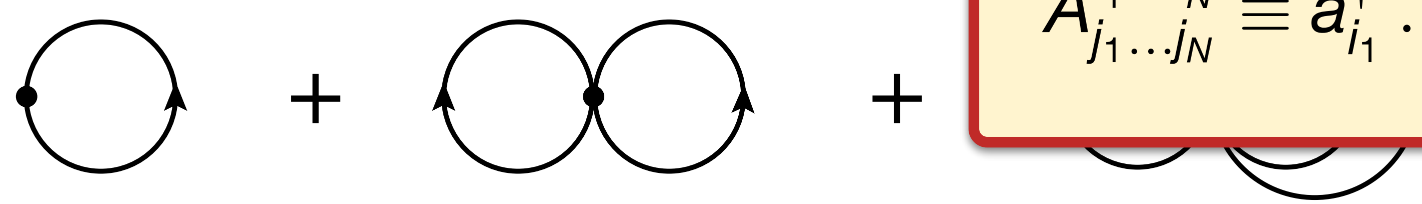
- reference state: **single Slater determinant**

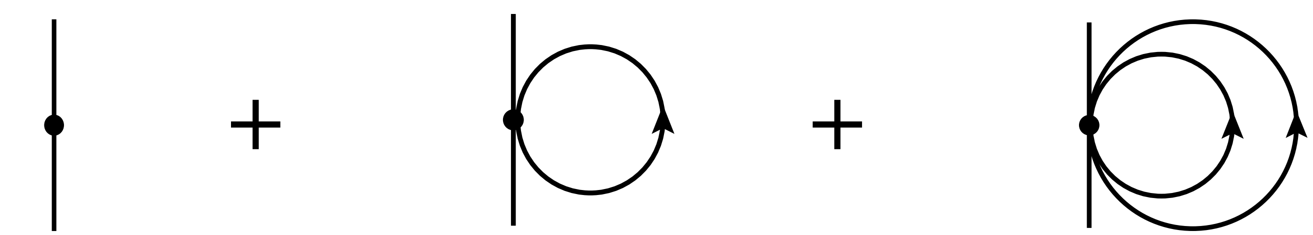
Normal-Ordered Hamiltonian

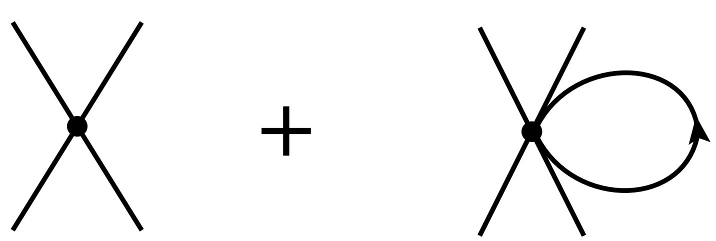
Normal-Ordered Hamiltonian

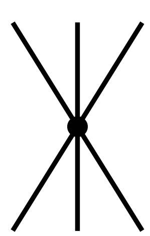
$$H = E_0 + \sum_{kl} f^k_l :A^k_l: + \frac{1}{4}\sum_{klmn}\Gamma^{kl}_{mn} :A^{kl}_{mn}: + \frac{1}{36}\sum_{ijklmn} W^{ijk}_{lmn} :A^{ijk}_{lmn}:$$

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

$E_0 =$ 

$f =$ 

$\Gamma =$ 

$W =$ 

Normal-Ordered Hamiltonian

Normal-Ordered Hamiltonian

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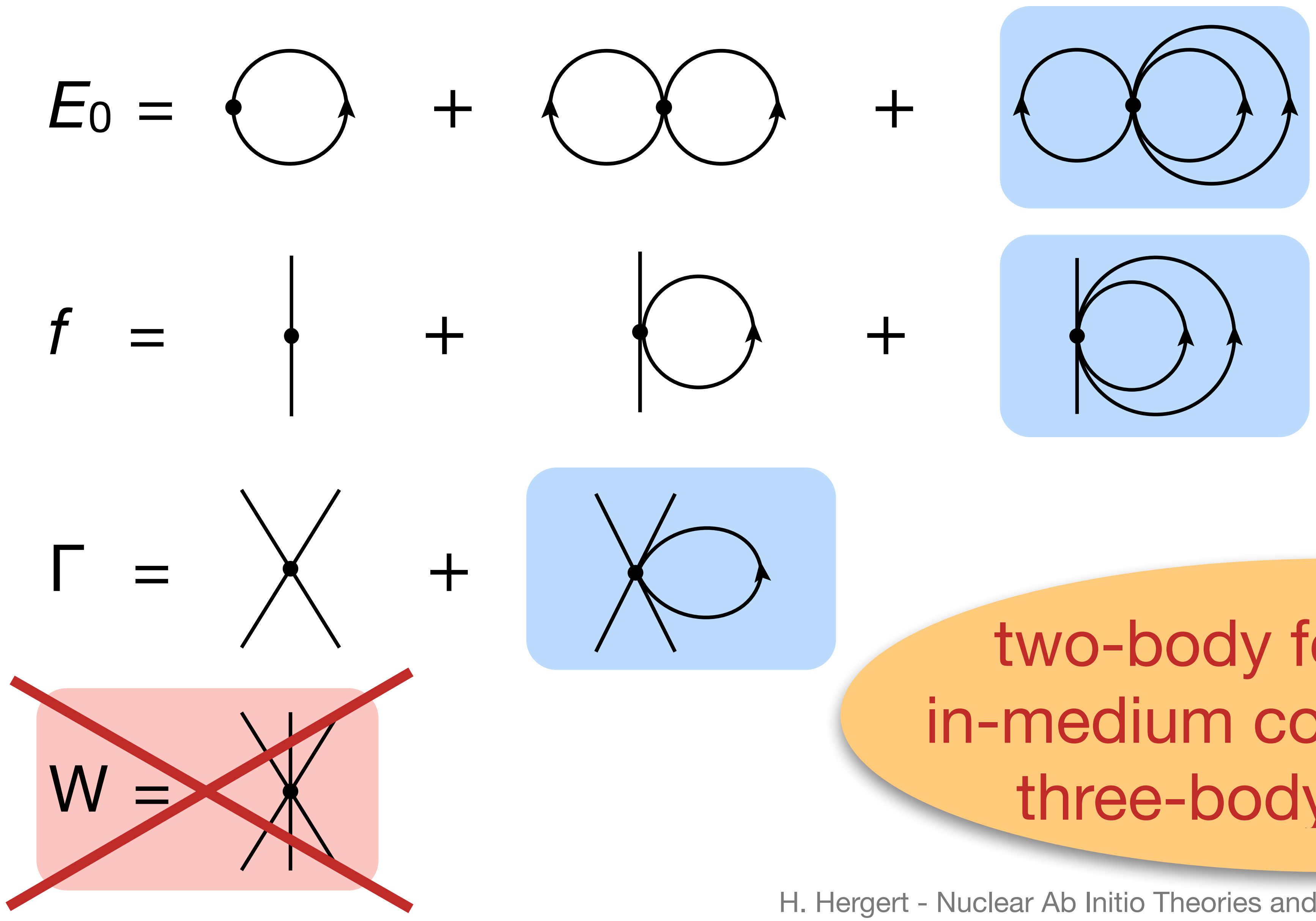
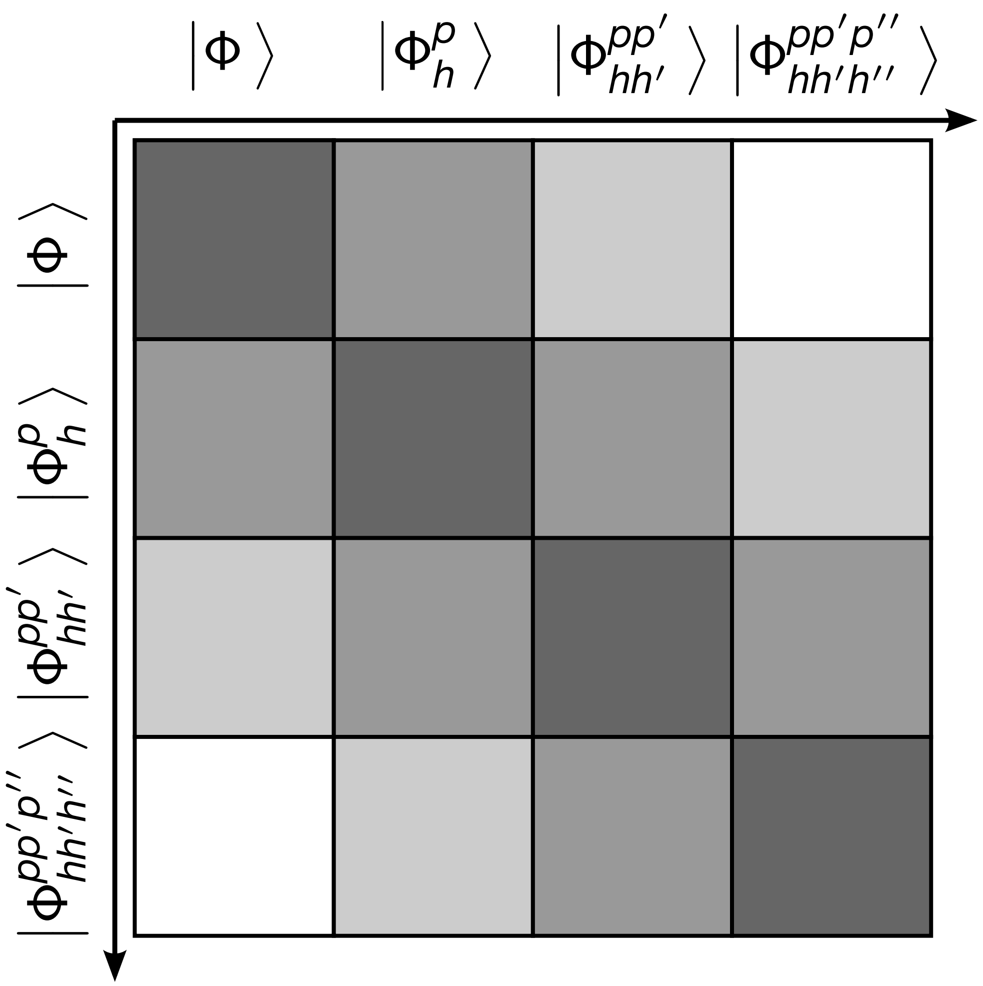


two-body formalism with in-medium contributions from three-body interactions

Single-Reference Case



$\langle i | H | j \rangle$

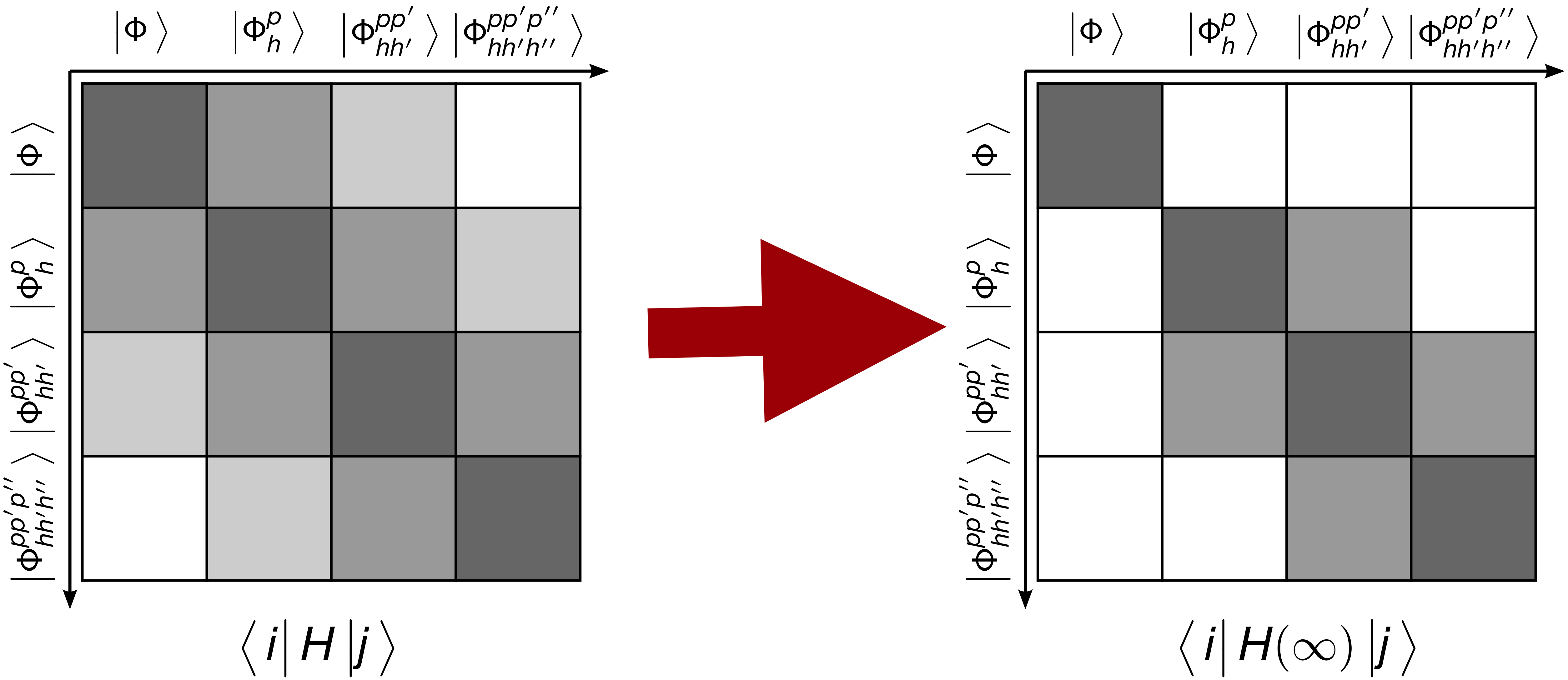
$$A^{i_1\ldots i_N}_{j_1\ldots j_N} \equiv a^\dagger_{i_1}\ldots a^\dagger_{i_N} a_{j_N}\ldots a_{j_1}$$

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

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

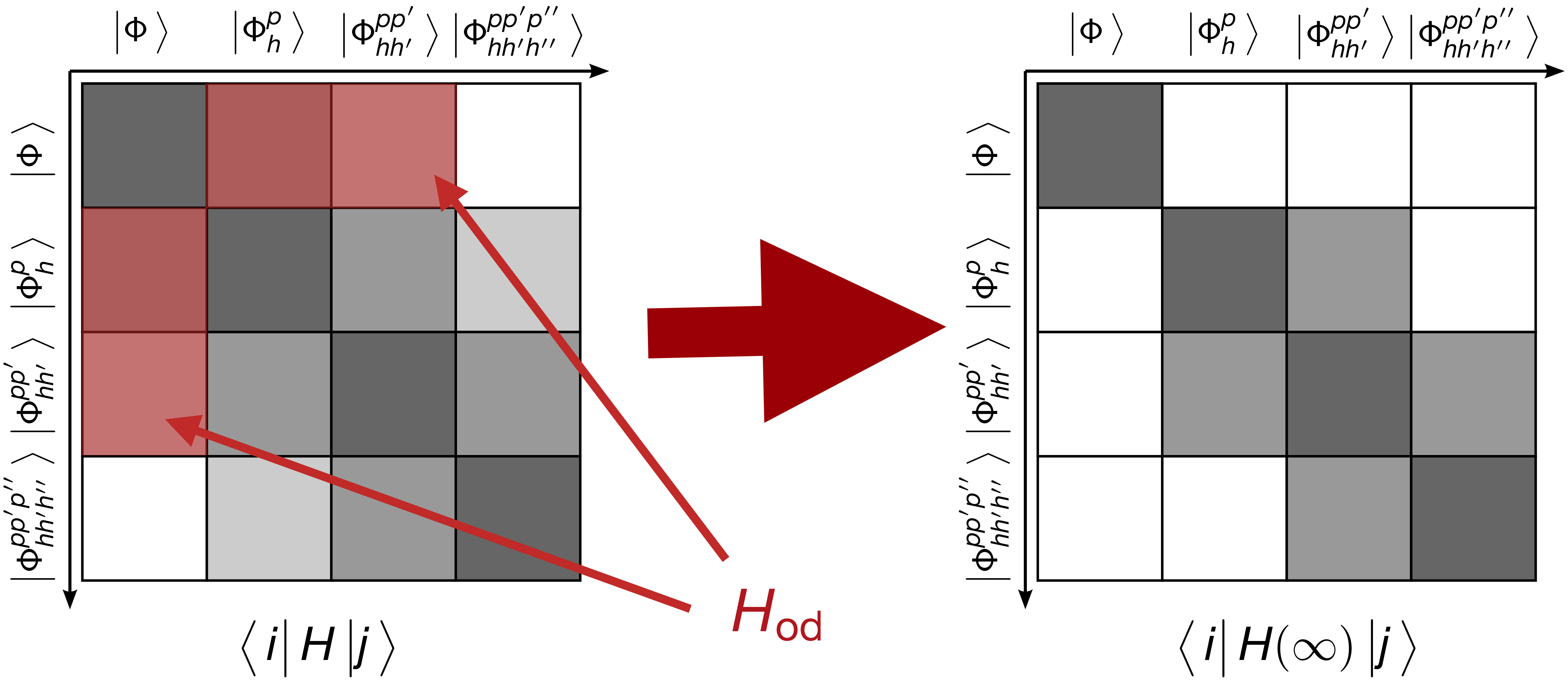
- reference state: **Slater determinant**
- normal-ordered operators **depend on occupation numbers (one-body density)**

Decoupling in A-Body Space



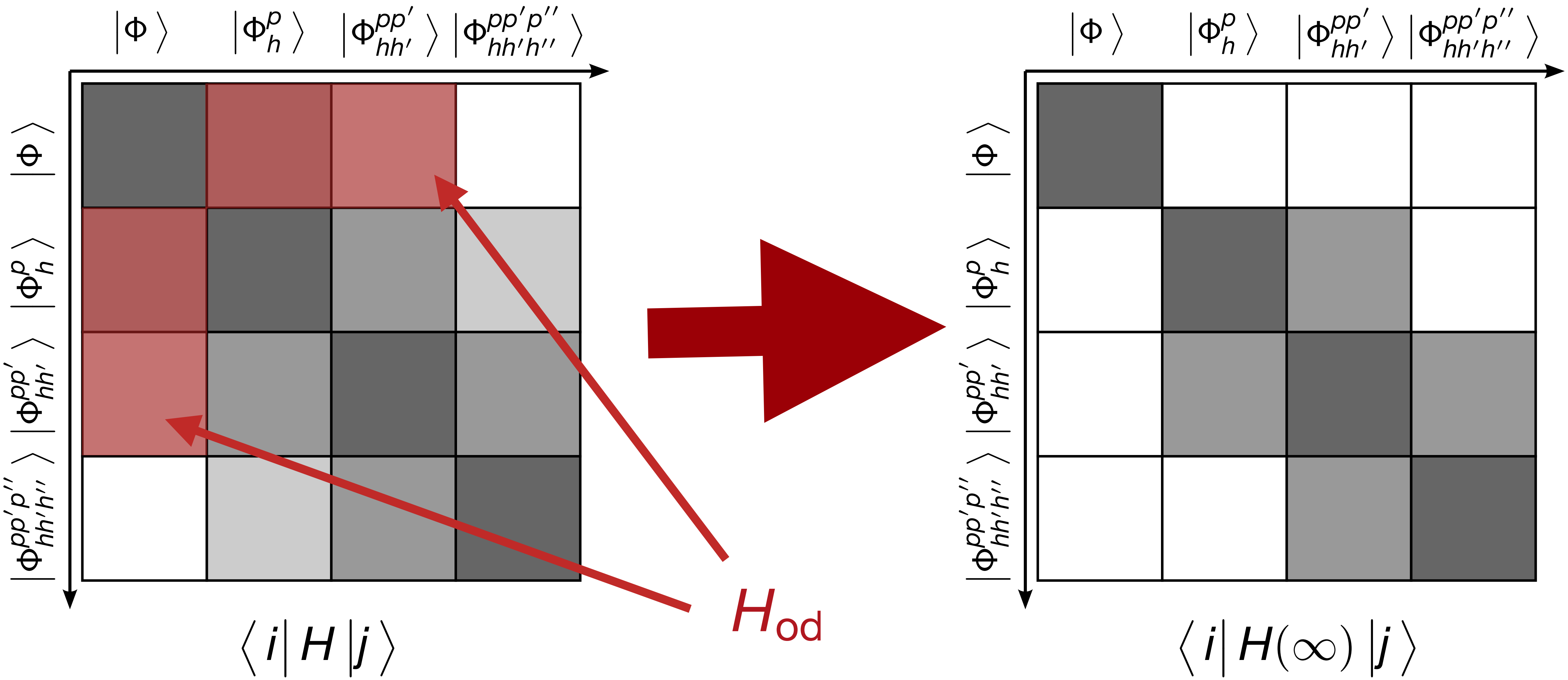
aim: decouple reference state $|\Phi\rangle$
from excitations

Flow Equation



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

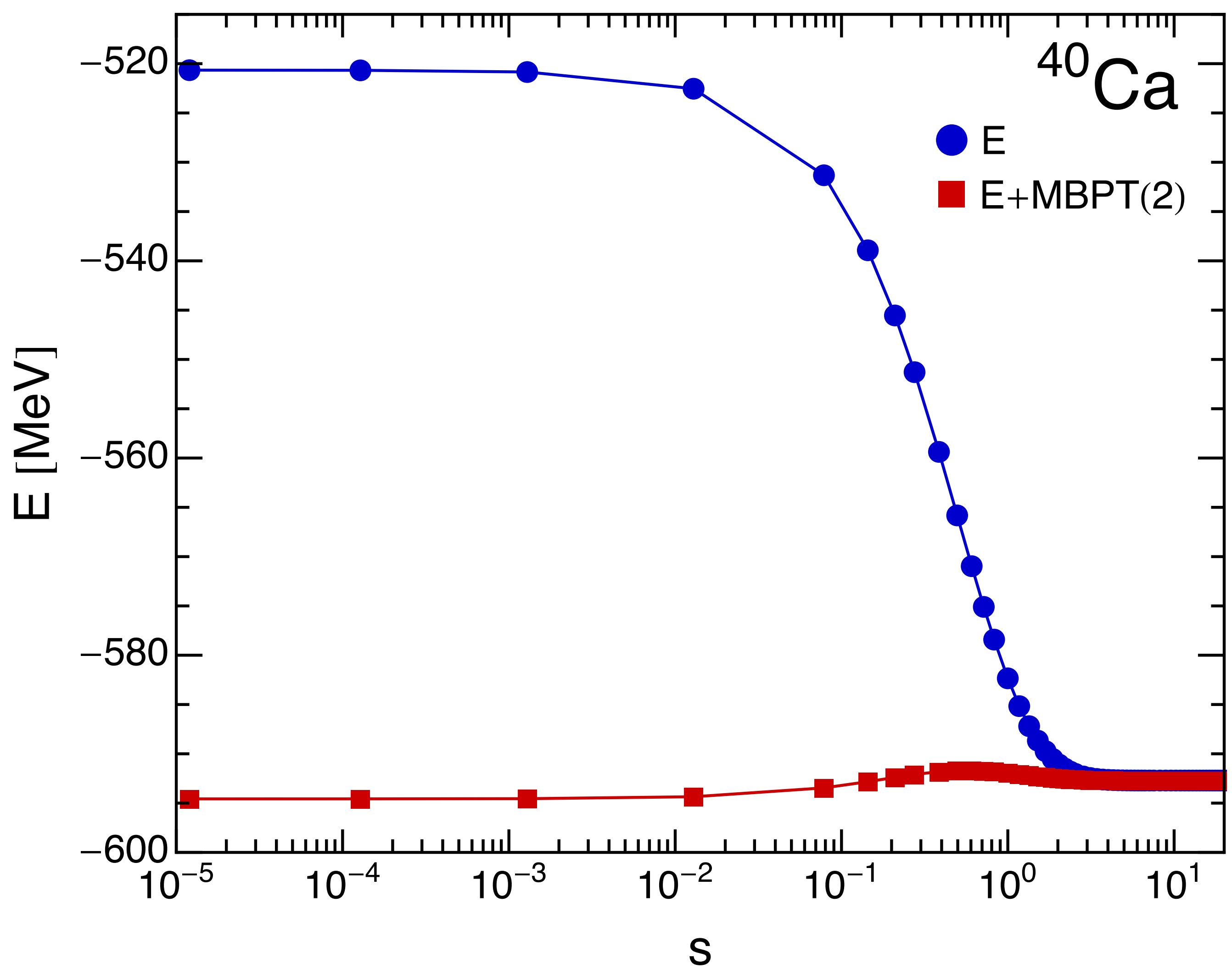
Flow Equation

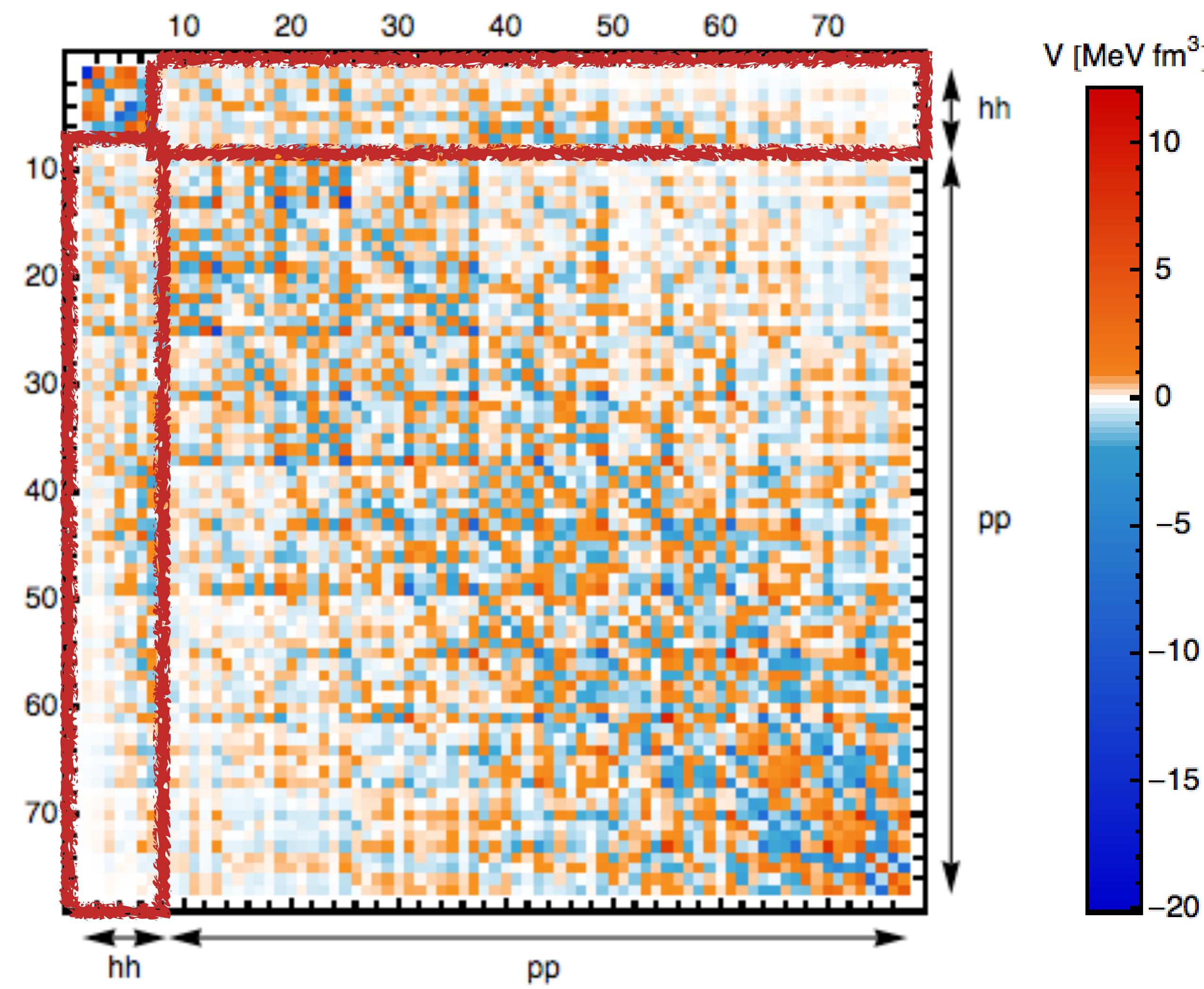


$$\frac{d}{ds}H(s) = \left[\eta(s), H(s)\right], \quad \text{e.g}$$

Matrix is never constructed explicitly!

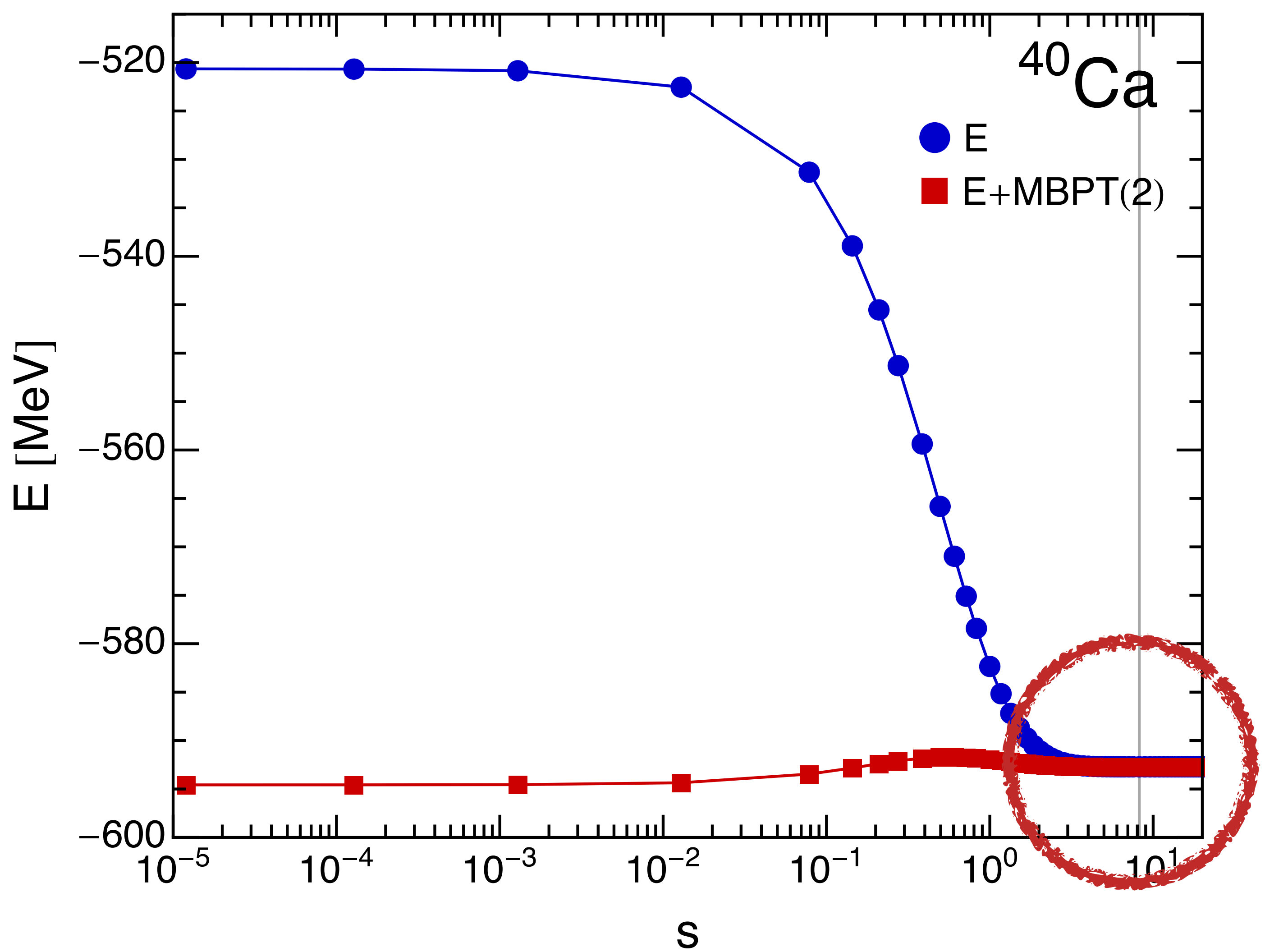
Decoupling

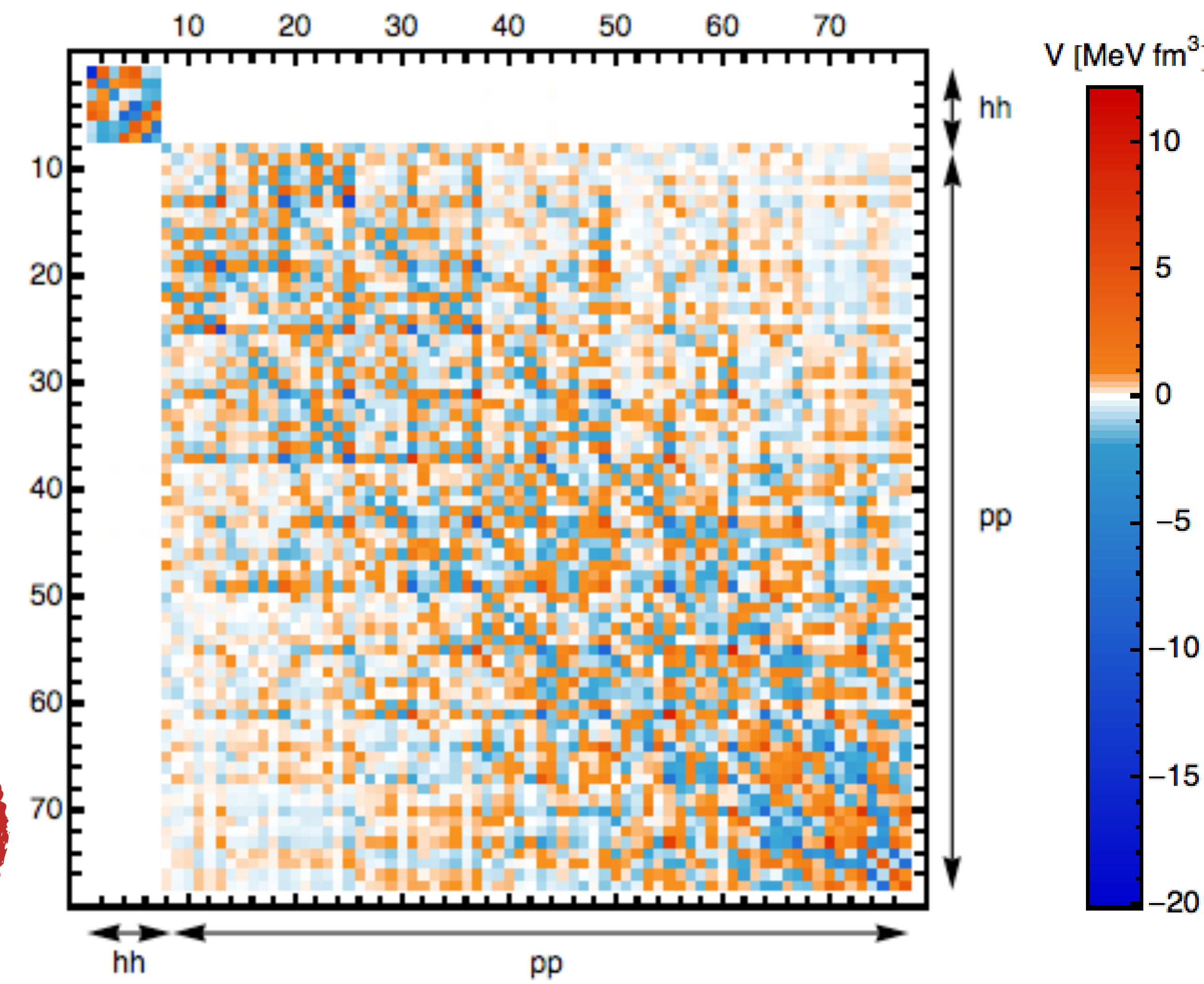




N3LO, $\lambda = 2.0\ \text{fm}^{-1}, e_{\text{Max}} = 8$

Decoupling



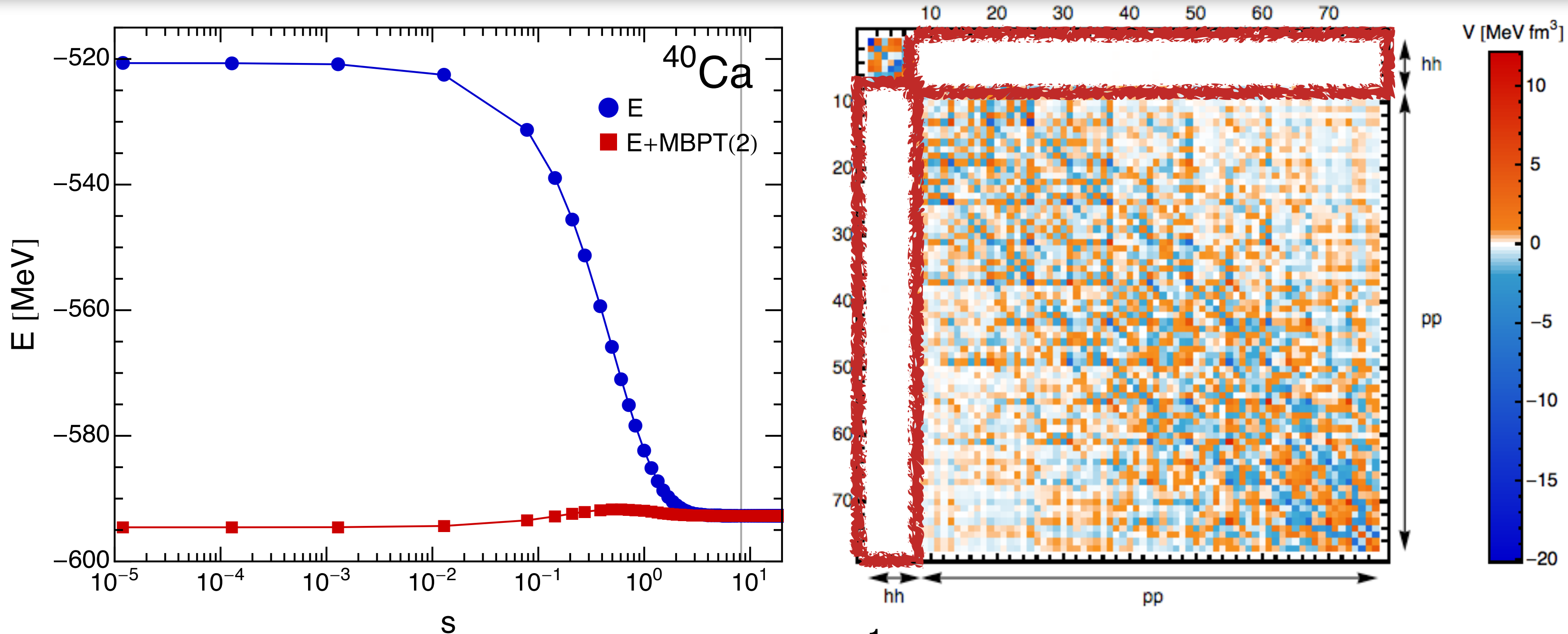


N3LO, $\lambda = 2.0\ \mathrm{fm}^{-1}, e_{\mathrm{Max}} = 8$

non-perturbative resummation of MBPT series (correlations)

off-diagonal couplings are rapidly driven to zero

Decoupling



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

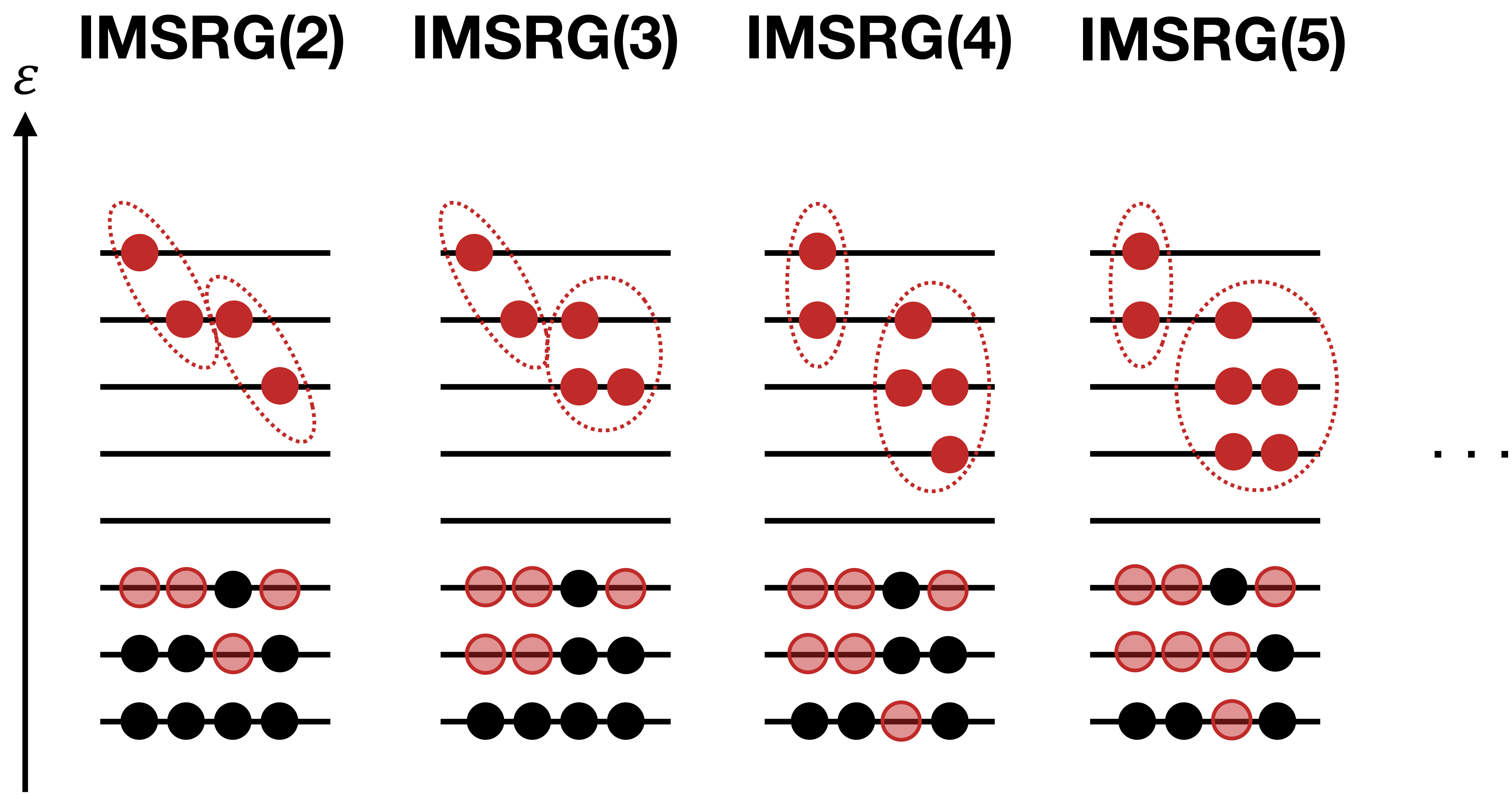
- absorb correlations into **RG-improved Hamiltonian**

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

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

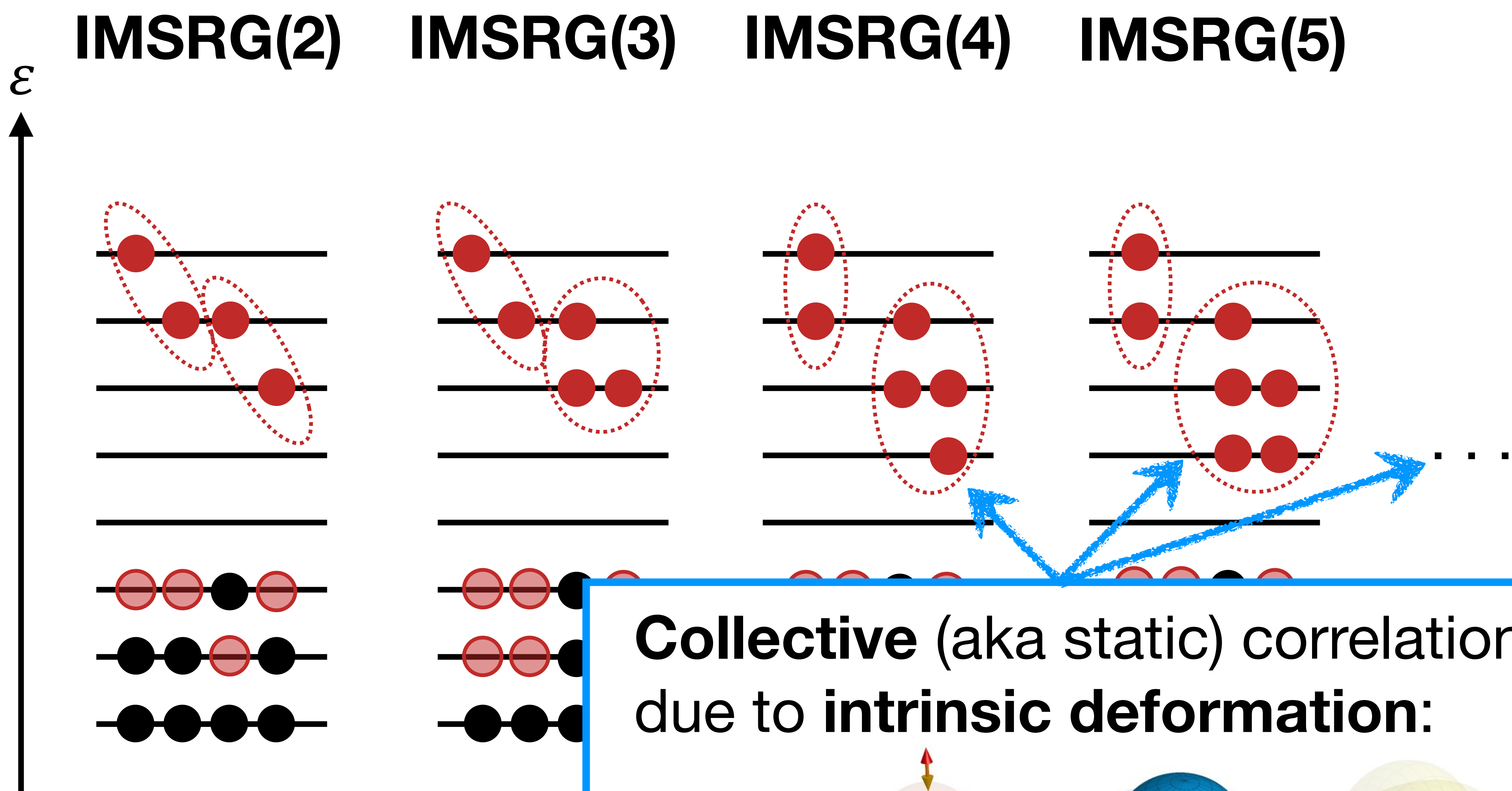
$$U(s)\left|\Psi_n\right\rangle \stackrel{!}{=} \left|\Phi\right\rangle$$

Correlated Reference States



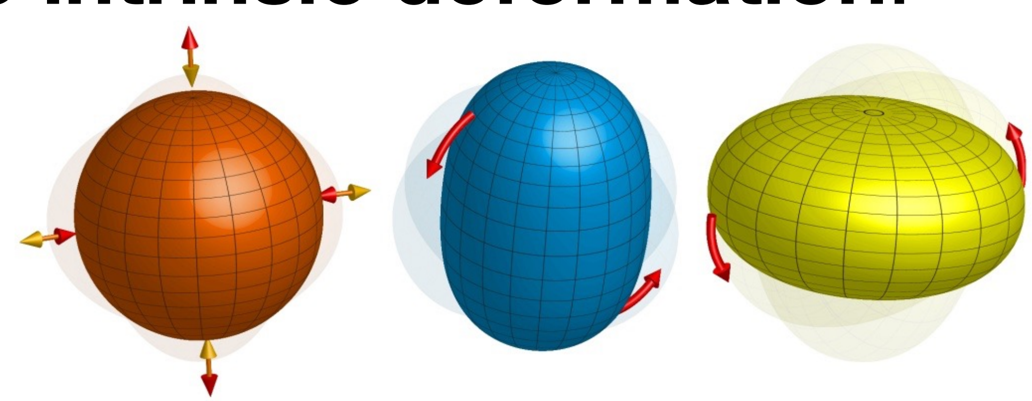
“standard” IMSRG: build correlations on top of Slater determinant (=**independent-particle state**)

Correlated Reference States

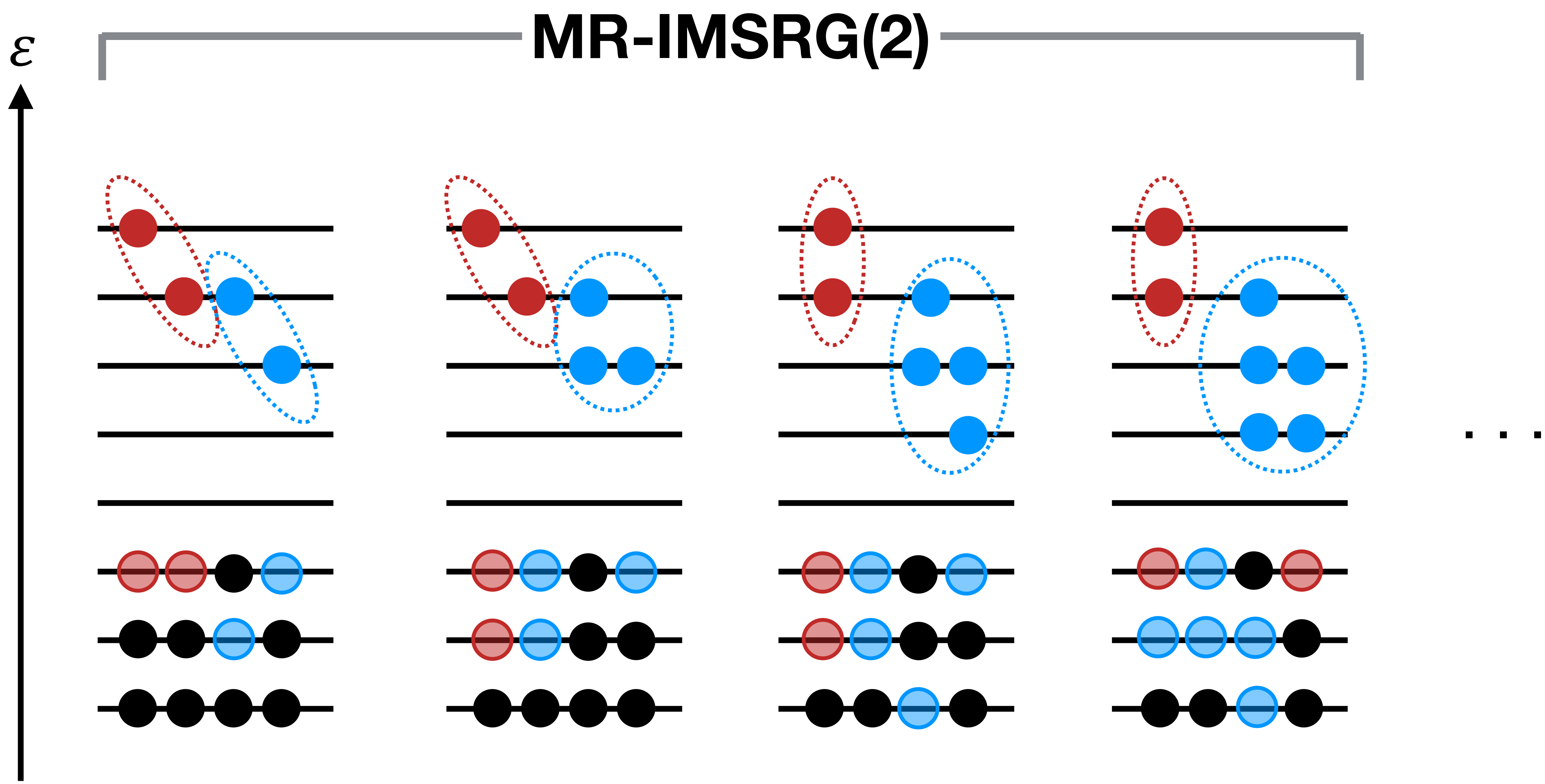


“standard” IMS
Slater determinan

Collective (aka static) correlations, e.g. due to **intrinsic deformation**:

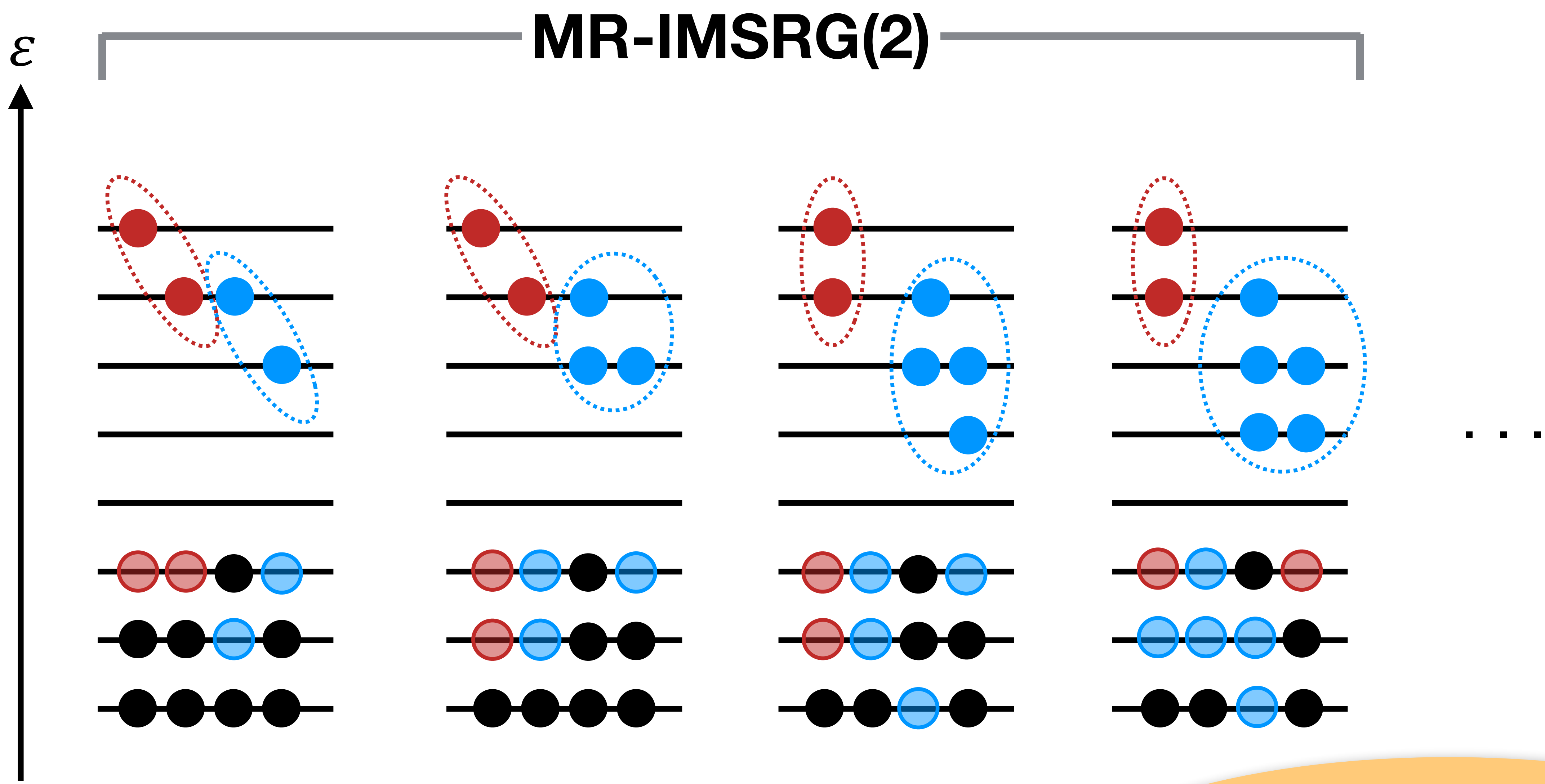


Correlated Reference States



MR-IMSRG: build correlations on top of **already correlated** state (e.g., from a method that describes static correlation well)

Correlated Reference States



MR-IMSRG: build correlations
already correlated state (e.g., fro
describes static correlation

use generalized normal ordering with 2B,... densities

MR-IMSRG References States

available

- Slater determinants (uncorrelated)
- number-projected Hartree-Fock Bogoliubov vacua
- Generator Coordinate Method (with projections)
- small-scale No-Core Shell Model
- symmetry-adapted NCSM, clustered states, Density Matrix Renormalization Group, tensor networks etc.

future

SA-NCSM: see talk by K. Launey

MR-IMSRG References States

available

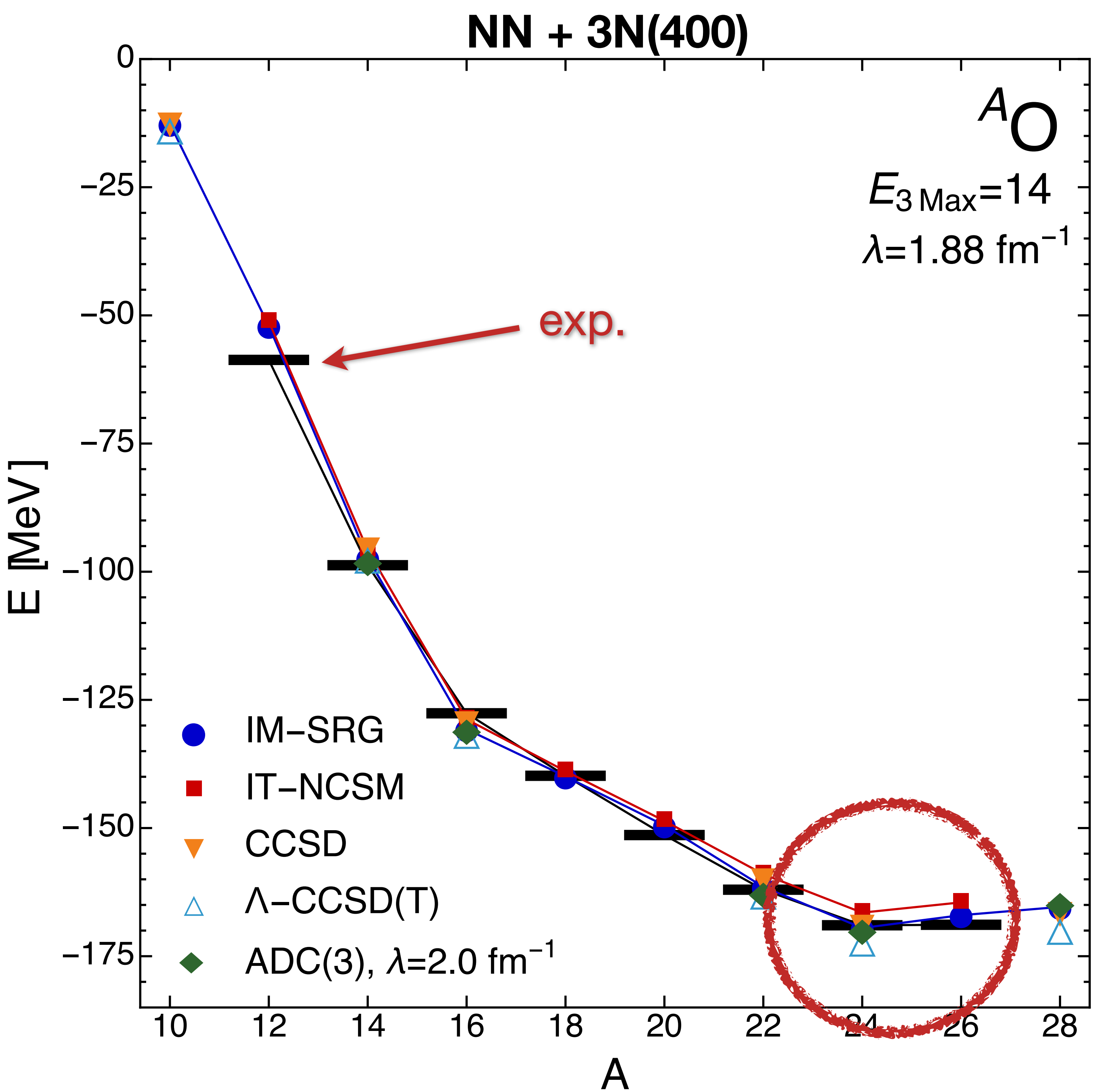
- **Slater determinants (uncorrelated)**
- **number-projected Hartree-Fock Bogoliubov vacua**
- Generator Coordinate Method (with projections)
- small-scale No-Core Shell Model

future

- symmetry-adapted NCSM, clustered states, Density Matrix Renormalization Group, tensor networks etc.

Oxygen Isotopes

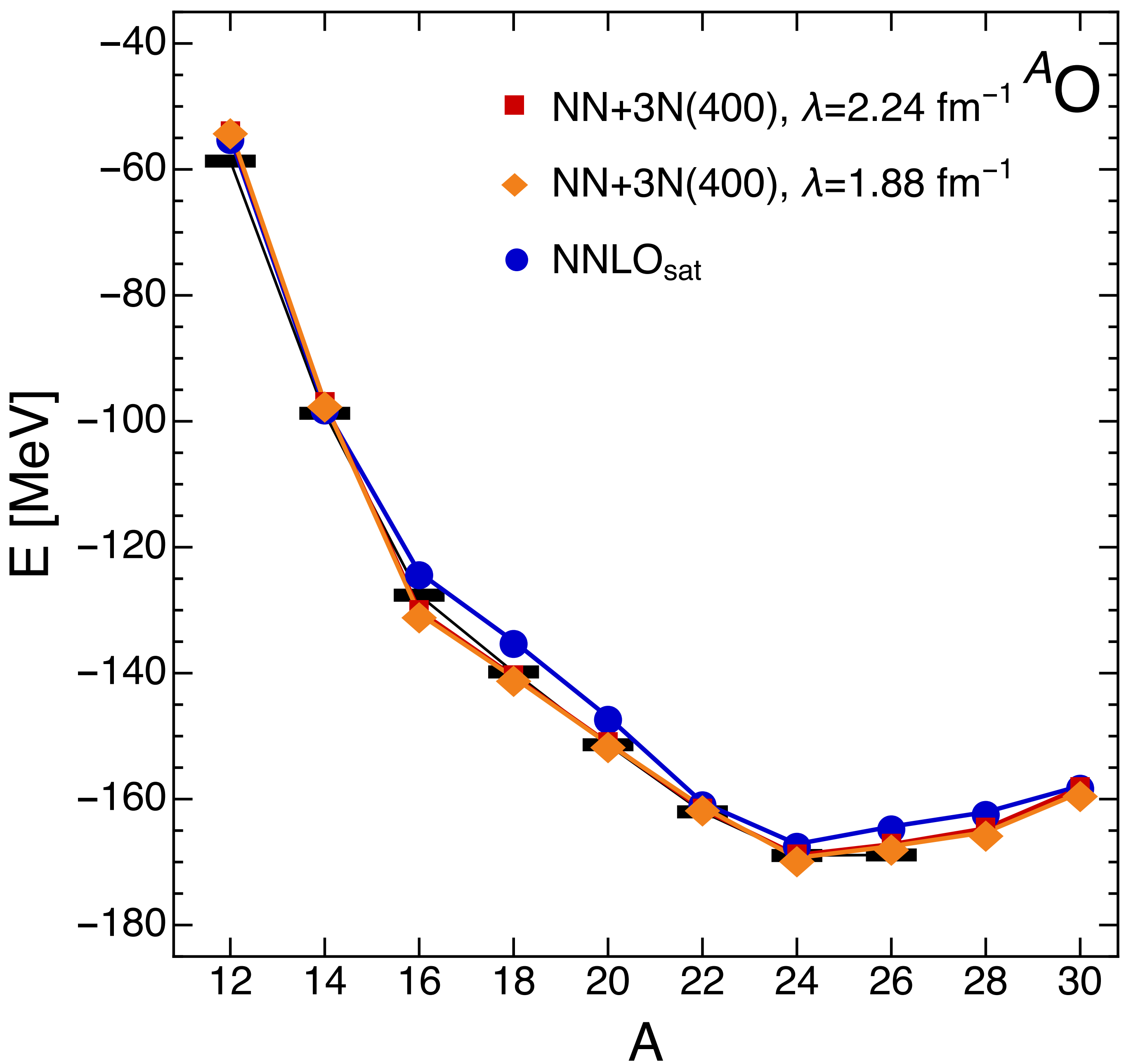
*HH et al., PRL **110**, 242501 (2013), ADC(3): A. Cipollone et al., PRL **111**, 242501 (2013)*

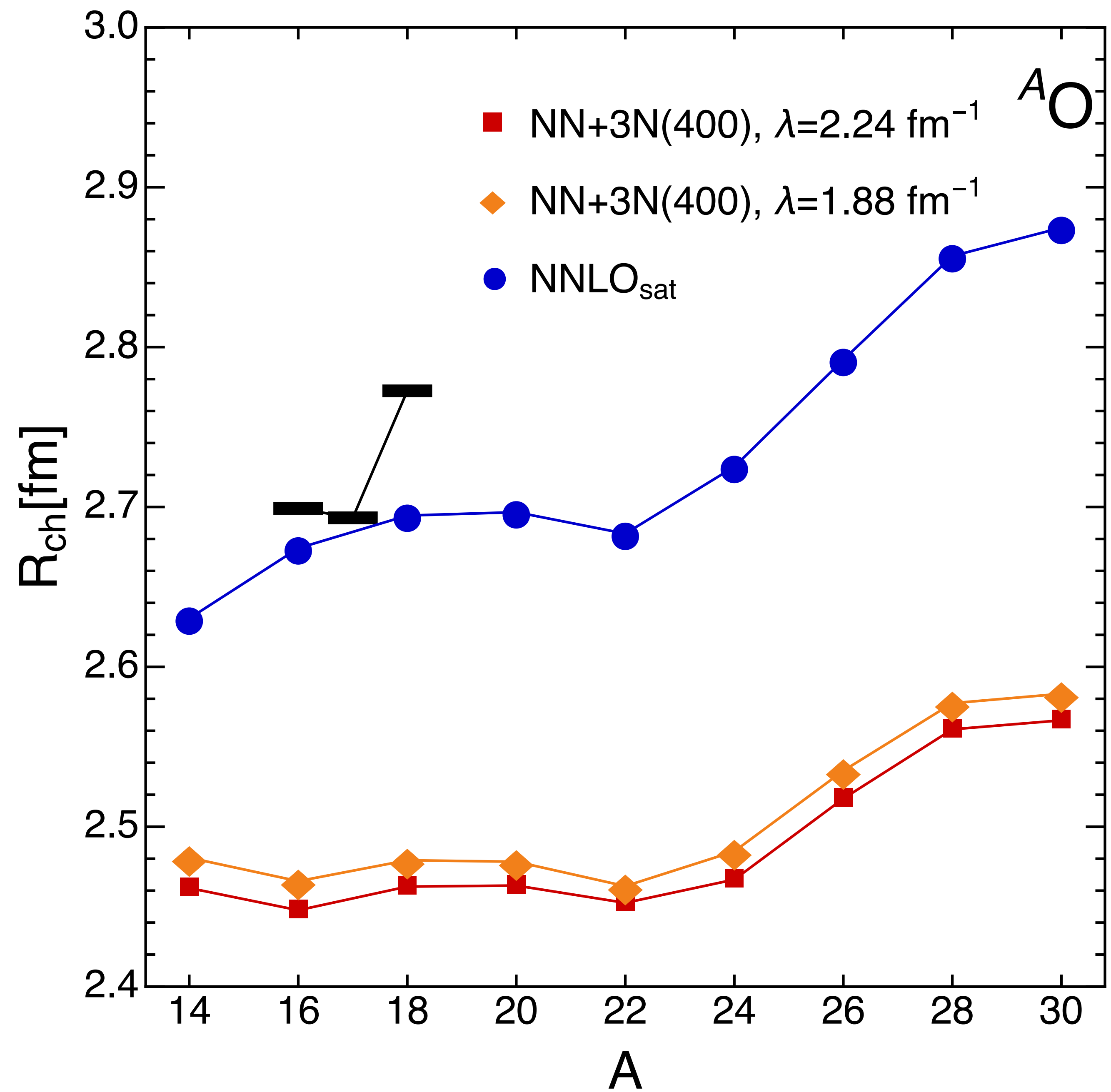


- **MR-IMSRG** with particle-number projected HFB reference state
- **consistency between many-body methods**
- ^{24}O drip line, but ^{25,26}O g.s. resonances too high: continuum and interaction

Oxygen Radii

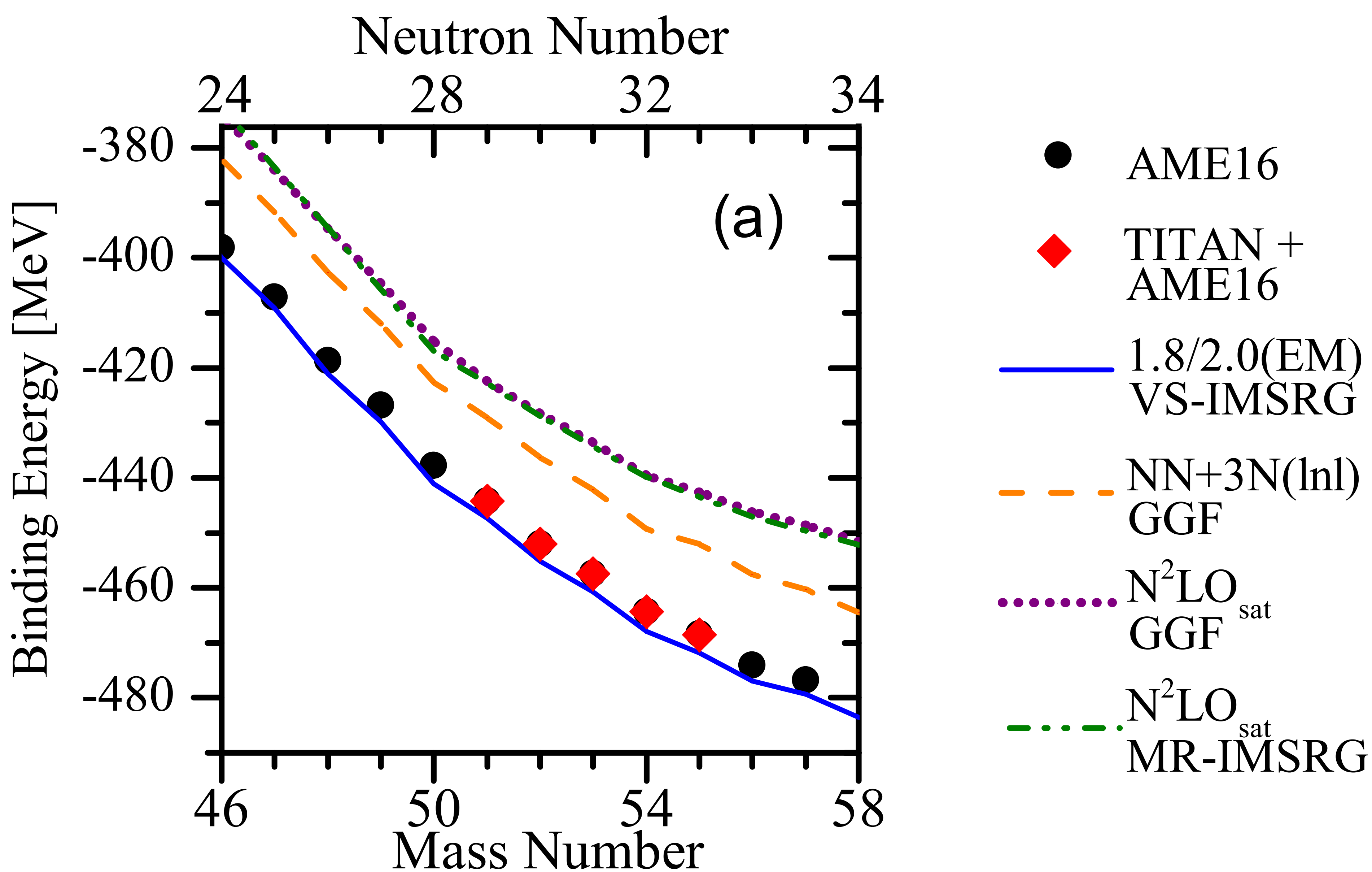
V. Lapoux, V. Somà, C. Barbieri, HH, J. D. Holt, and S. R. Stroberg, PRL 117, 052501 (2016)





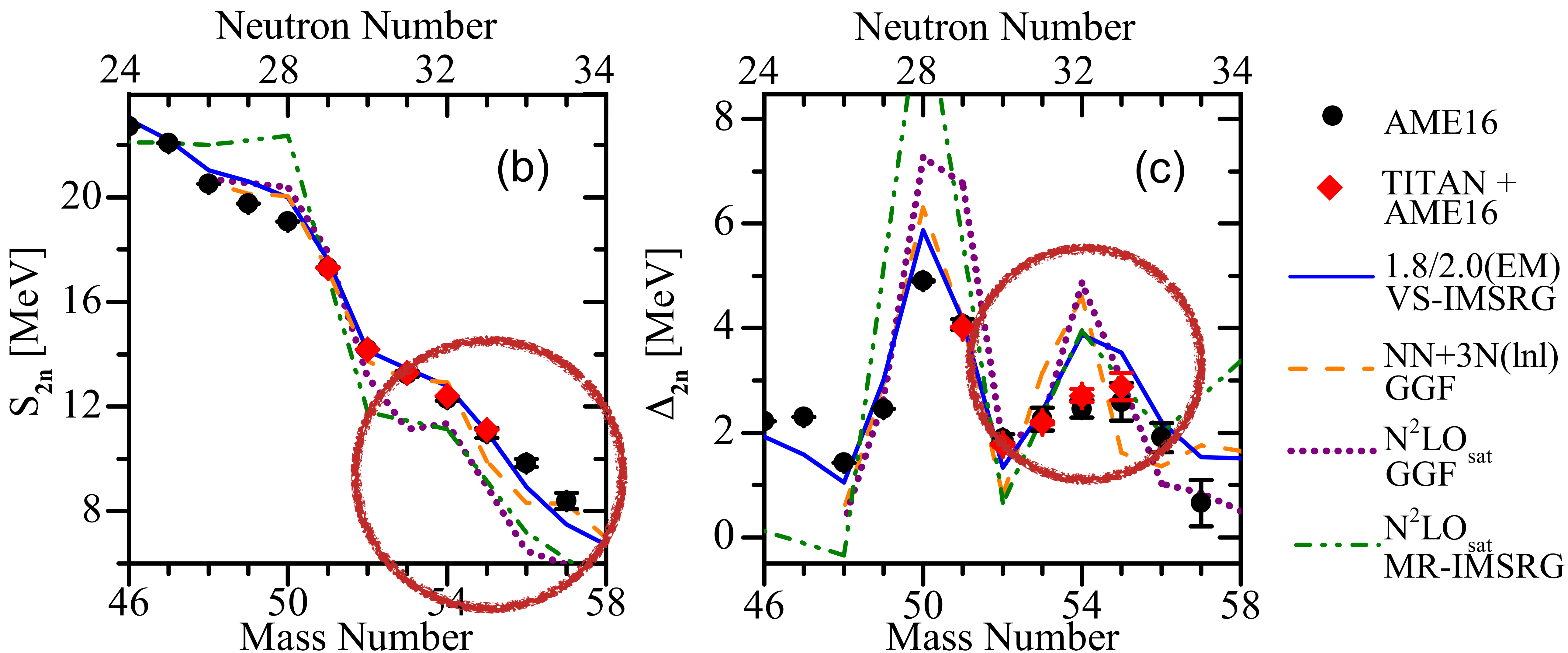
Titanium Isotopes

*E. Leistenschneider et al., PRL **120**, 062503 (2018)*



Titanium Isotopes

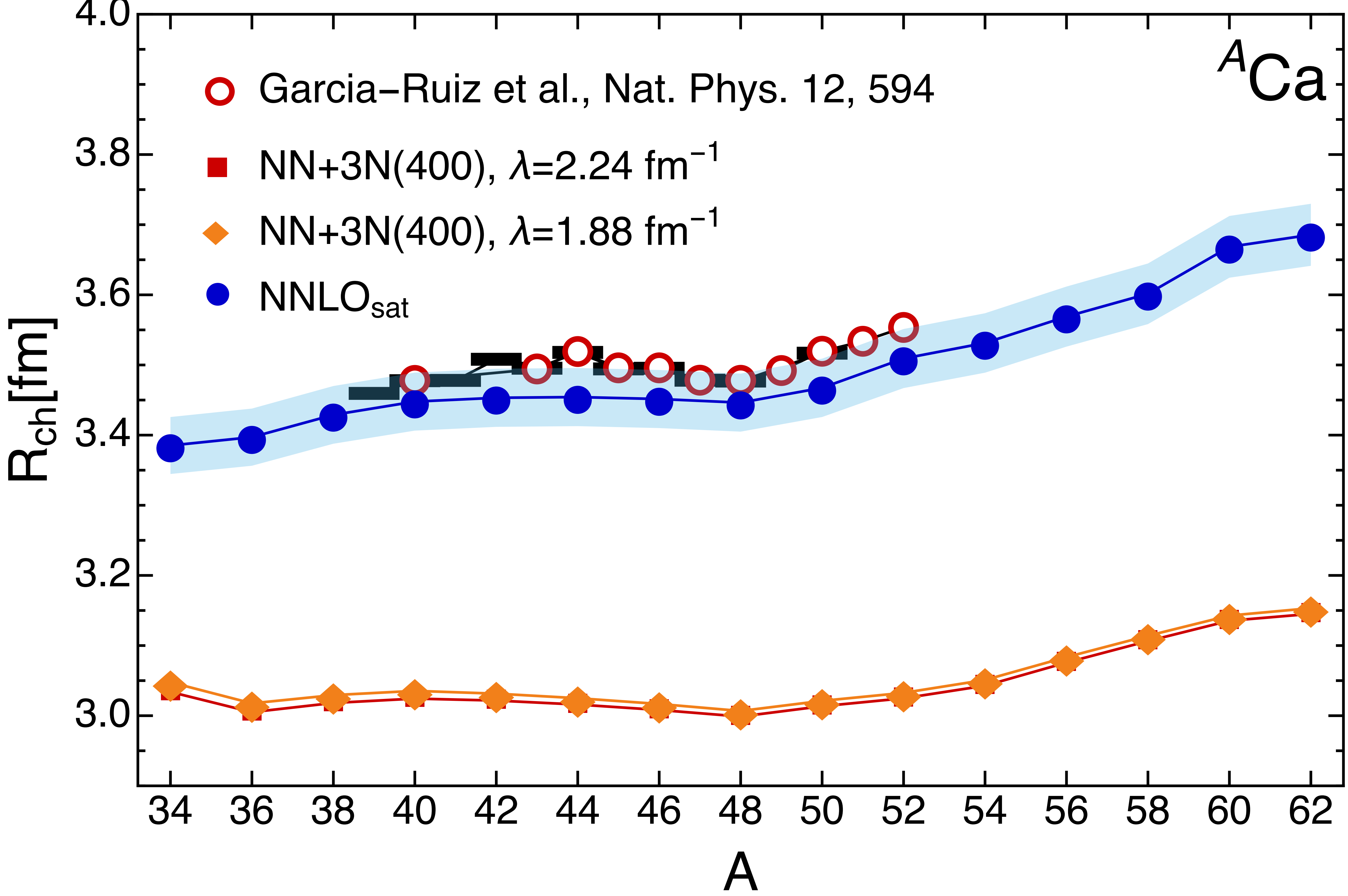
*E. Leistenschneider et al., PRL **120**, 062503 (2018)*



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

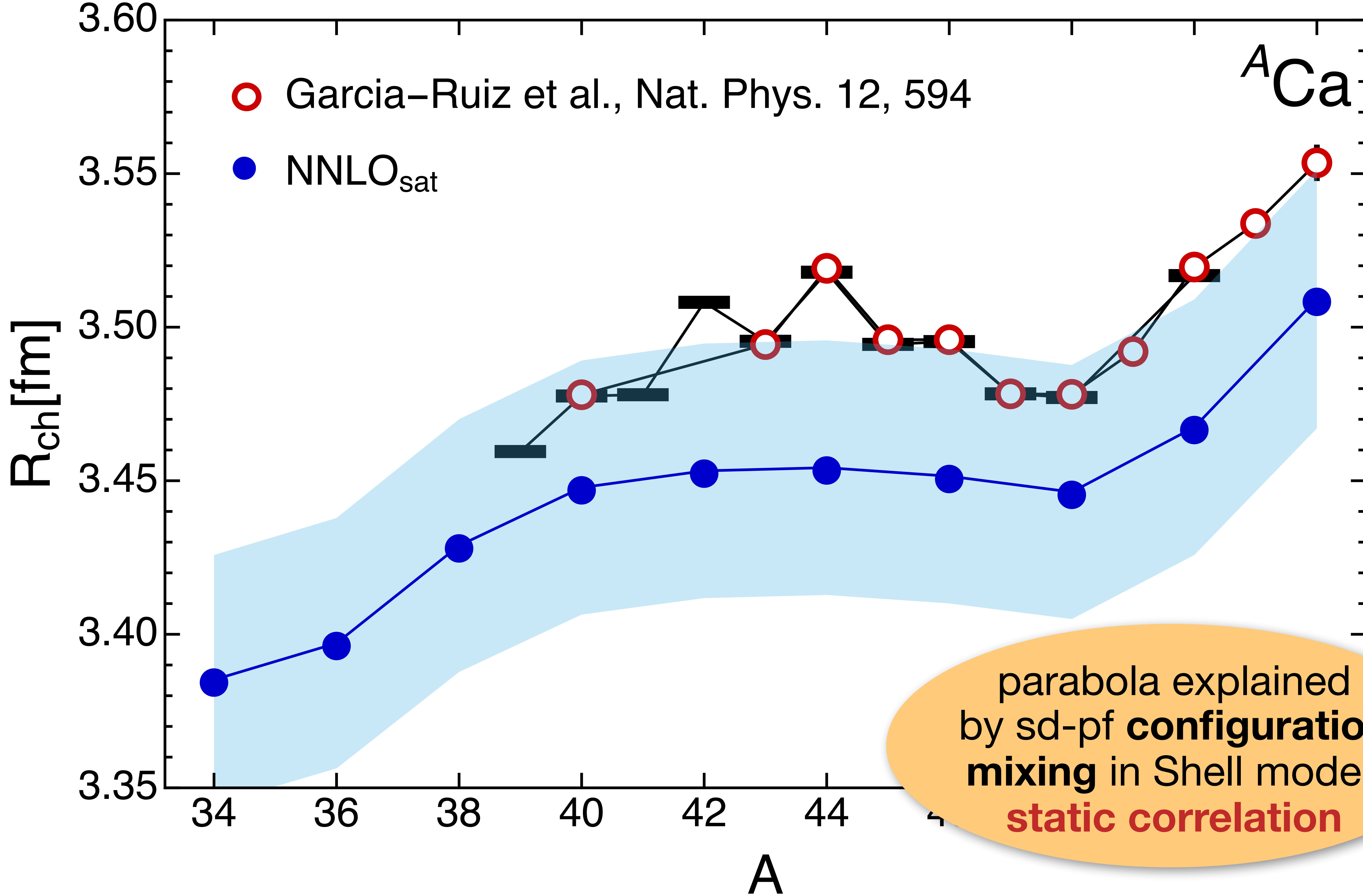
Calcium Isotopes

HH, in preparation



Calcium Isotopes

HH, in preparation



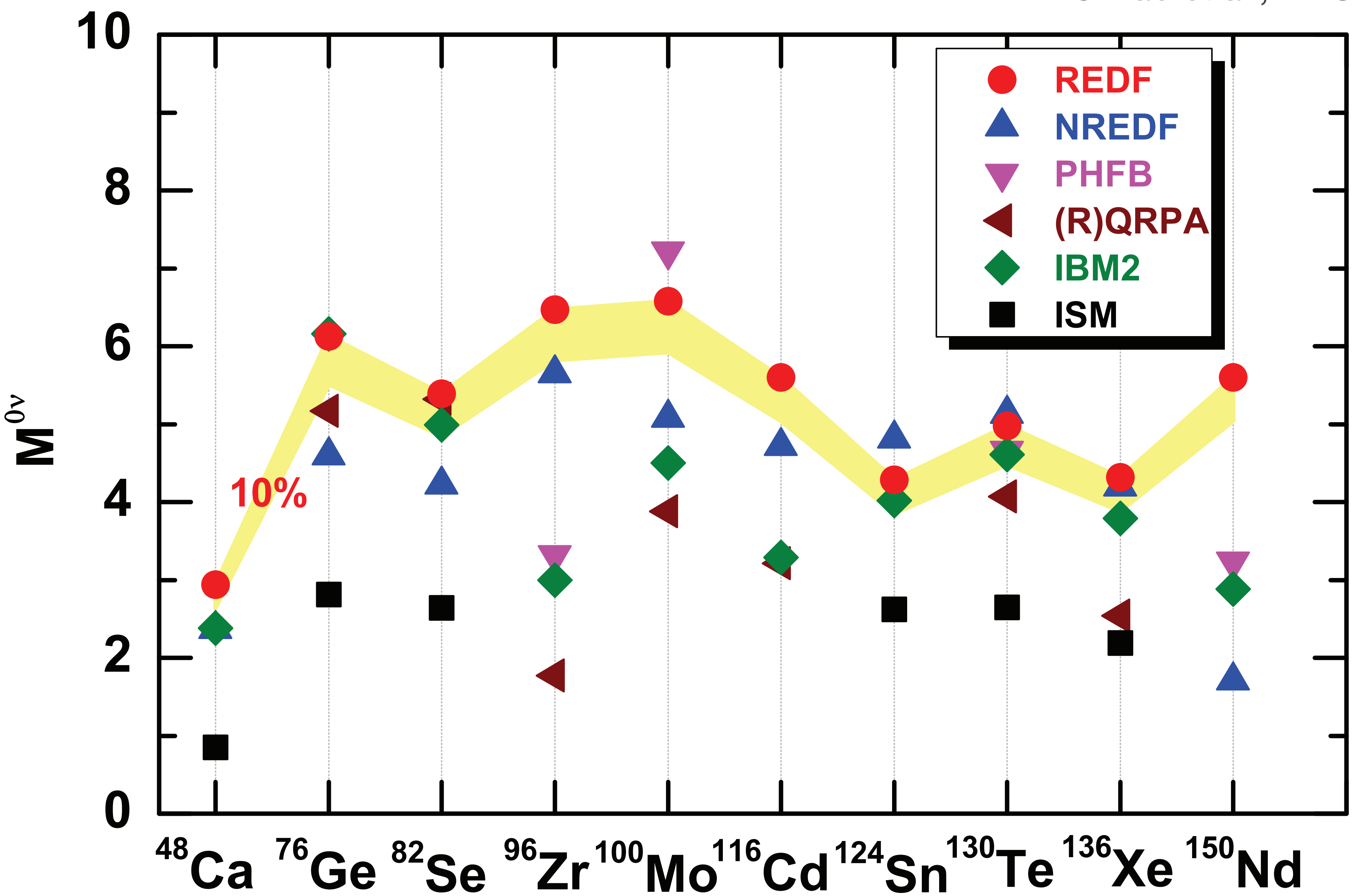
parabola explained by sd-pf **configuration mixing** in Shell model: **static correlation**

Ground-State to Ground-State Decay

with **J. Yao**, J. Engel, …

Nuclear Matrix Elements

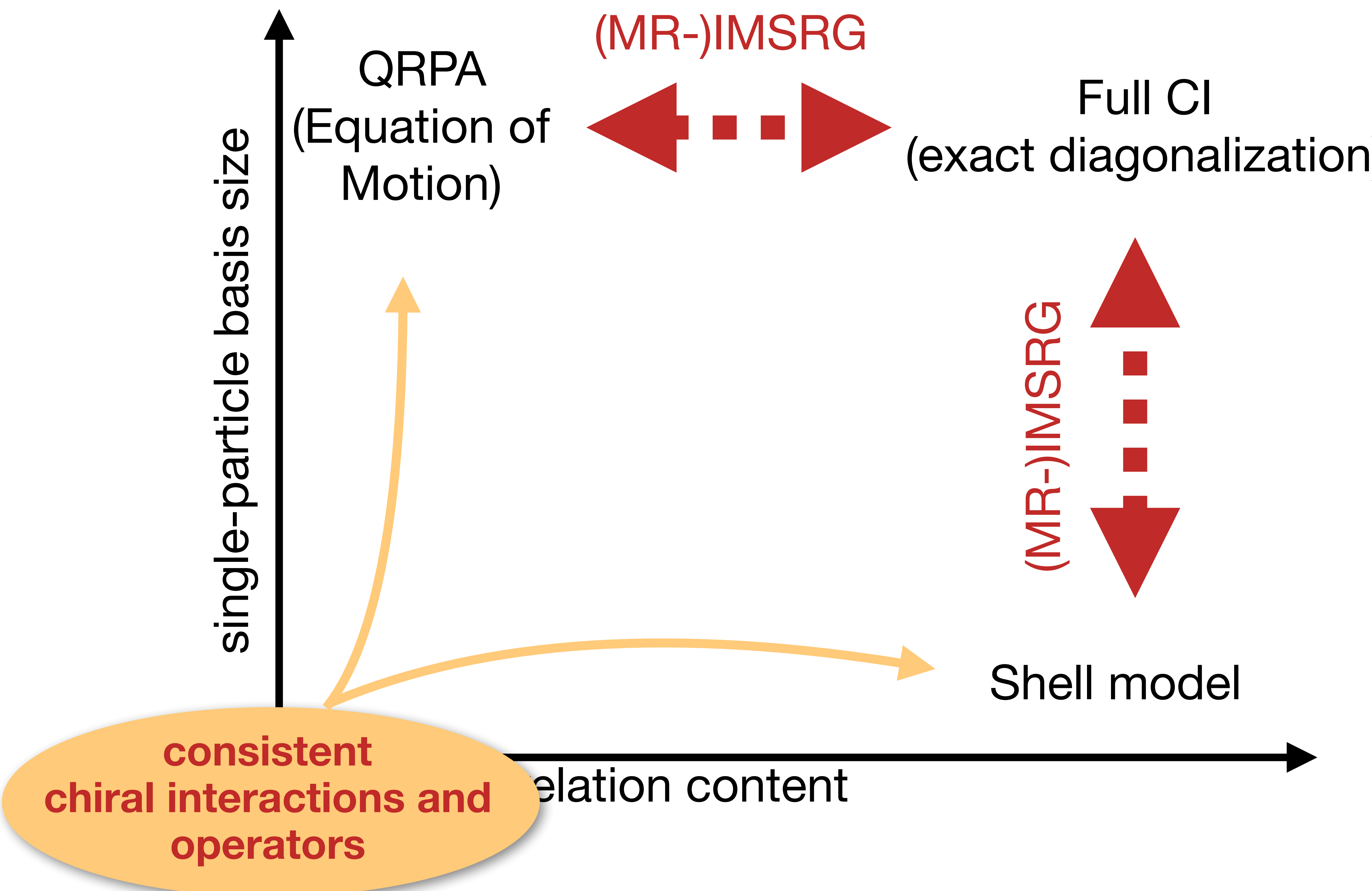
J. Yao et al., PRC **91**, 024316 (2015)



- 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

- Slater determinants (uncorrelated)
- number-projected Hartree-Fock Bogoliubov vacua
- **Generator Coordinate Method (with projections)**
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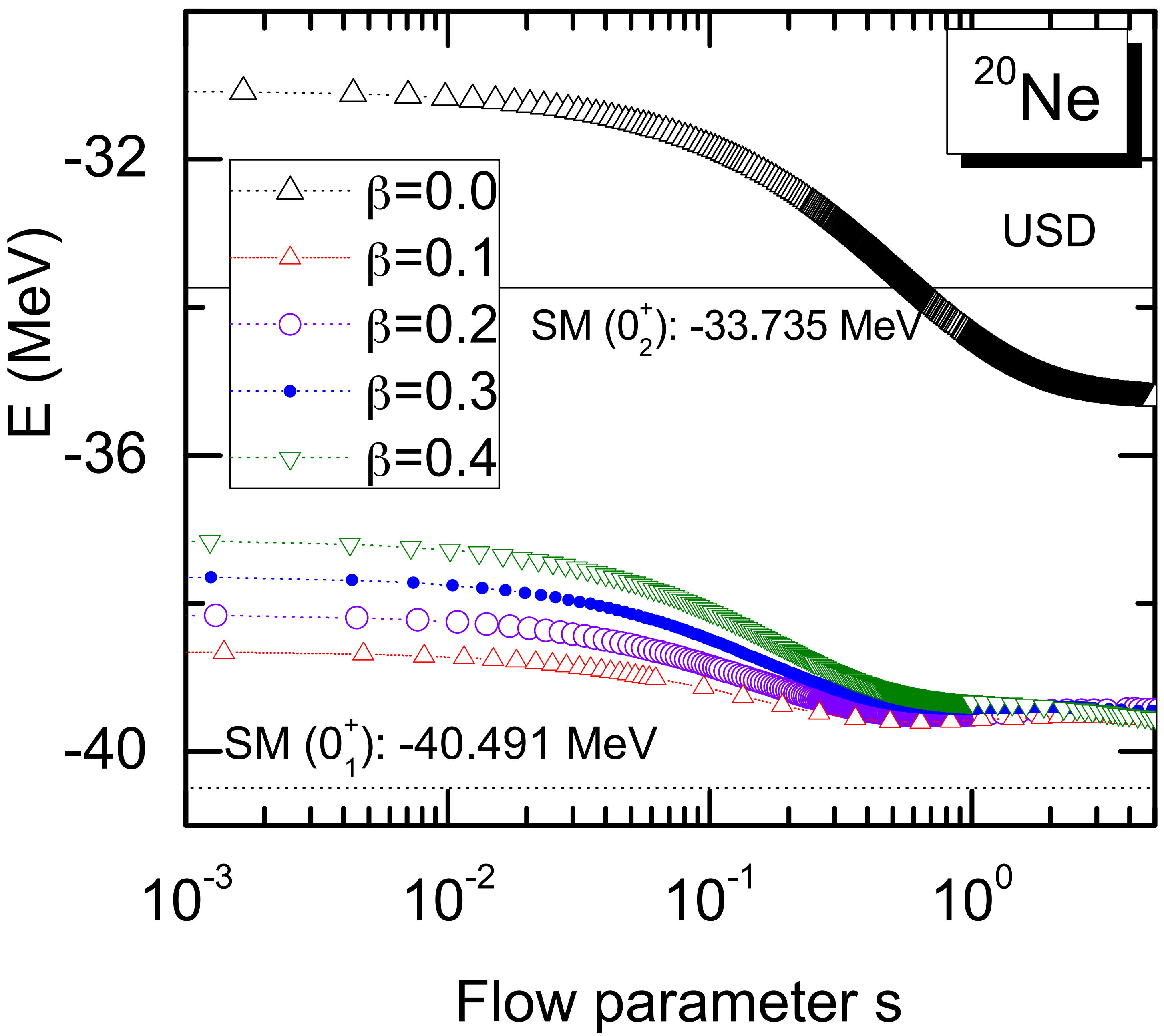
- symmetry-adapted NCSM, clustered states, Density Matrix Renormalization Group, tensor networks etc.

future

Example: ^{20}Ne

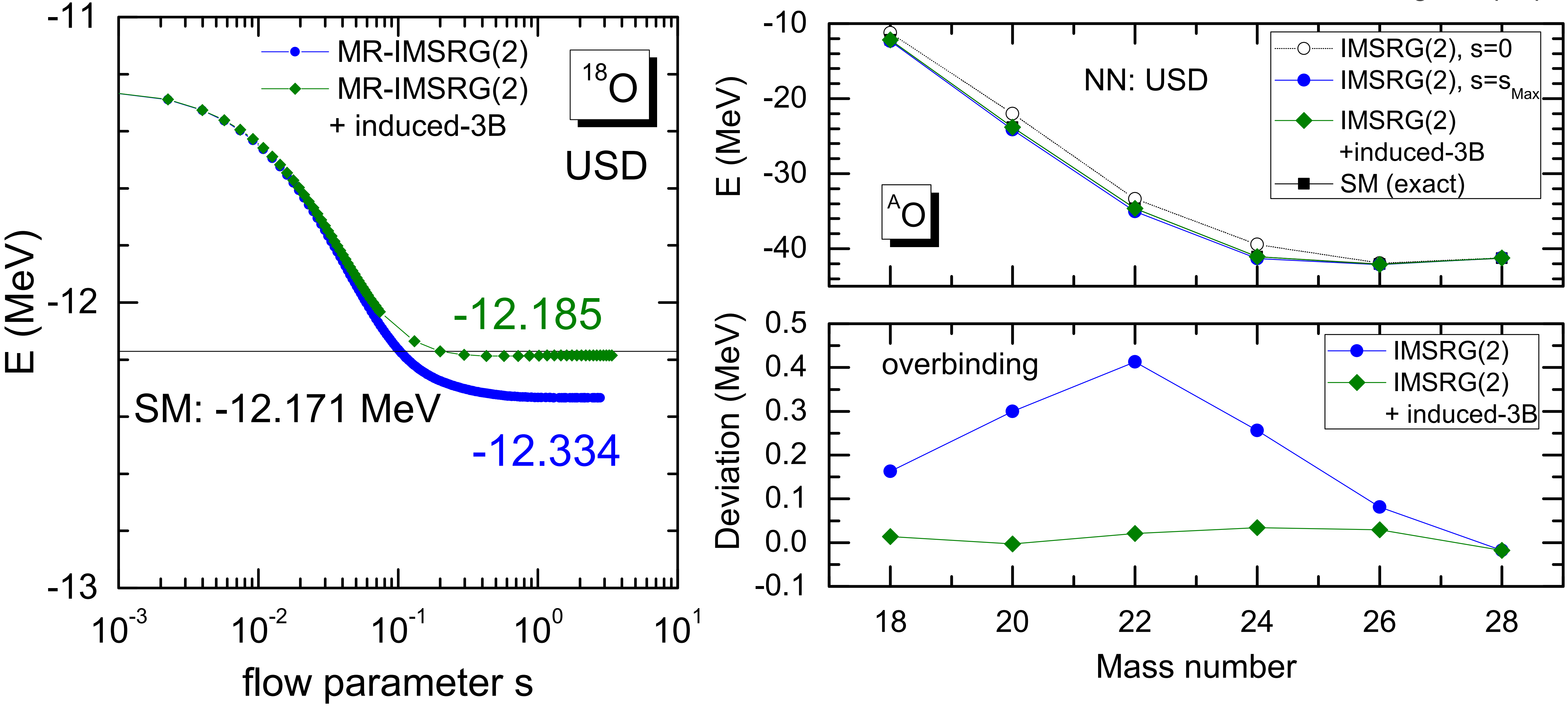
J. Yao, T. D. Morris, HH, J. Engel, in prep.



- 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
- 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**:

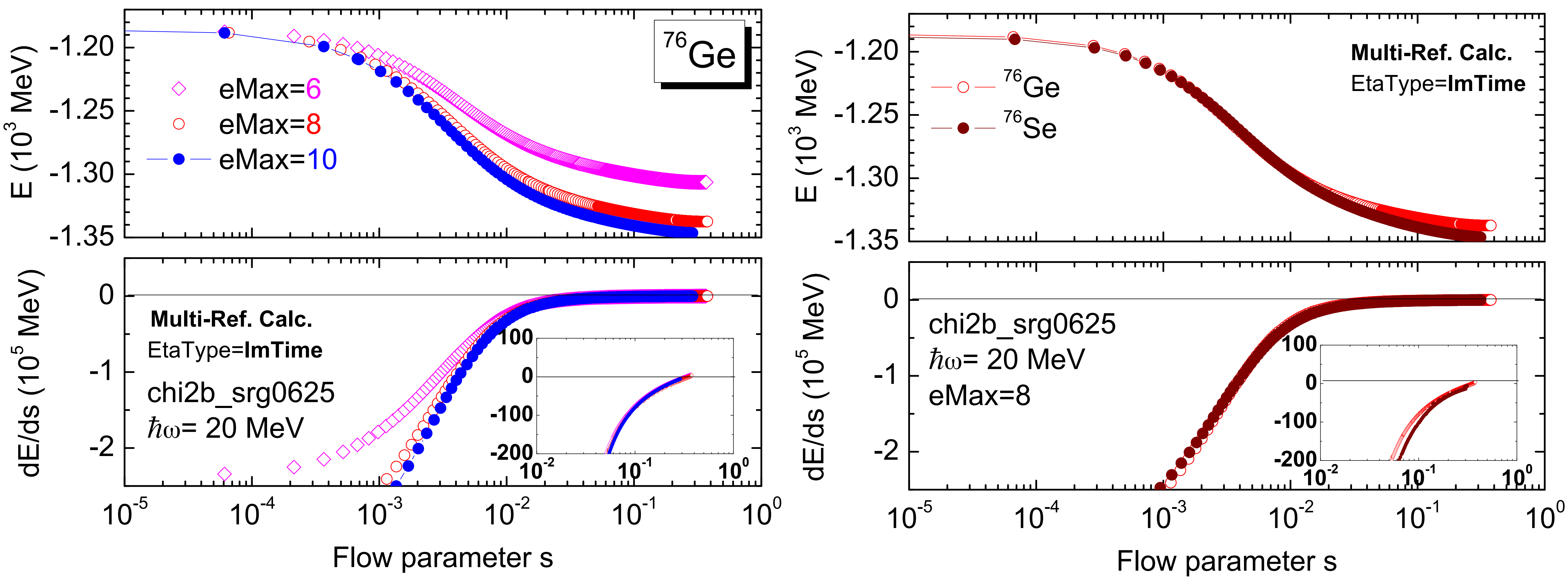
$$M_{0\nu\beta\beta} = \left\langle \Phi_F\right| e^{-\overline{\Omega}_F} O_{0\nu\beta\beta} e^{\overline{\Omega}_I}\left|\Phi_I\right\rangle$$

- 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

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



proof of principle: MR-IM-SRG based on **(intrinsically deformed) GCM state converges** ^{76}Ge,^{76}Se ground-state energies

Explicit Treatment of Excited States

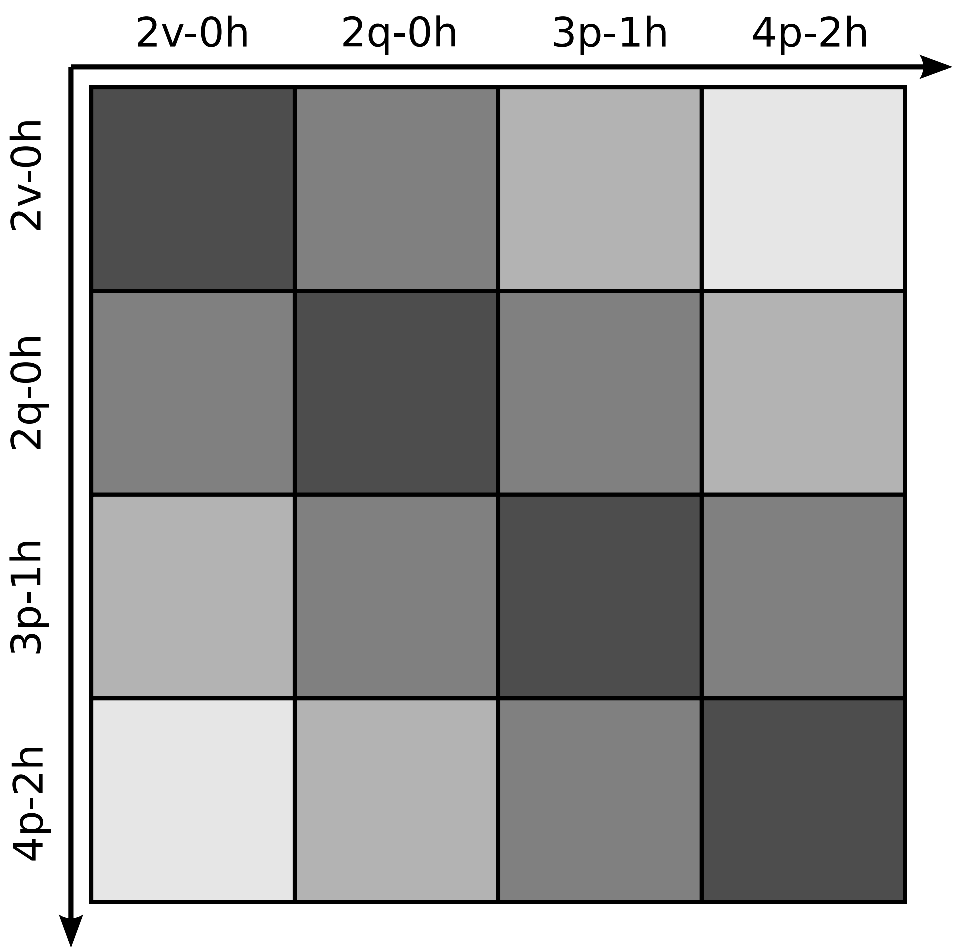
N. M. Parzuchowski, **S. R. Stroberg**, P. Navratil, H. H., S. K. Bogner, PRC **96**, 034324 (2017)

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, PRC93, 051301(R) (2016)

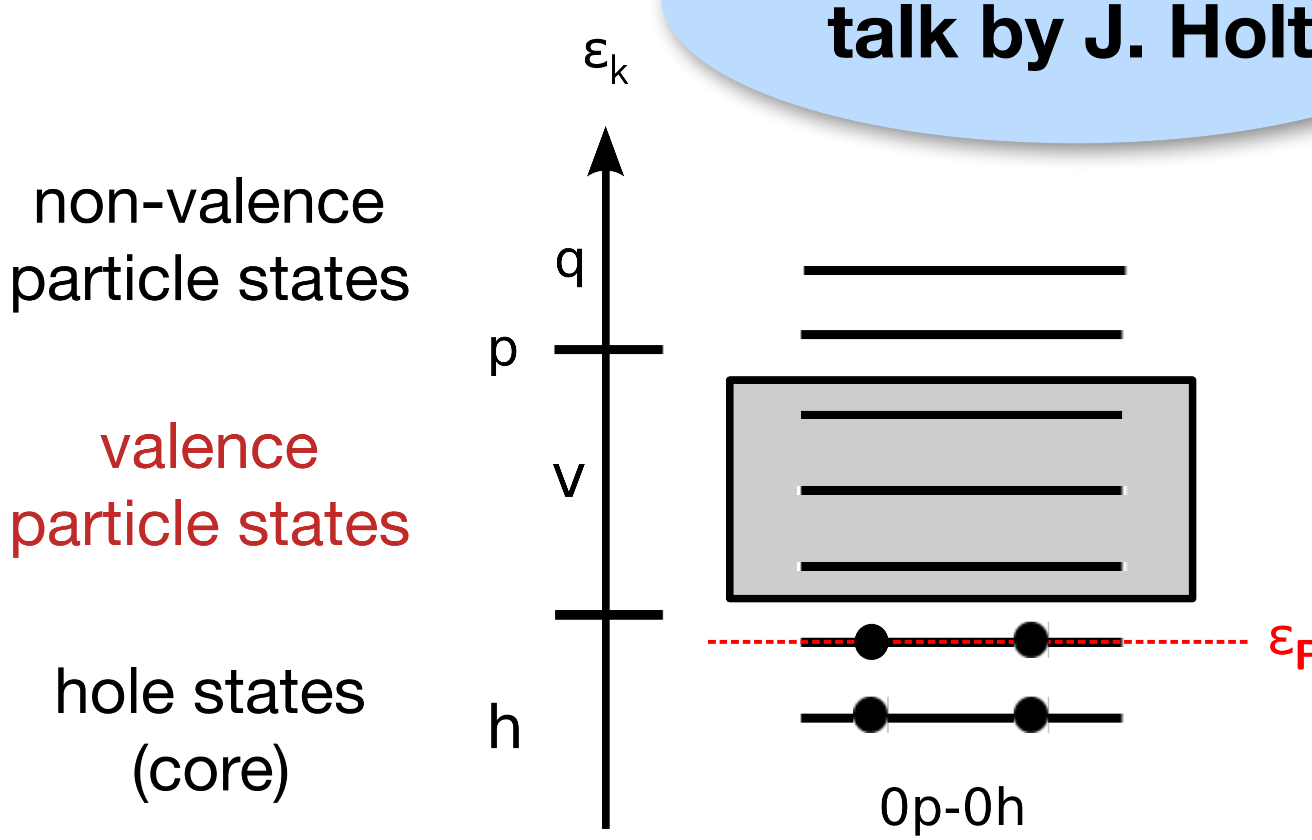
S. K. Bogner, H. H., J. D. Holt, A. Schwenk, S. Binder, A. Calci, J. Langhammer, R. Roth, Phys. Rev. Lett. 113, 142501 (2014)

Valence Space Decoupling

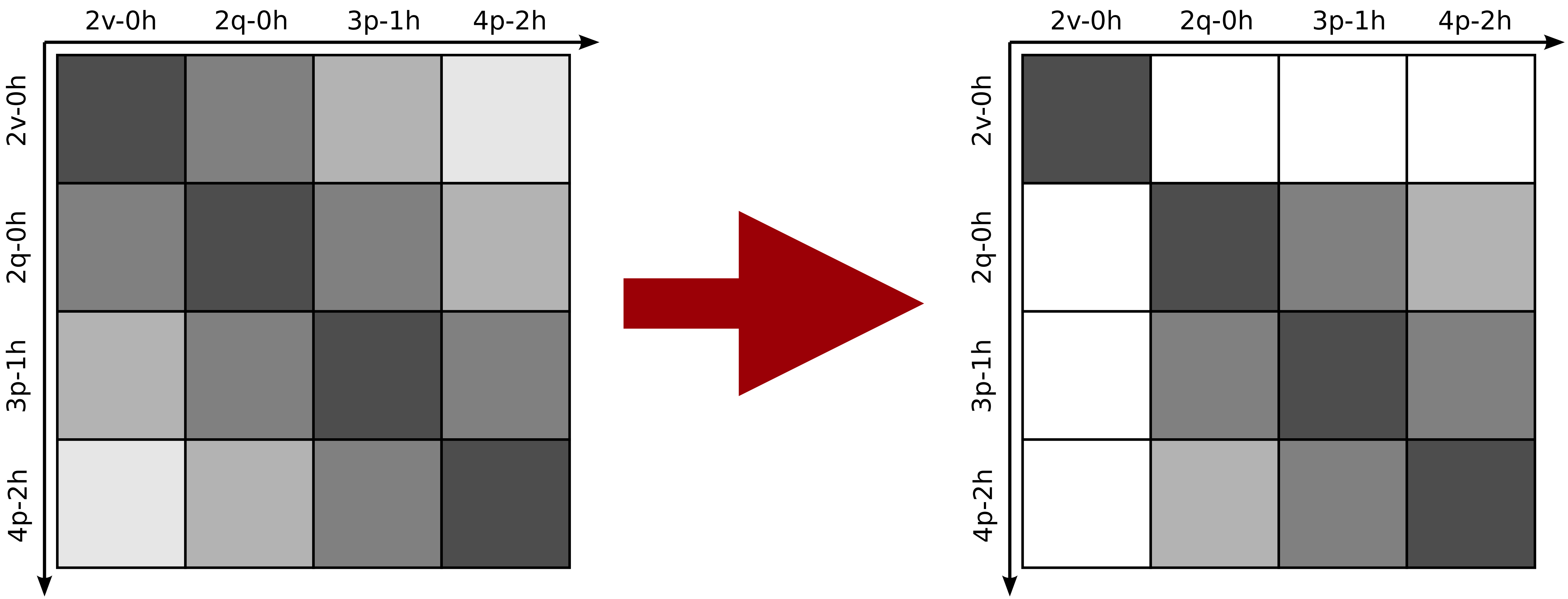


$\langle i | H | j \rangle$

also see talk by J. Holt



Valence Space Decoupling



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

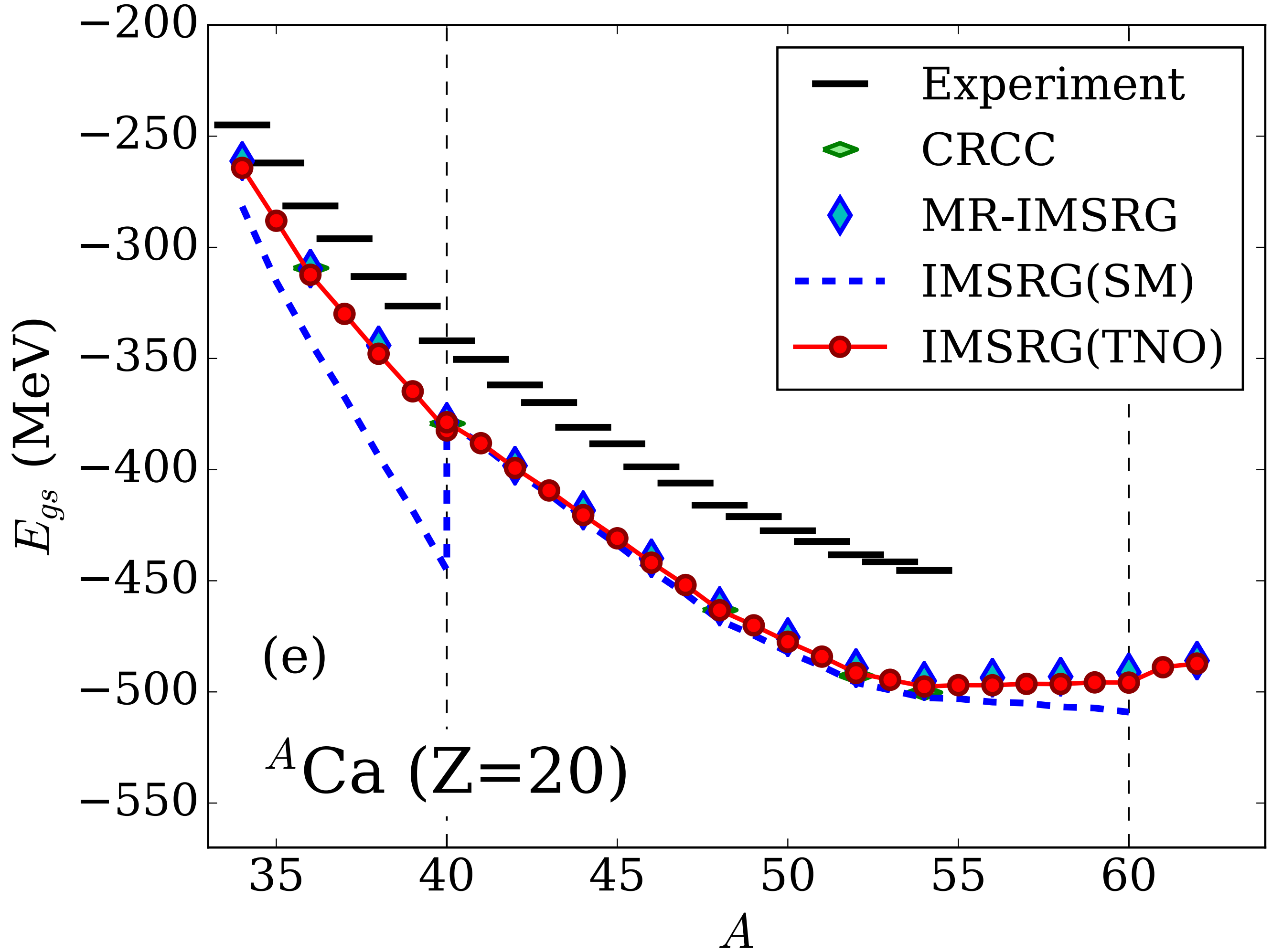
change definition of off-diagonal

$$\left\{ H^{od} \right\} = \{ f^{h}_{h'}, f^{p}_{p'}, f^{p}_{h}, f^{q}_{v}, \Gamma^{pp'}_{hh'}, \Gamma^{pp'}_{hv}, \Gamma_{vv'} \}$$

consistent interaction and DBD operator for Shell Model

Ground-State Energies

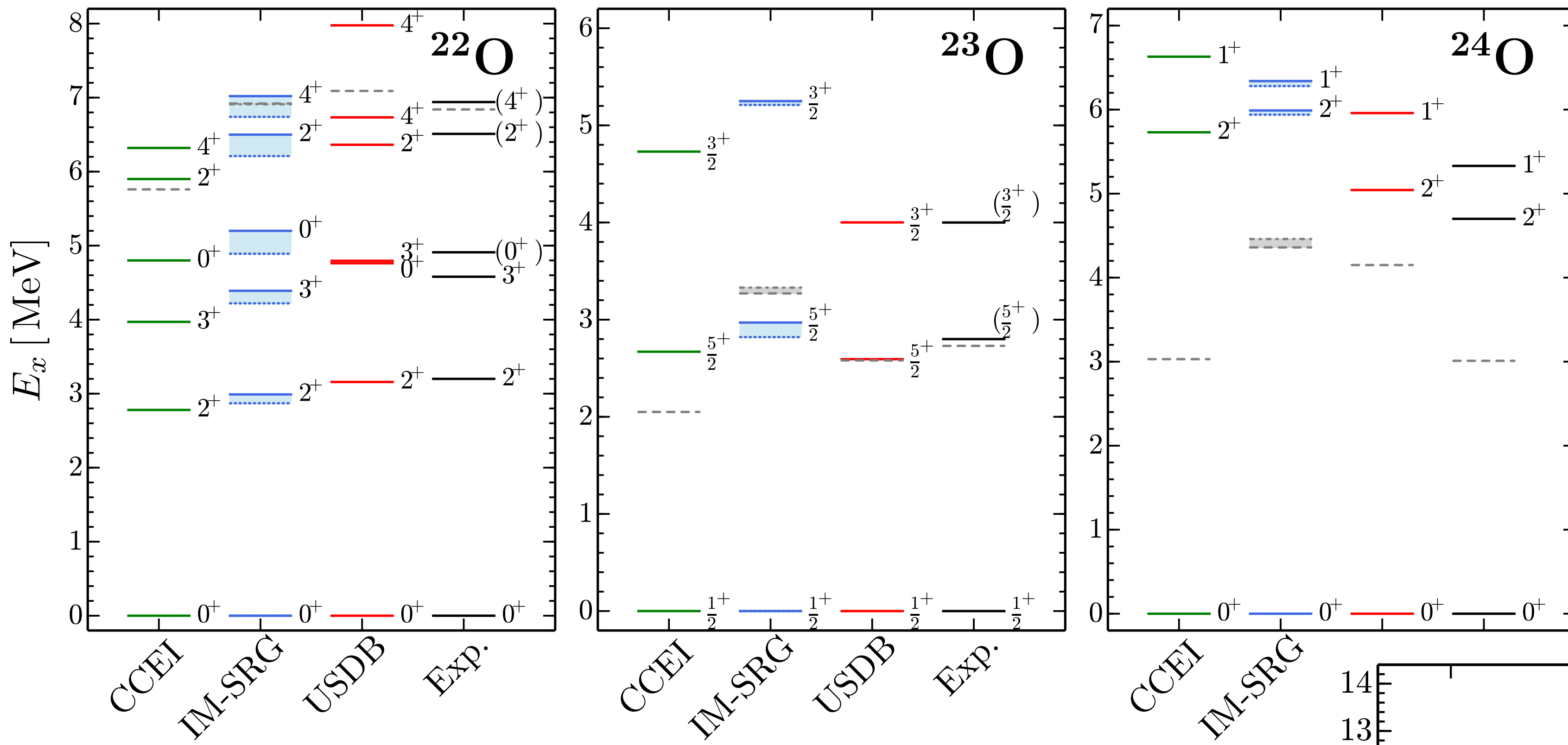
*S. R. Stroberg, A. Calci, HH, J. D. Holt, S. K.Bogner, R. Roth, A. Schwenk, PRL **118**, 032502 (2017)*

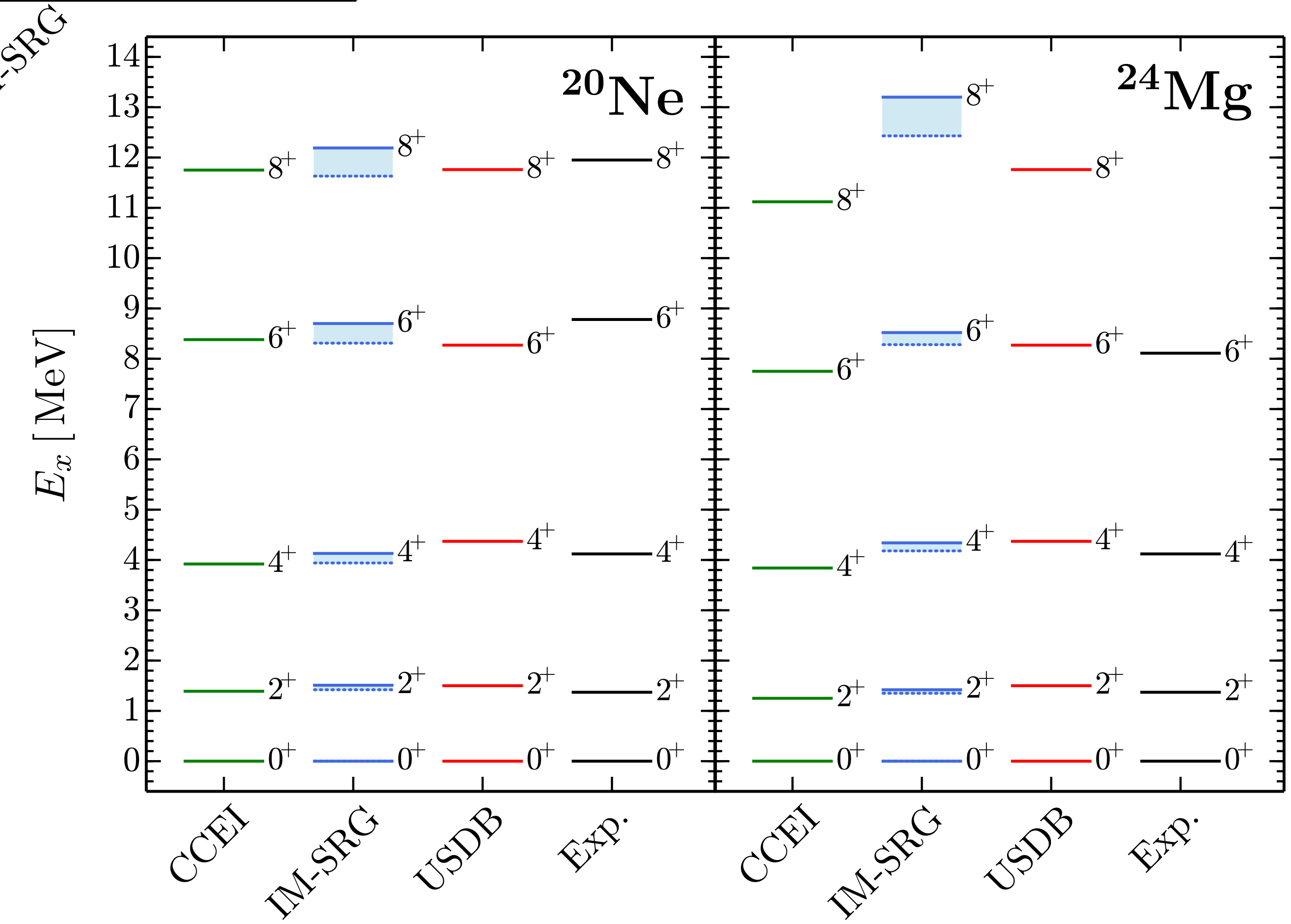


- (initial) normal ordering and IMSRG decoupling in the **target nucleus**
- **consistent with (MR-)IMSRG ground state energies** (and CC, SCGF, …) for the **same Hamiltonian**

Excitation Spectra

*S. K. Bogner et al., PRL **113**, 142501 (2014), S. R. Stroberg et al., PRC **93**, 051301(R) (2016)*





sd-shell spectra agree very well with experiment and USDA/B…

… for NN+3N(400) with c_D = -0.2.

Equations-of-Motion for Excitations

N. M. Parzuchowski, T. D. Morris, S. K. Bogner, PRC 95, 044304 (2017)

- describe **excited states** based on ground state:

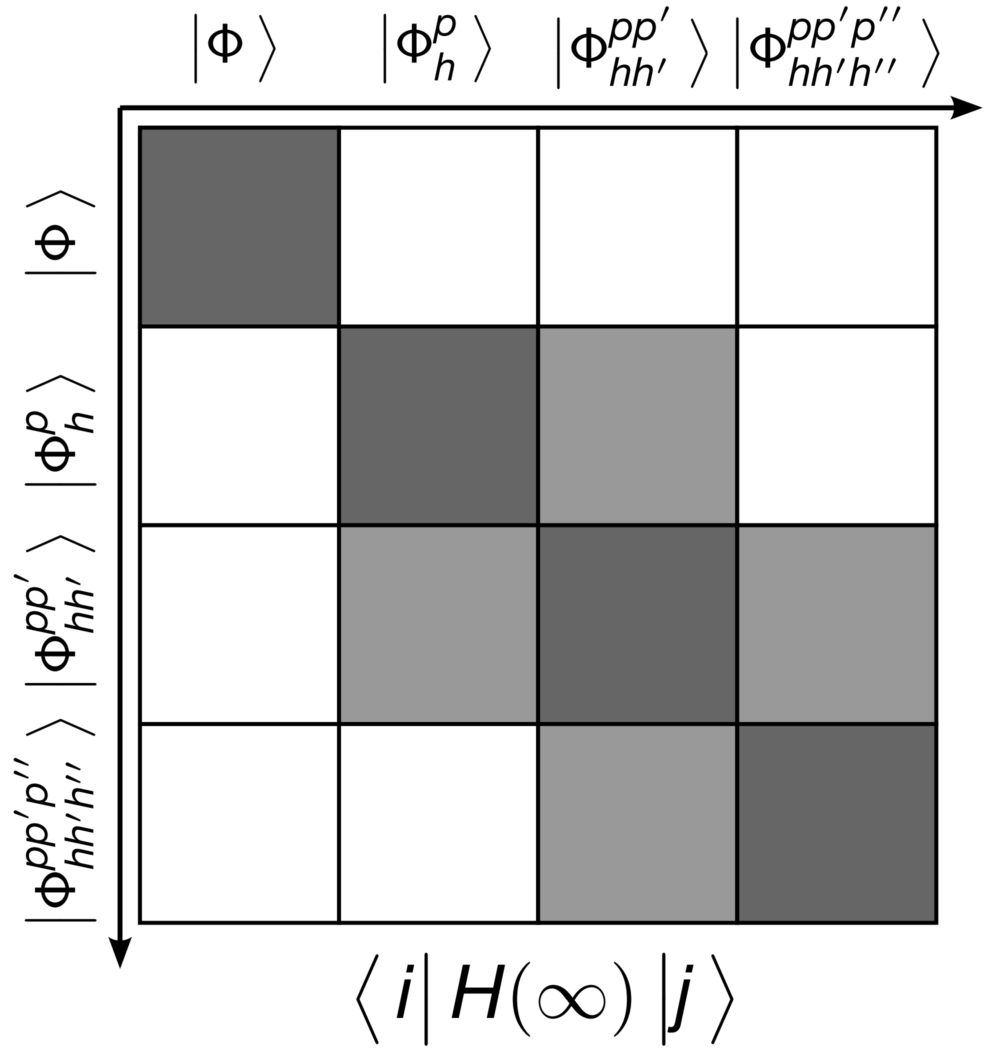
$$\left|\Psi_k\right\rangle \equiv R_k \left|\Psi_0\right\rangle$$

- apply **IMSRG transformation**:

$$U(s)\left|\Psi_k\right\rangle = U(s) R_k U^\dagger(s) U(s)\left|\Psi_0\right\rangle = R_k(s)\left|\Phi\right\rangle$$

- ansatz for excitation operator:

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

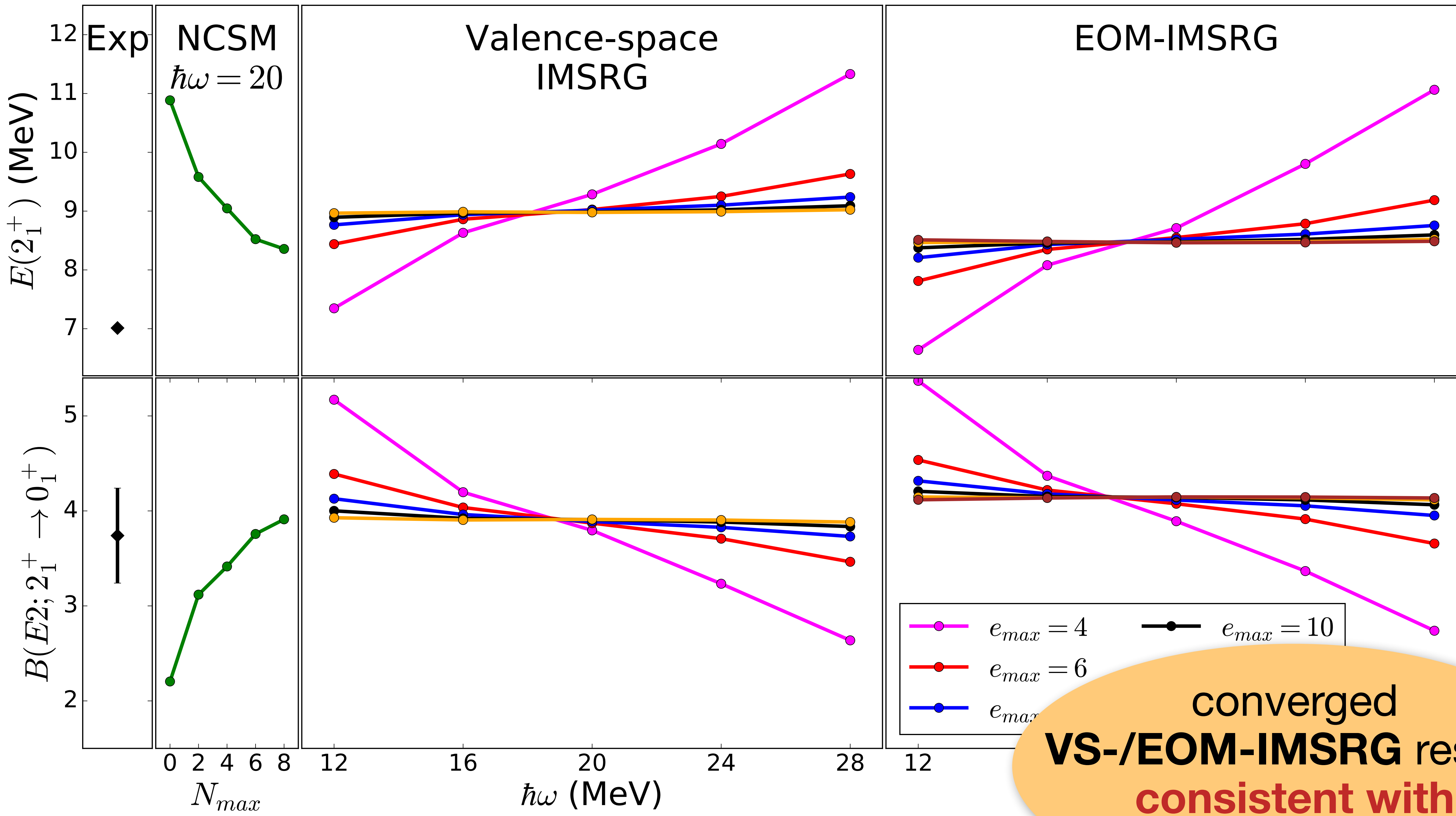


- solve EoM by diagonalization (**polynomial effort**):

$$\left[H(s), R_k(s)\right] = \omega_k R_k(s), \quad \omega_k = E_k - E_0$$

E2 Transitions

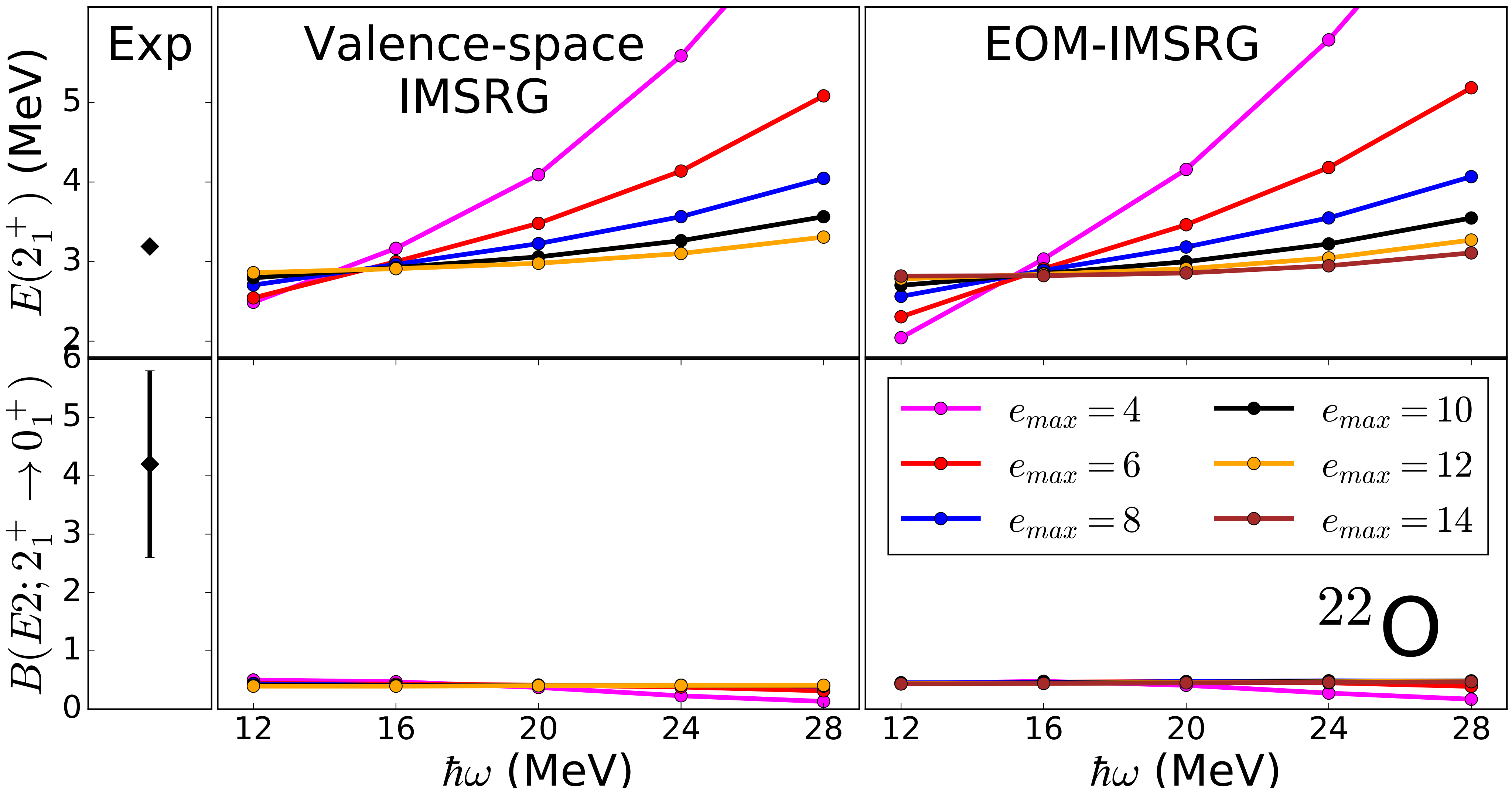
N. M. Parzuchowski, S. R. Stroberg, P. Navratil, HH, S. K. Bogner, PRC 96, 034324 (2017)



converged
VS-/EOM-IMSRG results
consistent with NCSM

E2 Transitions

N. M. Parzuchowski, S. R. Stroberg, P. Navratil, HH, S. K. Bogner, PRC 96, 034324 (2017)

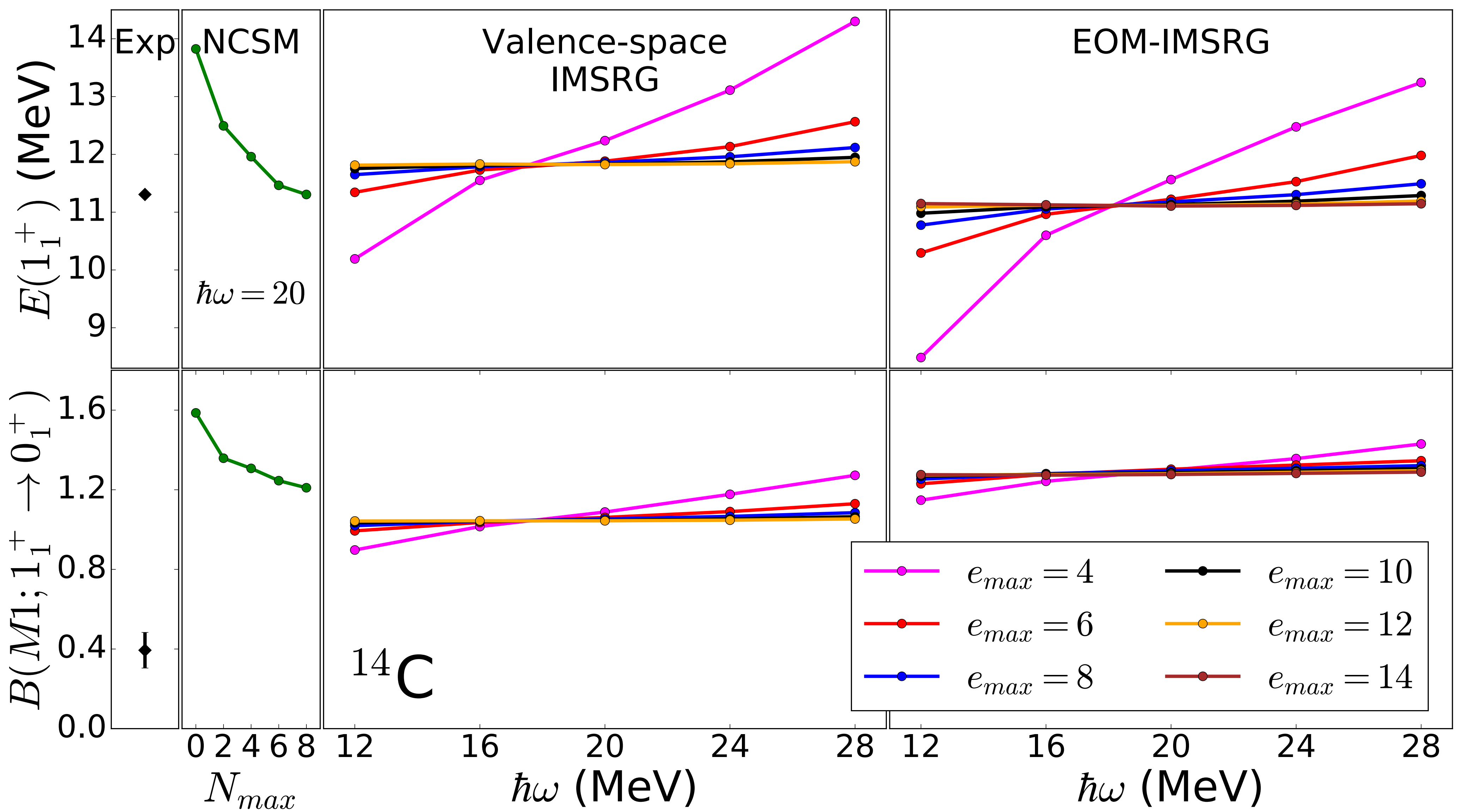


- non-zero B(E2) from Shell model: **VS-IMSRG induces effective neutron charge**
- **B(E2) much too small:** effect of intermediate 3 states that are truncated in IMSRG evolution

MR-IMSRG + EOM, CI, ...

M1 Transitions

N. M. Parzuchowski, S. R. Stroberg, P. Navratil, HH, S. K. Bogner, PRC 96, 034324 (2017)



- M1 transitions **consistent** between methods, but **generally too large** - include currents in initial operator

Epilogue

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

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NERSC

NSF

NUCLEI
Nuclear Computational Low-Energy Initiative

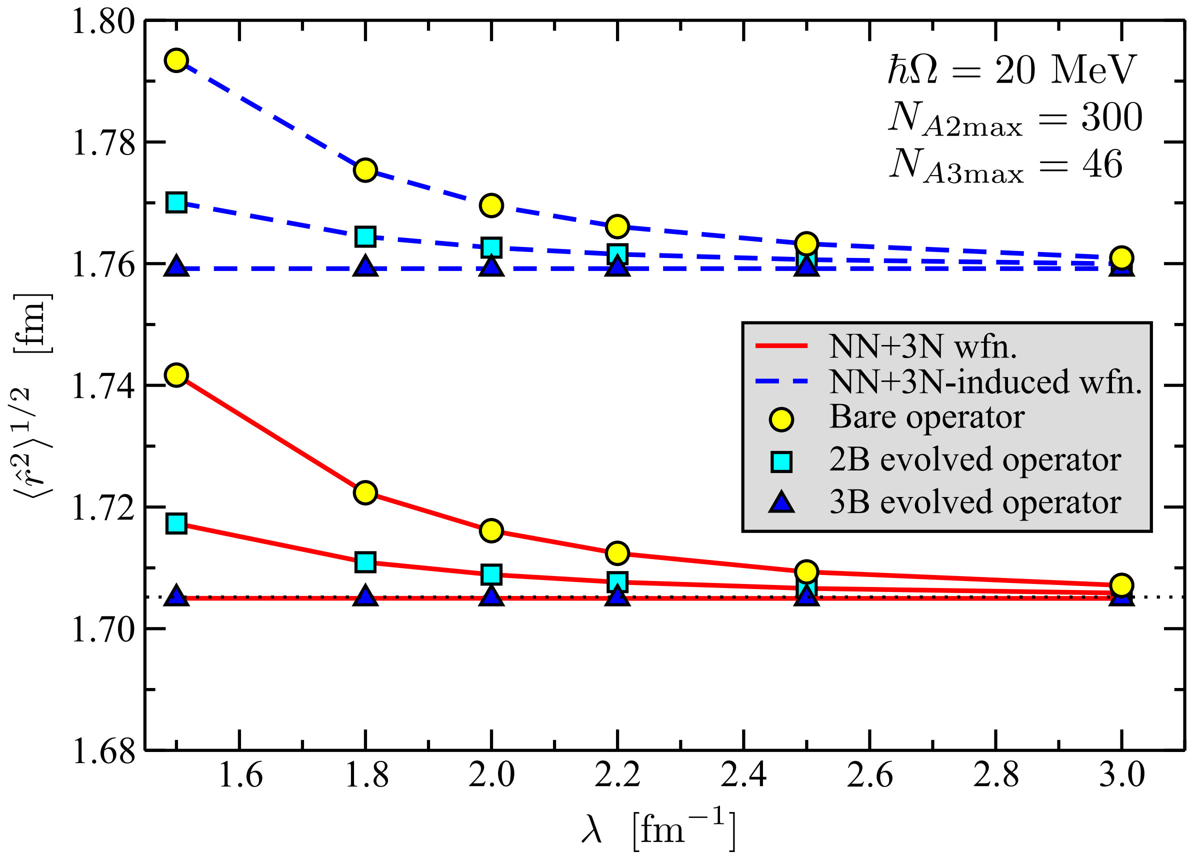
Ohio Supercomputer Center

ICER

Supplements

Free-Space Evolution of Operators

^{3}H rms matter radius

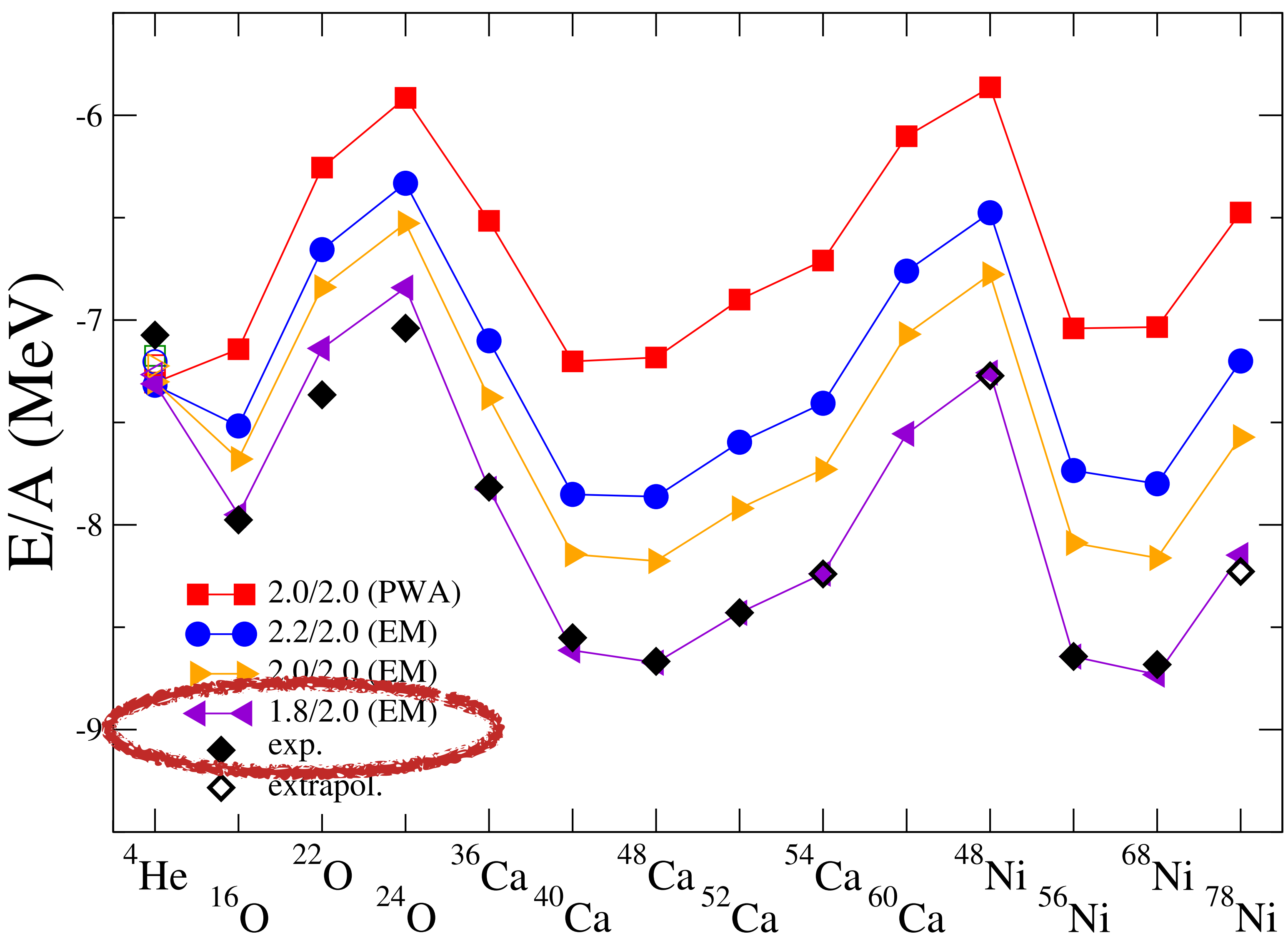


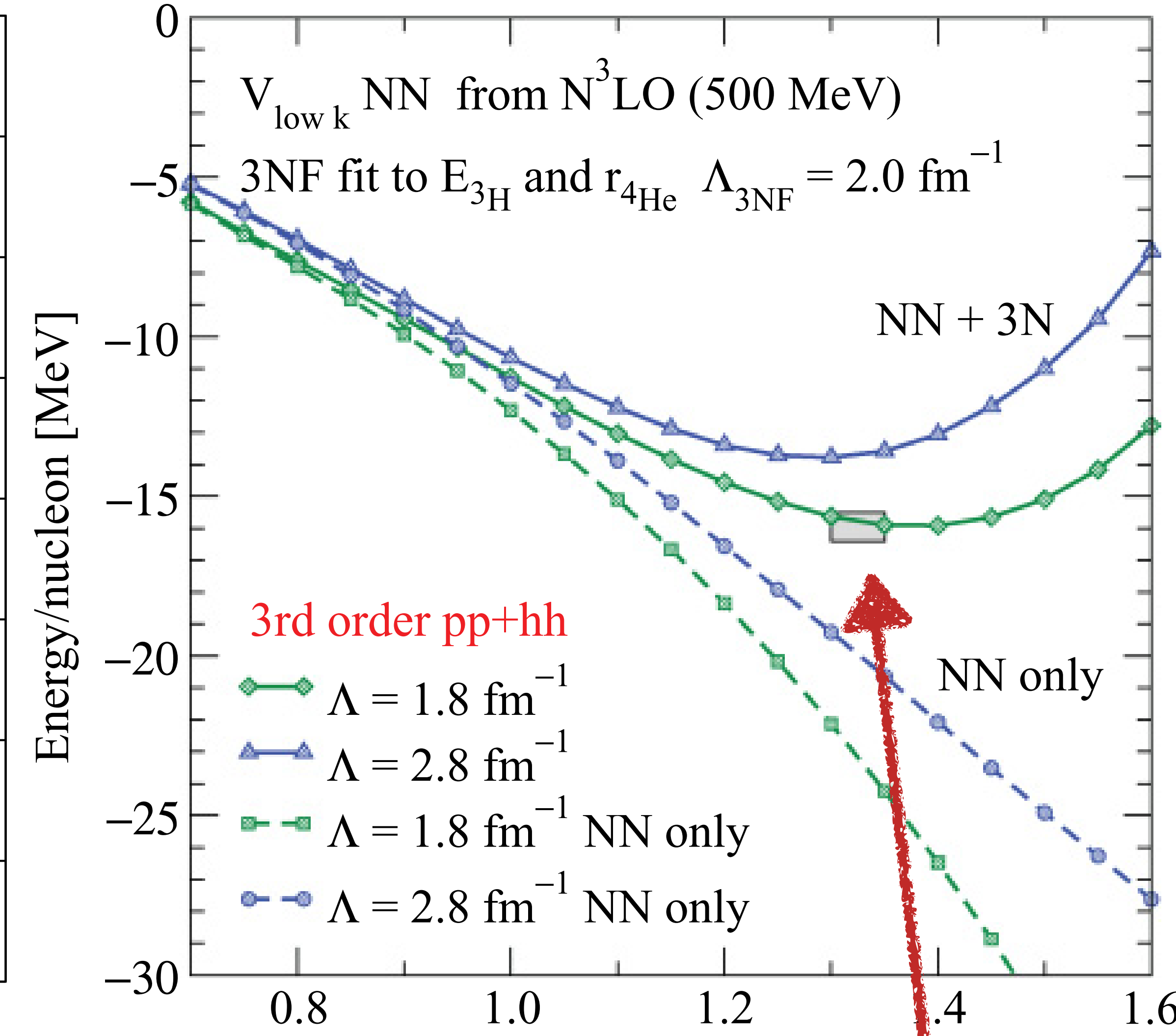
from: Schuster et al., PRC90, 011301 (2014)

- derive operators from chiral EFT, including currents
- optimize LECs together with interaction
- evolve to desired resolution scale
- evaluate operator (1B+2B +...) in IM-SRG (and Shell Model)
- (most) existing ab initio & Shell model codes lack capabilities for many-body observables

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

Hebeler et al., PRC83, 031301