Oak Ridge National Laboratory | LEADERSHIP COMPUTING FACILITY

# Perturbative treatment of subleading interactions in ab initio calculations

**MH**, König, Hergert, preliminary

Matthias Heinz, ORNL

*INT Workshop: "Chiral EFT: New Perspectives"*
*Seattle, WA, March 19, 2025*

Work supported by:

U.S. DEPARTMENT OF ENERGY

NUCLEI
Nuclear Computational Low-Energy Initiative

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# Goals for many-body theory

- We want to solve many-body Schrödinger equation…
- … **precisely** to describe emergent phenomena…
- … in **light, medium-mass, and heavy nuclei** and **nuclear matter**…
- … **consistently** based on input **nuclear forces**…
- … with **quantified uncertainties**

**Low-resolution forces** + **qualitatively correct reference state**
allow for efficient expansion of many-body wave function

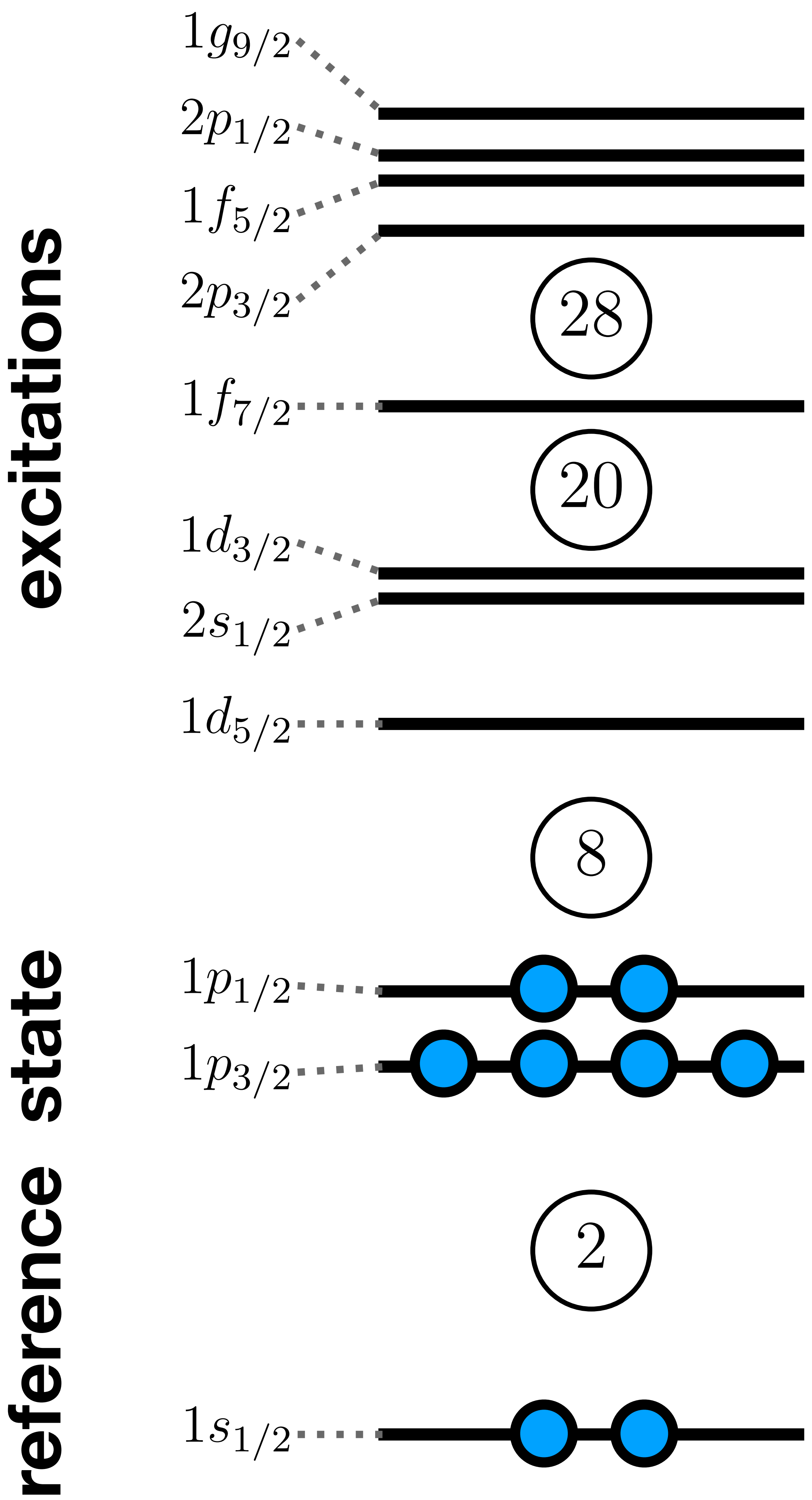
# Outline

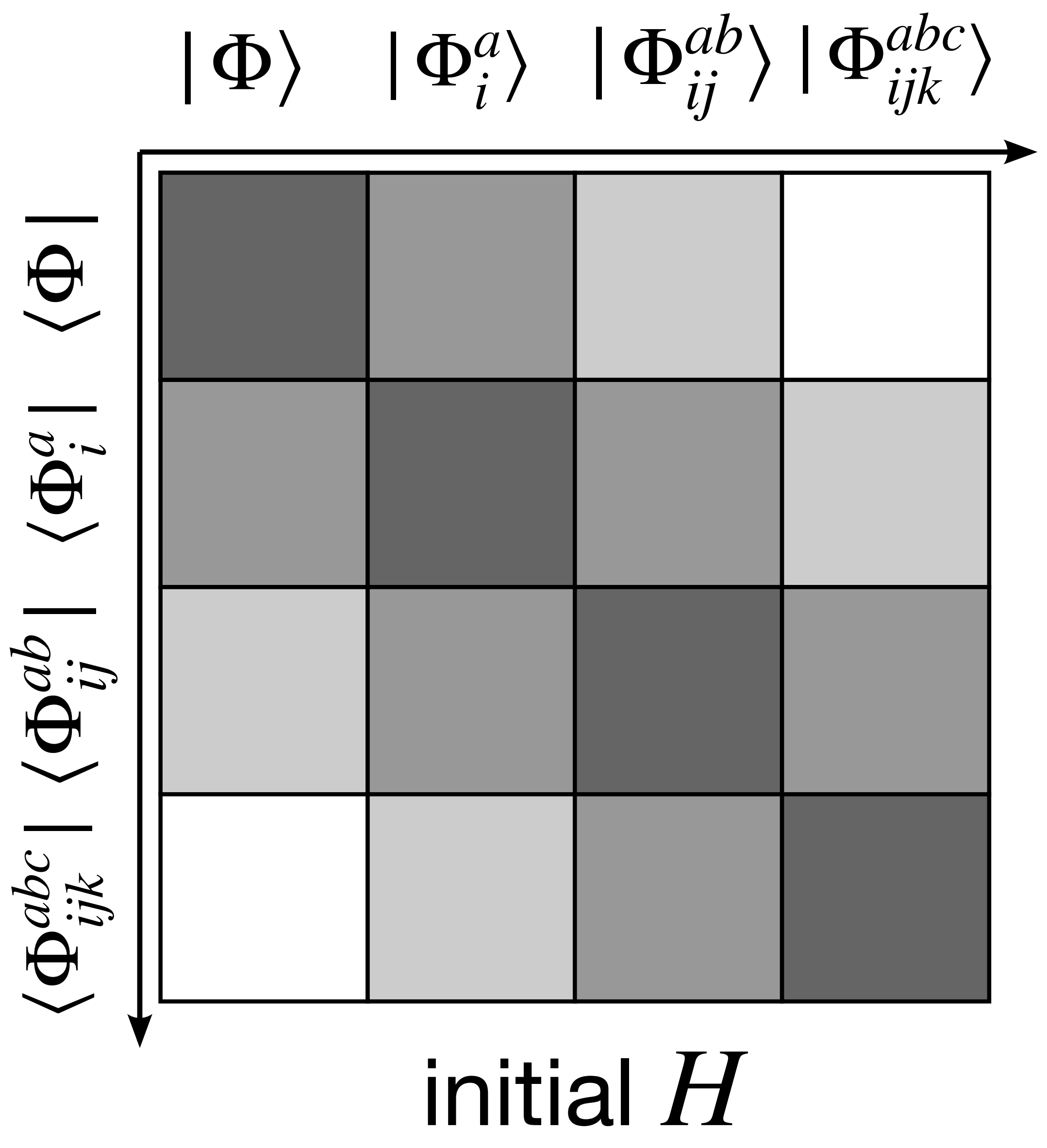
- Ab initio methods & chiral EFT: **Developments and growing pains**
- **IMSRG-based perturbation theory** for subleading terms
- **Preliminary explorations** in (medium-)light nuclei

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

# The IMSRG

in-medium similarity renormalization group



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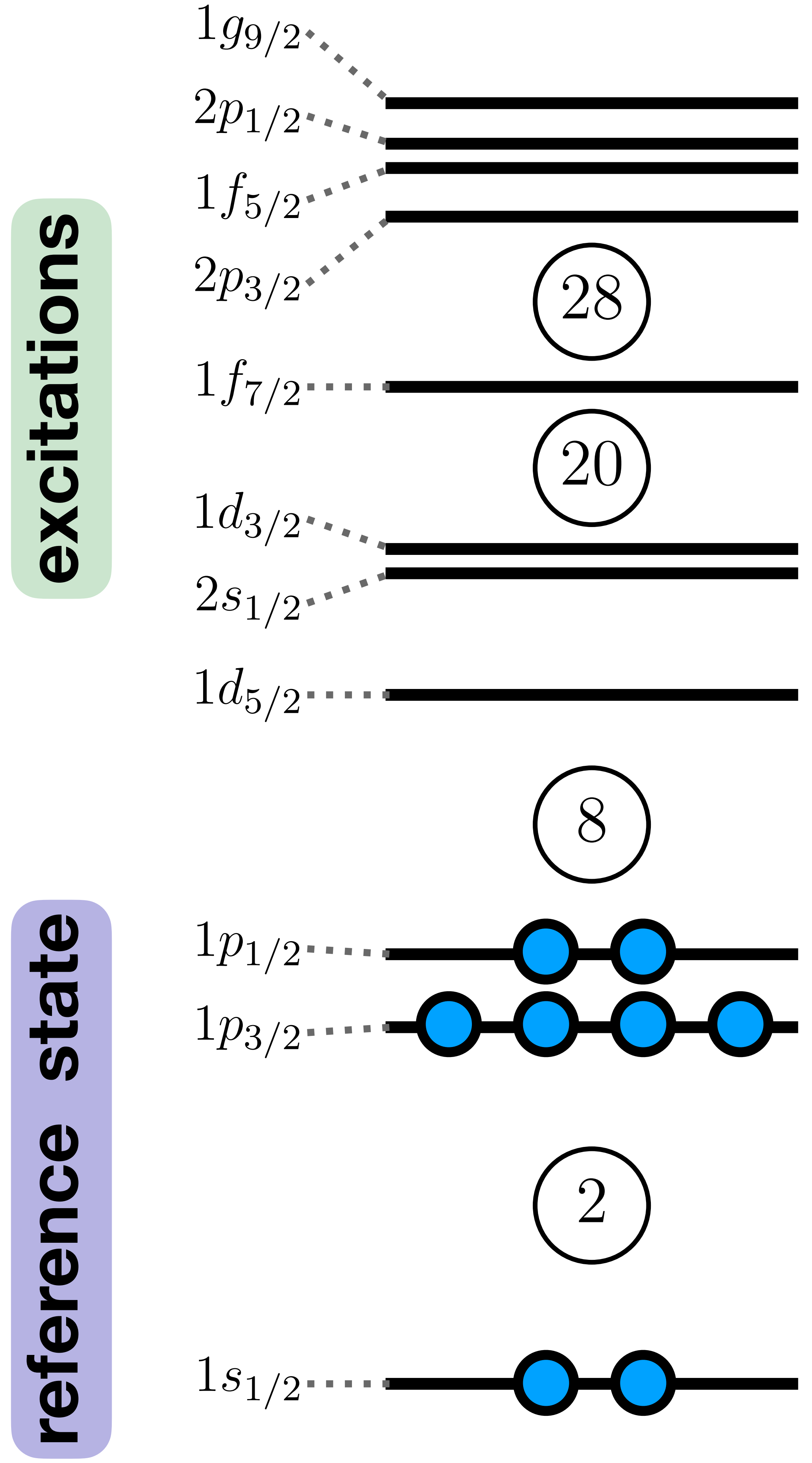


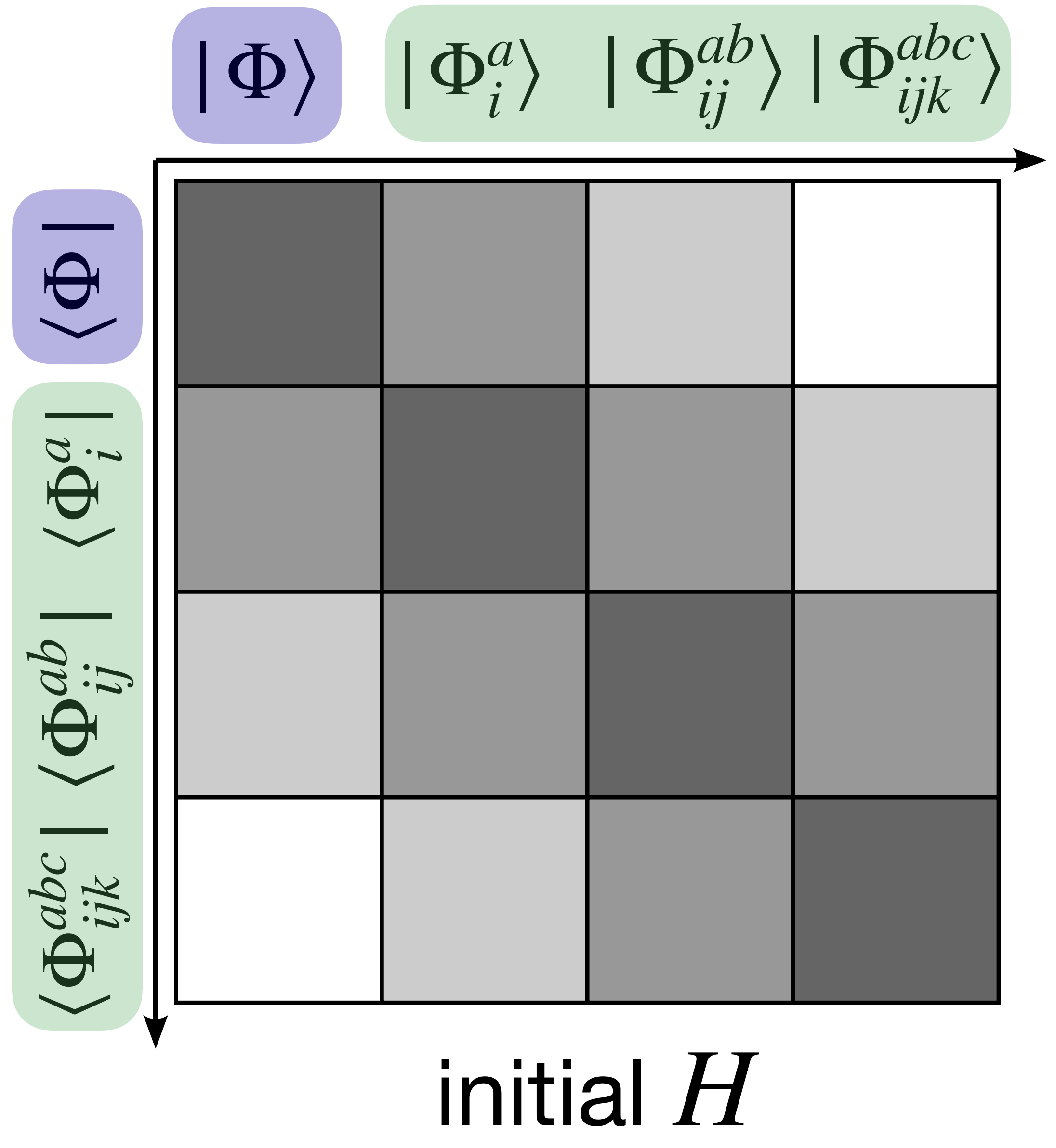

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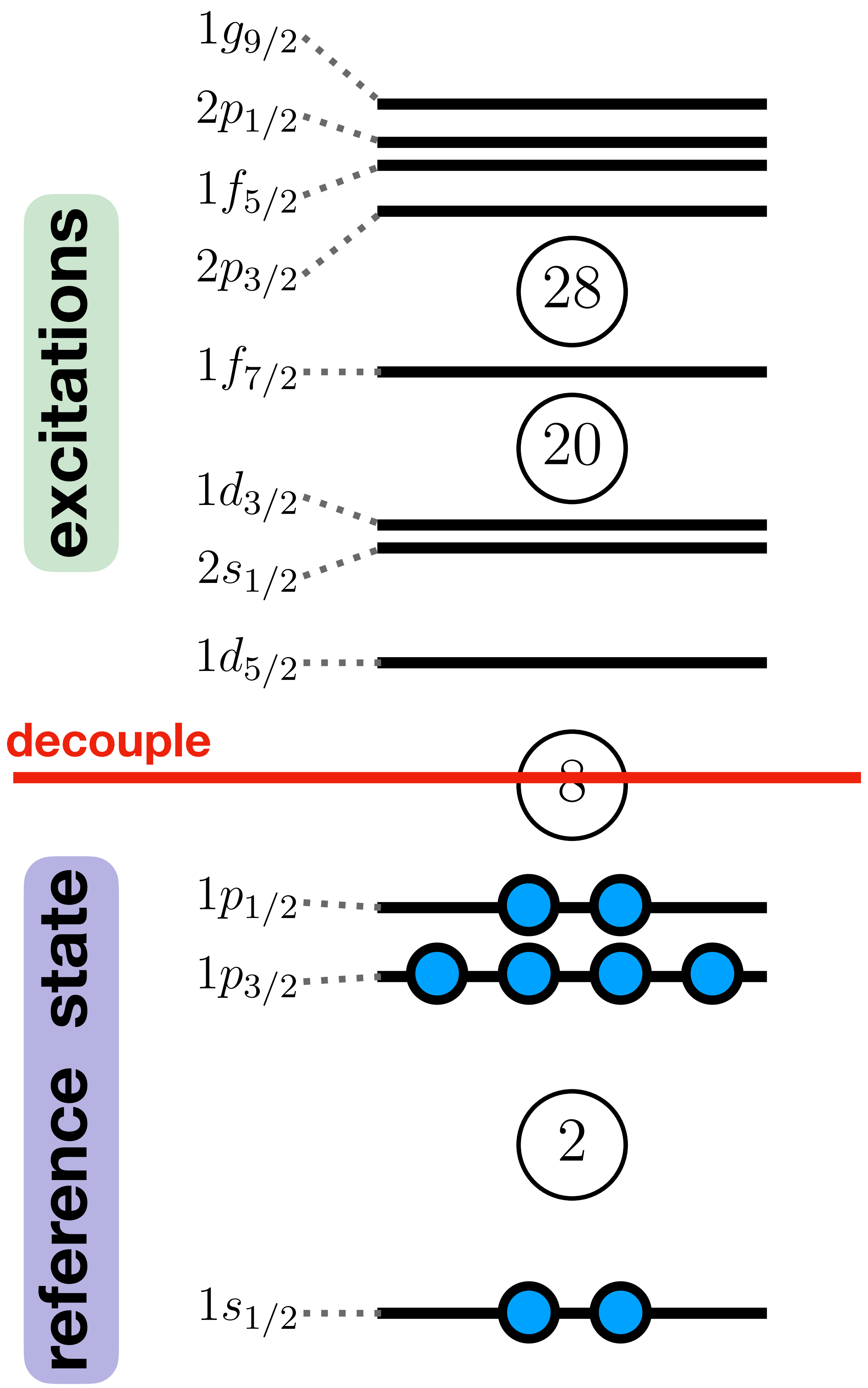


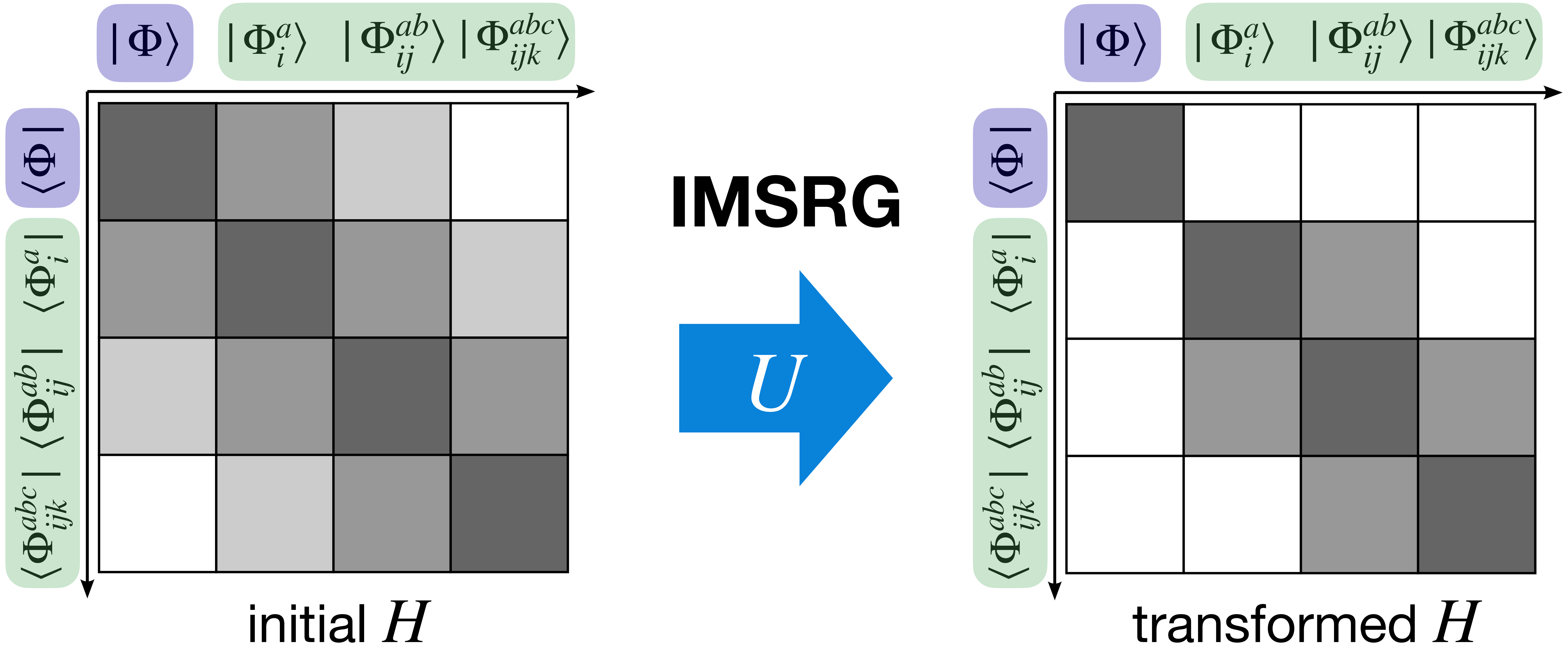


Hergert et al., Phys. Rep. **621** (2016)

- **IMSRG**: Unitary transformation $U = e^{\Omega}$ to decouple reference state from excitations

*Background*

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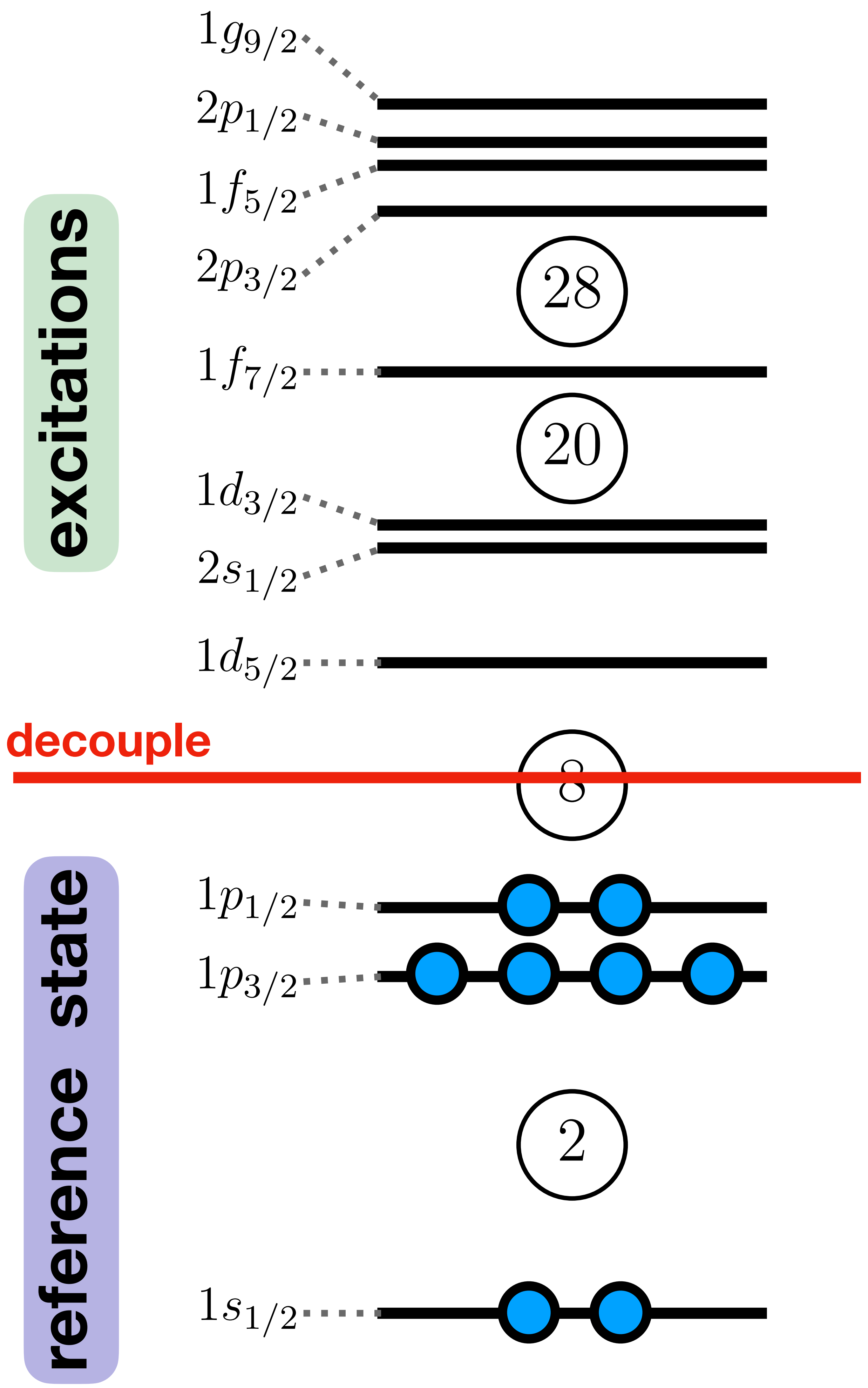
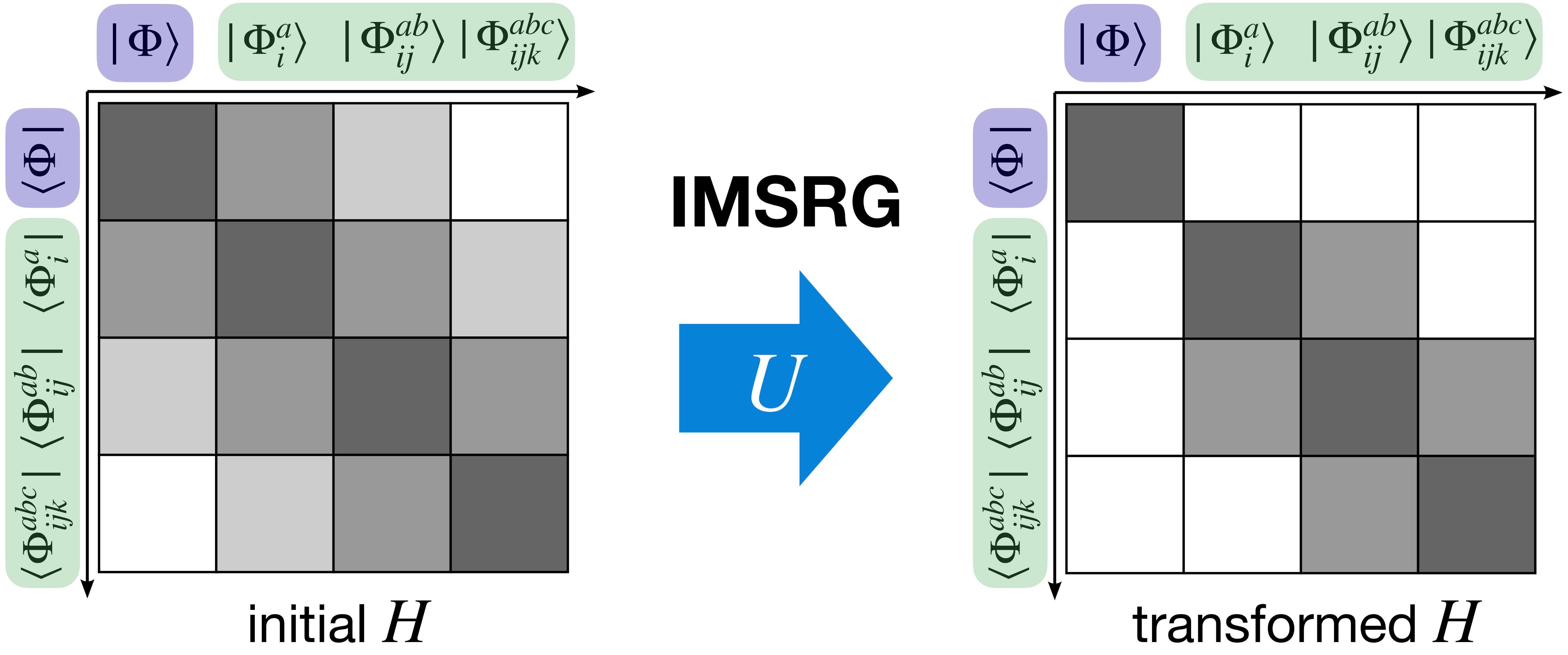



Hergert et al., Phys. Rep. **621** (2016)

- **IMSRG**: Unitary transformation $U = e^{\Omega}$ to decouple reference state from excitations
- Expansion and truncation in **many-body operators**

$$U = e^{\Omega} = e^{\Omega_1 + \Omega_2 + \Omega_3 + \dots}$$

**MH** et al., PRC **103** (2021)
PRC **111** (2025)
Stroberg, He (2024)

- **IMSRG(3)** for **precision** and **uncertainty quantification**

# The IMSRG decouples excitations

Solve SRG flow equation

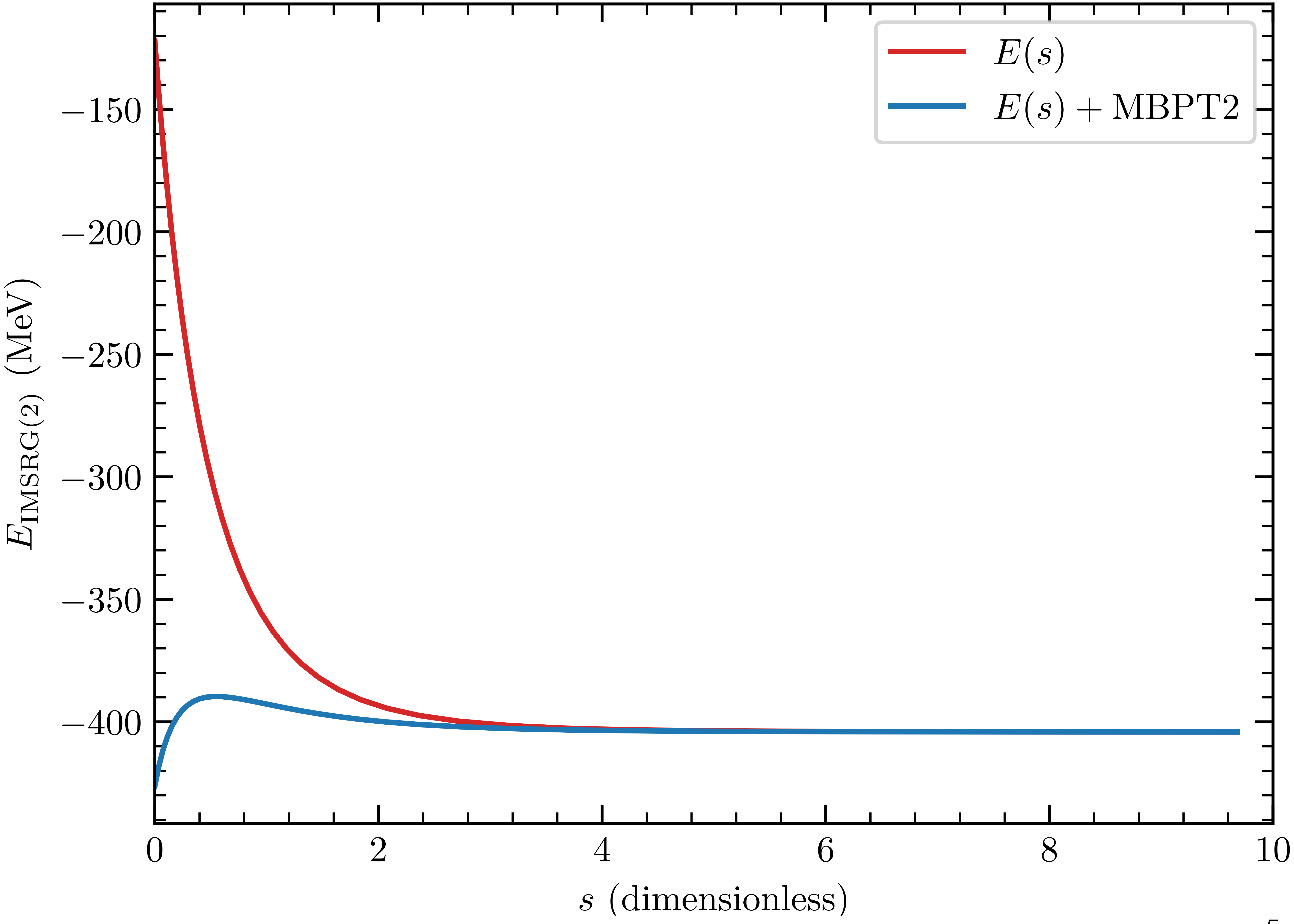
$$\frac{dH}{ds} = [\eta, H]$$

with condition that

$$\langle \Phi \,|\, H(s) \,|\, \Phi_i^a \rangle \to 0,$$

$$\langle \Phi \,|\, H(s) \,|\, \Phi_{ij}^{ab} \rangle \to 0$$

for $s \to \infty$



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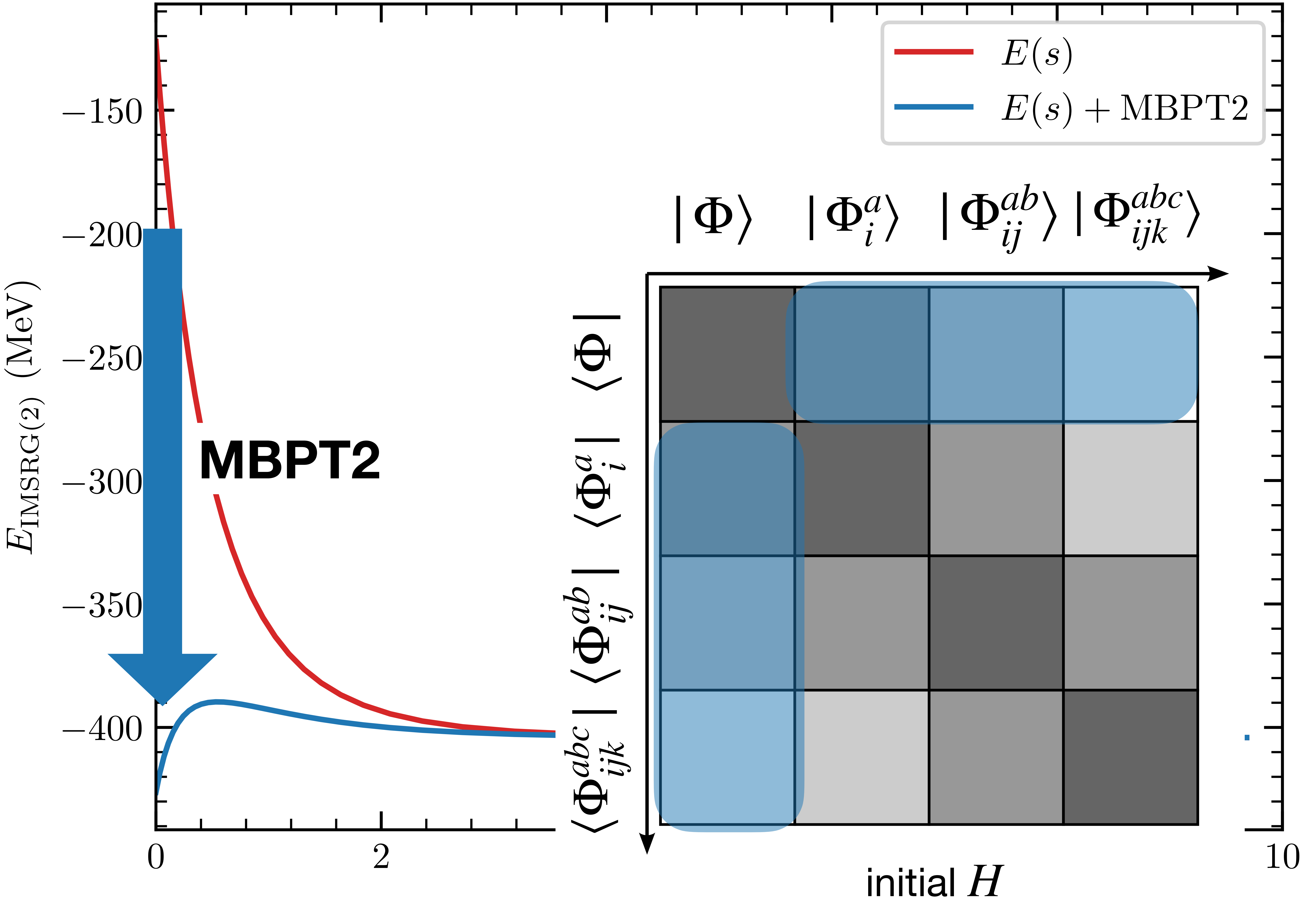

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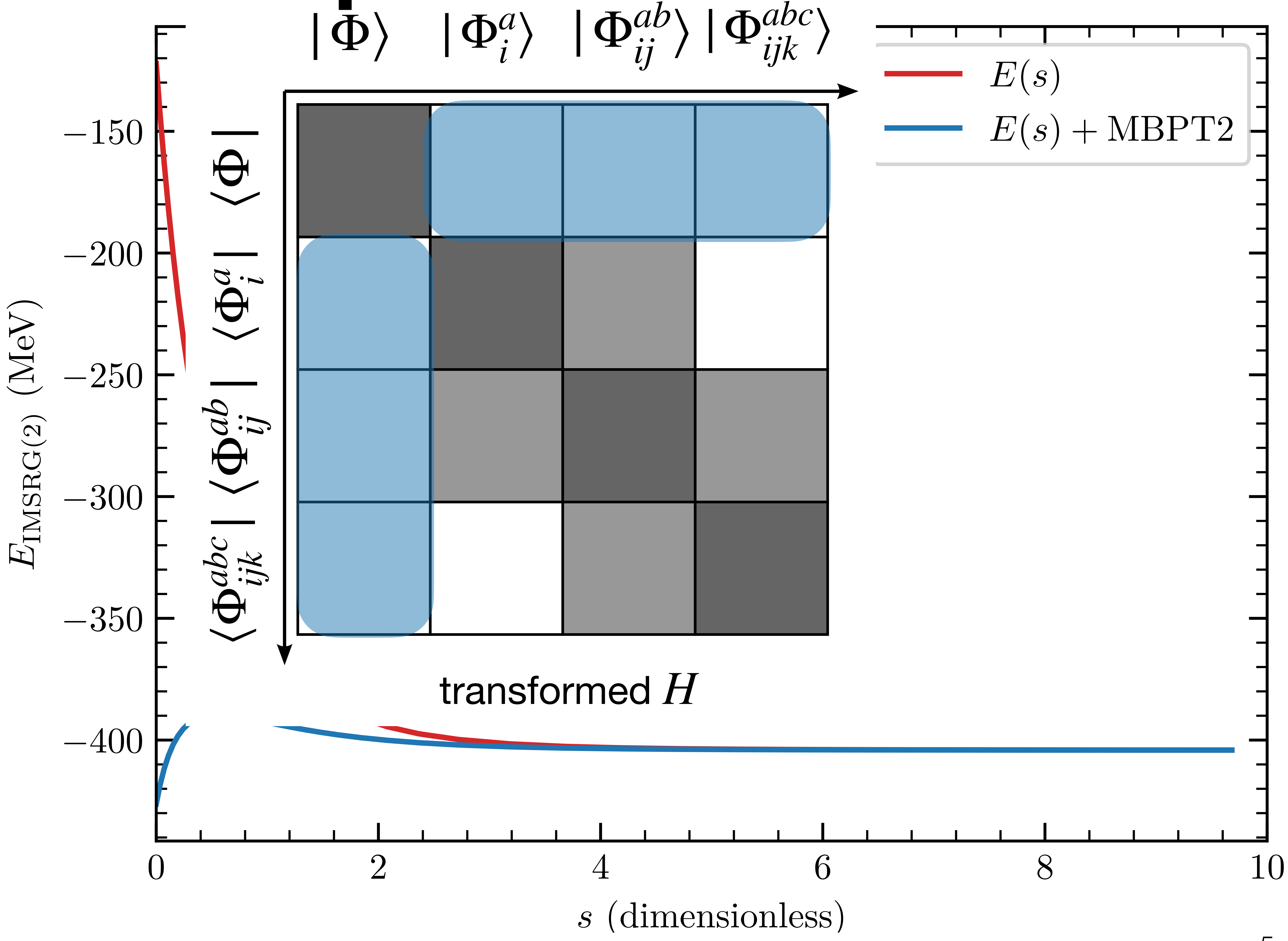

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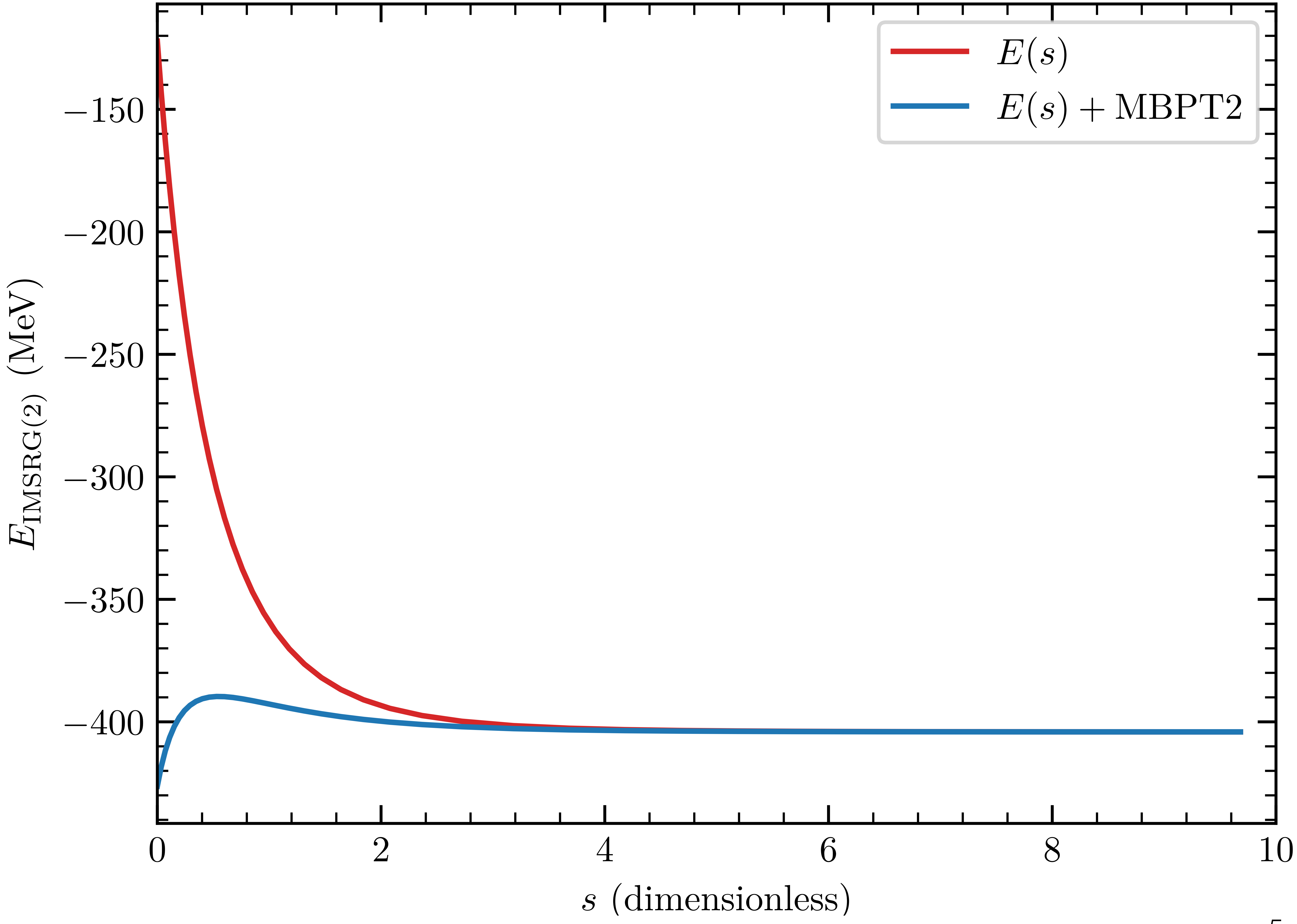
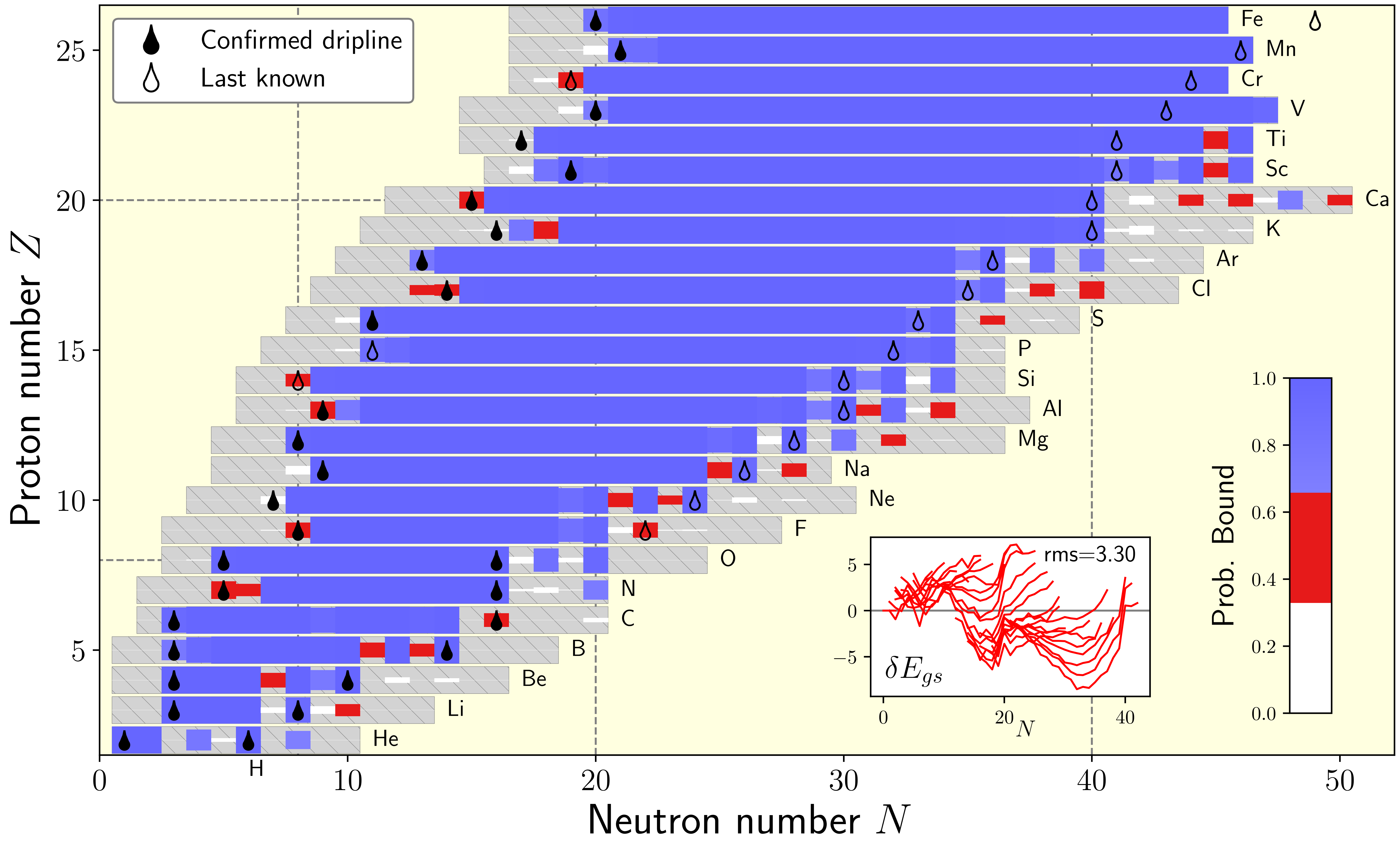


# Consistency and predictive power




Stroberg et al., PRL **126** (2021)

- **Global approaches** to nuclear structure
- **Nuclear deformation** from nuclear forces
- **Generally successful** in comparisons to experiment

# Reach to heavy nuclei

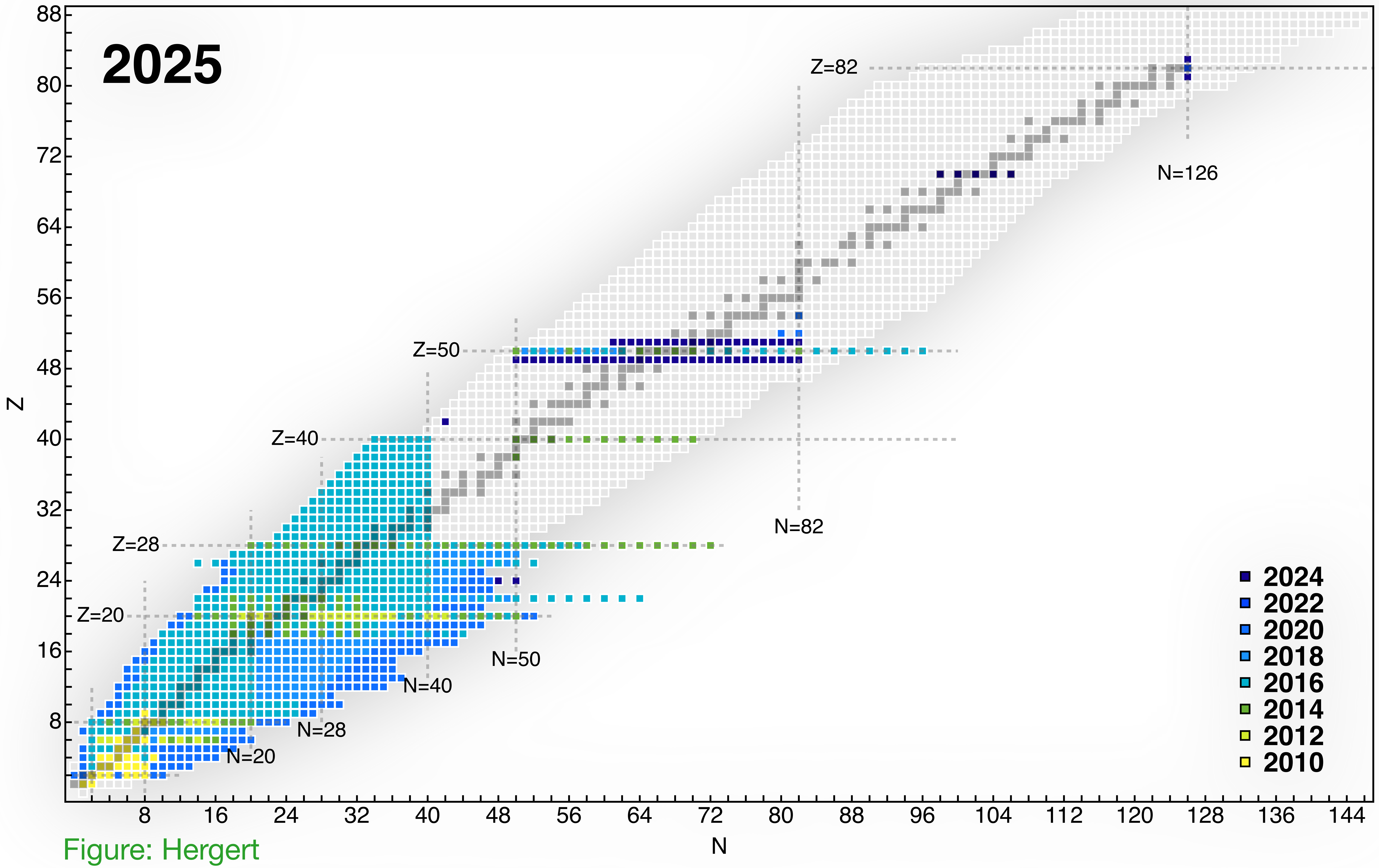



Figure: Hergert

*Successes and challenges*

# Reach to heavy nuclei

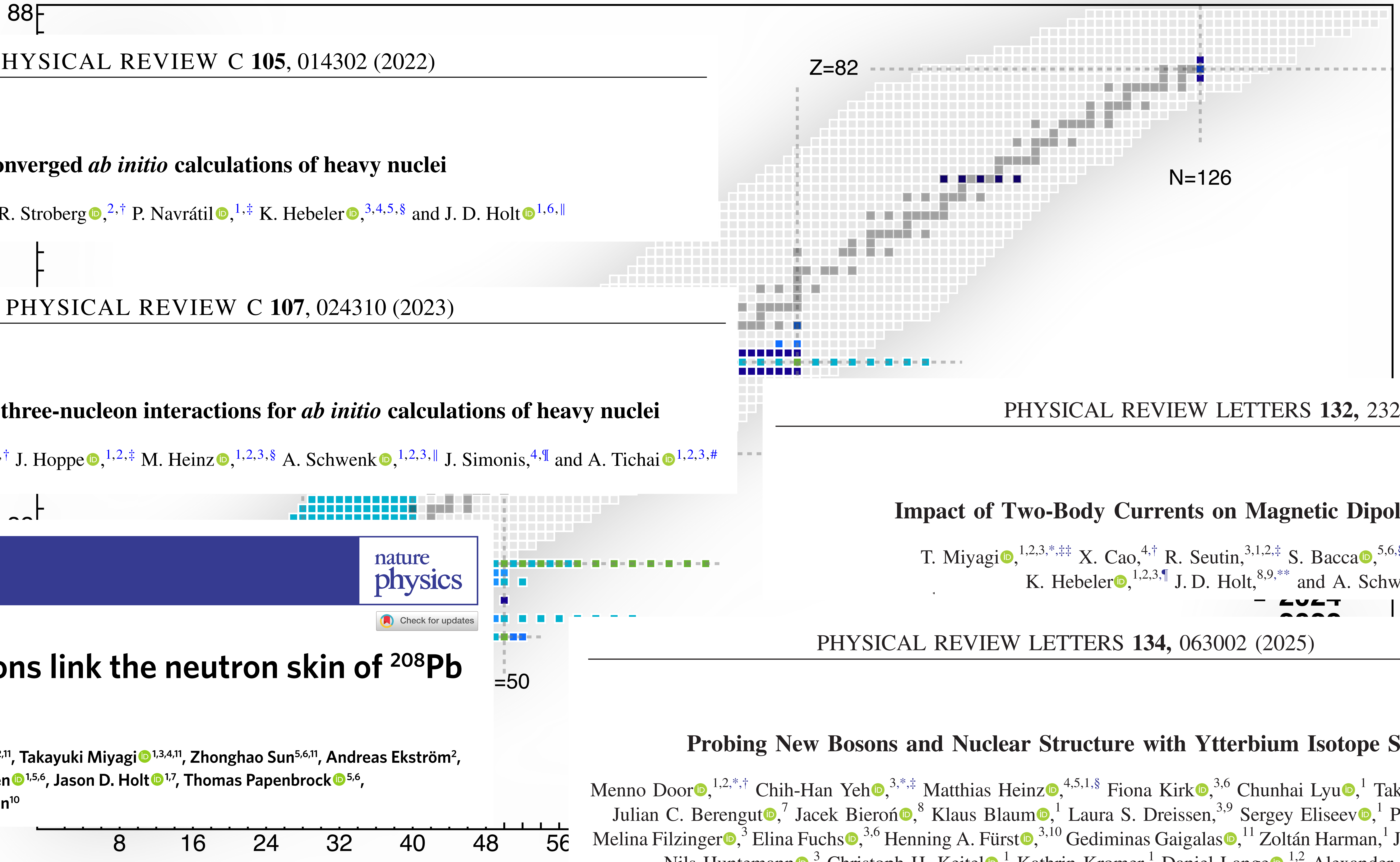



Figure: Hergert

PHYSICAL REVIEW C **105**, 014302 (2022)

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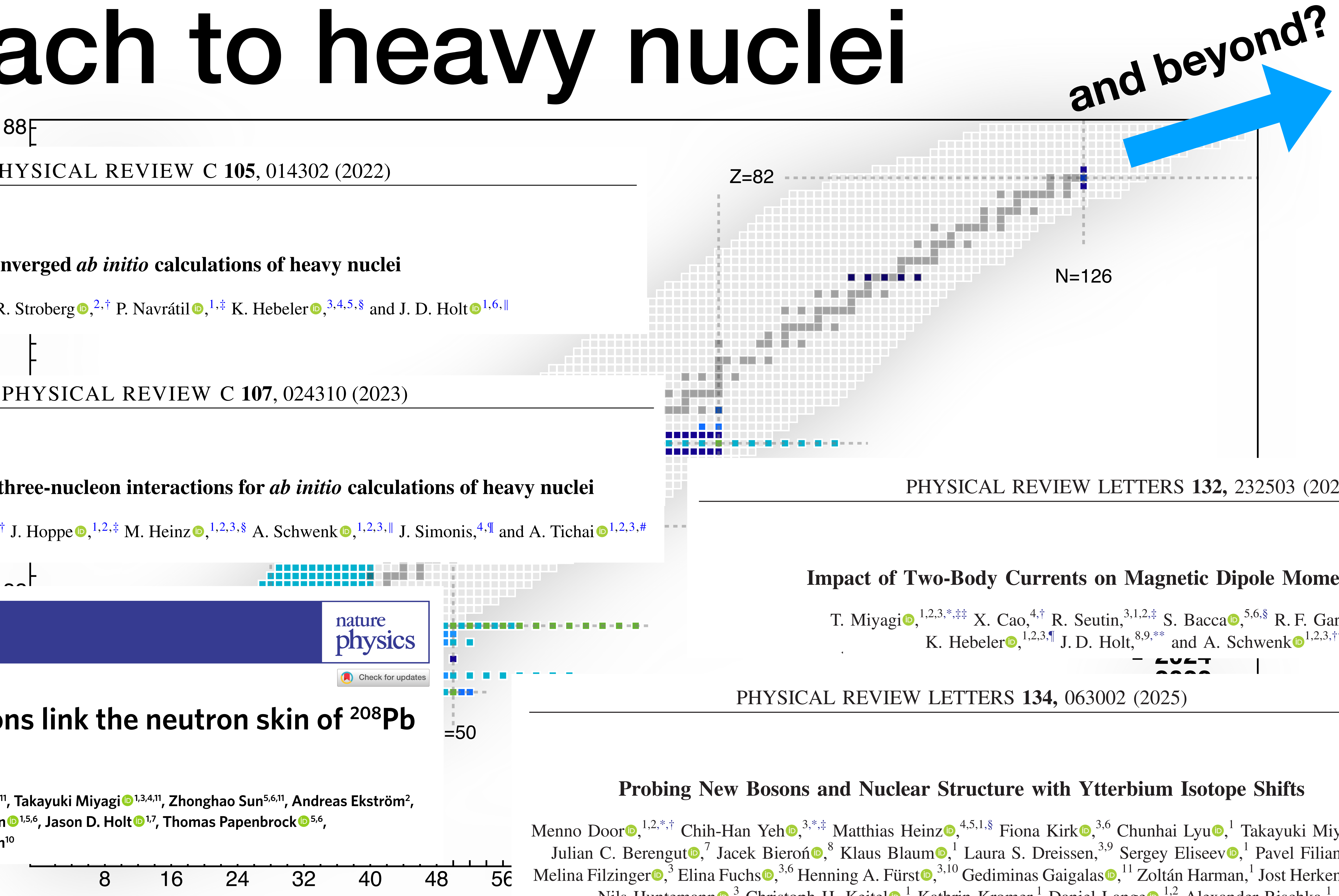


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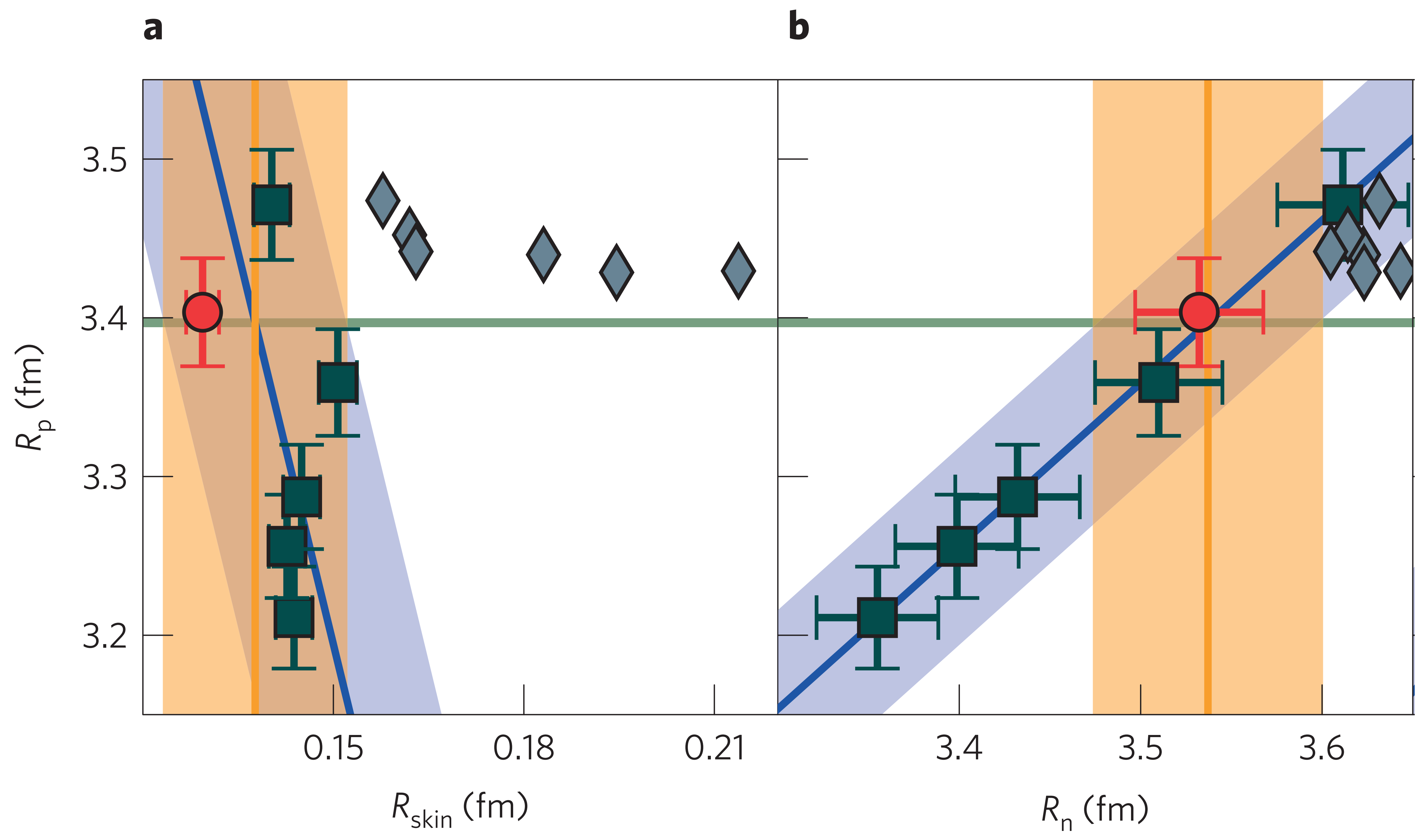
# Strong constraints for neutron densities




Hagen et al., Nat. Phys. **12** (2016)

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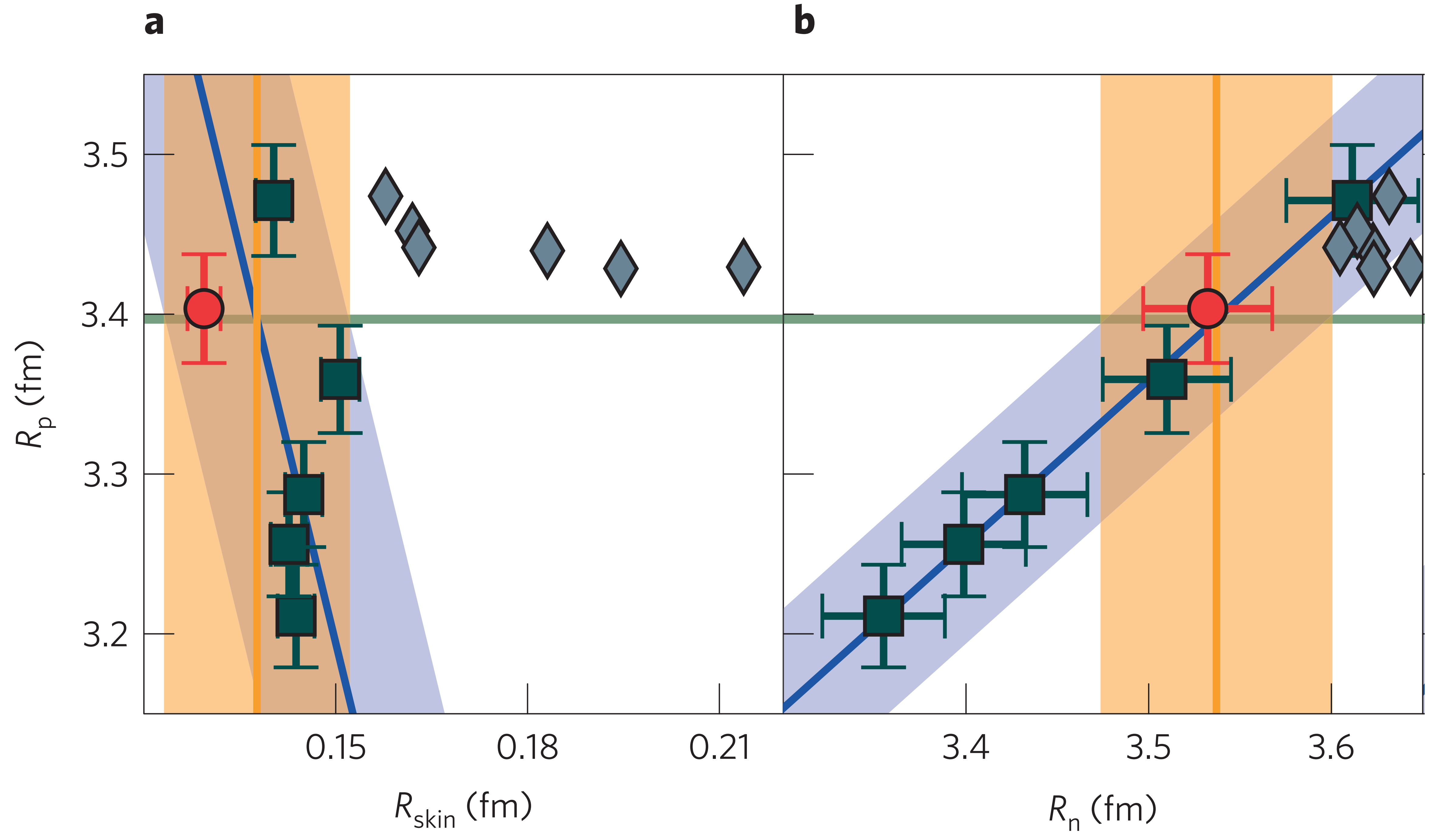
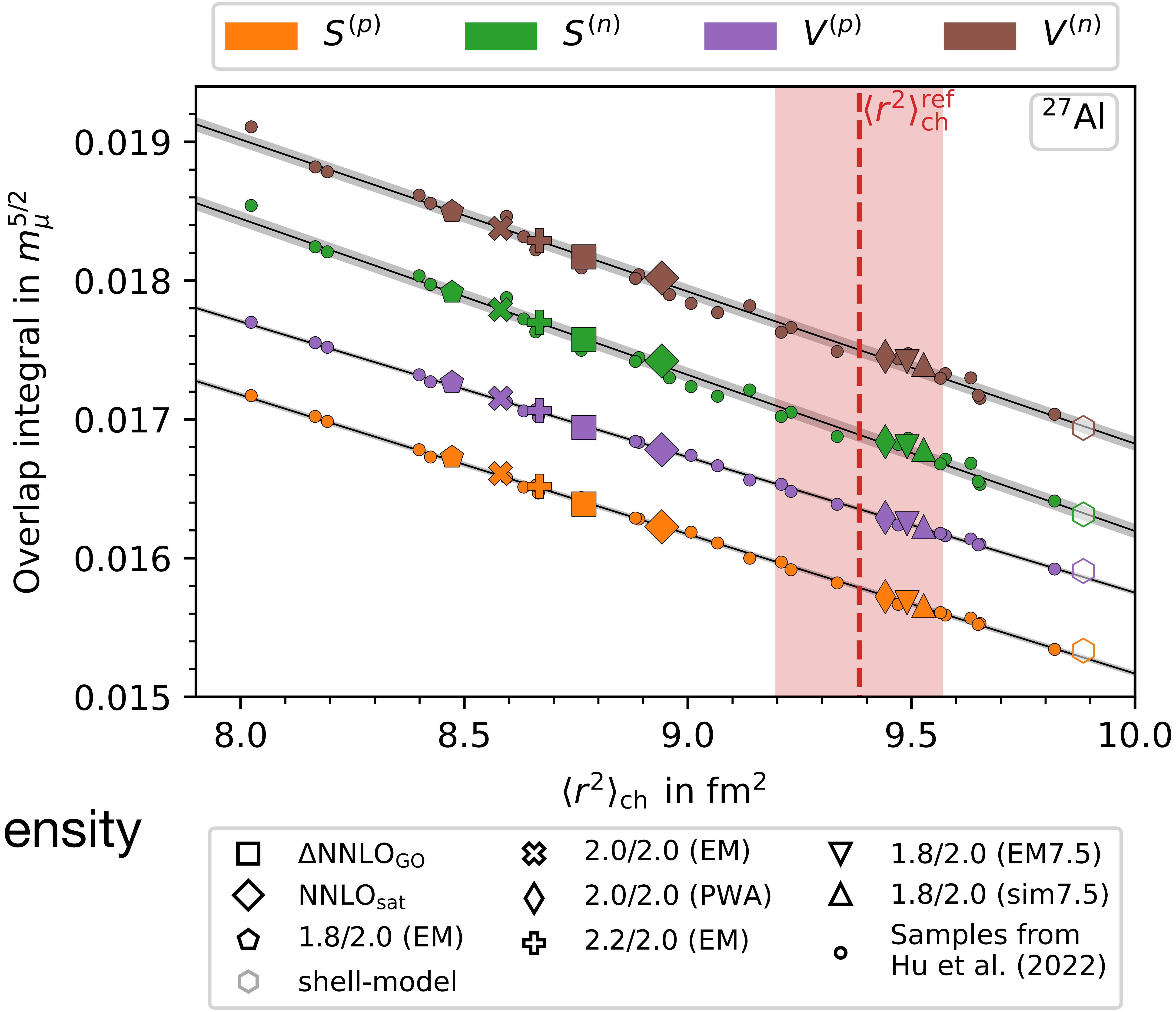



Hagen et al., Nat. Phys. **12** (2016)



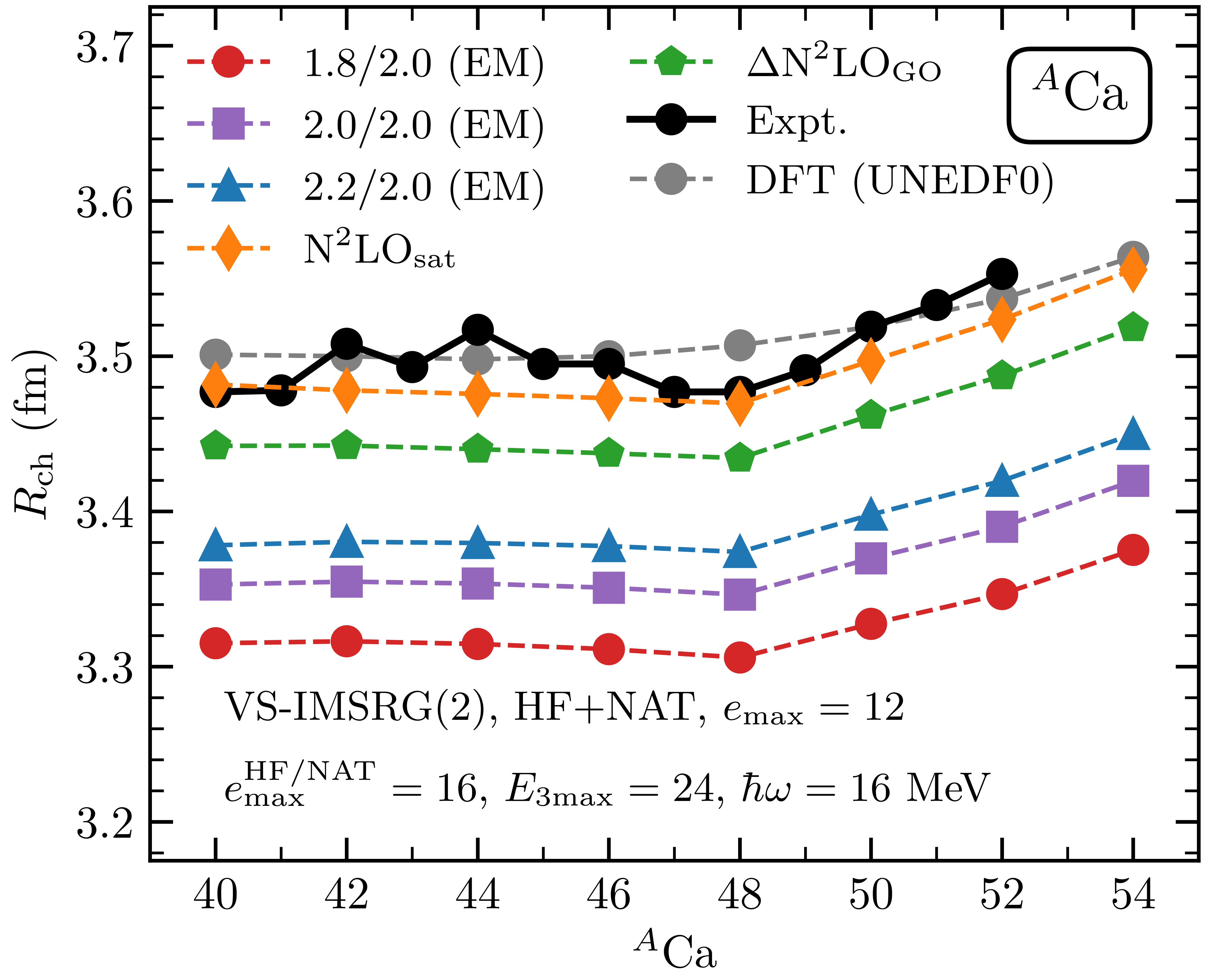

- $\mu \to e$ overlap integrals sensitive to neutron density

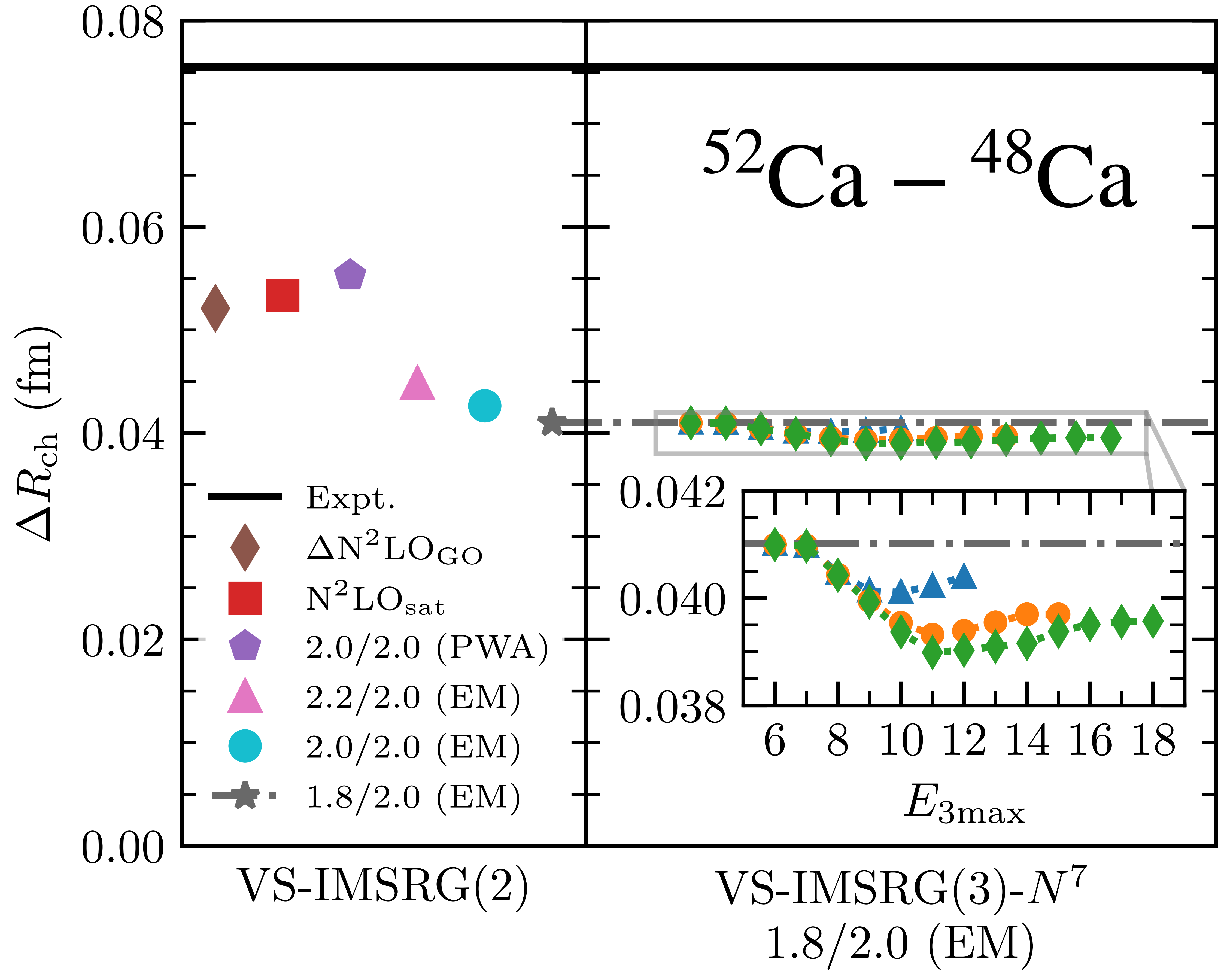
$$S^{(n)} \sim \int_0^\infty dr\, r^2 \rho_n(r)\, s(r)$$

**MH**, Hoferichter, Miyagi, Noël, Schwenk, arXiv:2412.04545

# Energies vs radii vs spectra

- Simultaneous reproduction of all observables challenging
- Various challenges in trends along isotopic chains




**MH** et al., PRC **111** (2025)

# Effective interactions

**Input** $T_{\mathrm{int}} + V_{\mathrm{LO}}$ $V_{\mathrm{NLO}}$ $V_{\mathrm{N^2LO}}$ **...**

# Effective interactions

**LO IMSRG(2)**

| | LO IMSRG(2) | | | |
|---|---|---|---|---|
| **Input** | $T_{\text{int}} + V_{\text{LO}}$ | $V_{\text{NLO}}$ | $V_{\text{N}^2\text{LO}}$ | ... |
| **Transformation** | $U_{\text{LO}}$ ↓ | | | |
| **Expectation value** | $E_{\text{LO}}$ | | | |

# Effective interactions

| | LO IMSRG(2) | Consistently evolved | | |
|---|---|---|---|---|
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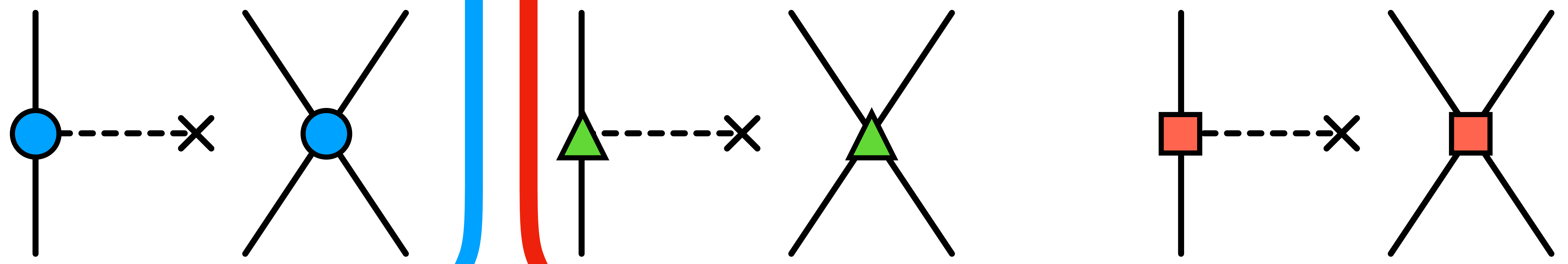
| **Effective residual interactions** | see diagrams below | see diagrams below | see diagrams below | |



# Setting up a PT expansion

**Notation:**

$$\overline{H} = H(s \to \infty) = U_{\mathrm{LO}} H U_{\mathrm{LO}}^\dagger$$

**Key ideas:**

1. Reference state $|\Phi\rangle$ **solves nonpert. Schrödinger equation** for $\overline{H}_{\mathrm{LO}}$

2. Treat $\overline{V}_{\mathrm{NLO}}$, $\overline{V}_{\mathrm{N^2LO}}$ as **perturbations**

3. Use **simple many-body perturbation theory** to compute corrections

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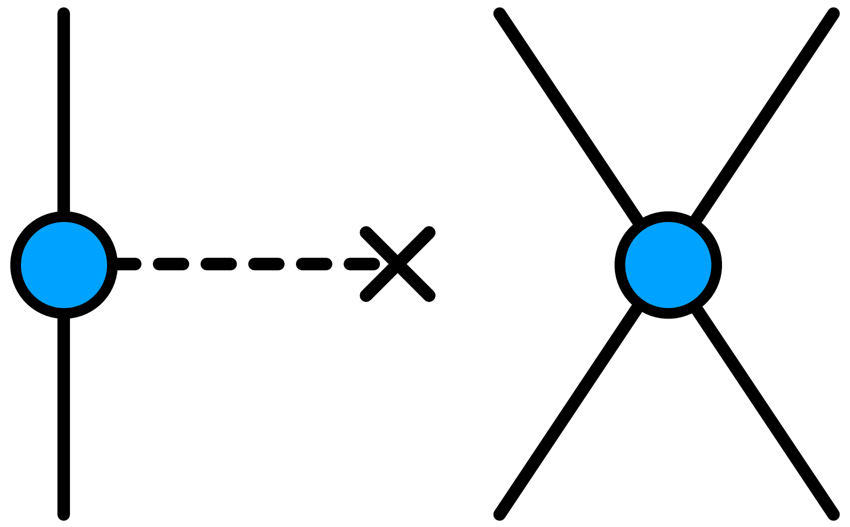

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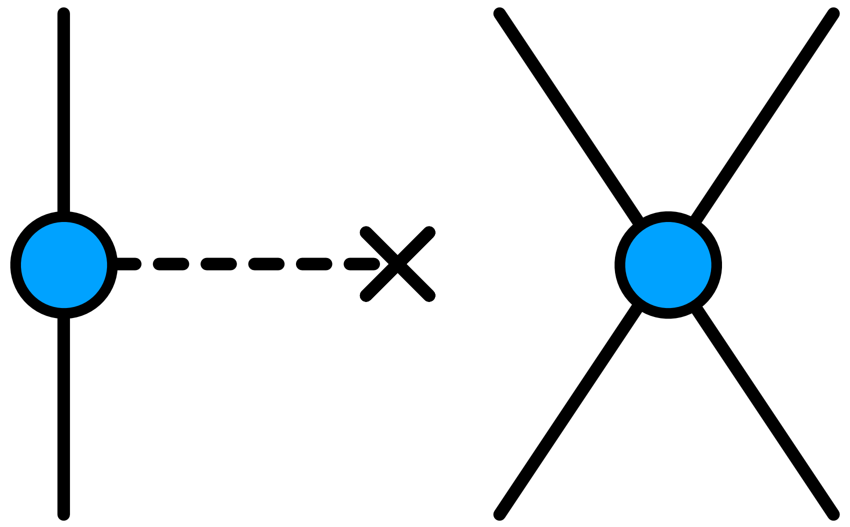

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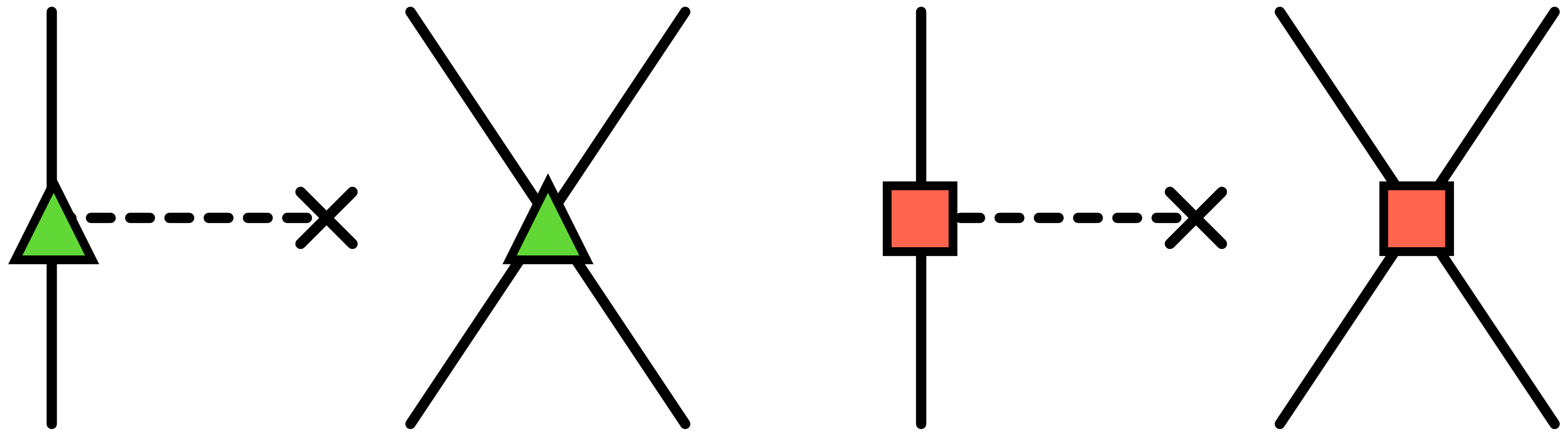
   - Nonzero expectation values…
   - … and nontrivial residual interactions

$\langle V_{\mathrm{NLO}} \rangle$ $\langle V_{\mathrm{N^2LO}} \rangle$



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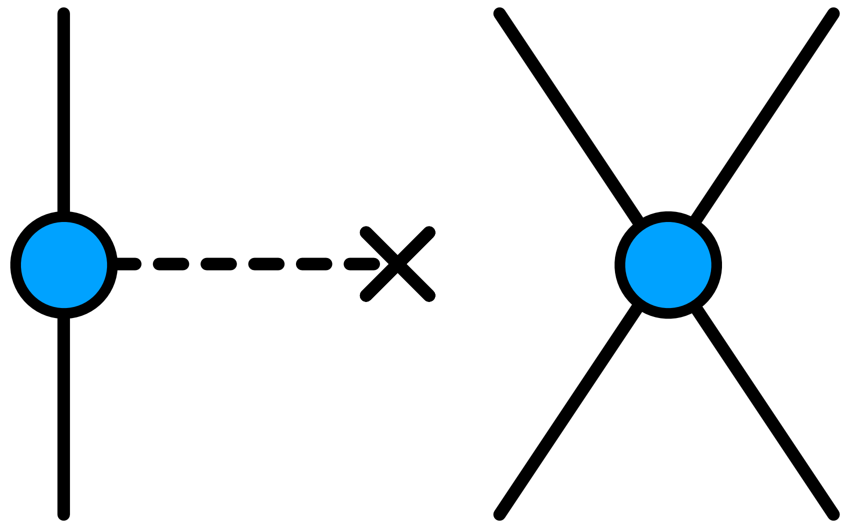

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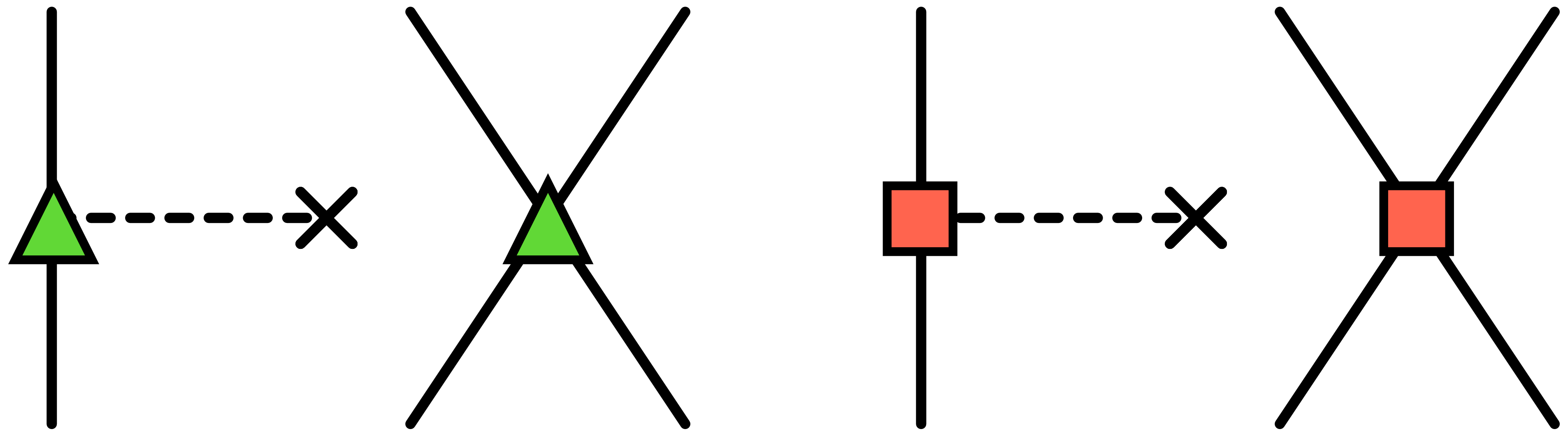

3. Use **simple many-body perturbation theory** to compute corrections

$$H = E_{\mathrm{LO}} + \mathrm{diag}\,\overline{H}_{\mathrm{LO}} + \lambda(\mathrm{offdiag}\,\overline{H}_{\mathrm{LO}} + \overline{H}_{\mathrm{NLO}}) + \lambda^2 \overline{H}_{\mathrm{N^2LO}}$$

# Putting the pieces together

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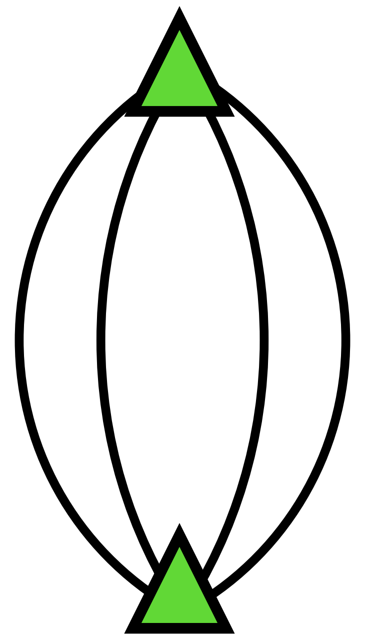
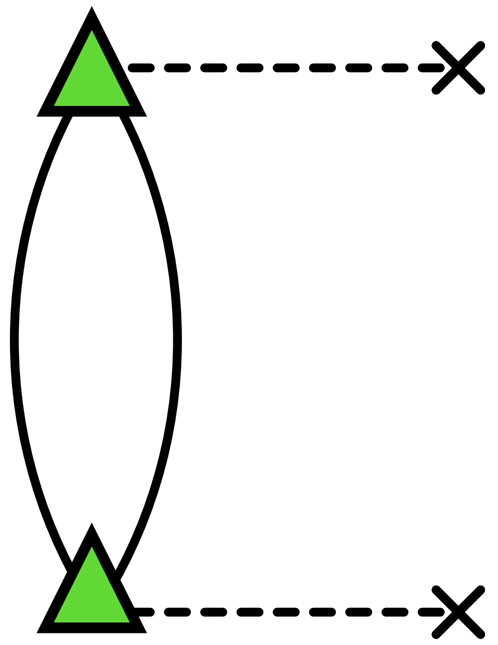
**N$^2$LO:** $\Delta E_{\mathrm{N^2LO}} = \langle V_{\mathrm{N^2LO}} \rangle$ $+$  $+$ 

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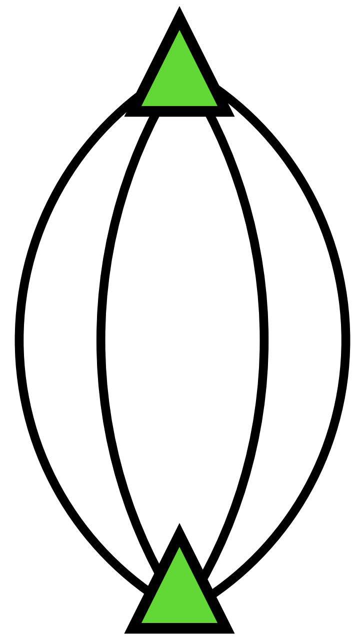
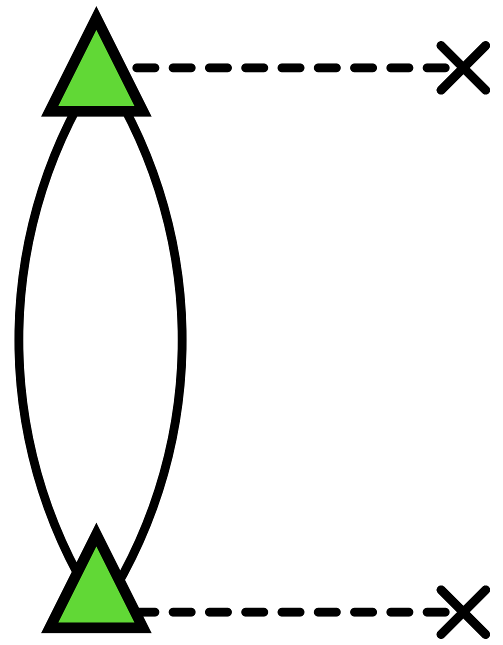
**N$^2$LO:** $\Delta E_{\mathrm{N^2LO}} = \langle V_{\mathrm{N^2LO}} \rangle$ $+$  $+$ 

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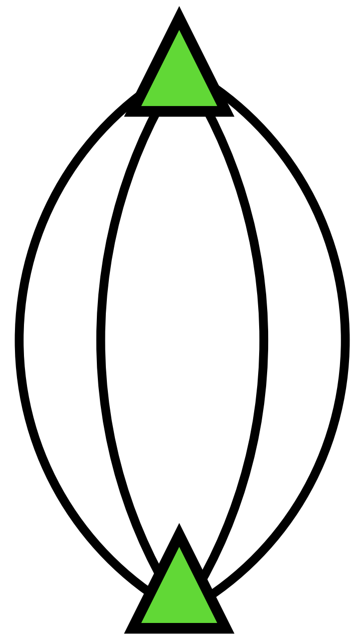
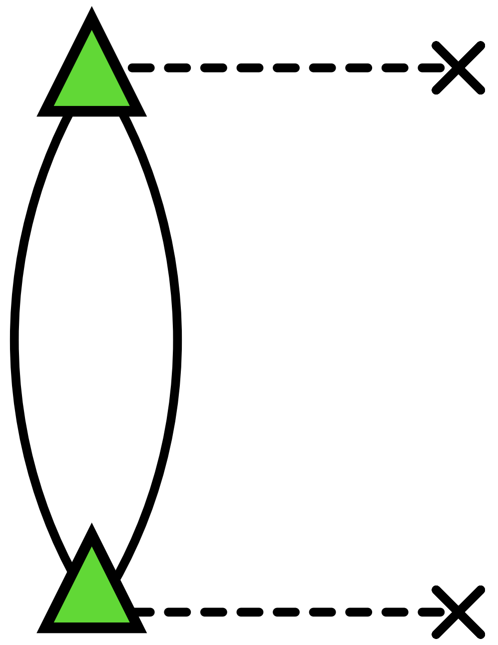
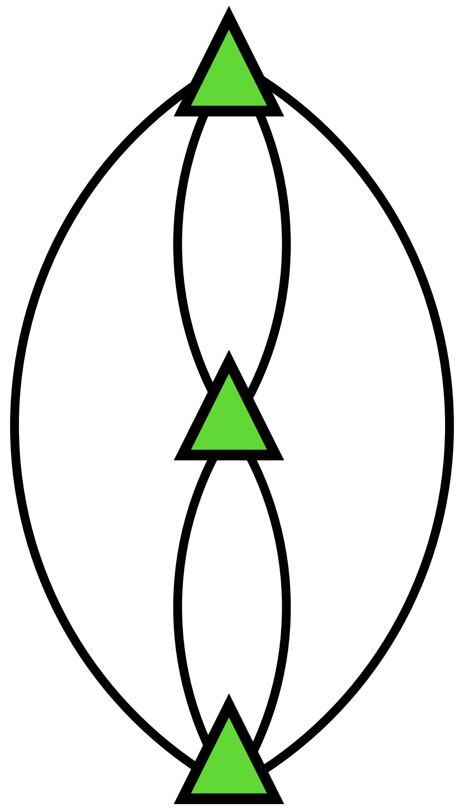
**LO:** $E_{\mathrm{LO}} = E_{\mathrm{LO}}$

**NLO:** $\Delta E_{\mathrm{NLO}} = \langle V_{\mathrm{NLO}} \rangle$

**N$^2$LO:** $\Delta E_{\mathrm{N^2LO}} = \langle V_{\mathrm{N^2LO}} \rangle$ $+$  $+$ 

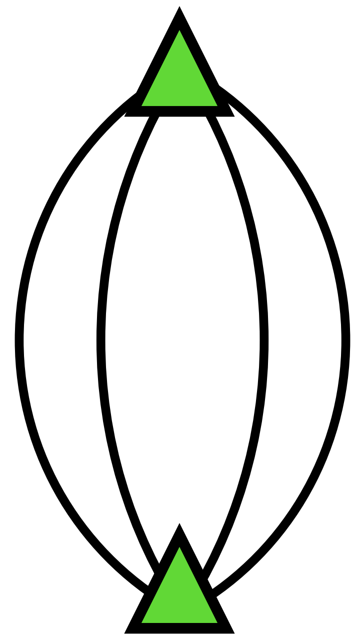
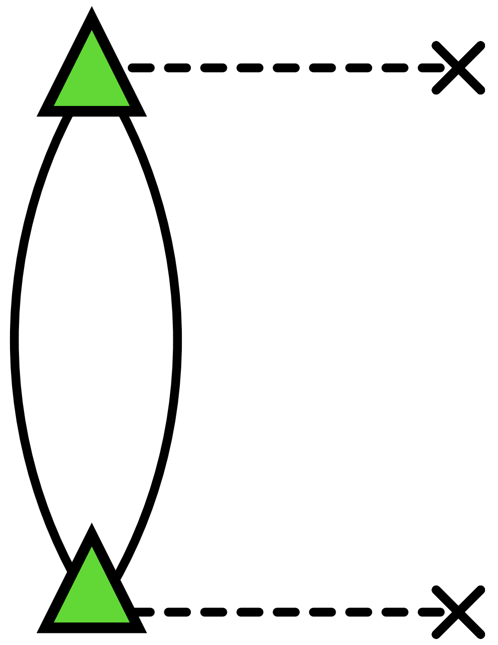
**N$^3$LO:** $\Delta E_{\mathrm{N^3LO}} = \langle V_{\mathrm{N^3LO}} \rangle$

$+$  **+ 3 other skeletons**

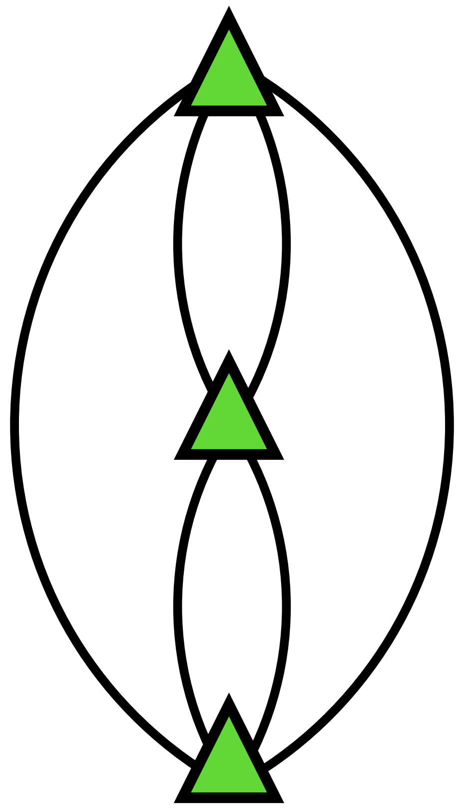
# Putting the pieces together

**LO:** $E_{\mathrm{LO}} = E_{\mathrm{LO}}$

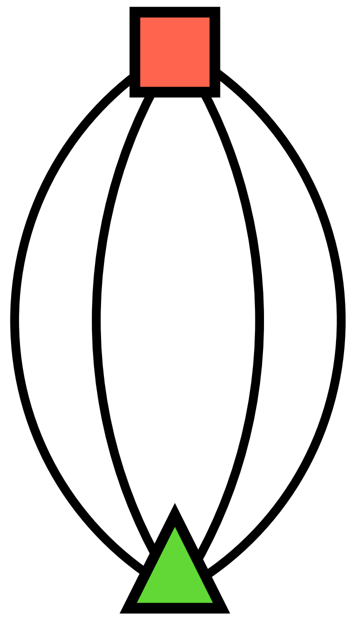
**NLO:** $\Delta E_{\mathrm{NLO}} = \langle V_{\mathrm{NLO}} \rangle$

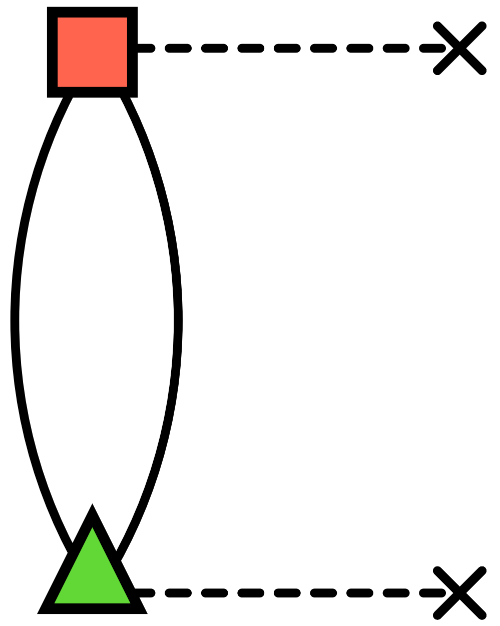
**N²LO:** $\Delta E_{\mathrm{N^2LO}} = \langle V_{\mathrm{N^2LO}} \rangle \quad +$  $+$ 

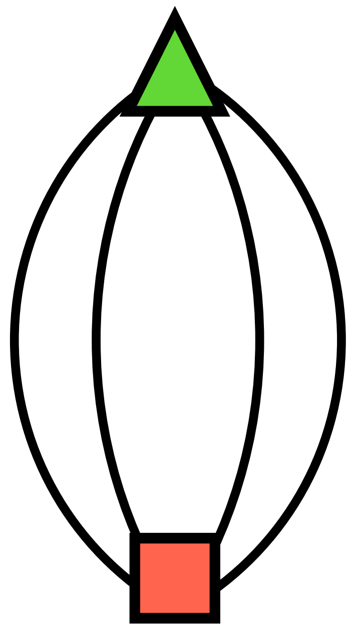
**N³LO:** $\Delta E_{\mathrm{N^3LO}} = \langle V_{\mathrm{N^3LO}} \rangle$

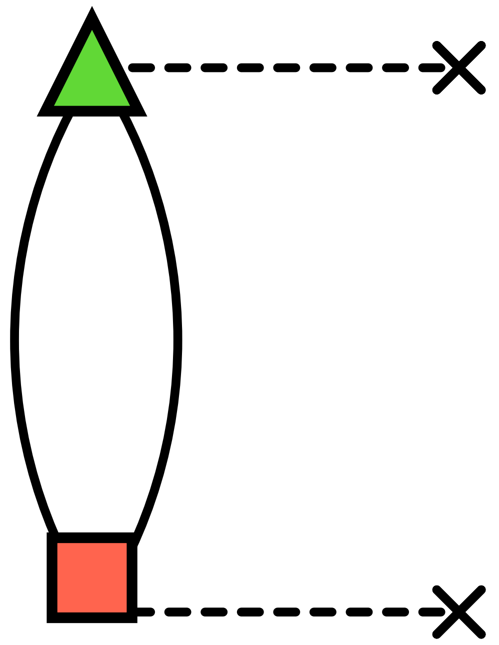
$+$ 

**+ 3 other skeletons**









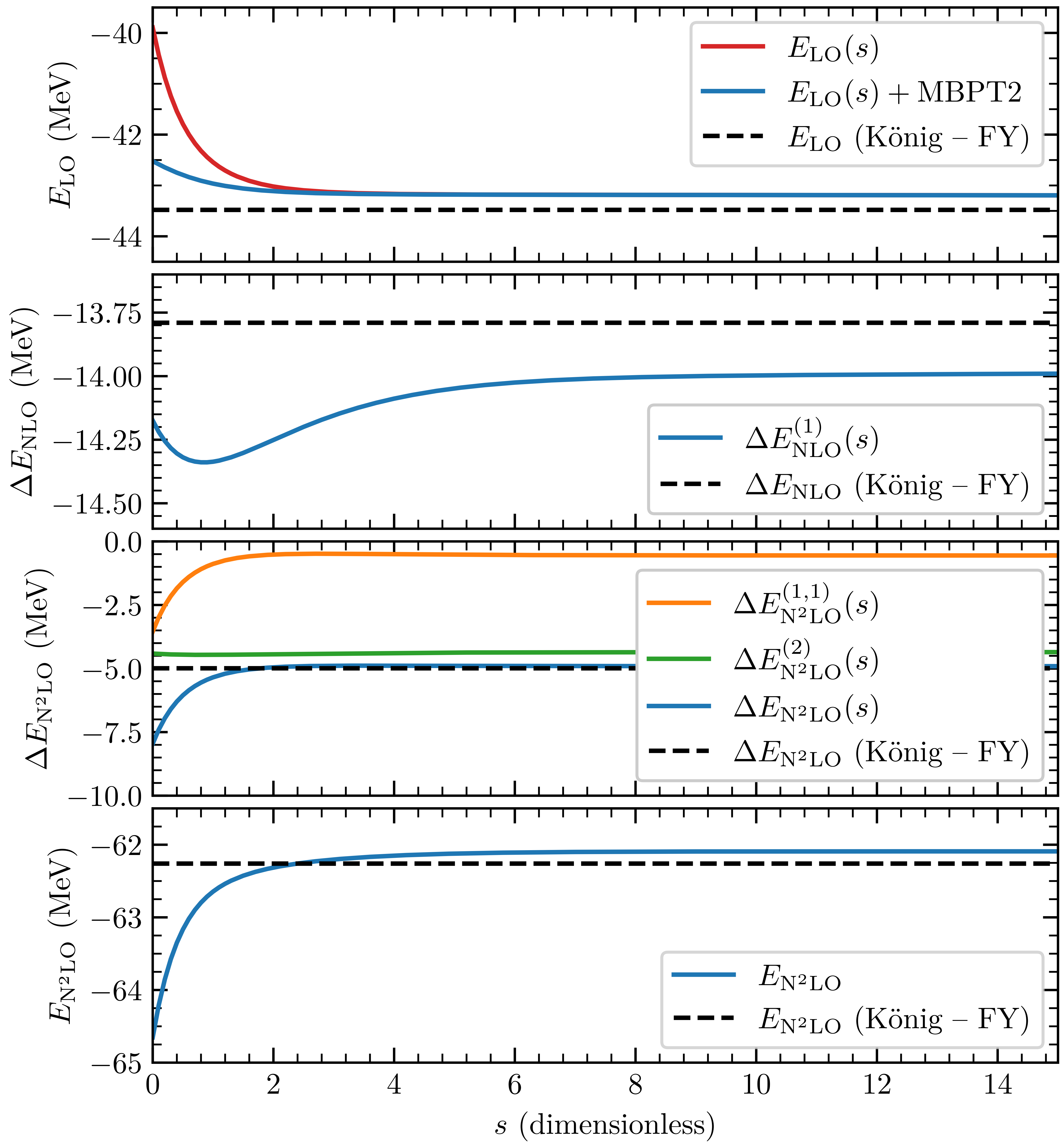
# Basic setup

- Input Hamiltonian:
  - NN-only pionless EFT up to $\mathrm{N^2LO}$, $\Lambda = 400\ \mathrm{MeV}$
  - Expansion around unitary limit König, EPJA **56** (2020)
  - Caveat: **No 3N force** at $\mathrm{LO}$, **no 4N force** at $\mathrm{NLO}$, **benchmarks only!**
- Comparison with results from Faddeev-Yakubovsky (FY) calculations by Sebastian König for $^4\mathrm{He}$
- Main goal: **Quantitative agreement** to validate approach and implementation
  - Keep in mind: IMSRG(2) and MBPT are not exact methods

*Preliminary explorations*

# IMSRG flow

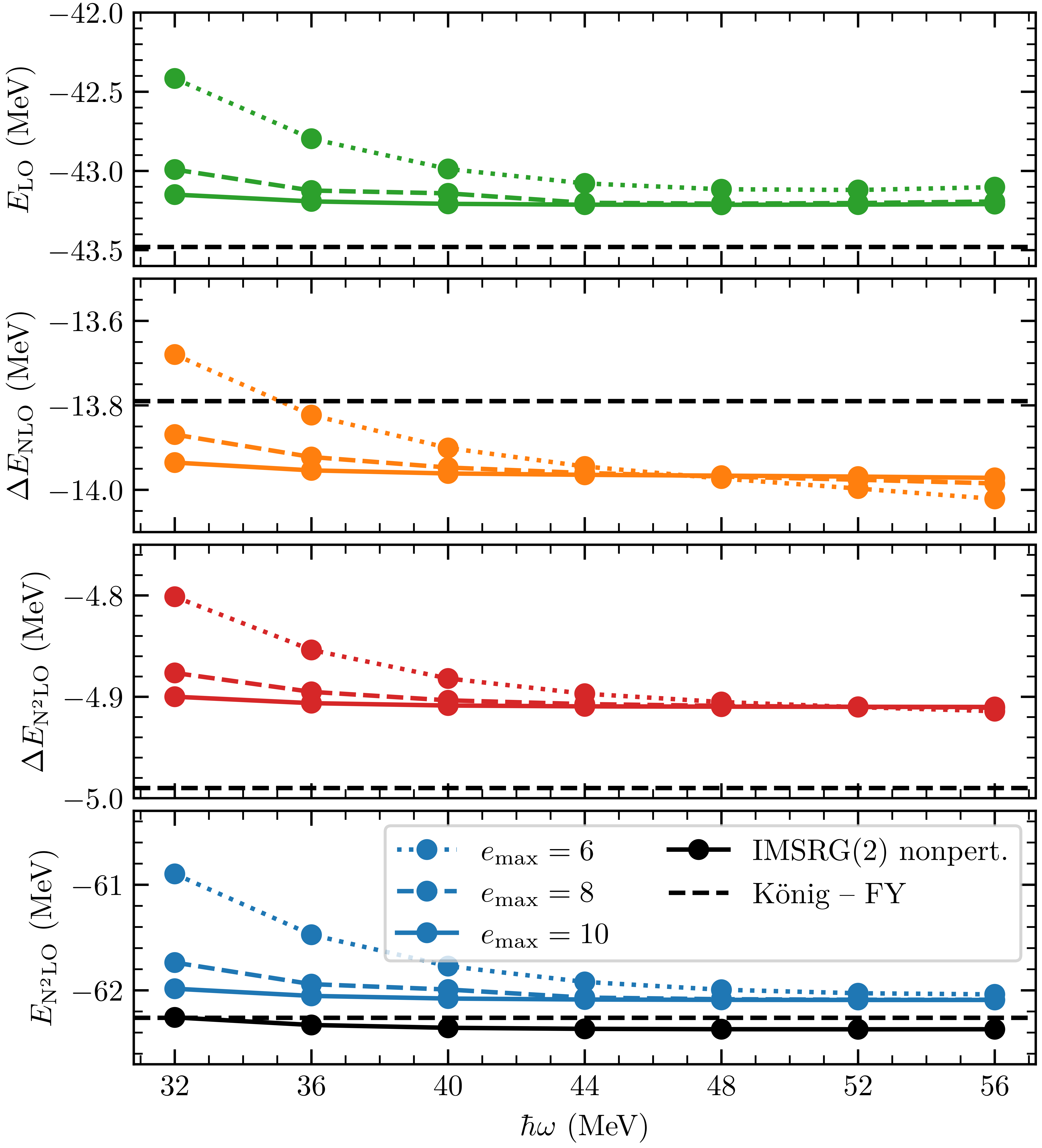
- **Good agreement with FY results** within expected uncertainties
  - Less than $300\ \mathrm{keV}$ at $\mathrm{LO}$
- IMSRG(2) solution seems to roughly decouple $\overline{V}_{\mathrm{NLO}}$
  - $\Delta E^{(1,1)}_{\mathrm{N^2LO}} \ll \Delta E^{(2)}_{\mathrm{N^2LO}}, s \to \infty$
- **LO IMSRG(2) solution** dominates many-body uncertainty



***Preliminary explorations***

# Convergence behavior

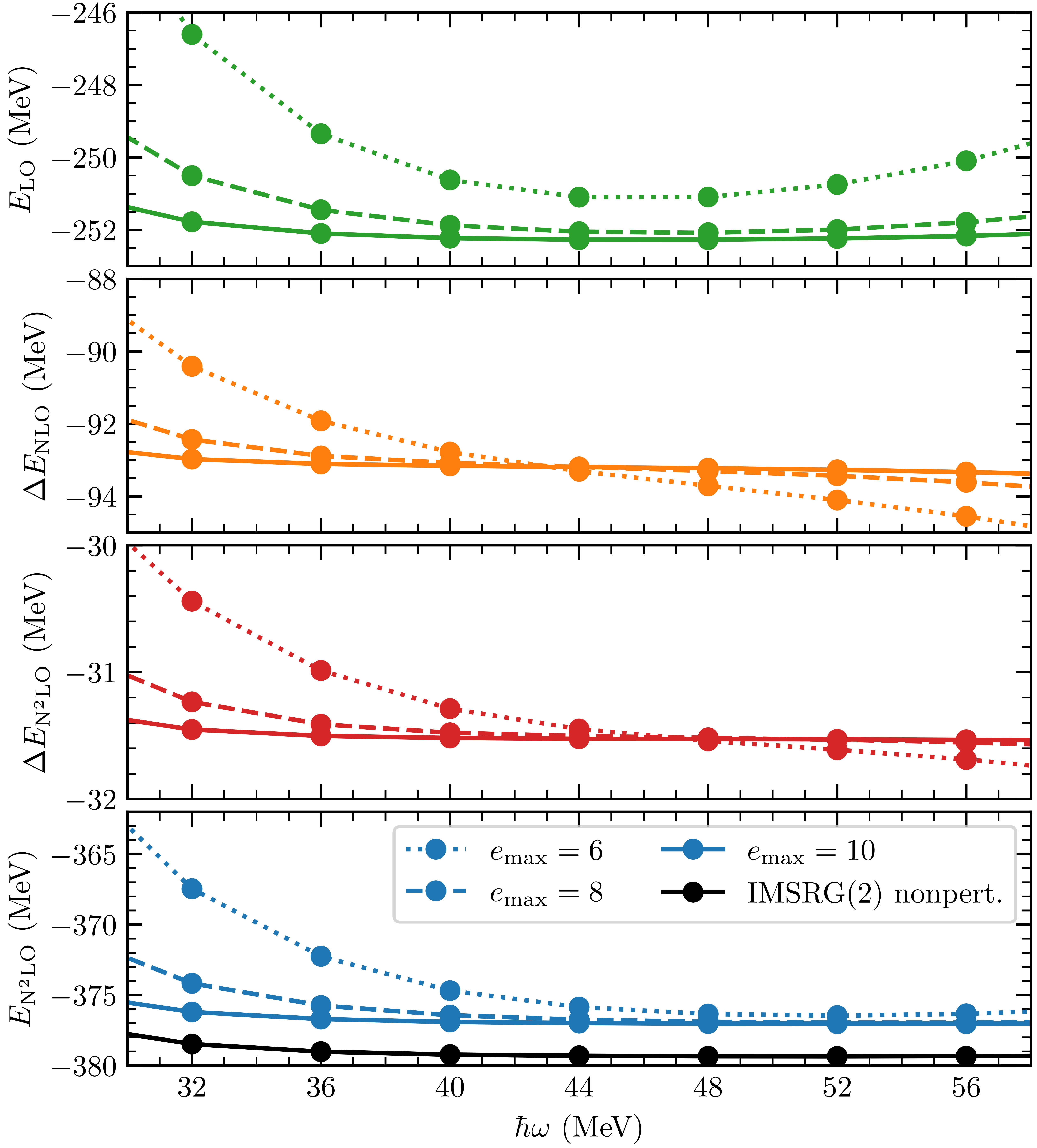
- Reasonable model-space convergence
  - Flat in $\hbar\omega$ at $e_{\max} = 10$
- Trends for $\Delta E_{\mathrm{NLO}}$ suggest that $\mathrm{LO}$ reference state may be suboptimal
- Full nonperturbative IMSRG(2) solution very compatible



## *Preliminary explorations*

# $^{16}$O

- LO → NLO relative correction looks similar to Yang et al.
- Model-space convergence behavior still reasonable
  - Can consider larger cutoffs, but not too large
- Overall promising approach, N$^3$LO also feasible



# What about larger cutoffs?

- Many-body methods have errors that scale with **correlation energy** $E_{\text{corr}}$
- Hard interactions → large correlation energies → large uncertainties
- Operate at **moderate cutoffs** to keep many-body uncertainties low

| IMSRG | IMSRG(2) | ΔIMSRG(3)-$N^7$ | % |
|---|---|---|---|
| $E_{\text{corr}}(^{40}\text{Ca})$ | −96.9 | −1.7 | 1.7 |
| $E_{\text{corr}}(^{48}\text{Ca})$ | −112.2 | −1.8 | 1.6 |
| $E_{\text{corr}}(^{52}\text{Ca})$ | −119.9 | −2.0 | 1.6 |

| VS-IMSRG | VS-IMSRG(2) | ΔVS-IMSRG(3)-$N^7$ | % |
|---|---|---|---|
| $E_{\text{corr}}(^{44}\text{Ca})$ | −108.2 | −1.4 | 1.3 |
| $E_{\text{corr}}(^{48}\text{Ca})$ | −113.5 | −1.2 | 1.1 |
| $E_{\text{corr}}(^{52}\text{Ca})$ | −121.4 | −1.3 | 1.1 |

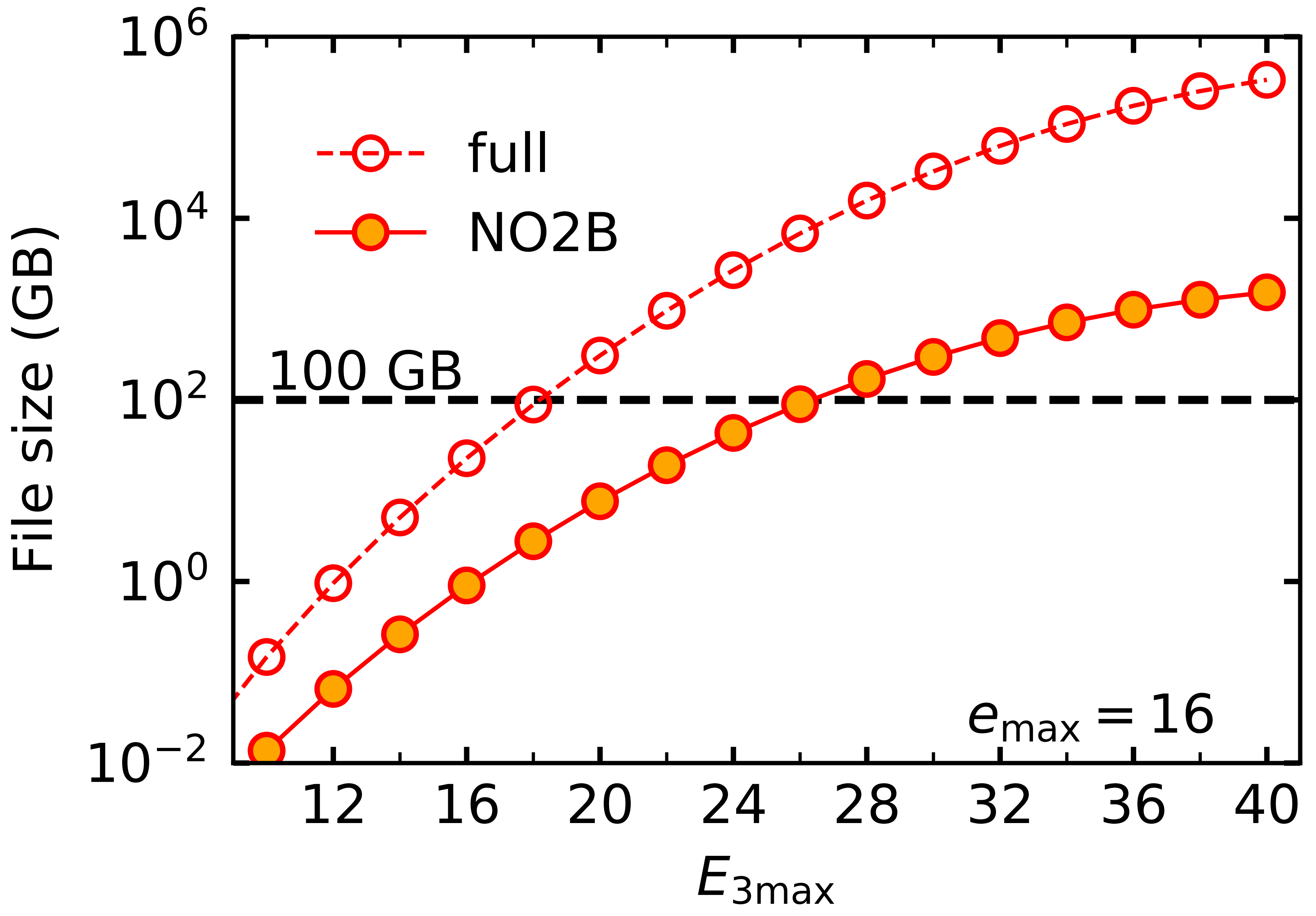
**MH** et al., PRC **111** (2025)

# What about 4N forces?

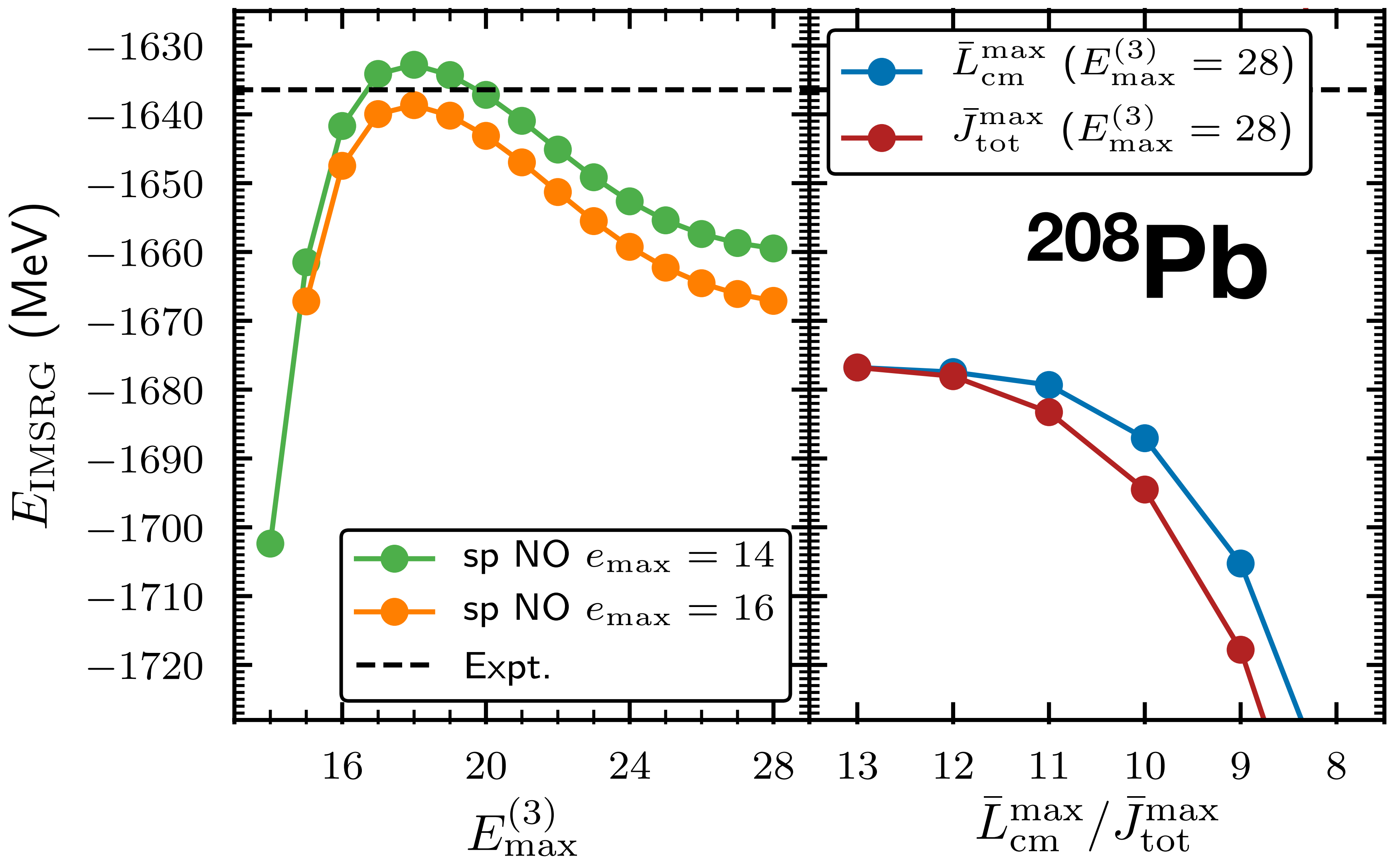
- Normal ordering of 3N forces

$$V^{(3,\mathrm{NO})}_{1234} = \sum_{ij} \rho_{ij} V^{(3)}_{12i34j}$$

- Reformulation in terms of Jacobi momenta
- Similar approach would work for short-range 4N forces, **but not long-range**



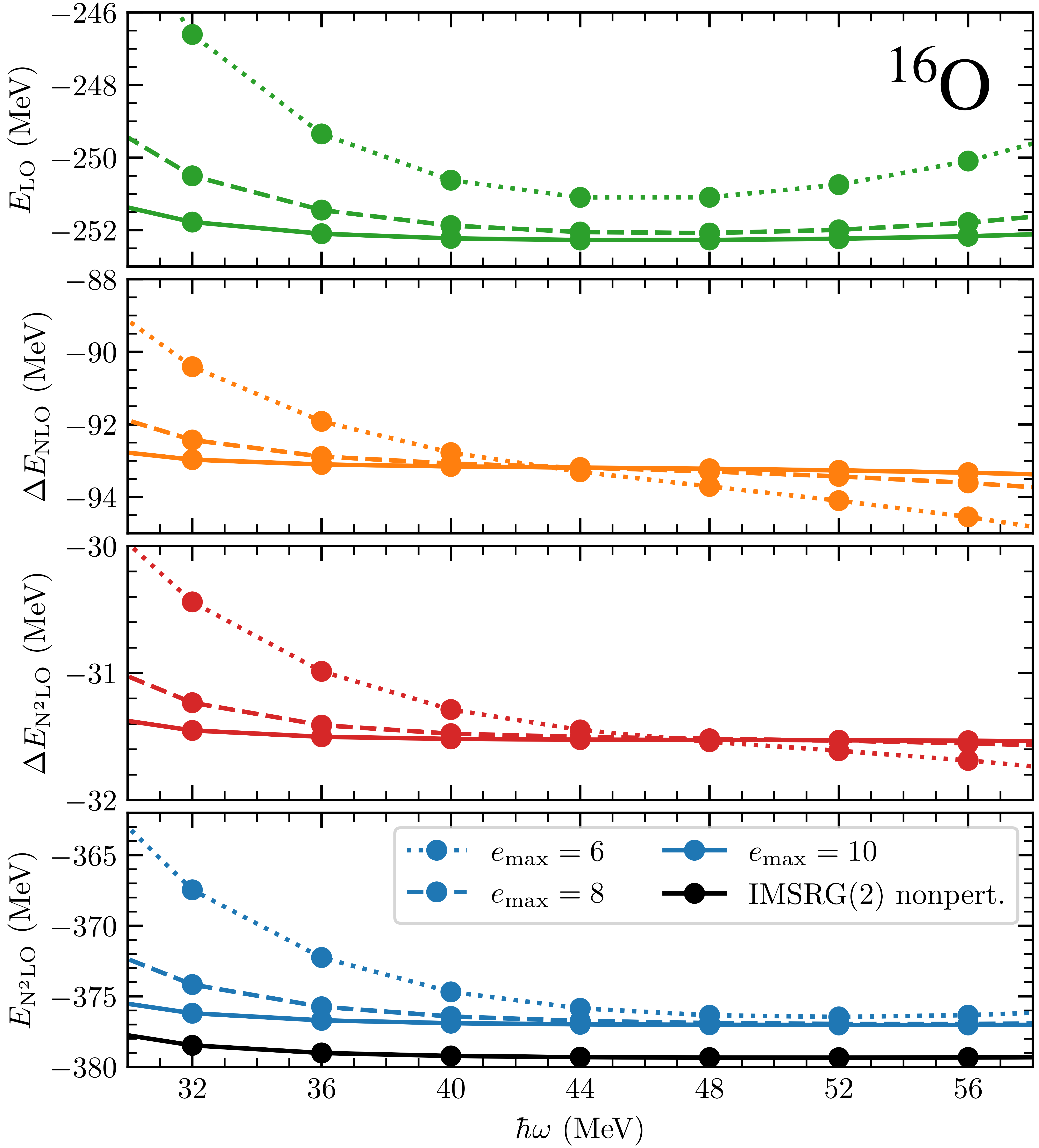

Miyagi et al., PRC **105** (2022)




Hebeler et al., PRC **107** (2023)

# Conclusions

- Combination of IMSRG & MBPT to treat **subleading potentials perturbatively**
- **Scalable** to medium-mass and heavy systems
- Still challenged by large cutoffs, 4N interactions



# Open challenges and questions

- Need to be clear about our goals, cost/benefit analysis
  - **Where can we improve? Where does current nonpert. approach fail?**
- LO reference state is probably pretty poor, need to test validity of PT
  - **Can we actually reasonably do perturbation theory in this case?**
- Similar approach not possible with valence space calculations yet
  - **How do we do PT in large-scale diagonalizations?**
- Considering other operators is more challenging
  - **How to evaluate PT for other operators?**
- **Overall, it is unclear what precision we can expect from this treatment; need to stay at moderate cutoffs b/c of many-body approximation**

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