Improved medium-mass nuclear structure and responses with the IMSRG

Matthias Heinz

*with **Tom Plies**, Jan Hoppe, Frederic Noël, Takayuki Miyagi, Alexander Tichai, Kai Hebeler, Martin Hoferichter, Ragnar Stroberg, Achim Schwenk*

TRIUMF

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The IMSRG

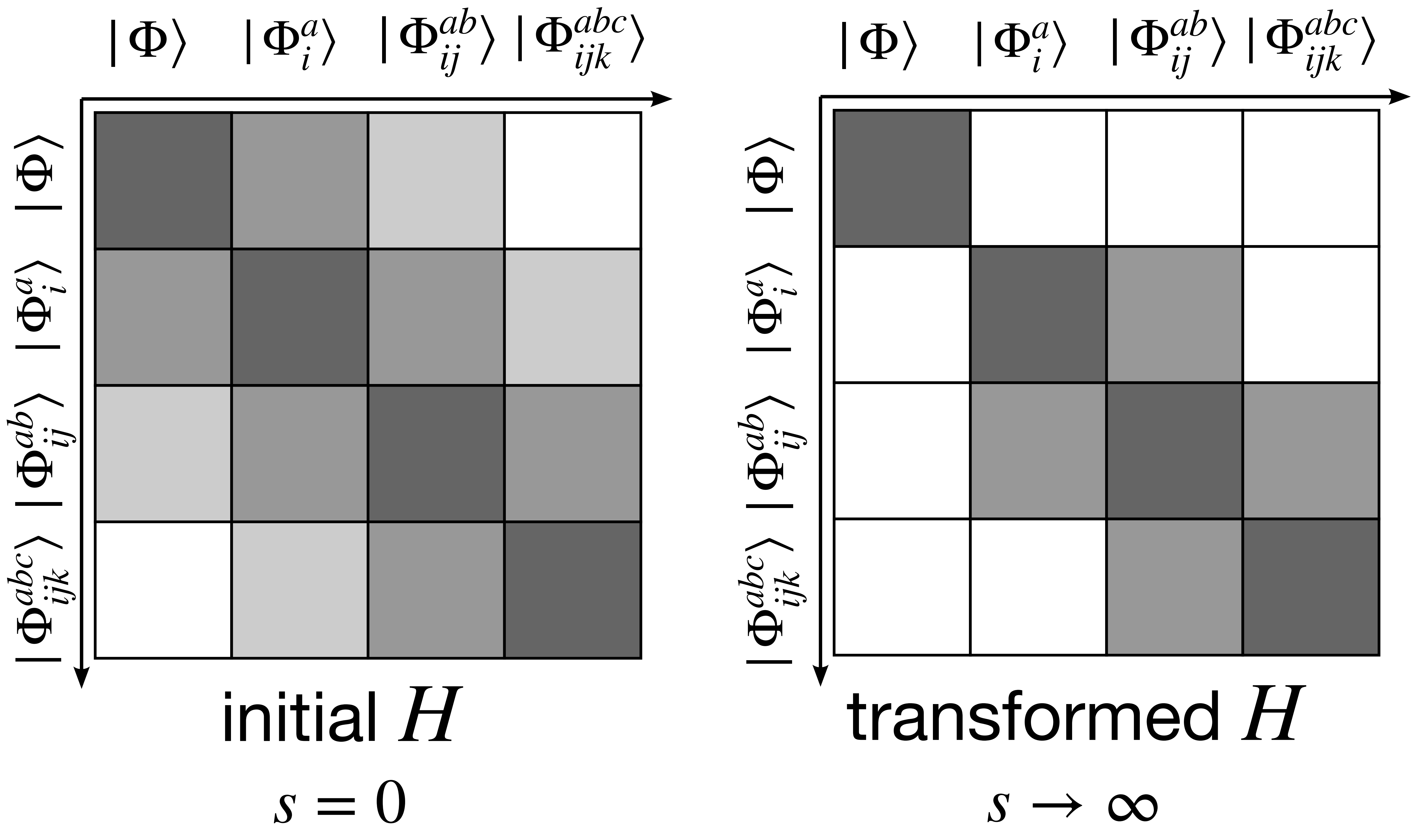
in-medium similarity renormalization group

- IMSRG generates unitary transformation of Hamiltonian

$$\frac{dH}{ds} = [\eta, H]$$

- Normal order with respect to $|\Phi\rangle$ approximately handles **3N forces** and **induced many-body forces**

Tsukiyama et al., PRL **106** (2011)
Hergert et al., Phys. Rep. **621** (2016)



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- Obtain $\overline{H} = UHU^\dagger$ with $|\Psi\rangle = U|\Phi\rangle = e^{\Omega}|\Phi\rangle$ and $\Omega = \Omega_1 + \Omega_2 + \ldots$

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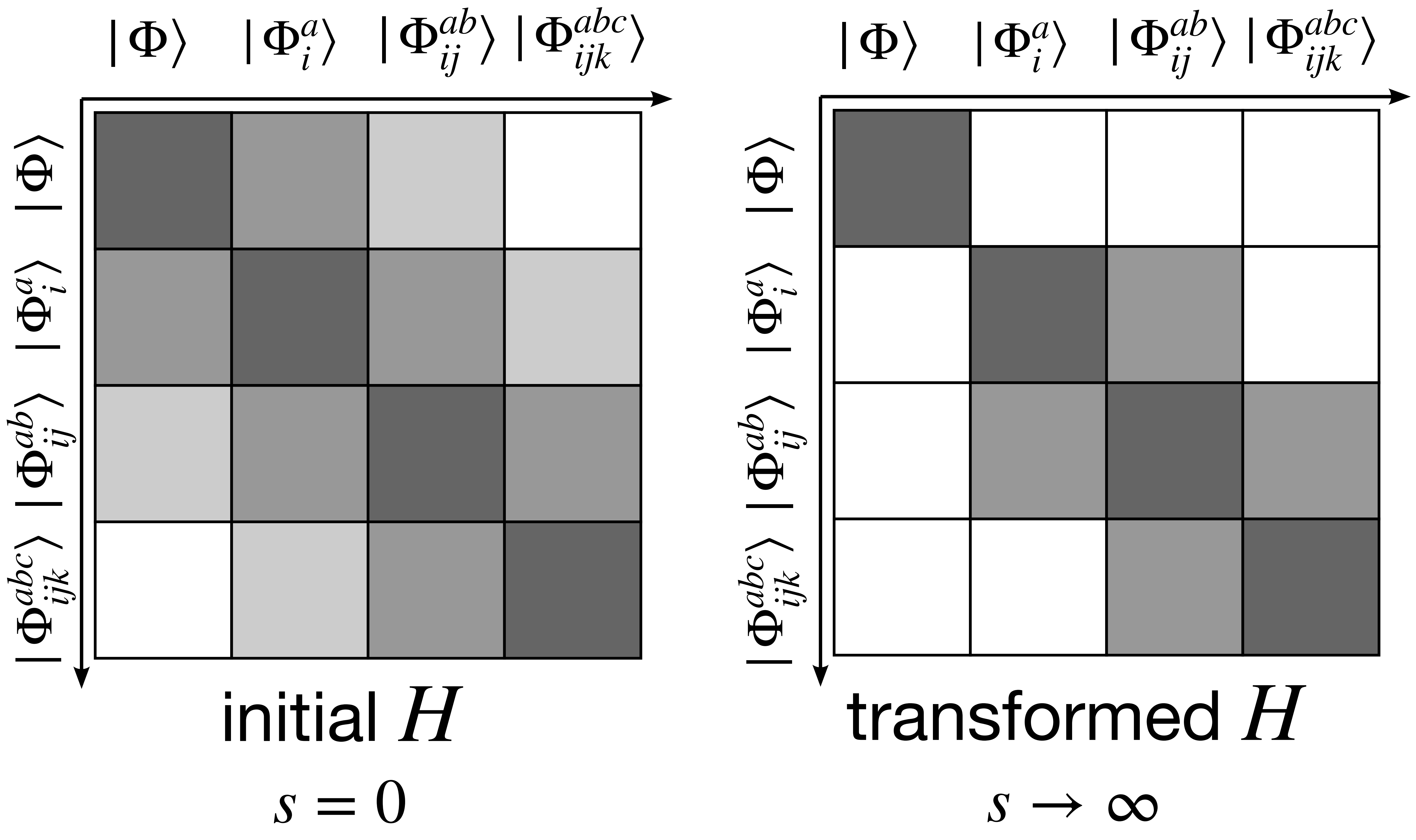

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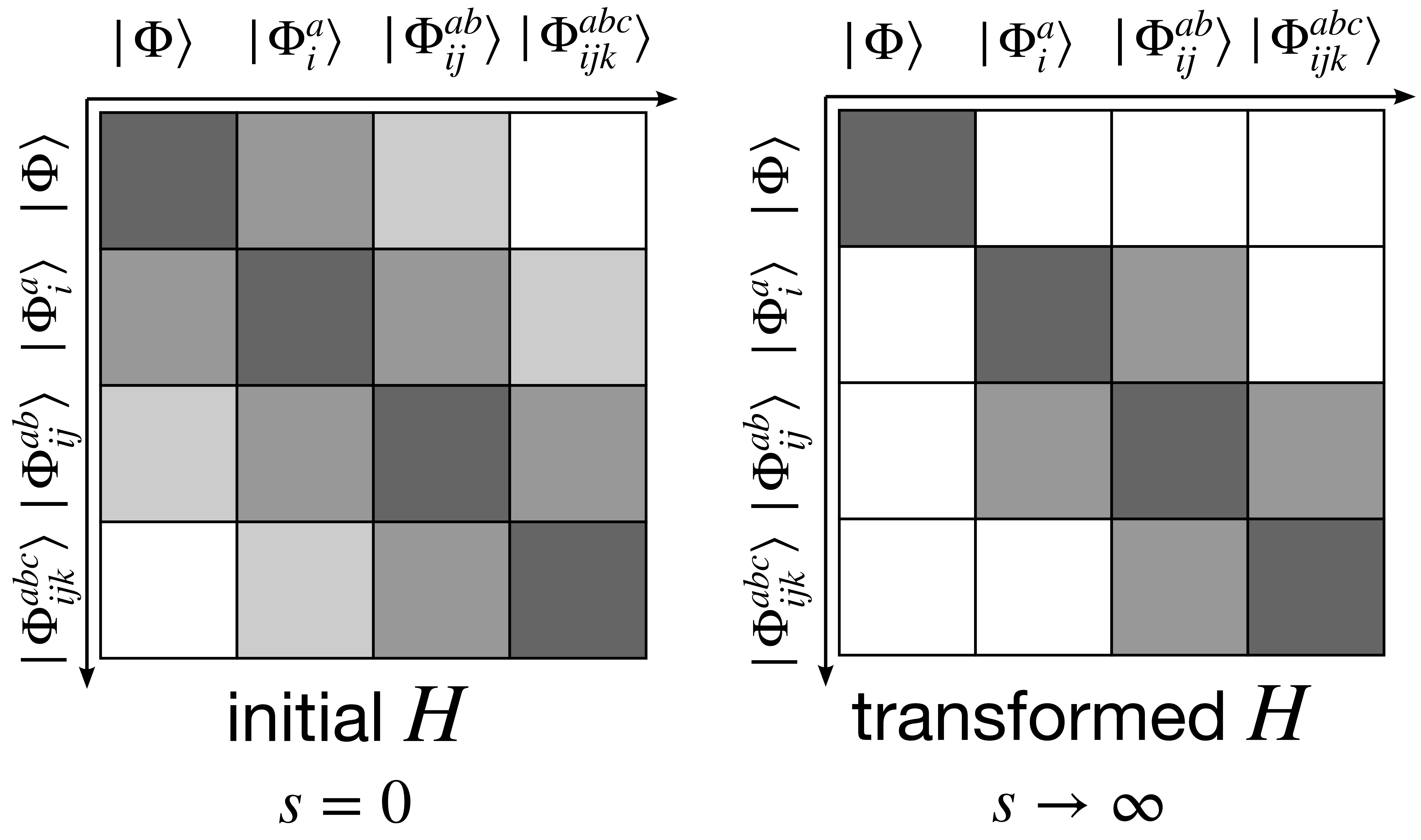
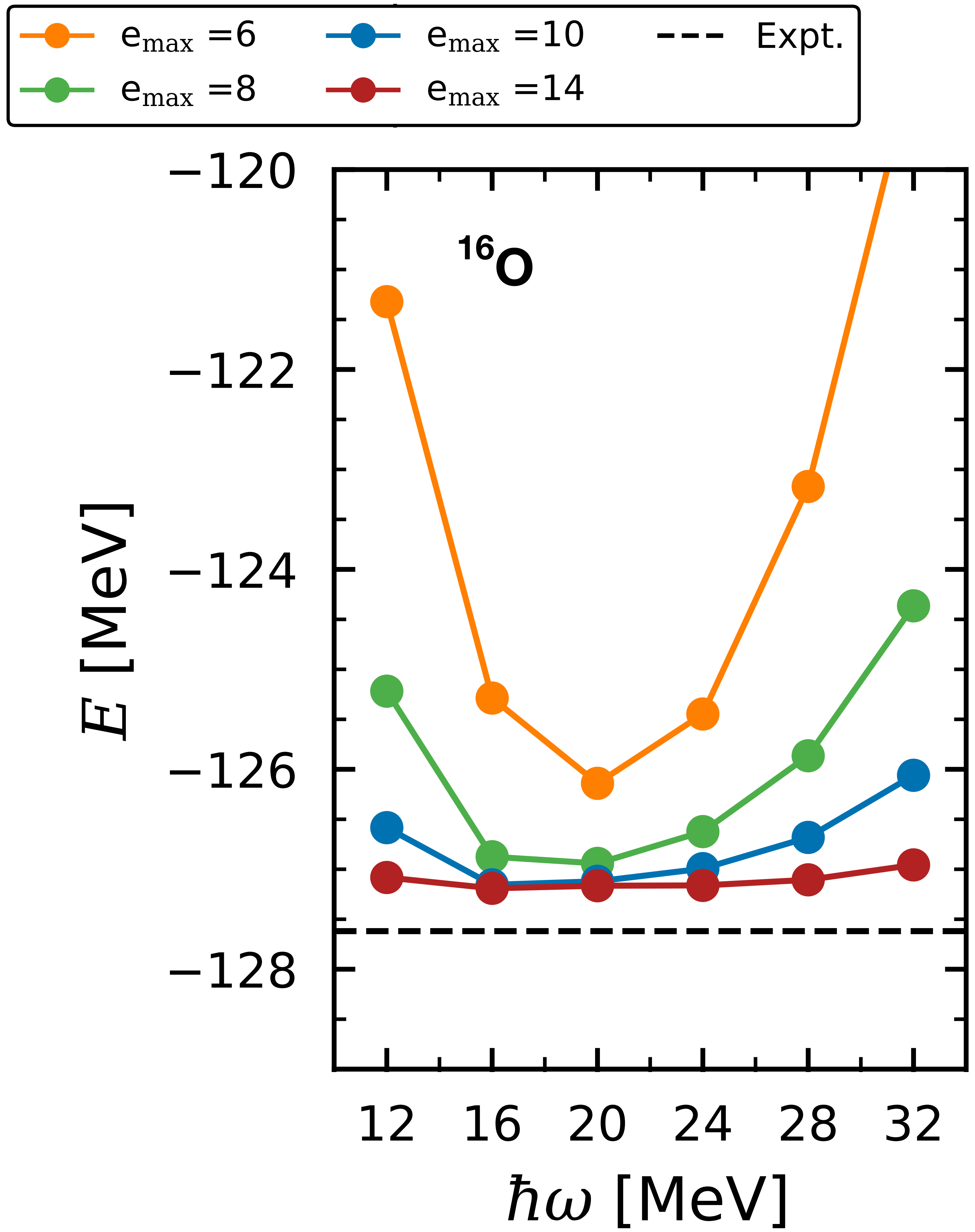


Hergert et al., Phys. Rep. **621** (2016)

Truncation necessary!
- Standard = IMSRG(2)
- More refined = **IMSRG(3)**

MH et al., PRC **103** (2021)

IMSRG ingredients



Hoppe, **MH**, et al., PRC **103** (2021)

1. Input Hamiltonian H
2. Solve for mean field (Hartree-Fock, NAT)
   - Input dependence: H, e_{max}, $E_{3\mathrm{max}}$, $\hbar\omega$
   - Output: reference state $|\Phi\rangle$, basis $\{\phi_p\}$
3. Solve for many-body correlations [IMSRG(2)/(3)]
   - Input dependence: $\underbrace{H, |\Phi\rangle}_{\text{normal ordering}}$, $\{\phi_p\}$, other ops ...

     normal ordering
     Hebeler, **MH**, et al., PRC **107** (2023)
   - Output: $|\Psi\rangle$, E, expectation values of ops ...

The commutator core of the IMSRG

$$[A^{(K)}, B^{(L)}] = \sum_M C^{(M)}$$

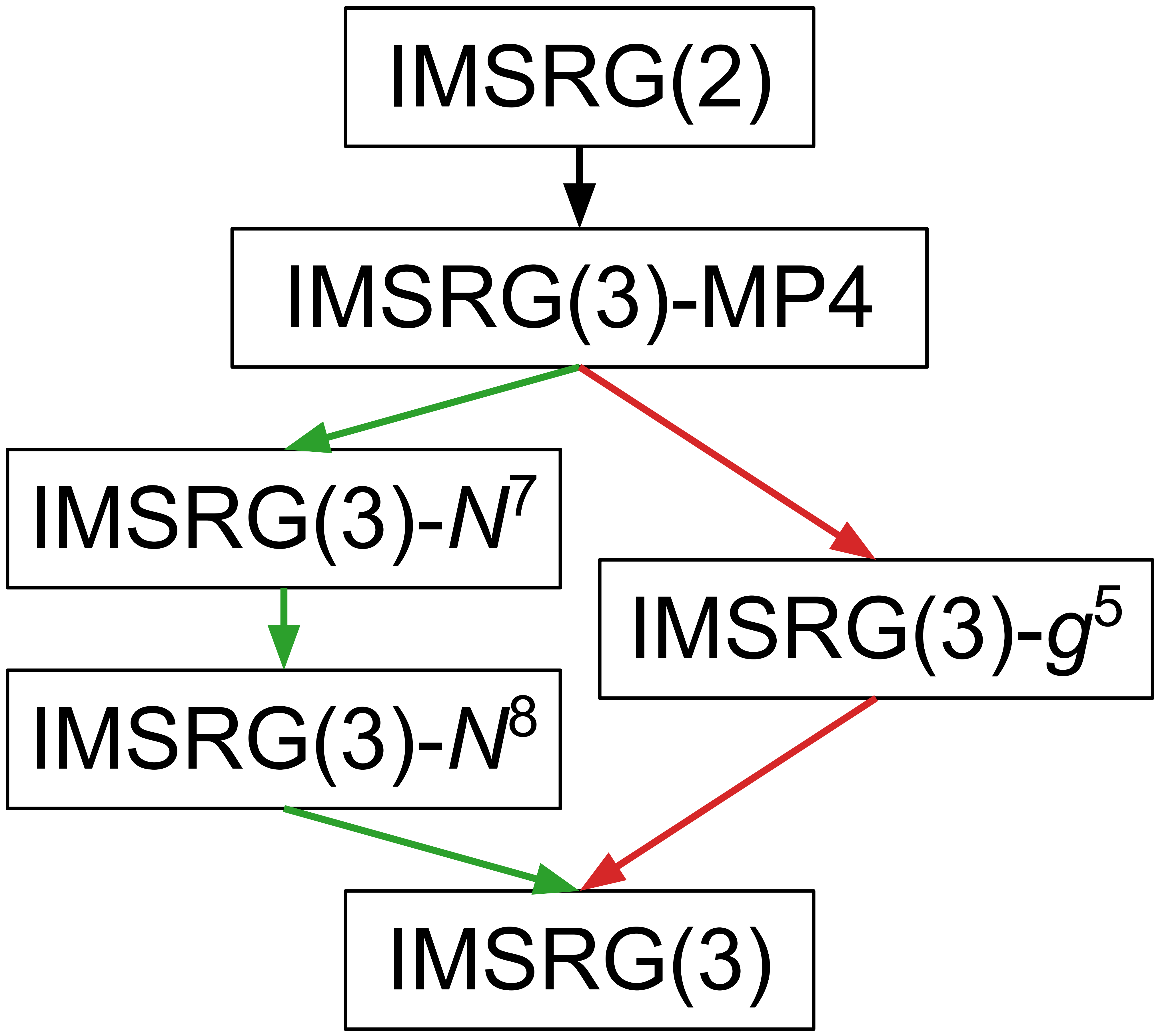
- Normal-ordered commutator induces many-body operators

  See talk by Ragnar Stroberg next

- Fundamental commutator $[A^{(K)}, B^{(L)}]^{(M)} = C^{(M)}$ with cost $\mathcal{O}(N^{K+L+M})$

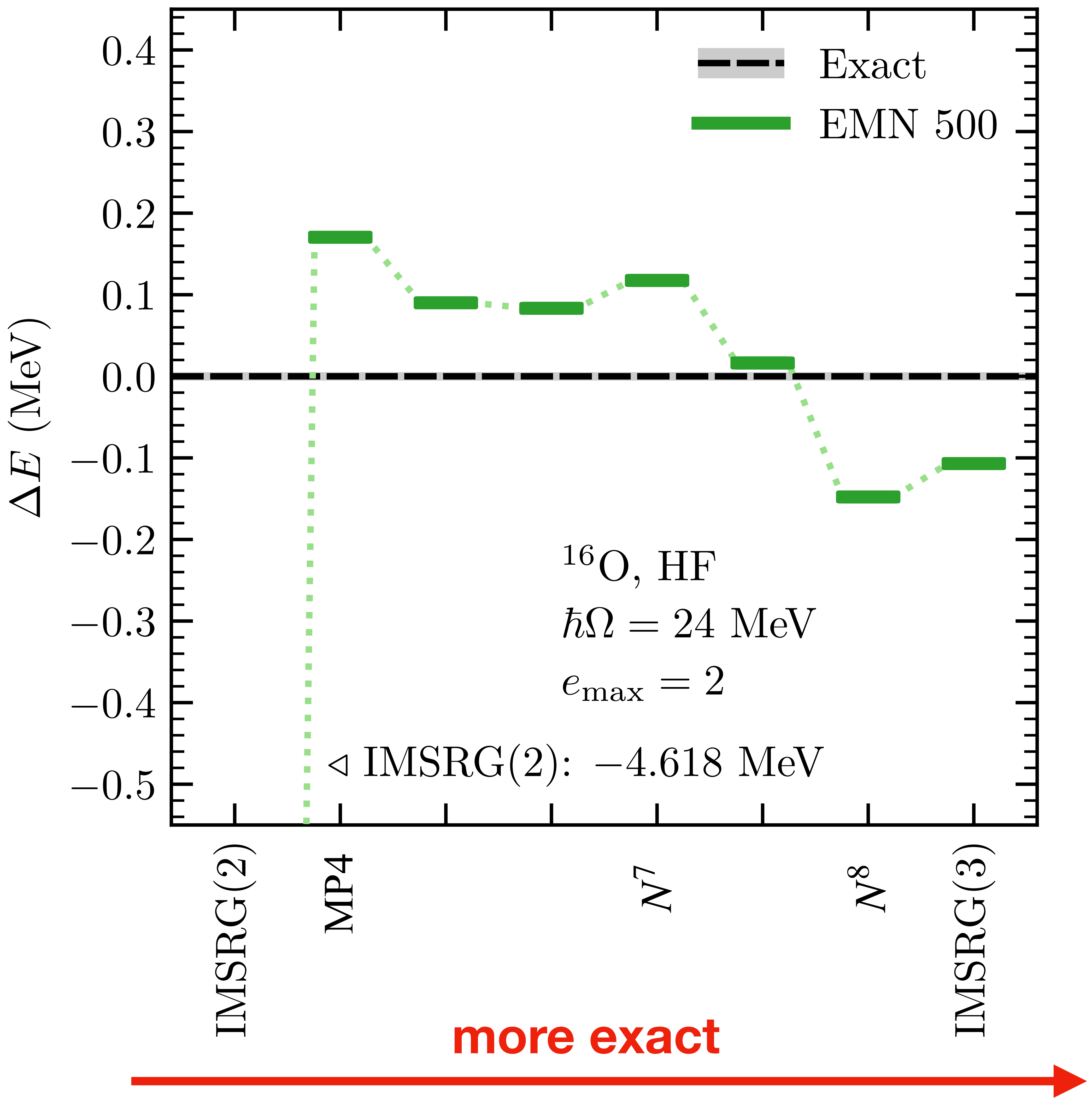
- IMSRG(3): 7 → 17 terms

- Organize based on **computational cost** and **perturbative importance**



MH et al., PRC **103** (2021)

The IMSRG(3) difference



MH et al., PRC **103** (2021)

- IMSRG(3) = next order in many-body expansion
- **Systematic improvement** towards exact results
- Benefit greatest for very nonperturbative problems
- **Excellent precision** on energies

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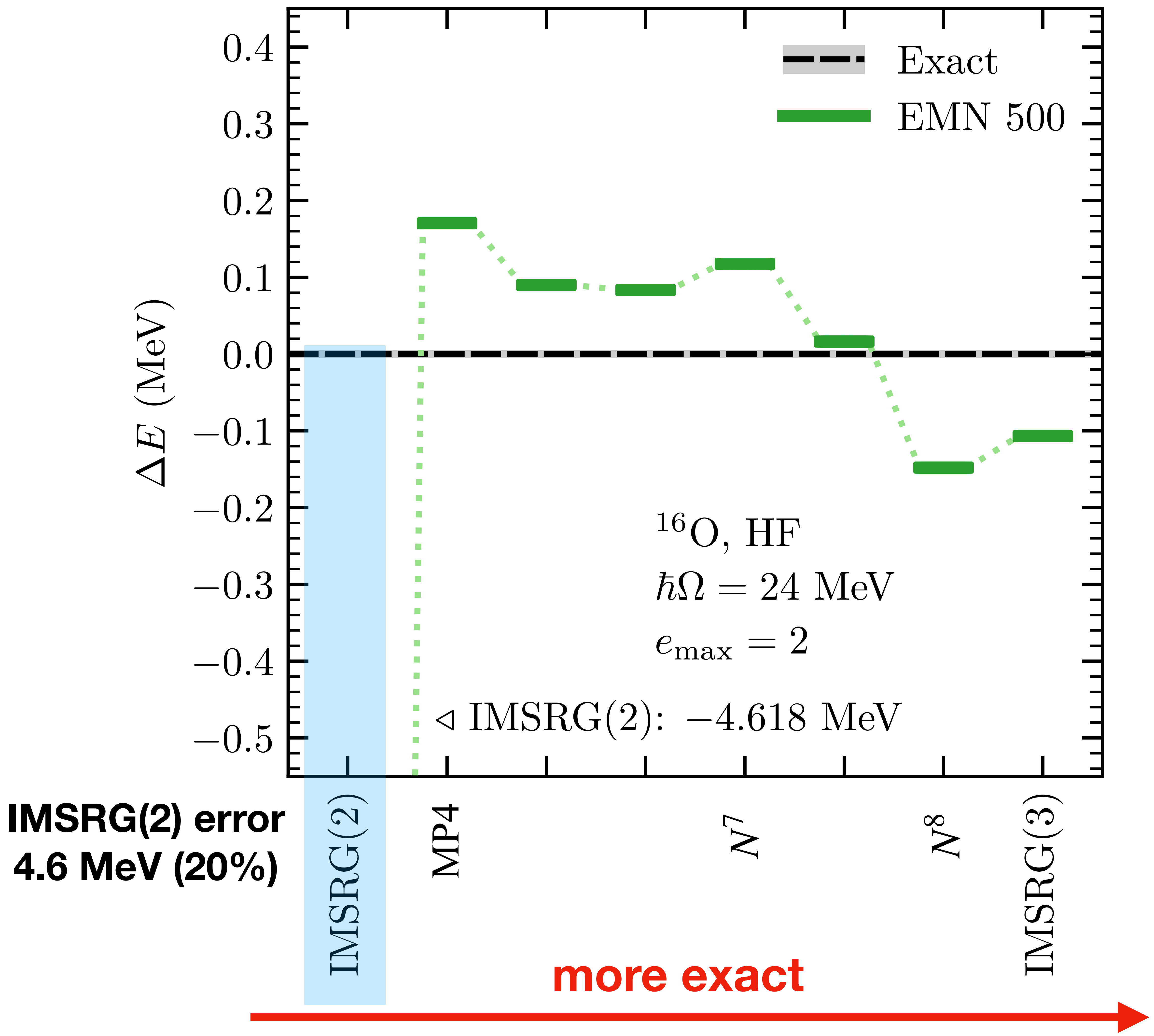

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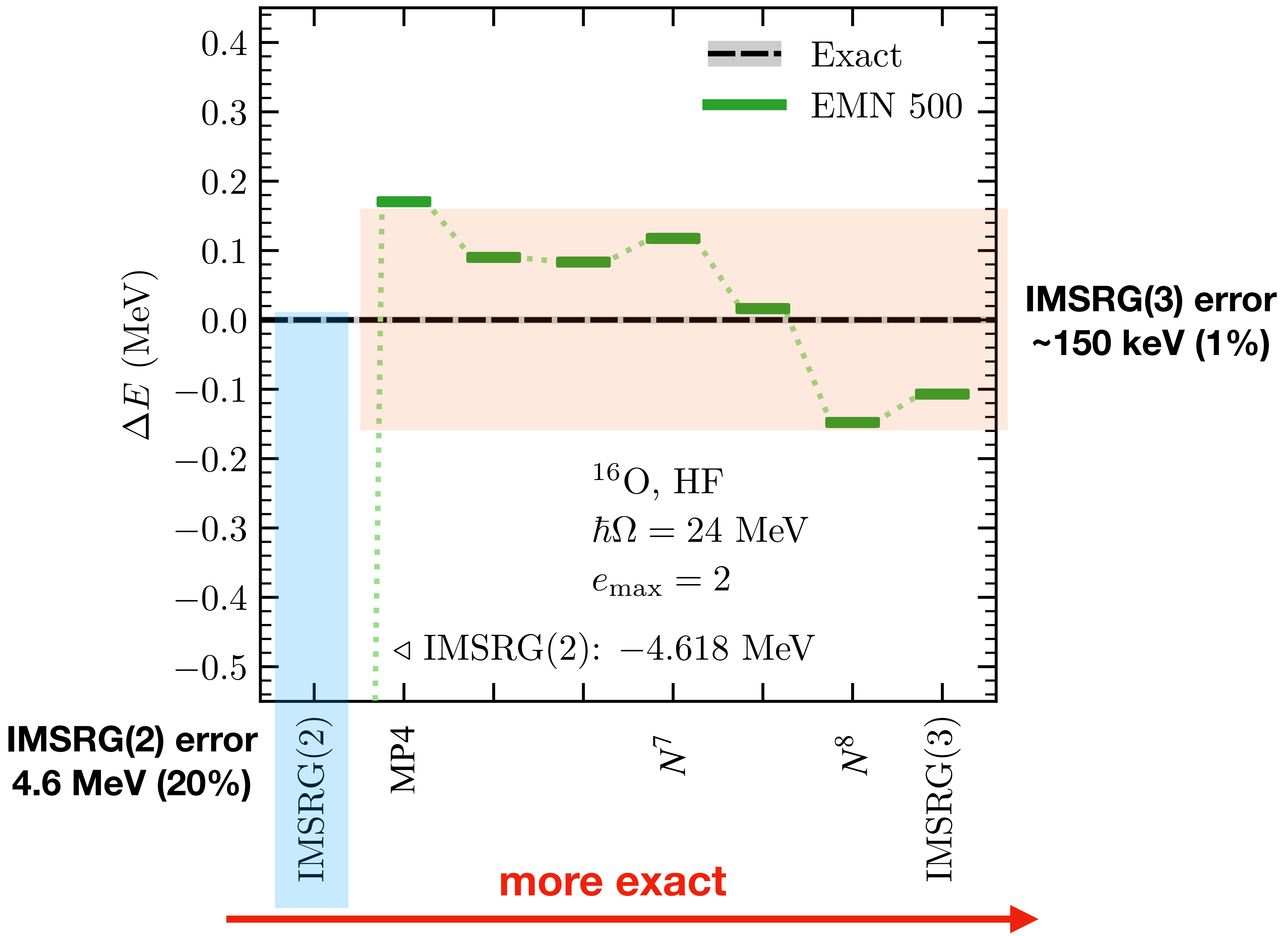

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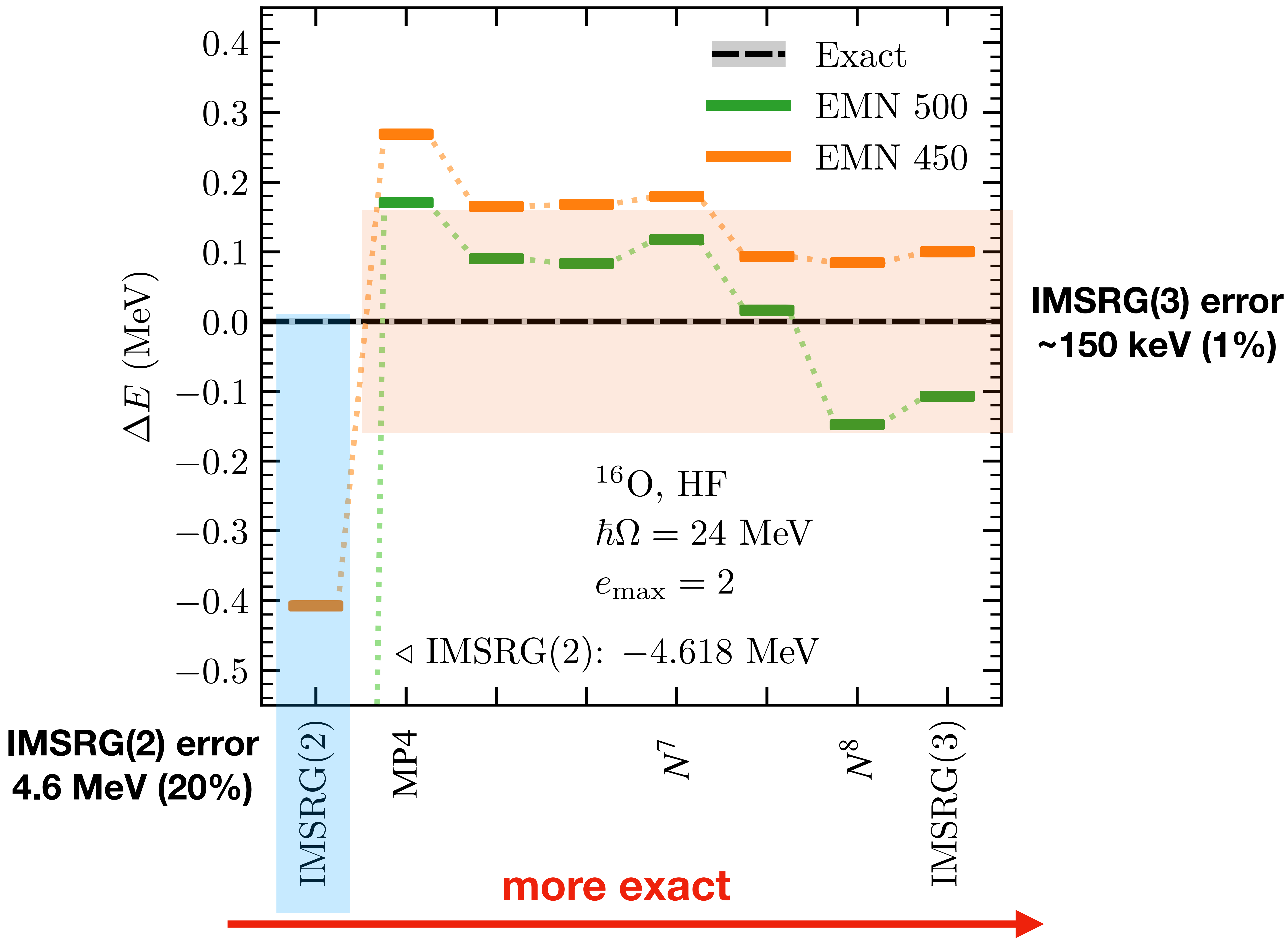

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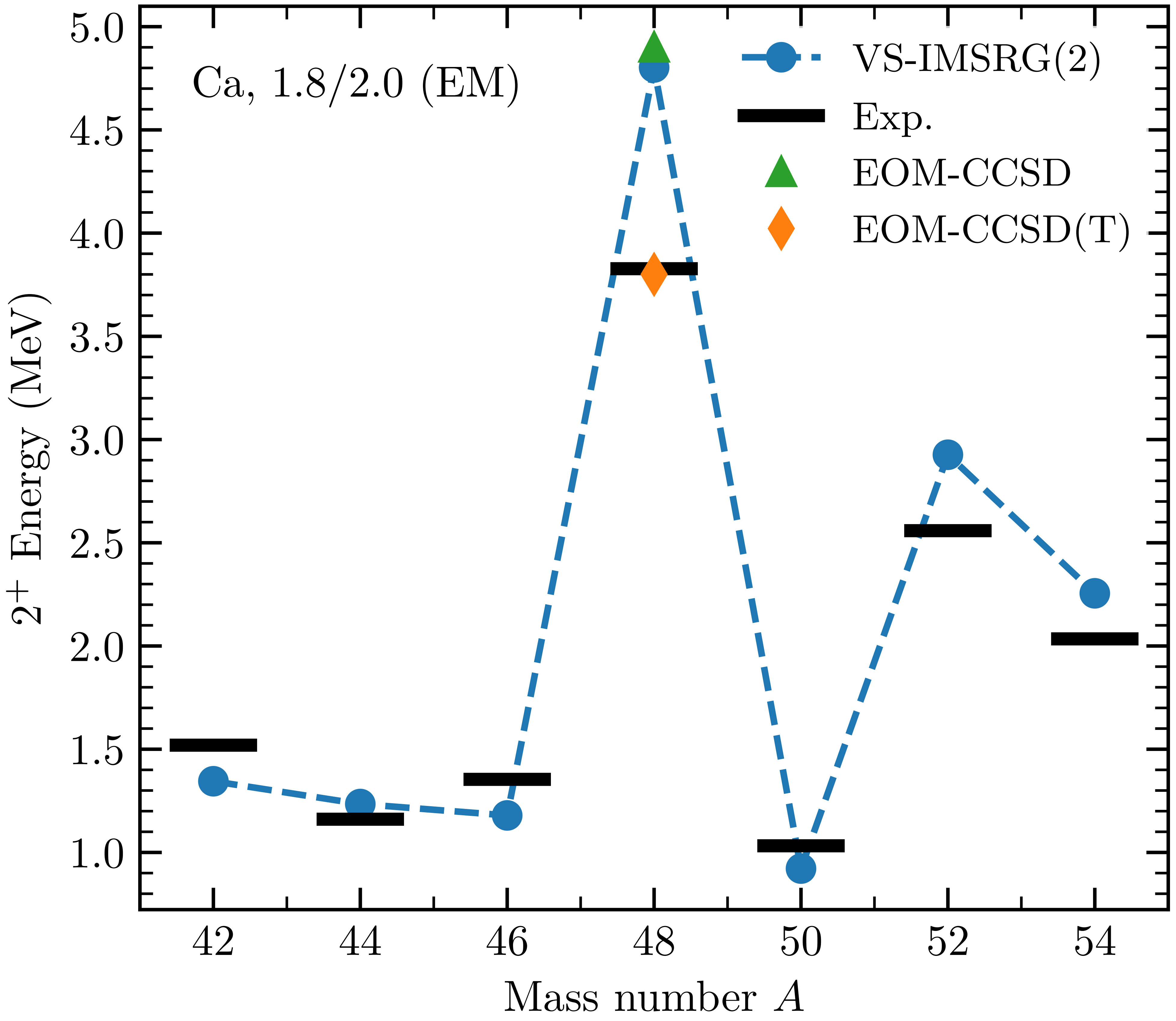
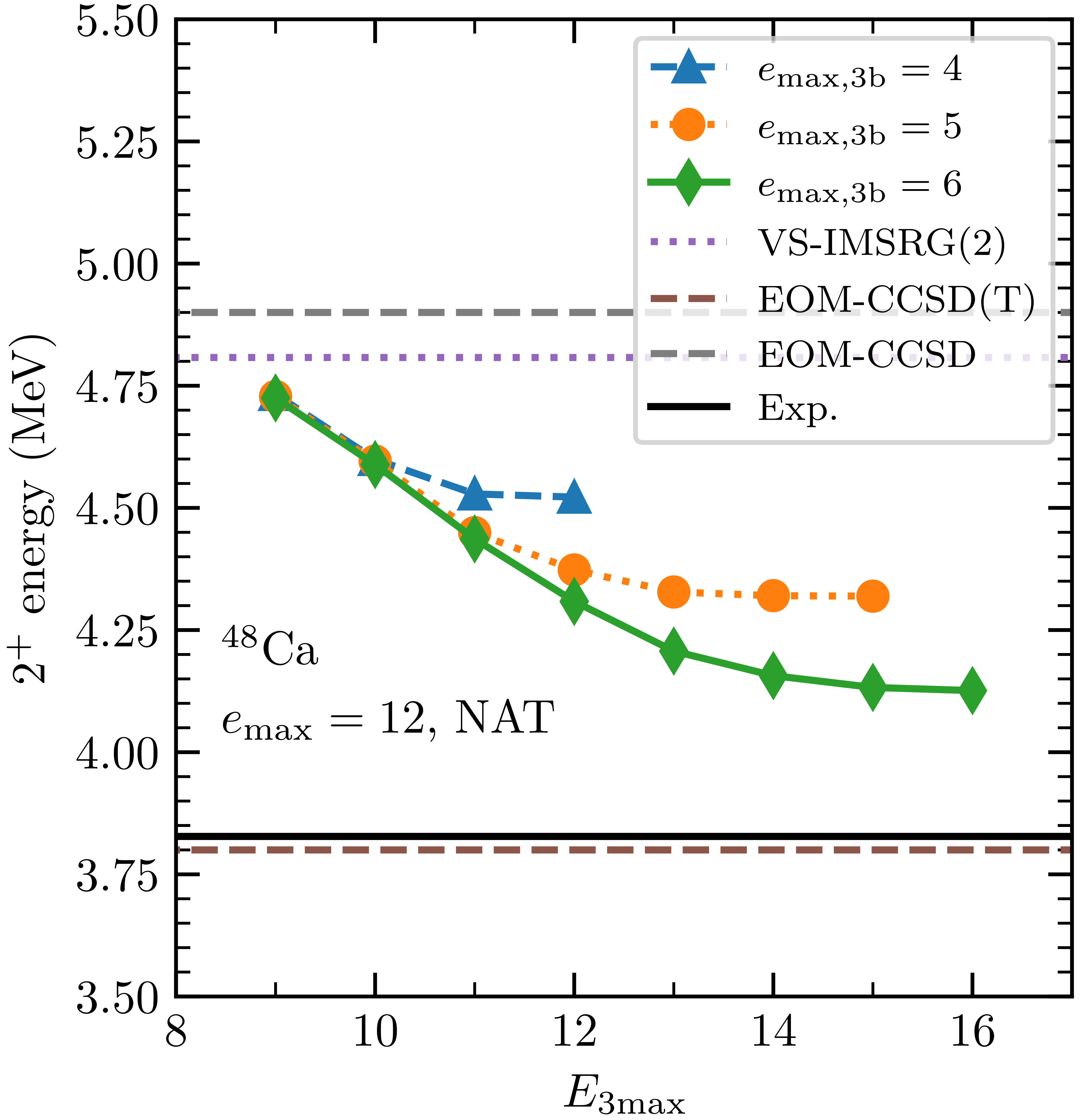
IMSRG(3) corrections for 2^+ of ^{48}Ca

- IMSRG(2) predictions for 2^+ energy in Ca follow experimental trends...
- **... except at ^{48}Ca**
- In CC, similar overprediction resolved by **3-body contributions**



Hagen et al., PRL **117** (2016)
Simonis et al., PRC **96** (2017)

IMSRG(3) corrections for 2^+ of ^{48}Ca



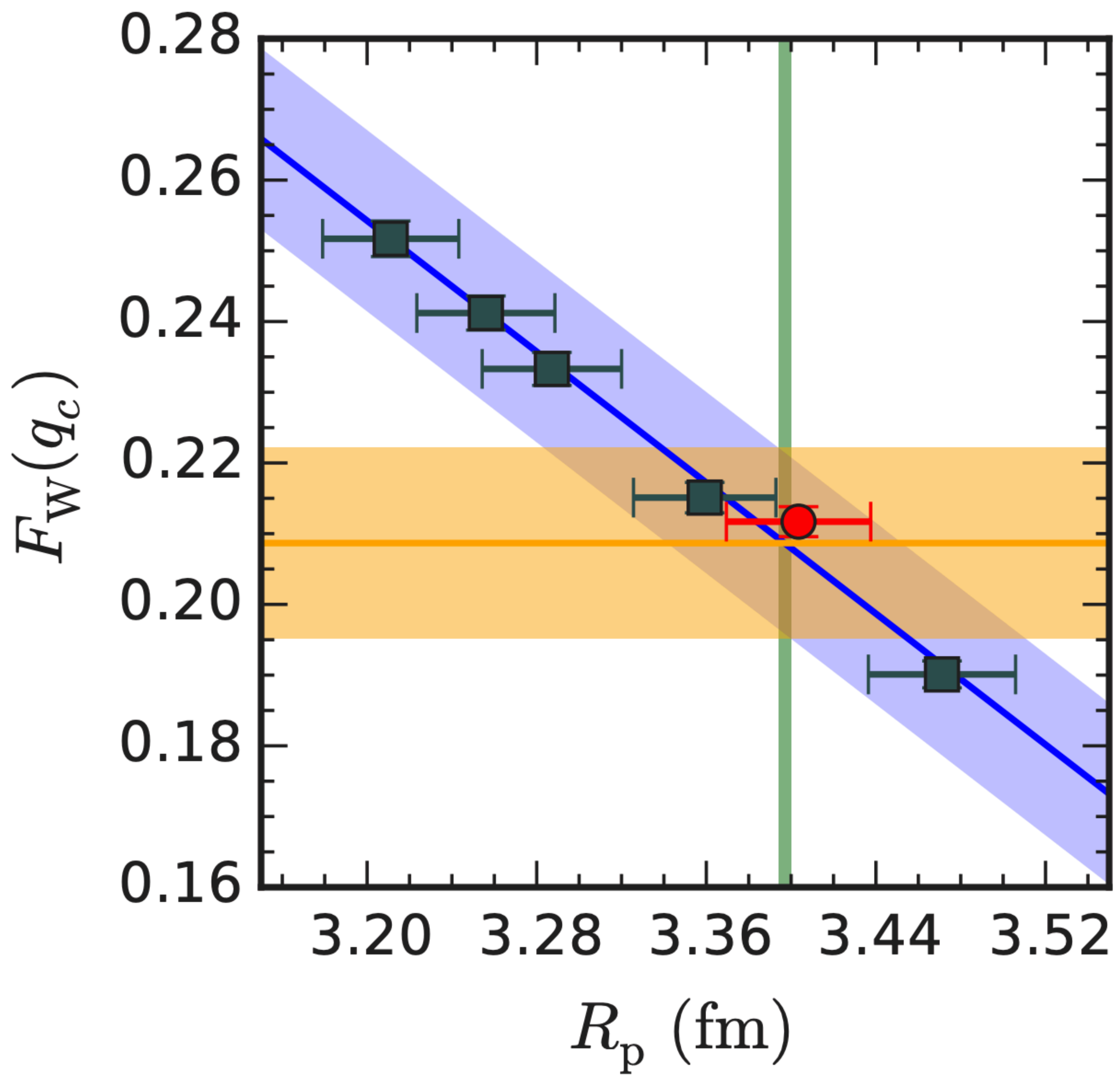
- Truncations on 3B operators necessary for realistic calculations: $e_{max,3b}$, E_{3max}
- Convergence in calcium challenging
- **Substantial corrections to 2^+ energy consistent with CC and experiment**
- Revamped numerical implementation to reach convergence
  Novario et al., PRC **102** (2020)

Precision IMSRG calculations in medium-mass nuclei possible soon!

Nuclear responses for elastic electron scattering

- Electron scattering data in ^{27}Al
- Longitudinal/Coulomb contributions: $M^J, \Phi''^J \, (J = 0, 2, 4)$
- Transverse contributions: $\Delta^J, \Sigma'^J \, (J = 1, 3, 5)$

Hagen et al., Nat. Phys. **12** (2015), Gazda et al., PRD **95** (2016), Hoferichter et al., PRD **102** (2020), Hu et al., PRL **128** (2022)



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- Center-of-mass corrections for responses Hagen et al., PRL **103** (2009)
- Fourier transform to obtain densities → expectation values

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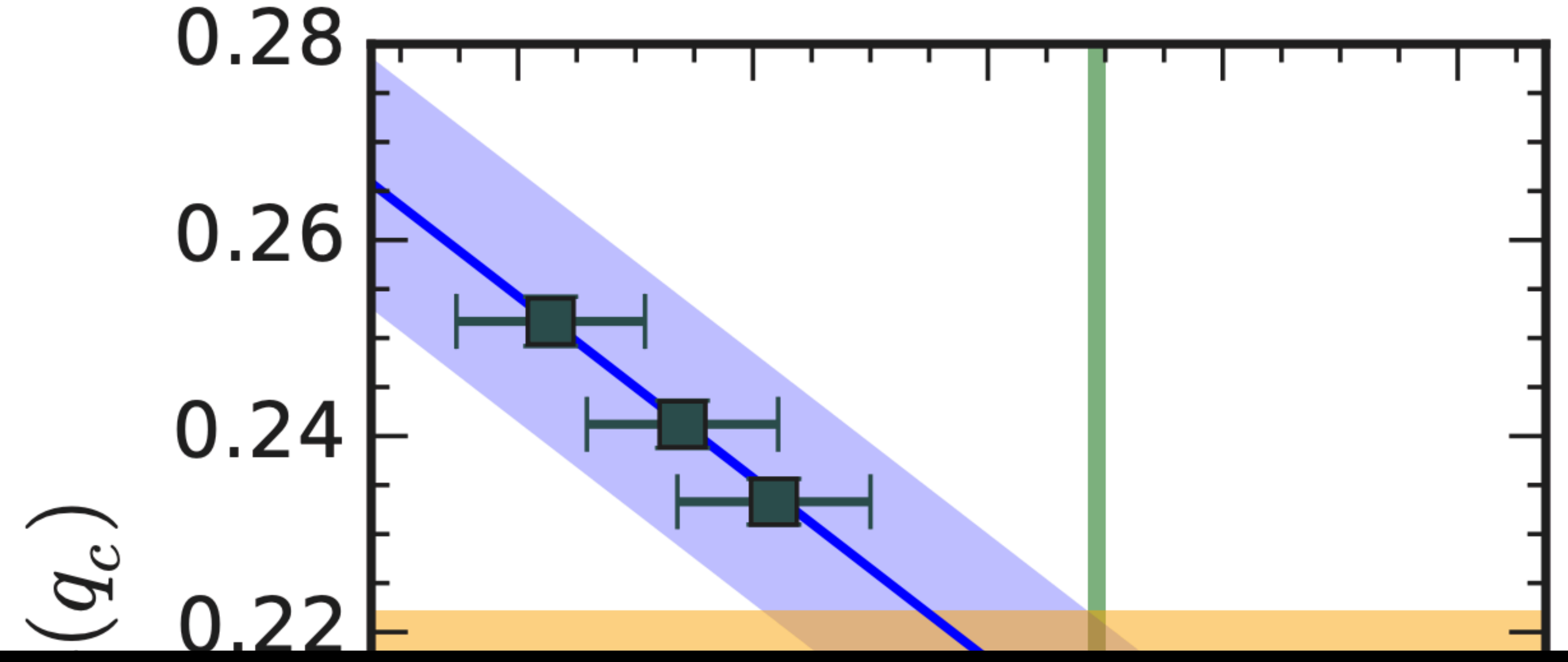

- Electron scattering data in ^{27}Al
- Longitudinal/Coulomb contributions:

PSA (Martin Hoferichter)

Error in r^2_{so} from Ong et al., PRC **82** (2010)

Fix: $r^2_{\text{so}} = \frac{1}{Z}\sum_i \frac{\mu_i - Q_i}{M^2}(\kappa_i + 1) \rightarrow \frac{1}{Z}\sum_i \frac{\mu_i - Q_i/2}{M^2}(\kappa_i + 1)$

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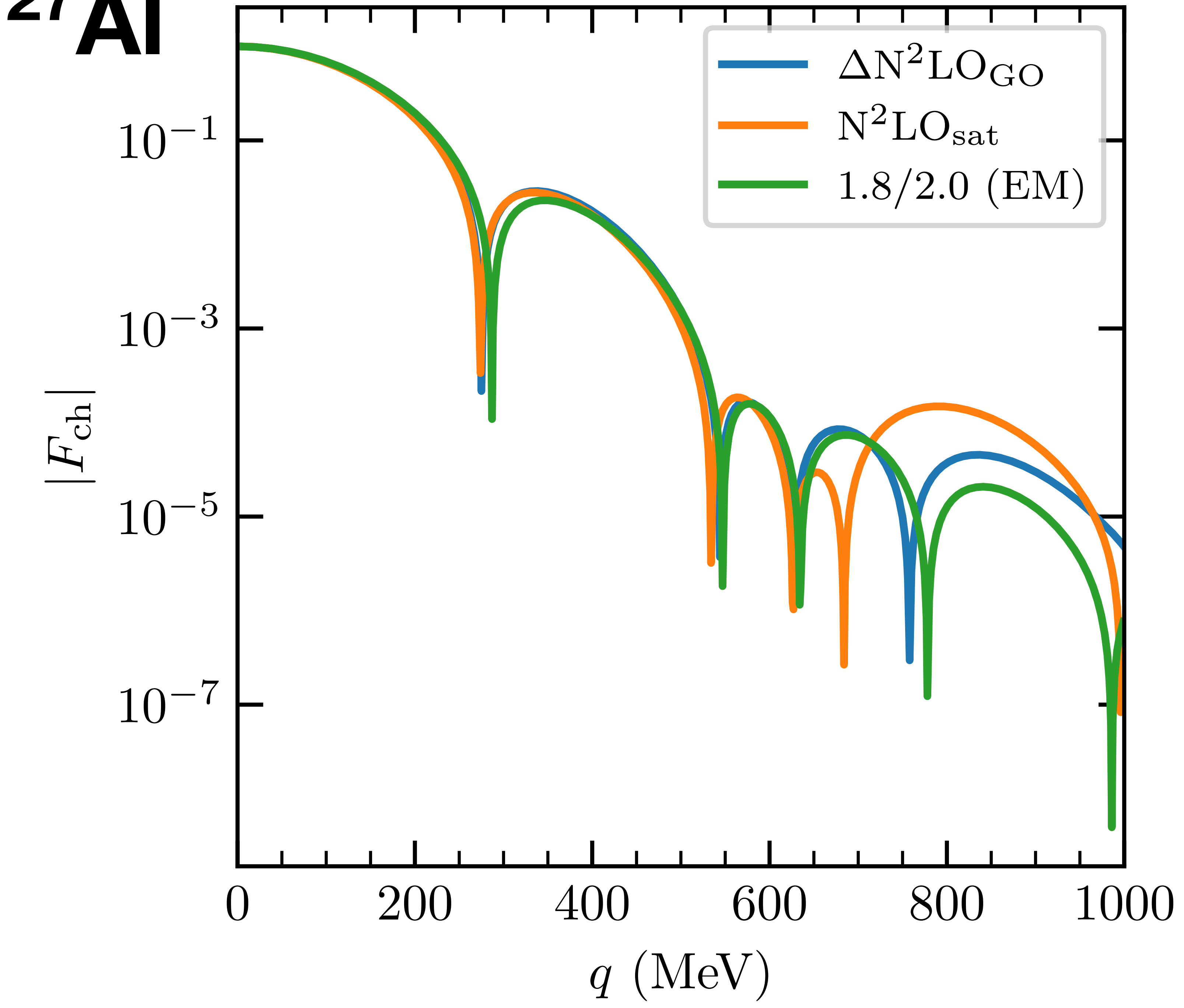
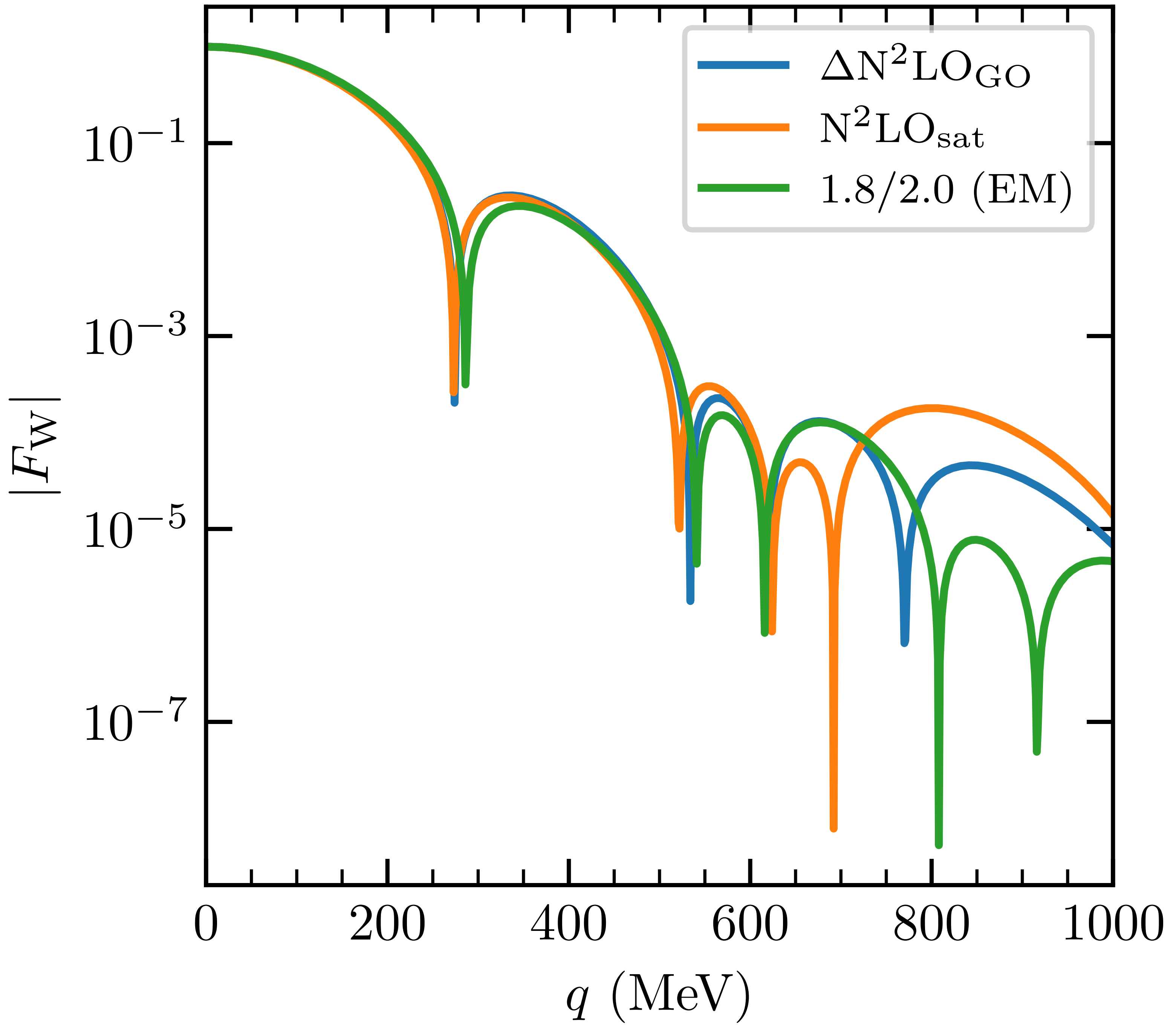
Neutron densities for $\mu \to e$ studies

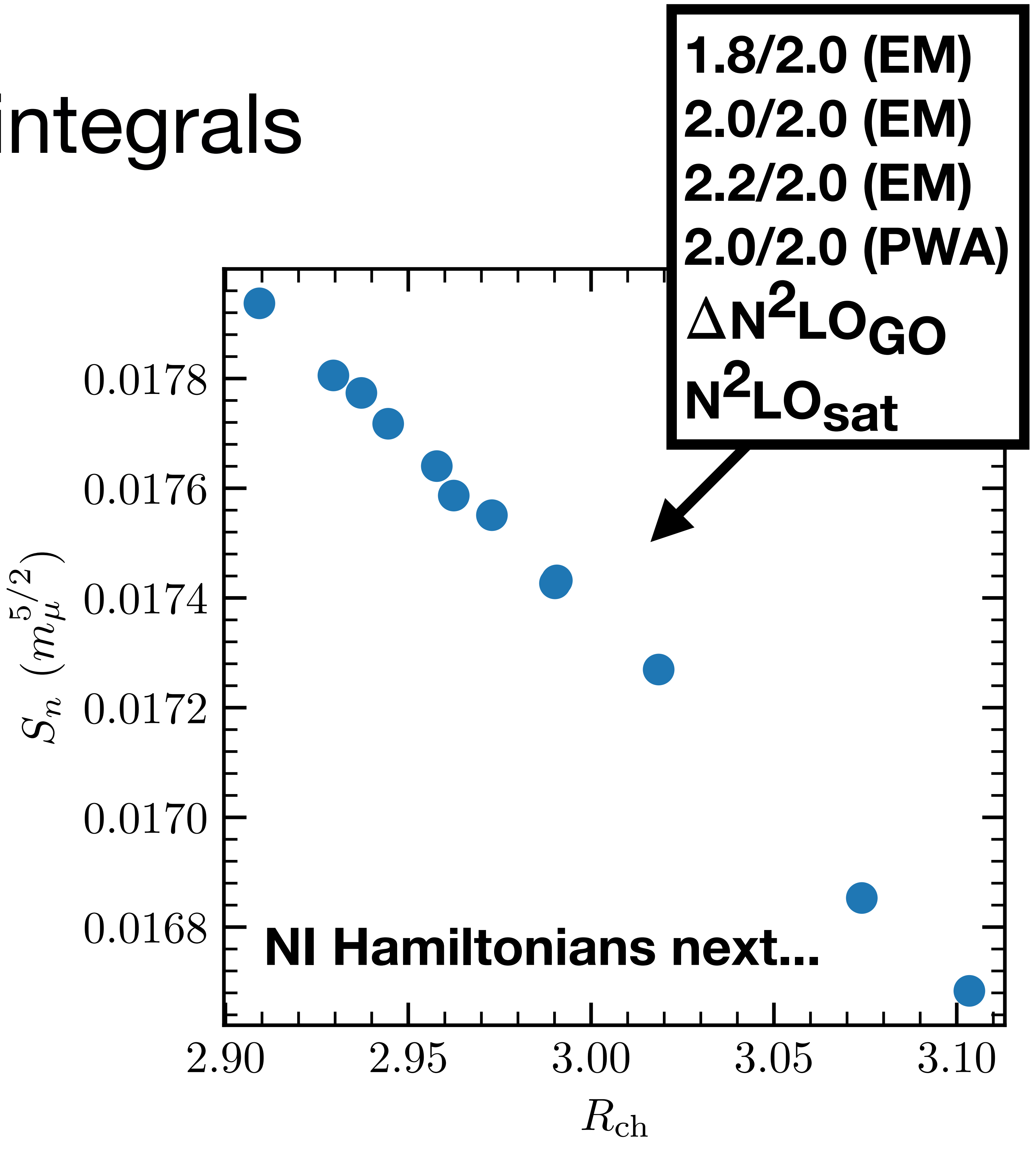
Noël, **MH**, Hoferichter, et al., preliminary

- Compute $F_{\rm ch}$, $F_{\rm W}$ for set of Hamiltonians ($J = 0$)
- Study **correlated uncertainties** in $R_{\rm ch}$, μ overlap integrals

^{27}Al





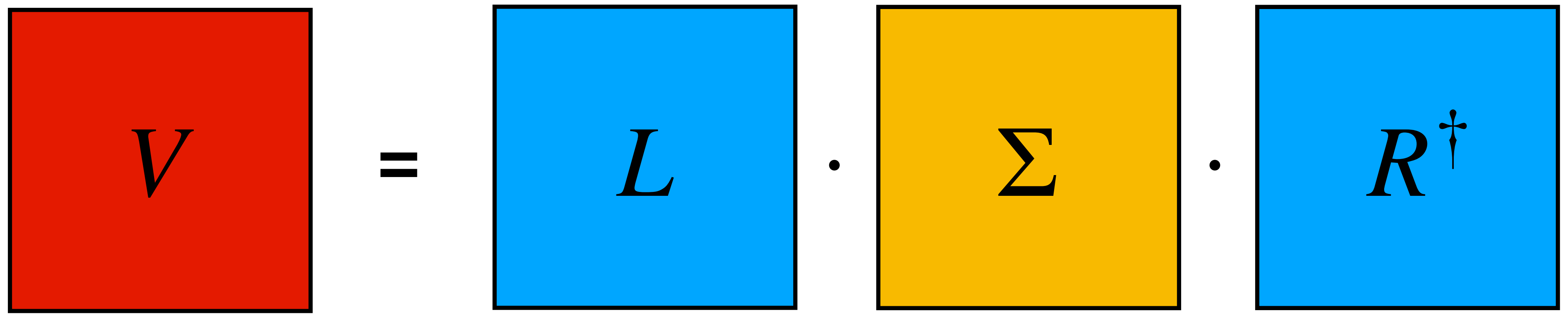


Weak scattering in nuclei strongly constrained by ab initio nuclear structure!

SVD for NN and 3N forces

singular value decomposition

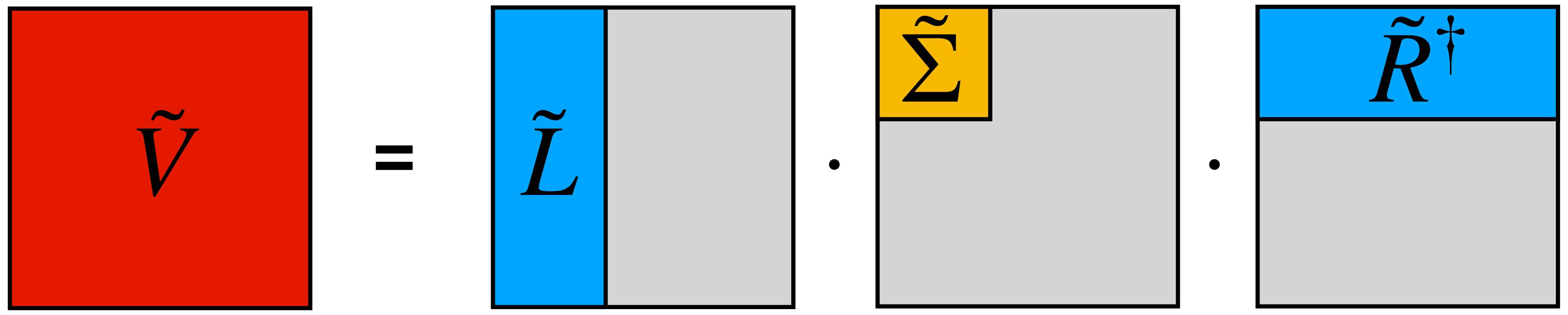
Tichai, **MH**, et al., PLB **821** (2021)
Tichai, **MH**, et al., arxiv:2307.15572

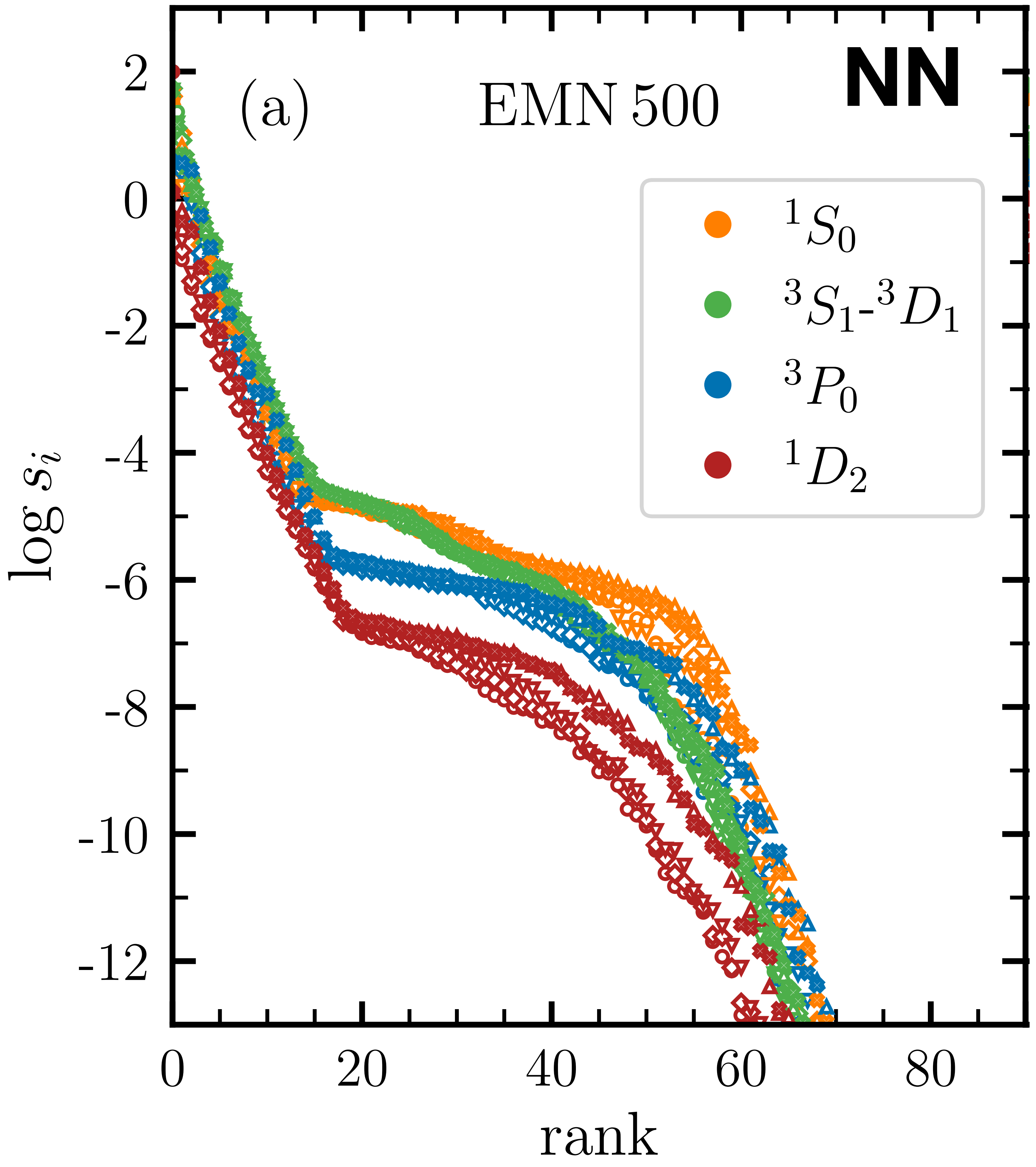


- **Largest singular values** are most important

$$\Sigma = \mathrm{diag}(s_i)$$

- **Low-rank approximation** via truncation (keeping largest singular values)





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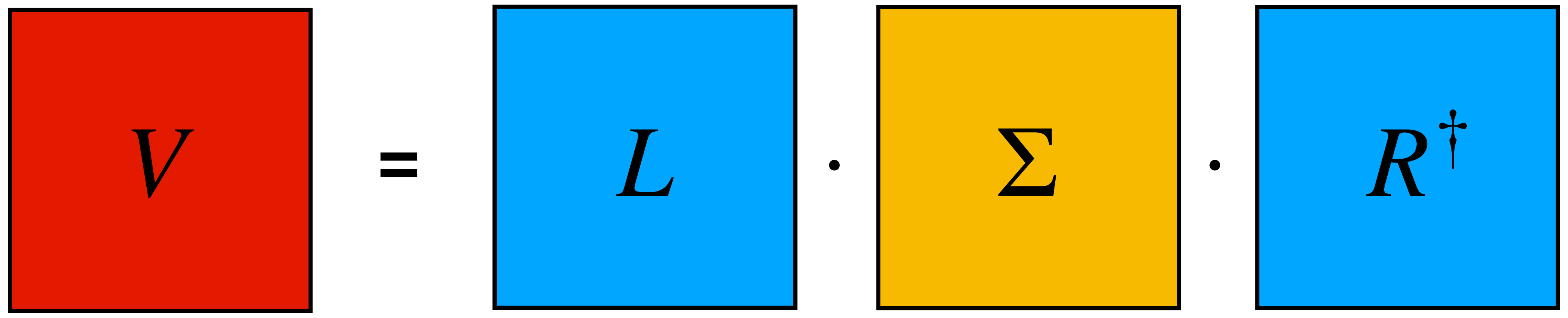

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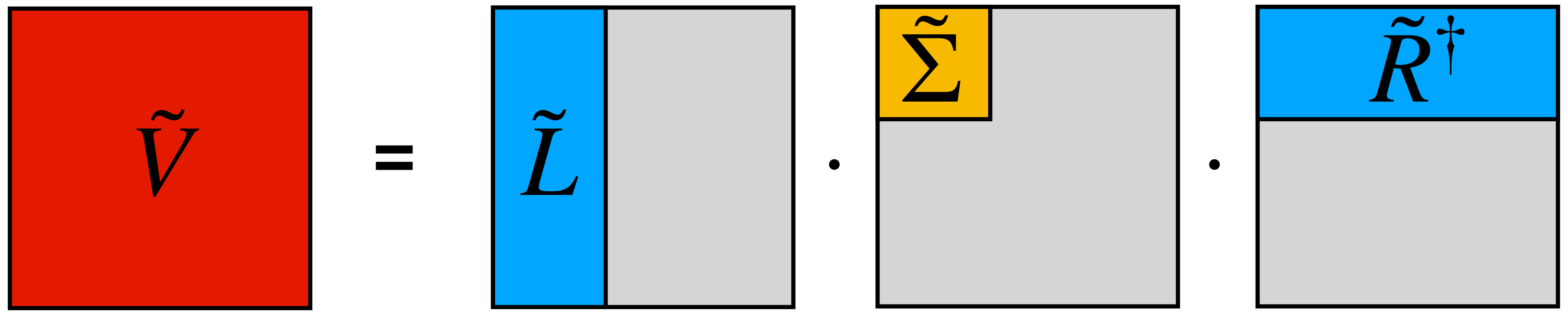
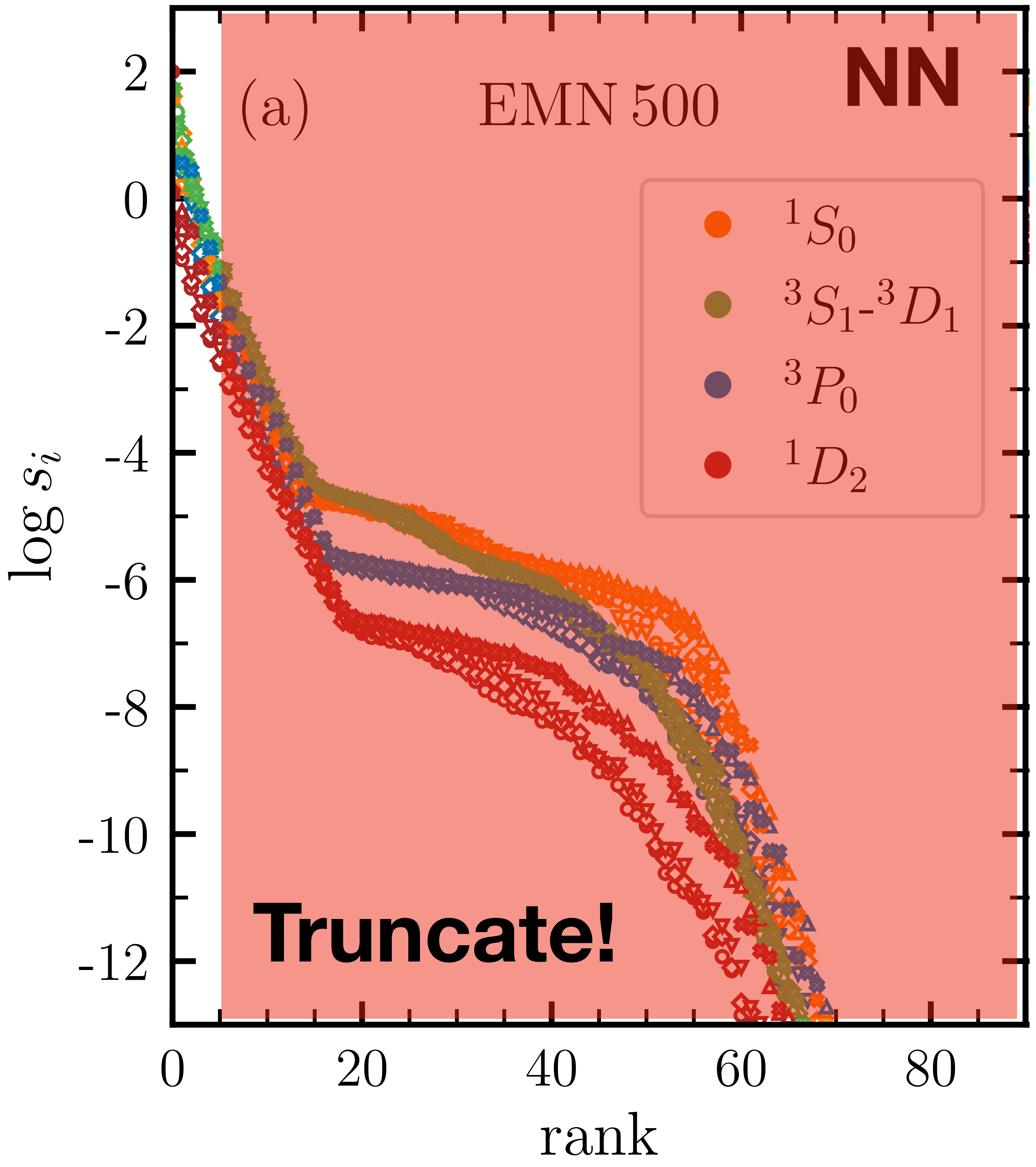
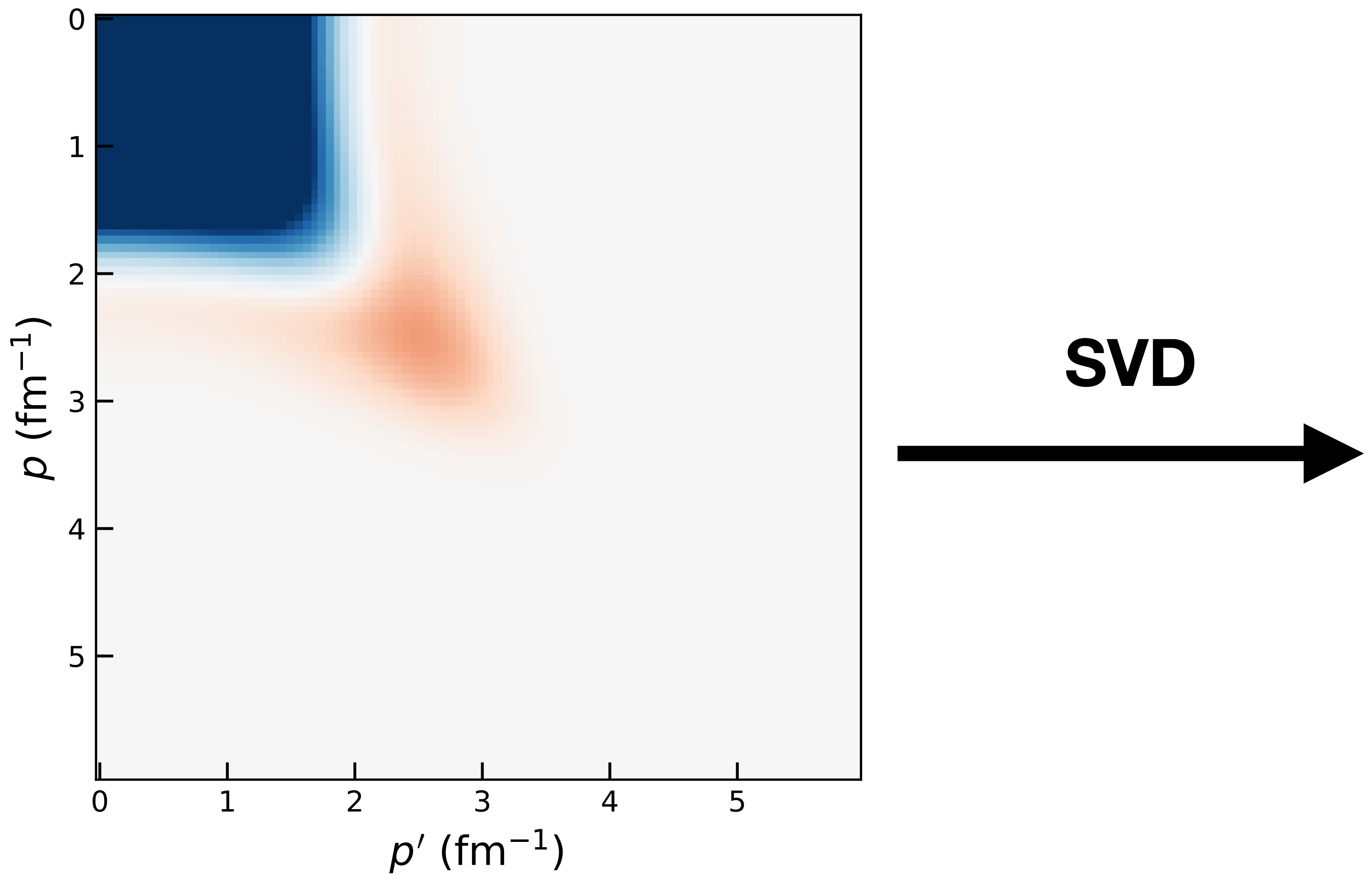


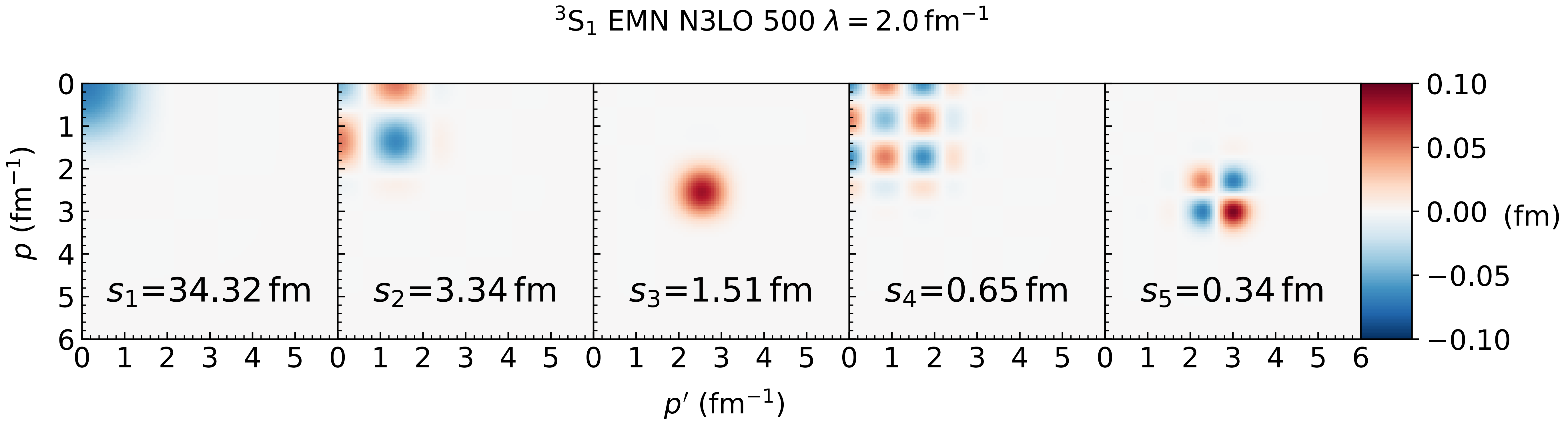


Operator basis for low-resolution potentials

Tom Plies @ TU Darmstadt

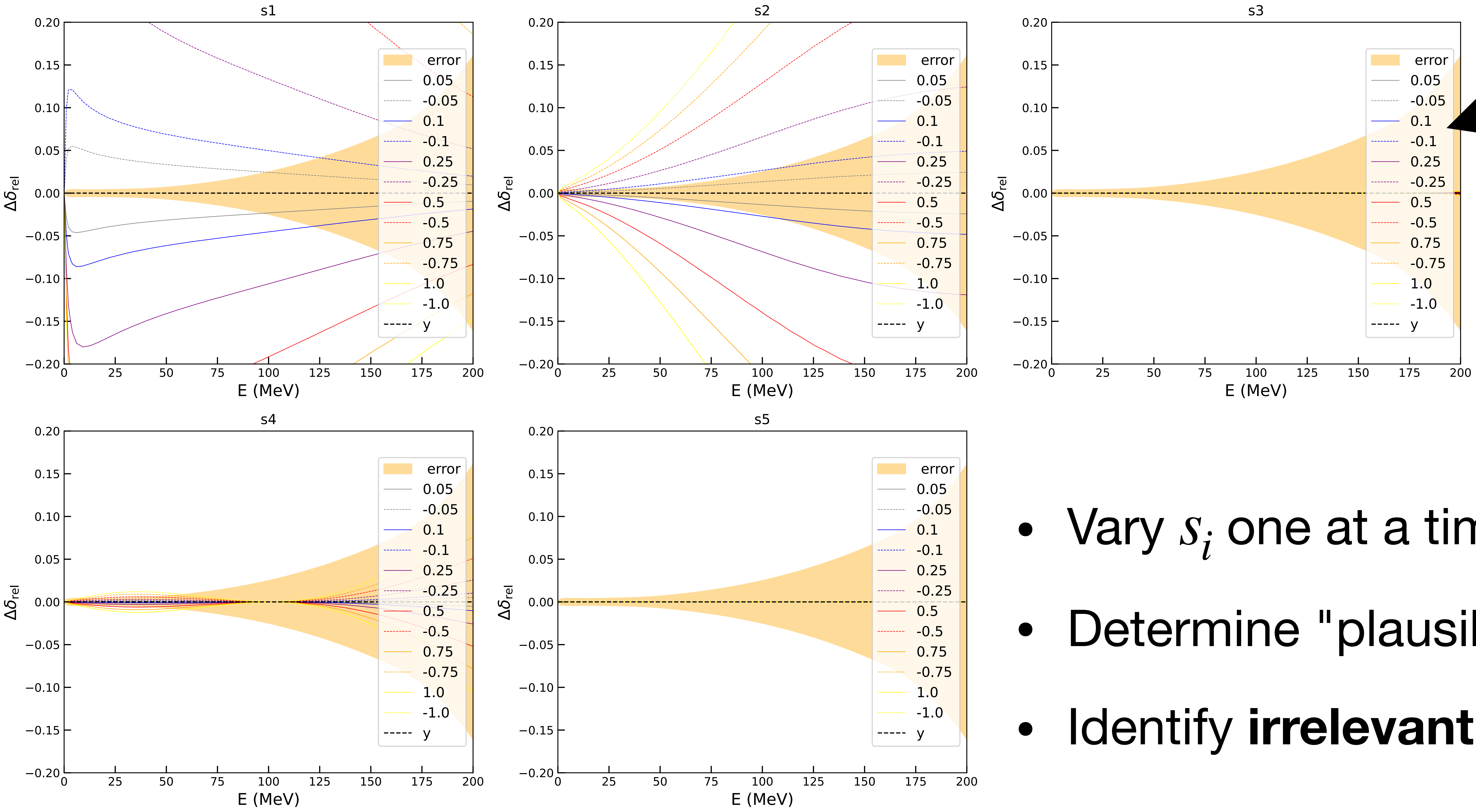
- Low-resolution potentials lack **linear operator structure** of chiral EFT
- **SVD** to recover **new operator basis:** $V = \sum_i s_i O_i = \sum_i s_i |l_i\rangle\langle r_i|$





- Treat singular values s_i as **free parameters (LECs)**
- Constrain based on chiral EFT uncertainties and **propagate to predictions**

Impact of singular values



5 to 100 percent

- Vary s_i one at a time
- Determine "plausible" range → prior
- Identify **irrelevant terms** (s_3, s_5)

Matching to low-energy phase shifts

Single partial wave

- Vary s_i within reasonable range: $\rightarrow \vec{s}$
- Constrain 10k samples based on likelihood

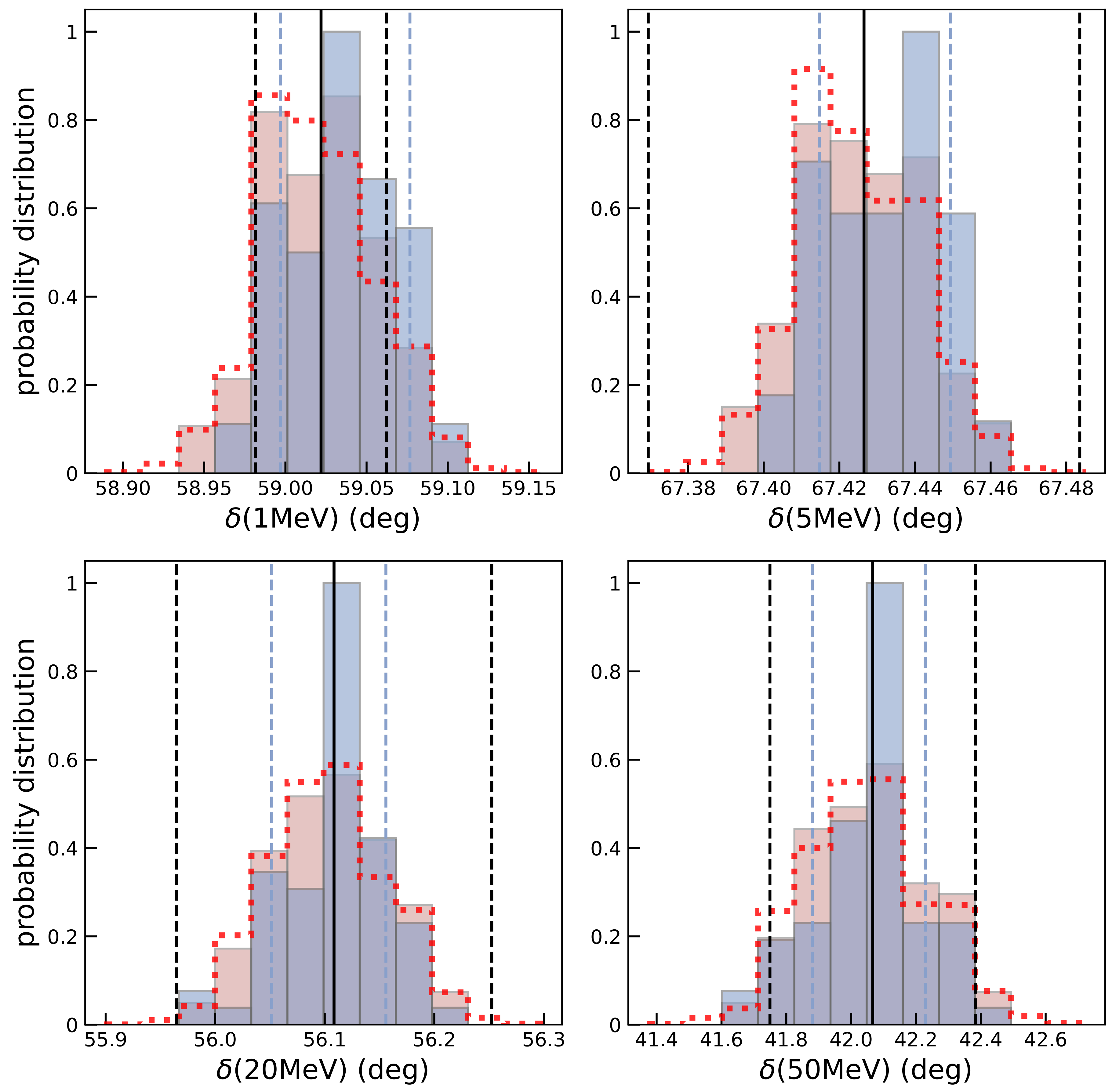
$$\mathscr{L}(\vec{s}) \sim \prod_E \mathcal{N}\left(\delta(\vec{s}, E) - \delta(\vec{s}_{\mathrm{ref}}, E), \sigma^2_{\mathrm{EKM}}\right)$$

- Resample to 100 samples based on likelihood

Multiple partial waves

$\left({}^1\mathrm{S}_0, {}^3\mathrm{S}_1, {}^1\mathrm{P}_1, {}^3\mathrm{P}_0, {}^3\mathrm{P}_1, {}^3\mathrm{P}_2\right)$ with charge indep.

- Product space of $\vec{s}$ in different partial waves
- Reduce to 64 samples



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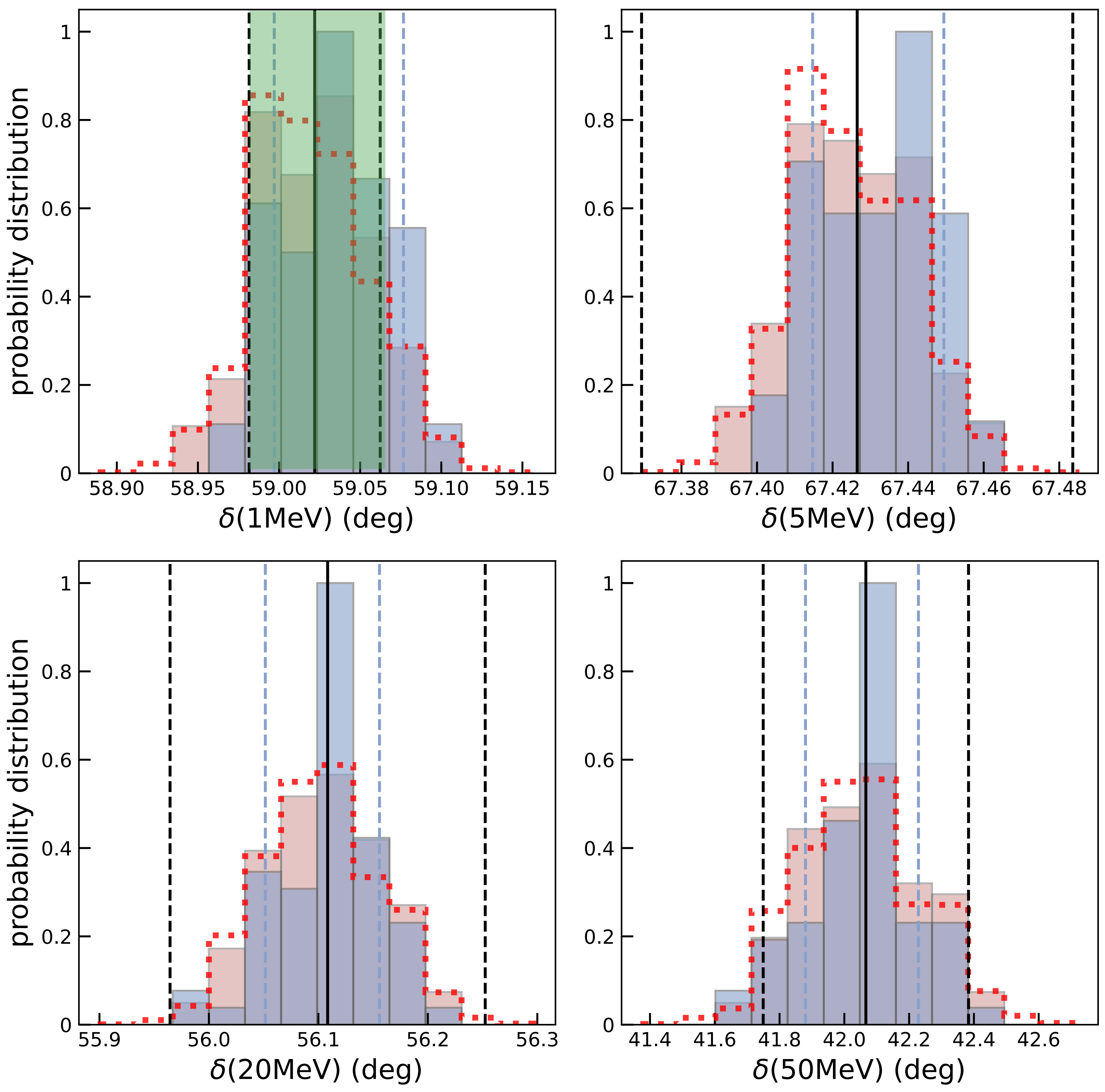

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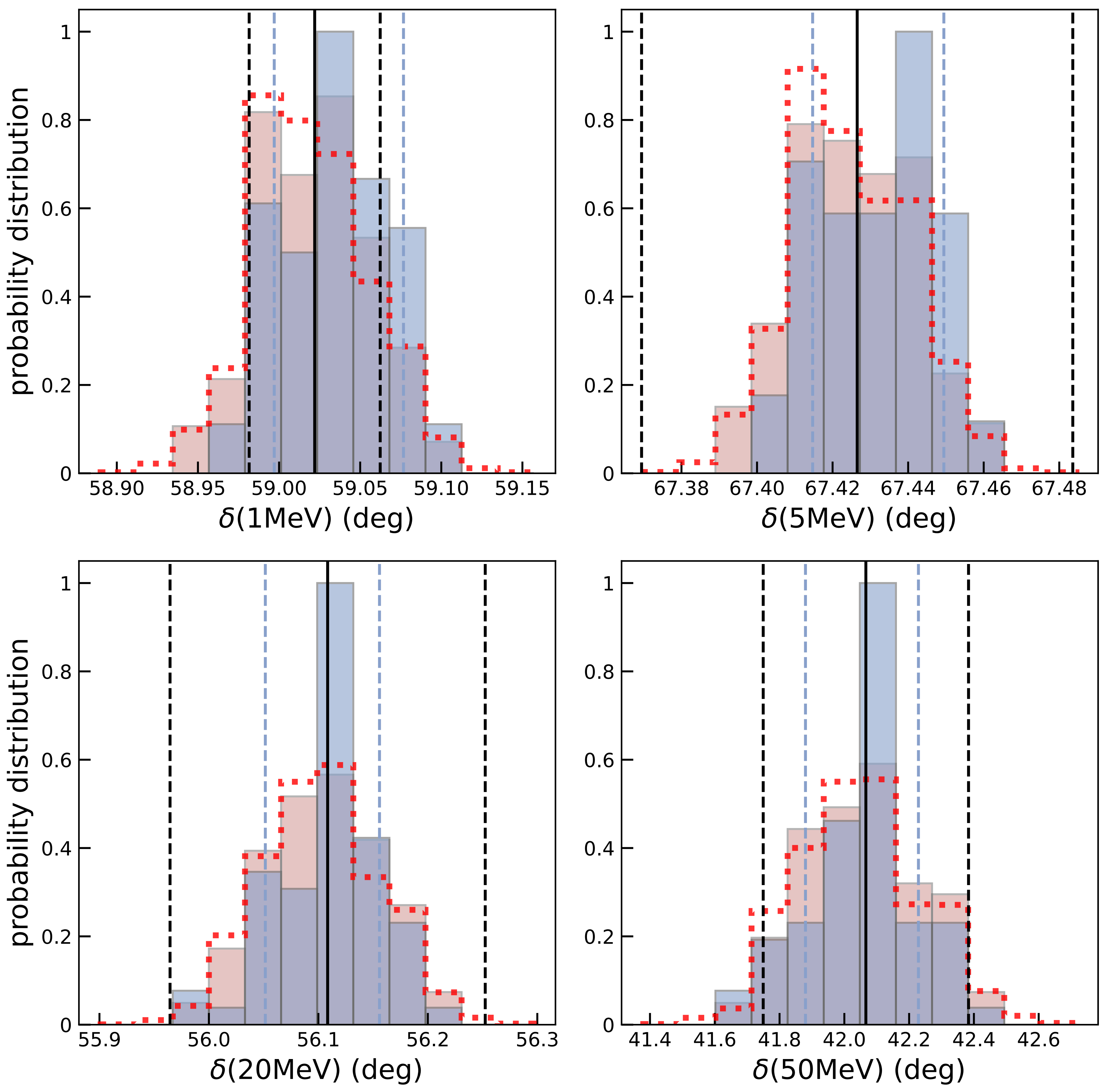

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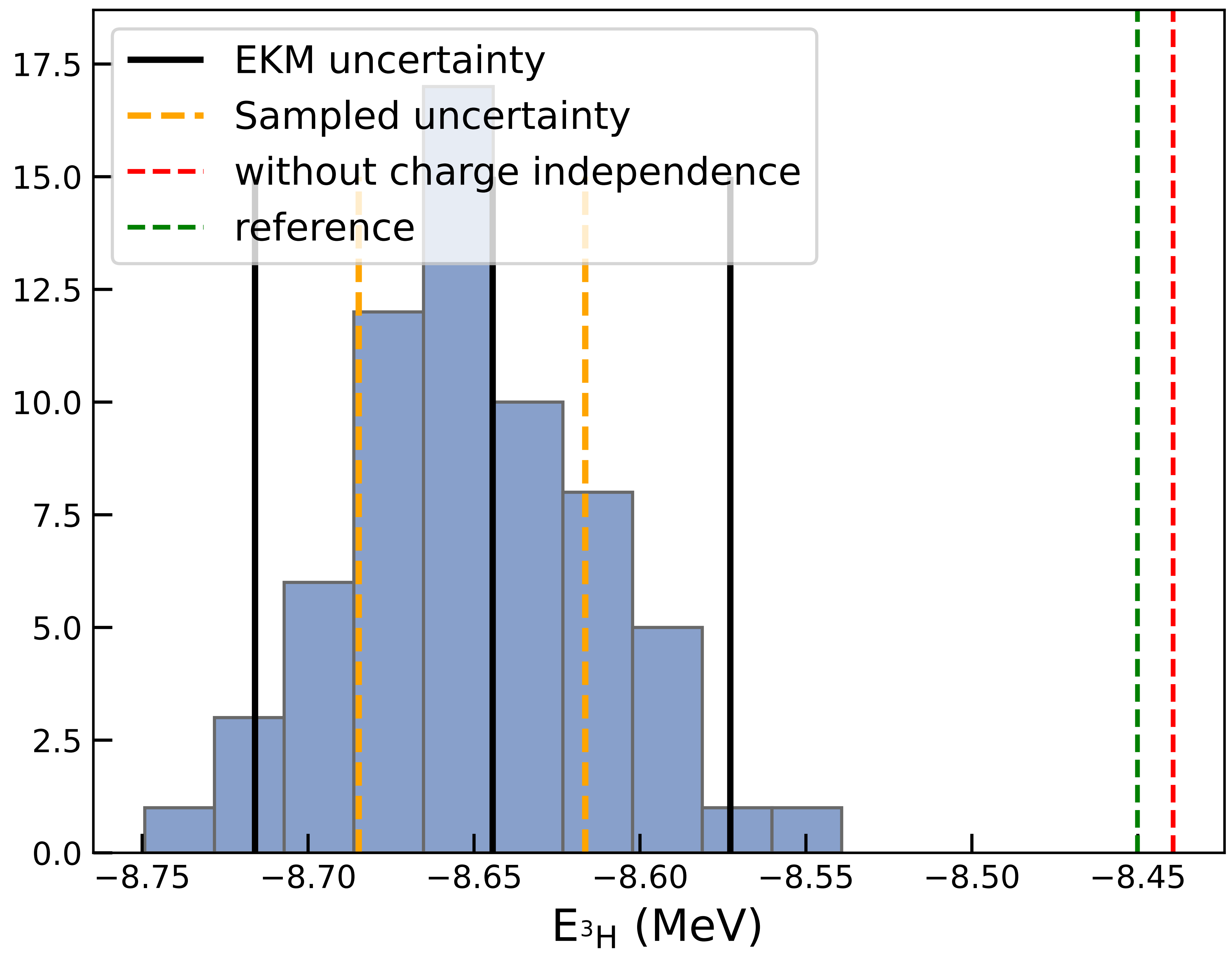
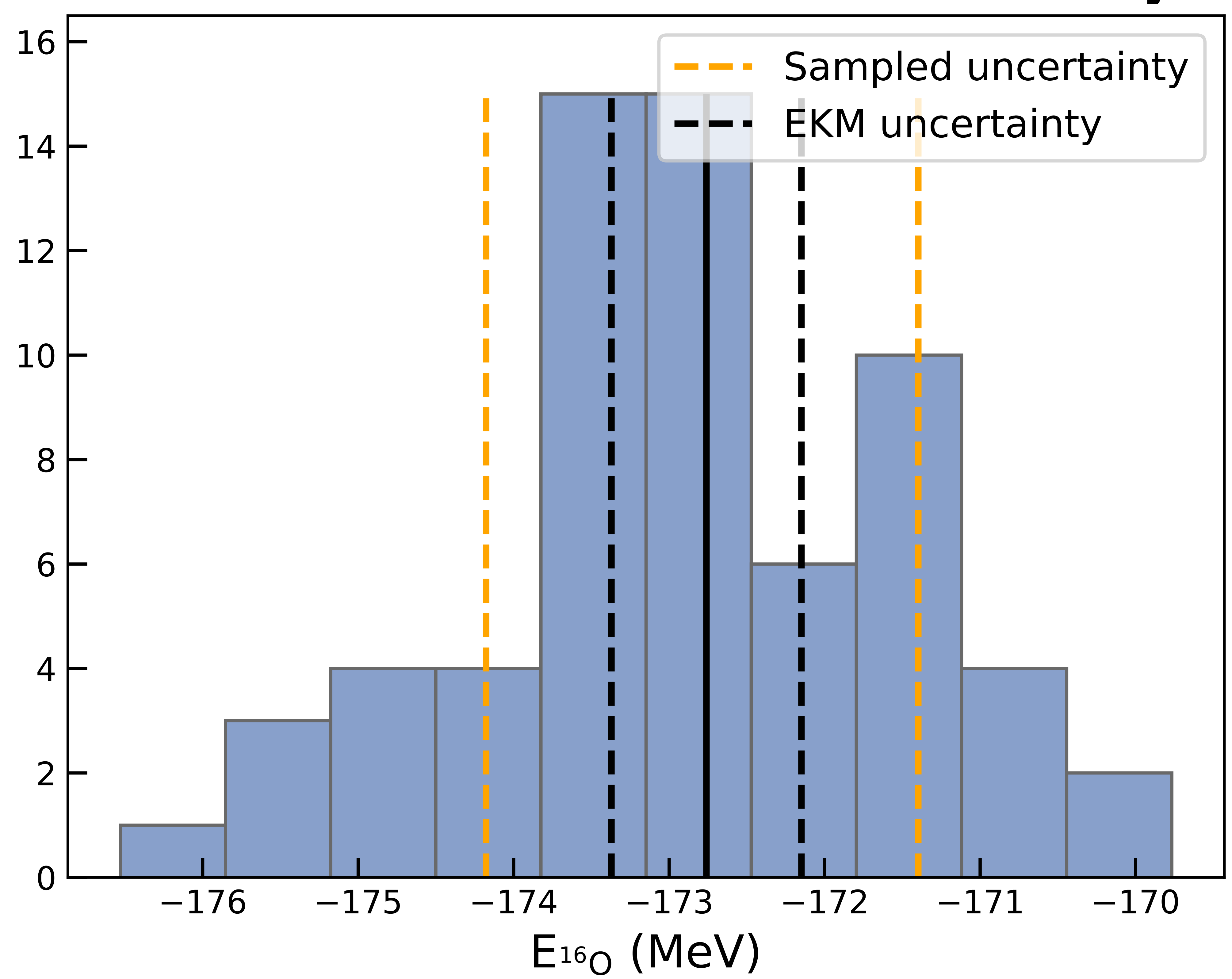
PPDs for ground-state energies

posterior predictive distributions

NN-only for now

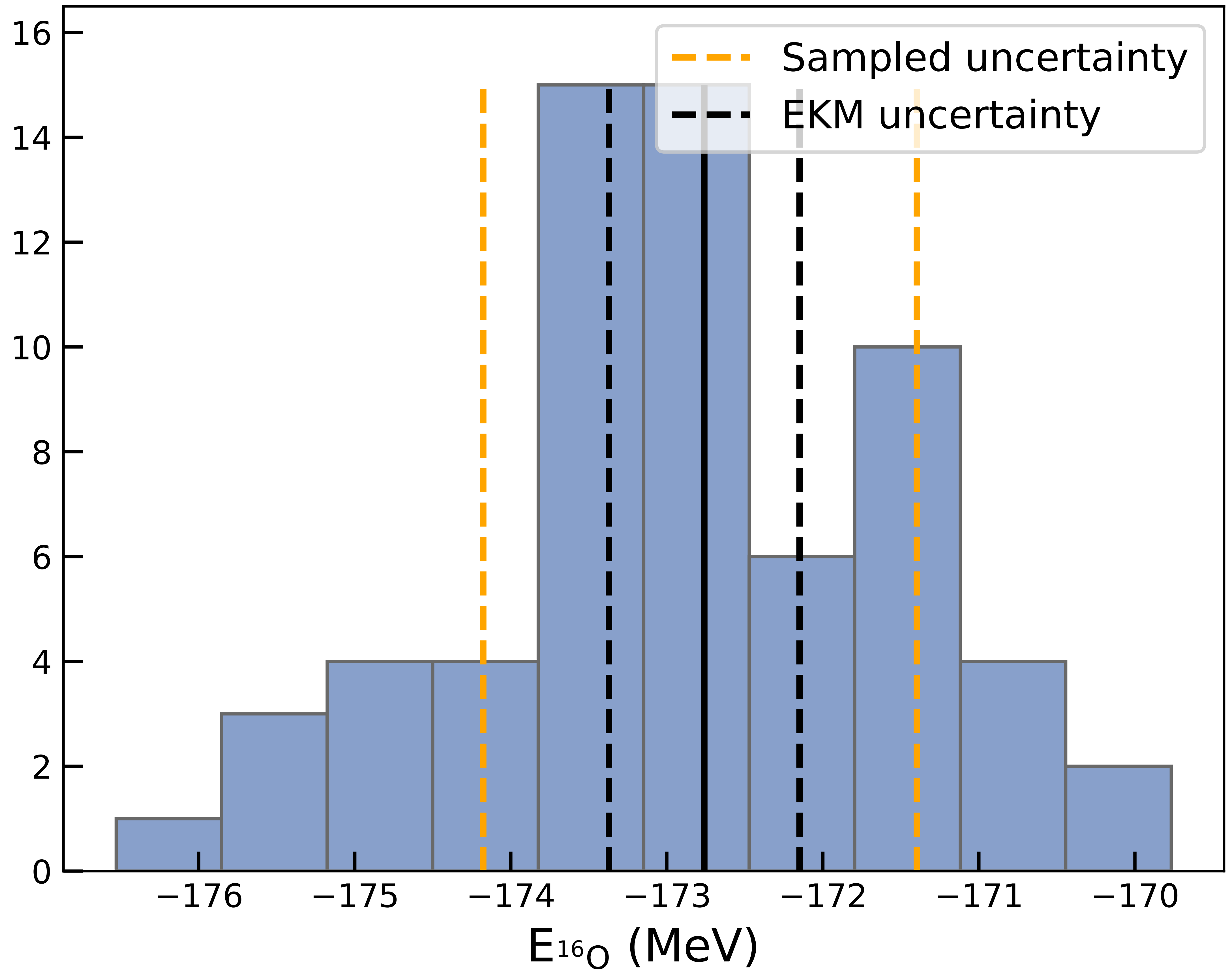




- Reproduction of EKM uncertainties good (improved by more samples)
- **EFT uncertainties for low-resolution potentials in nuclei**

Conclusion and outlook

- Establishing **IMSRG(3)** for high-precision description of medium-mass nuclei and uncertainty quantification
- Exploit **correlated uncertainties** to constrain difficult-to-measure and nonobservable quantities
- **New operator basis from SVD** for uncertainty quantification with low-resolution Hamiltonians



Acknowledgments

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Additional collaborators:

- **TU Darmstadt**: **Patrick Müller**, Wilfried Nörthershäuser
- **FRIB**: Scott Bogner, Heiko Hergert
- **TRIUMF**: **Antoine Belley**, Jason Holt
- **ORNL**: Gaute Hagen, Gustav Jansen, Thomas Papenbrock
- **University of Notre Dame**: Ragnar Stroberg
- **LANL**: **Brendan Reed**, Ingo Tews
- **NCSU**: Sebastian König
- **MPIK**: **Menno Door**, Klaus Blaum
- **PTB Braunschweig**: **Indy Yeh**, Tanja Mehlstäubler
- **Leibniz University Hannover**: **Fiona Kirk**, Elina Fuchs
- **UNSW**: Julian Berengut

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Thank you for your attention!