Ab initio nuclear structure calculations for new physics searches in ytterbium isotope shifts

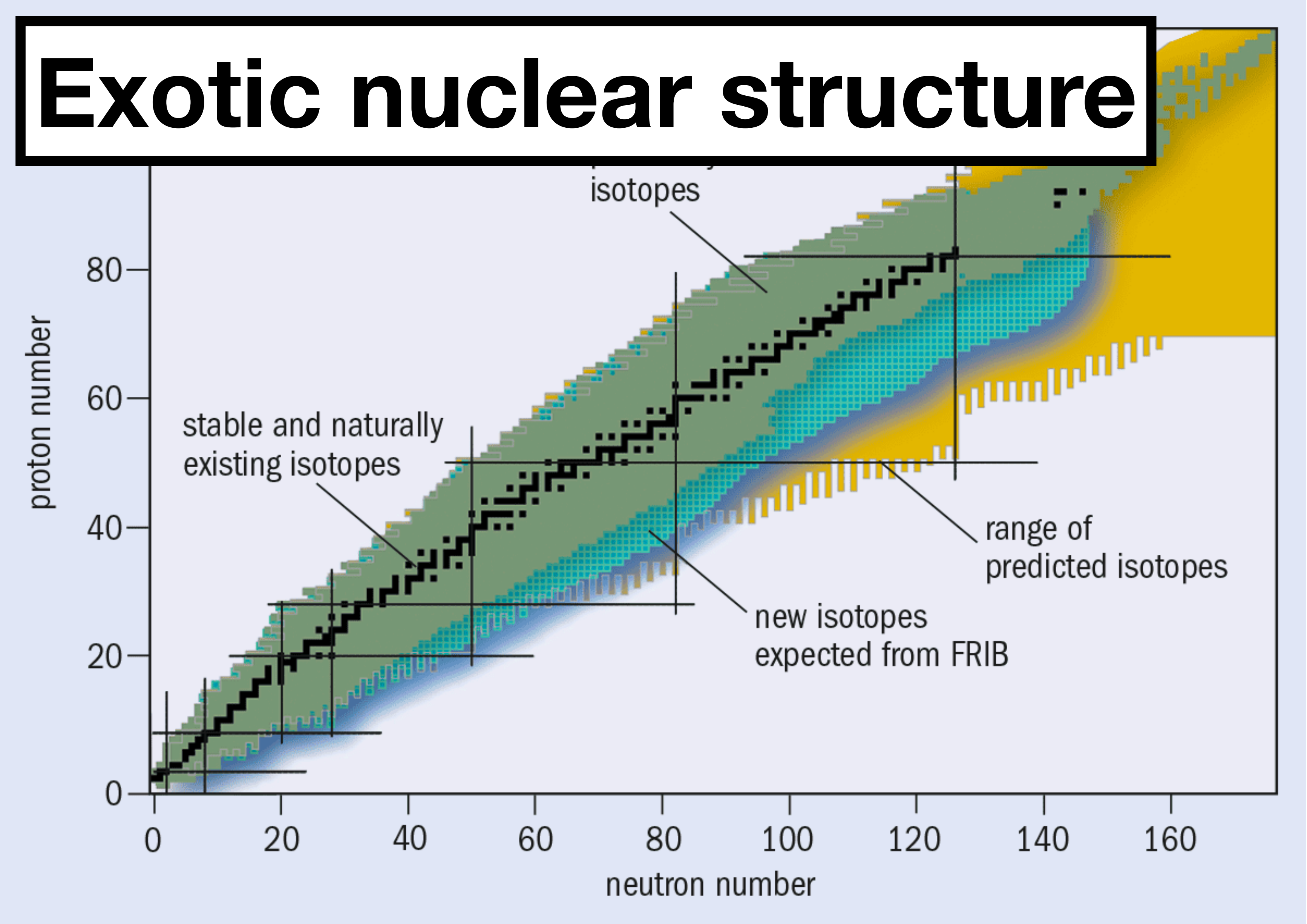
Door, Yeh, **MH**, et al., arXiv:2403.07792

Matthias Heinz

with ***Takayuki Miyagi*****,** ***Achim Schwenk*****,** ***Noritaka Shimizu*****,**
Menno Door, Klaus Blaum, Indy Yeh, Tanja Mehlstäubler, Fiona Kirk, Elina Fuchs,
Julian Berengut, Chunhai Lyu, Zoltán Harman, and others

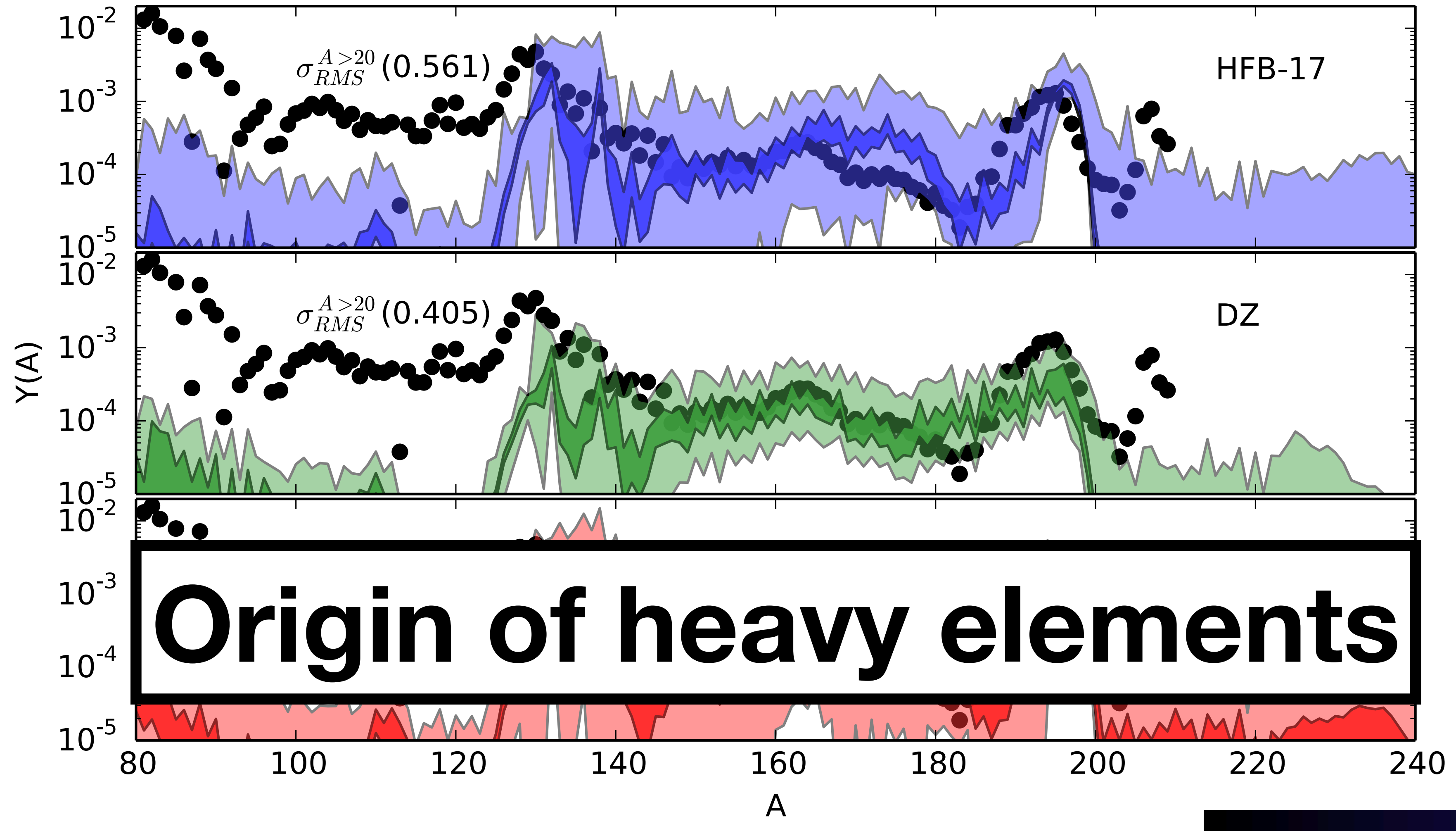
QCHSC 2024 - August 21, 2024

Nuclear structure motivations



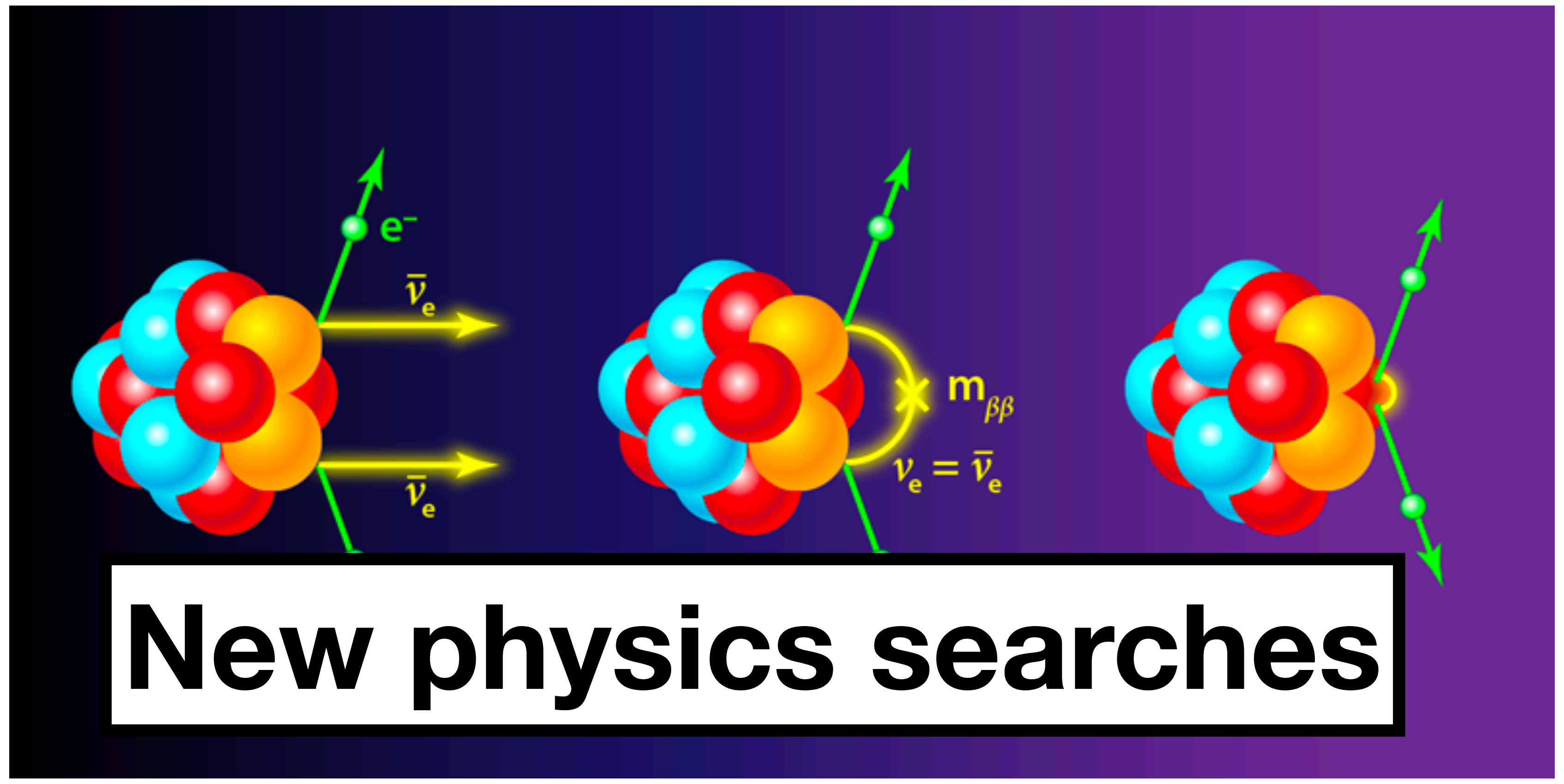
Exotic nuclear structure

Figure: FRIB



Origin of heavy elements

Mumpower et al., EPJ WoC **93** (2015)



New physics searches

Figure: LEGEND Collaboration

Theory predictions with quantified uncertainties essential!

Nonlinear King plot in ytterbium isotope shifts

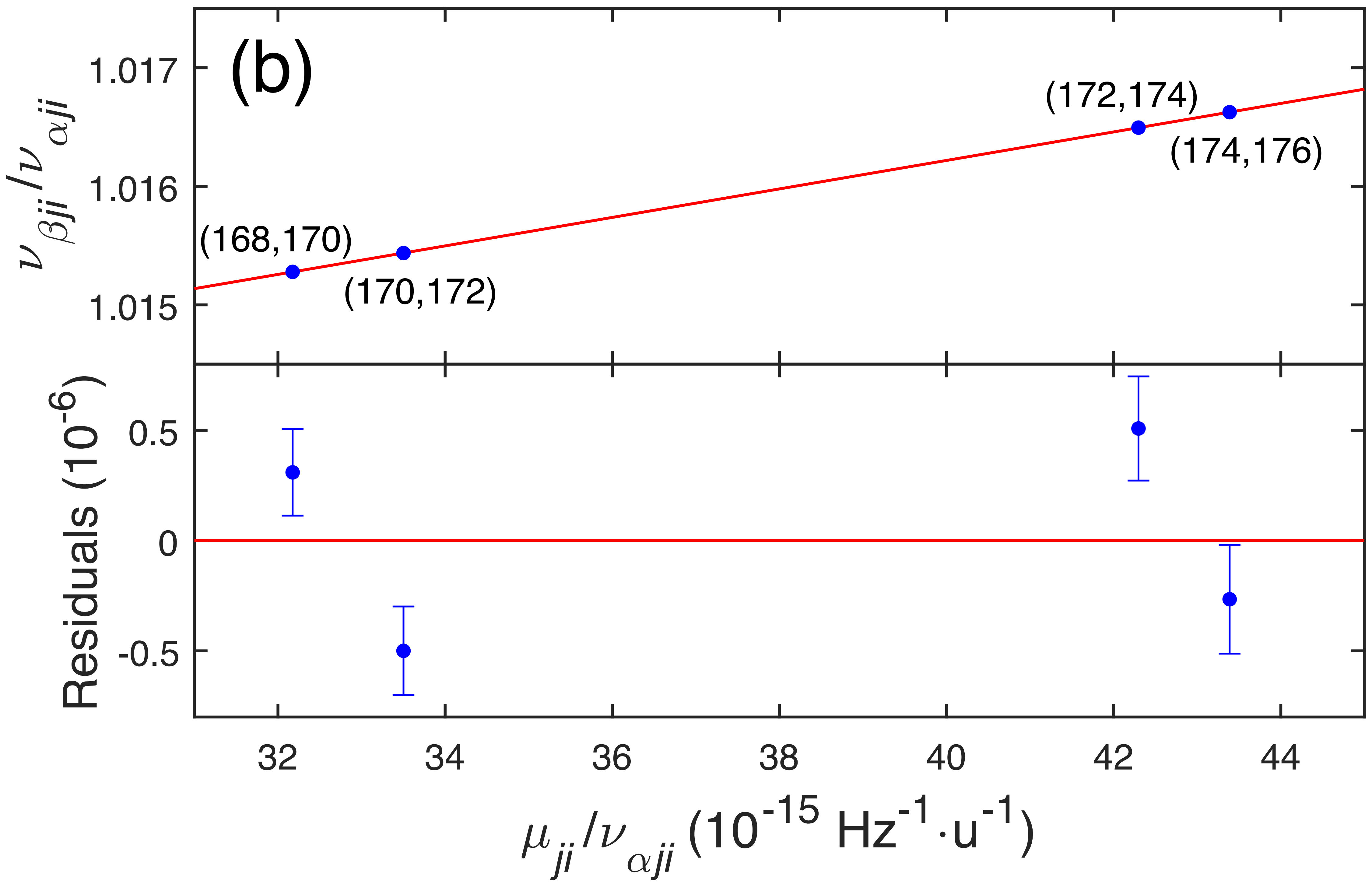
Delaunay et al., PRD **96** (2017)
Counts et al., PRL **125** (2020)
Allehabi et al., PRA **103** (2021)
Hur et al., PRL **128** (2022)
Figueroa et al., PRL **128** (2022)
Ono et al., PRX **12** (2022)
and more

Nonlinear King plot in ytterbium

- **Isotope shift** in atomic transition frequencies
- Leading order:

$$\nu_\tau^{A,A'} = \nu_\tau^{A} - \nu_\tau^{A'} \approx \underbrace{K_\tau w^{A,A'}}_{\textbf{mass shift}} + \underbrace{F_\tau \delta\langle r^2\rangle^{A,A'}}_{\textbf{field shift}}$$

- Leads to **linear King plot**



Counts et al., PRL **125** (2020)

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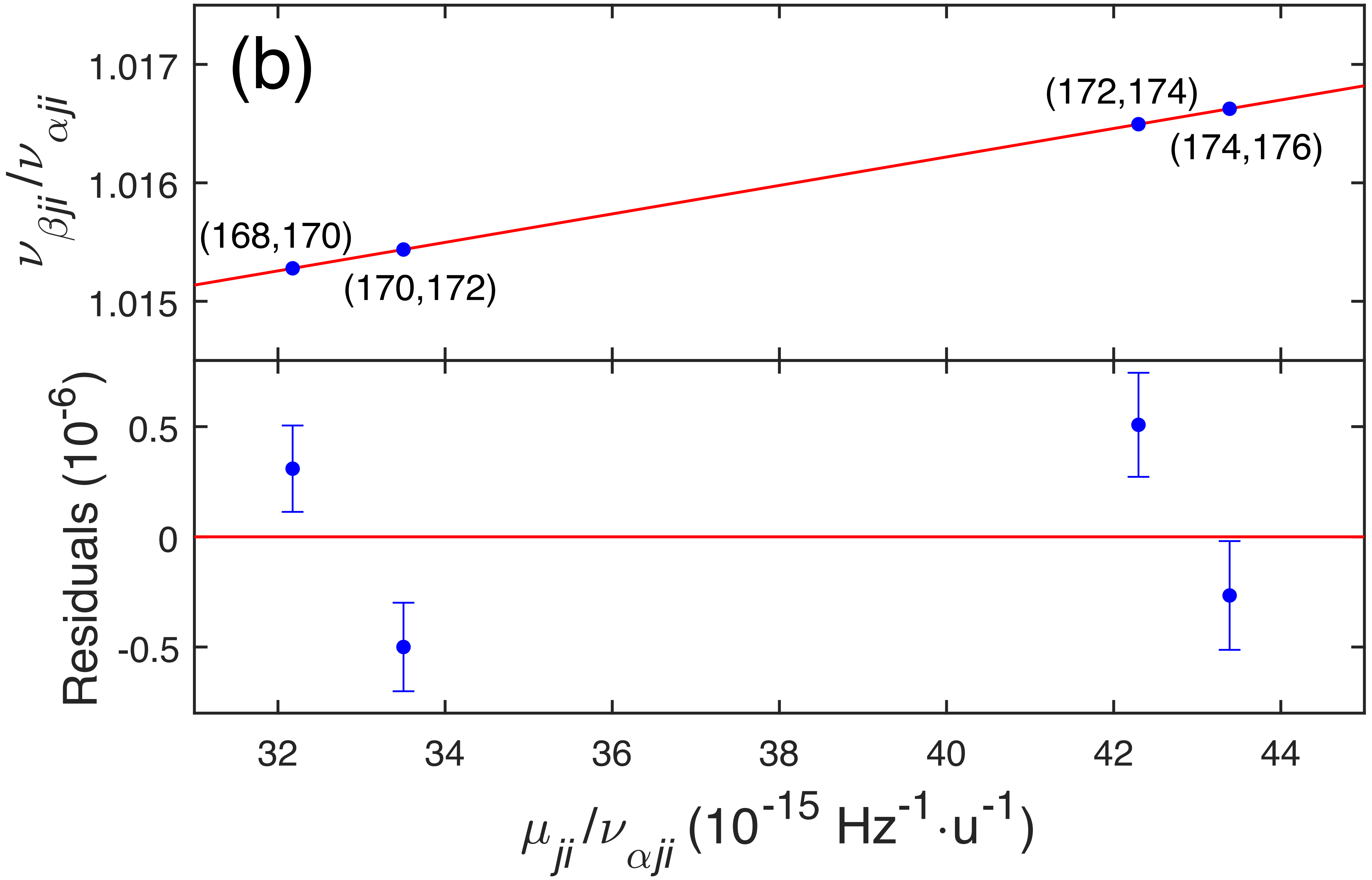

Counts et al., PRL **125** (2020)

Nonlinear King plot in ytterbium

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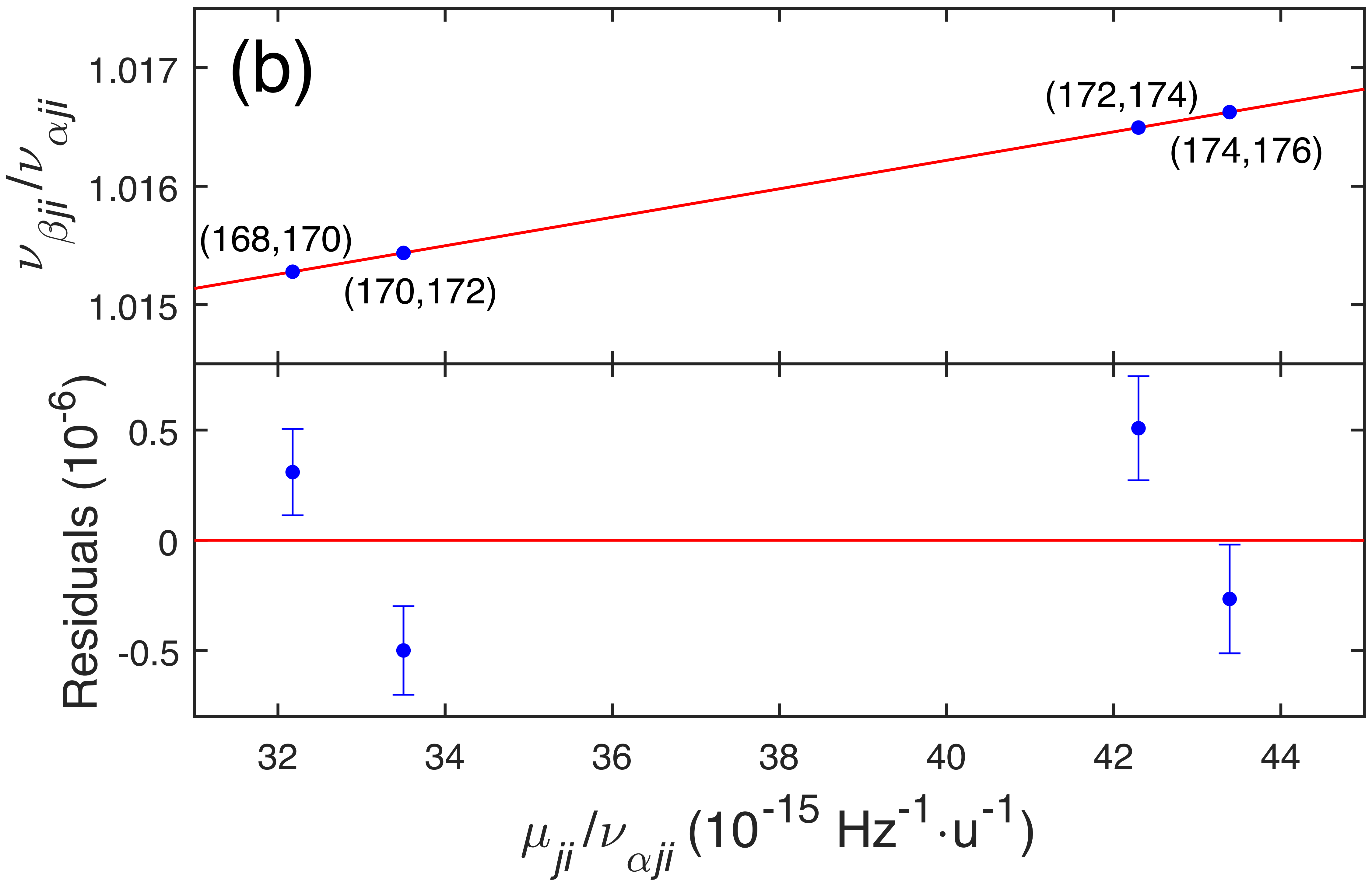
- Leads to **linear King plot**
- Nonlinear behavior due to other effects:

$$\nu_{\tau,\text{nonlin.}}^{A,A'} = \underbrace{G_\tau^{(2)}(\delta\langle r^2\rangle^2)^{A,A'} + G_\tau^{(4)}\delta\langle r^4\rangle^{A,A'}}_{\textbf{higher-order nuclear structure}}$$

$$\underbrace{+\frac{\alpha_{\text{NP}}}{\alpha_{\text{EM}}} D_\tau h^{A,A'}}_{\textbf{possible new boson}} + \ldots$$

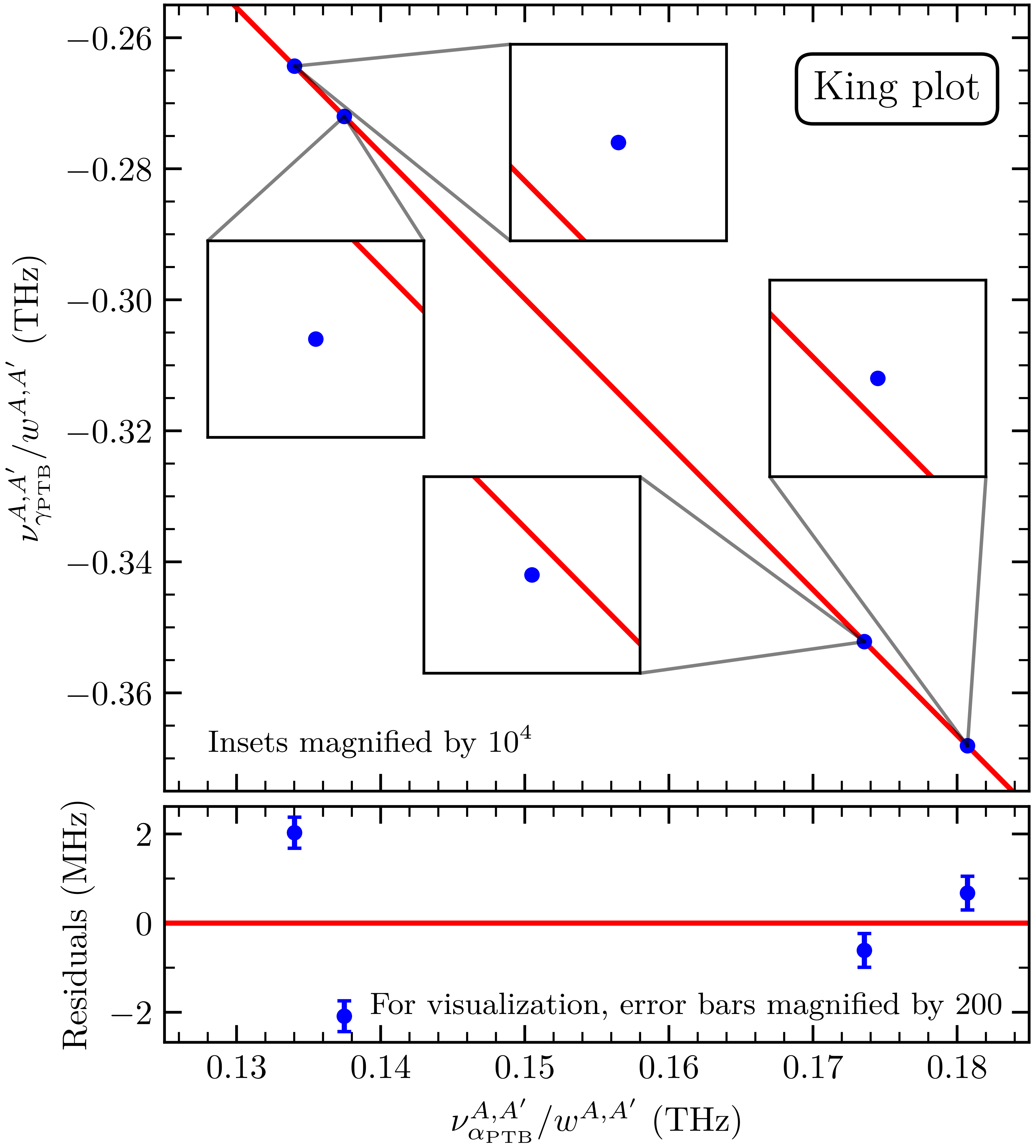


Counts et al., PRL **125** (2020)

Nonlinear King plot in ytterbium

New data:

- $^{168,170,172,174,176}\mathrm{Yb}$ (4 isotope pairs)
- Frequencies with 10^{-15} relative precision (Yeh, Mehlstäubler @**PTB Braunschweig**)
- Mass-ratios with 10^{-12} relative precision (Door, Blaum @**MPIK Heidelberg**)



Nonlinearity observed with high significance!
Is this new physics?

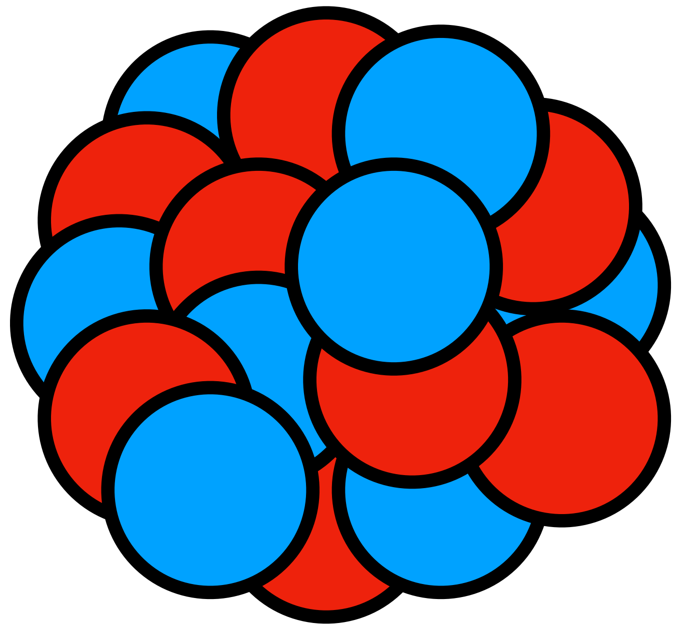
Ab initio nuclear structure theory

Ab initio nuclear structure

🔵 **N neutrons**

🔴 **Z protons**

A nucleons



$$H|\Psi\rangle = E|\Psi\rangle$$

Ab initio nuclear structure

🔵 N **neutrons**

🔴 Z **protons**

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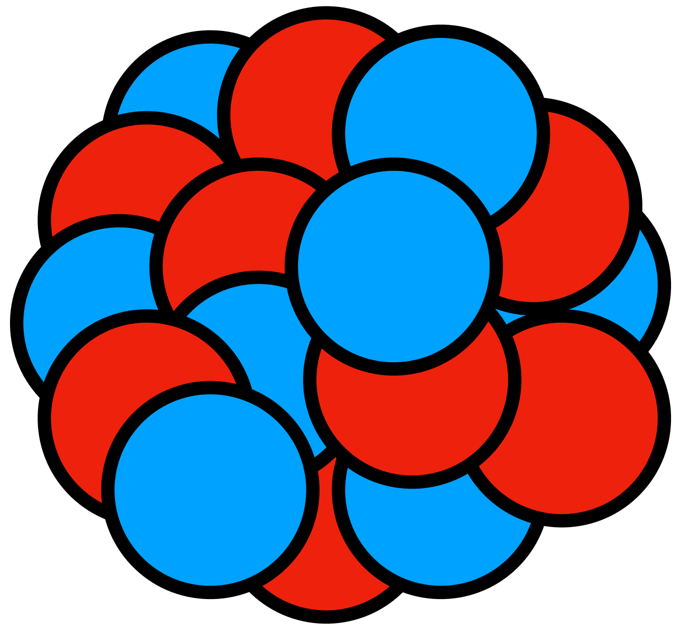
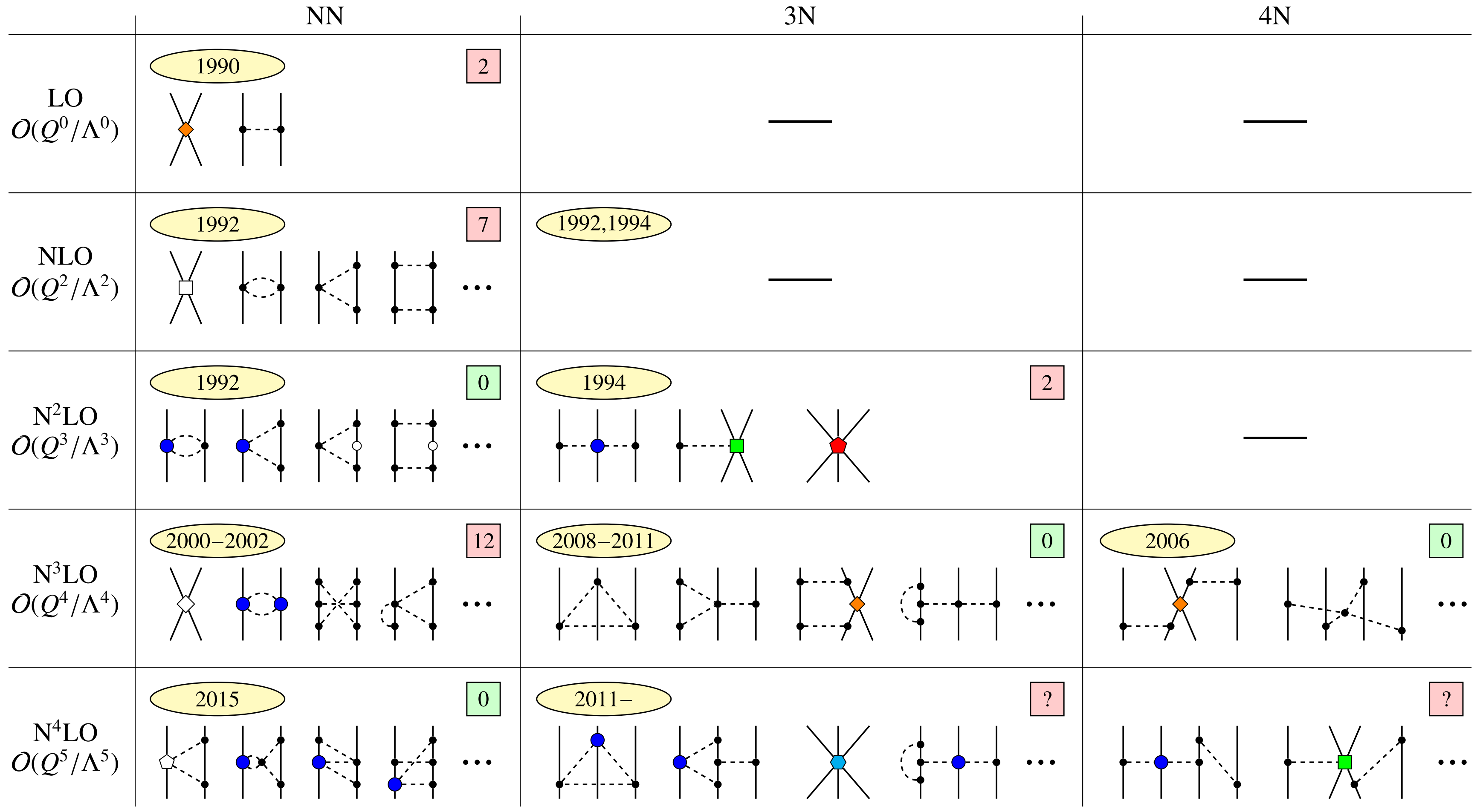


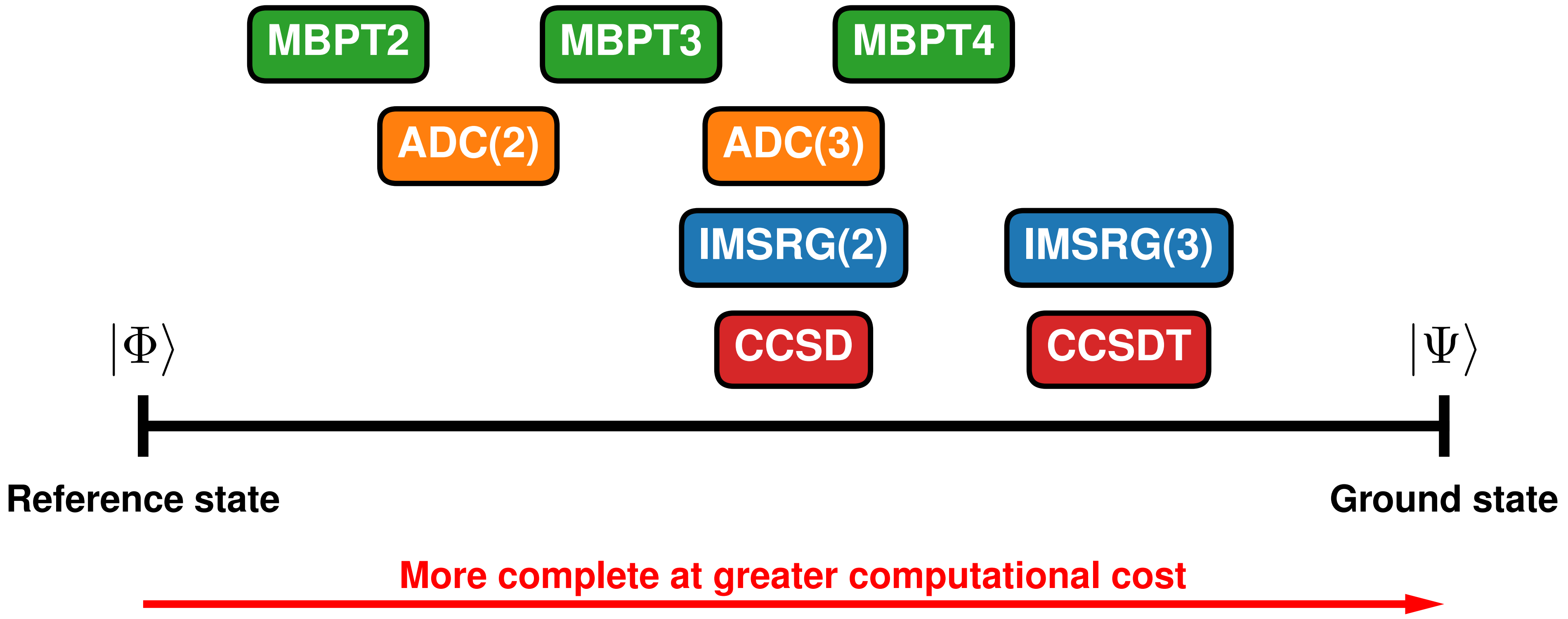
$$H|\Psi\rangle = E|\Psi\rangle$$

Nuclear forces



Hebeler, Phys. Rep. **890** (2021)

Many-body methods



MBPT2 MBPT3 MBPT4

ADC(2) ADC(3)

IMSRG(2) IMSRG(3)

CCSD CCSDT

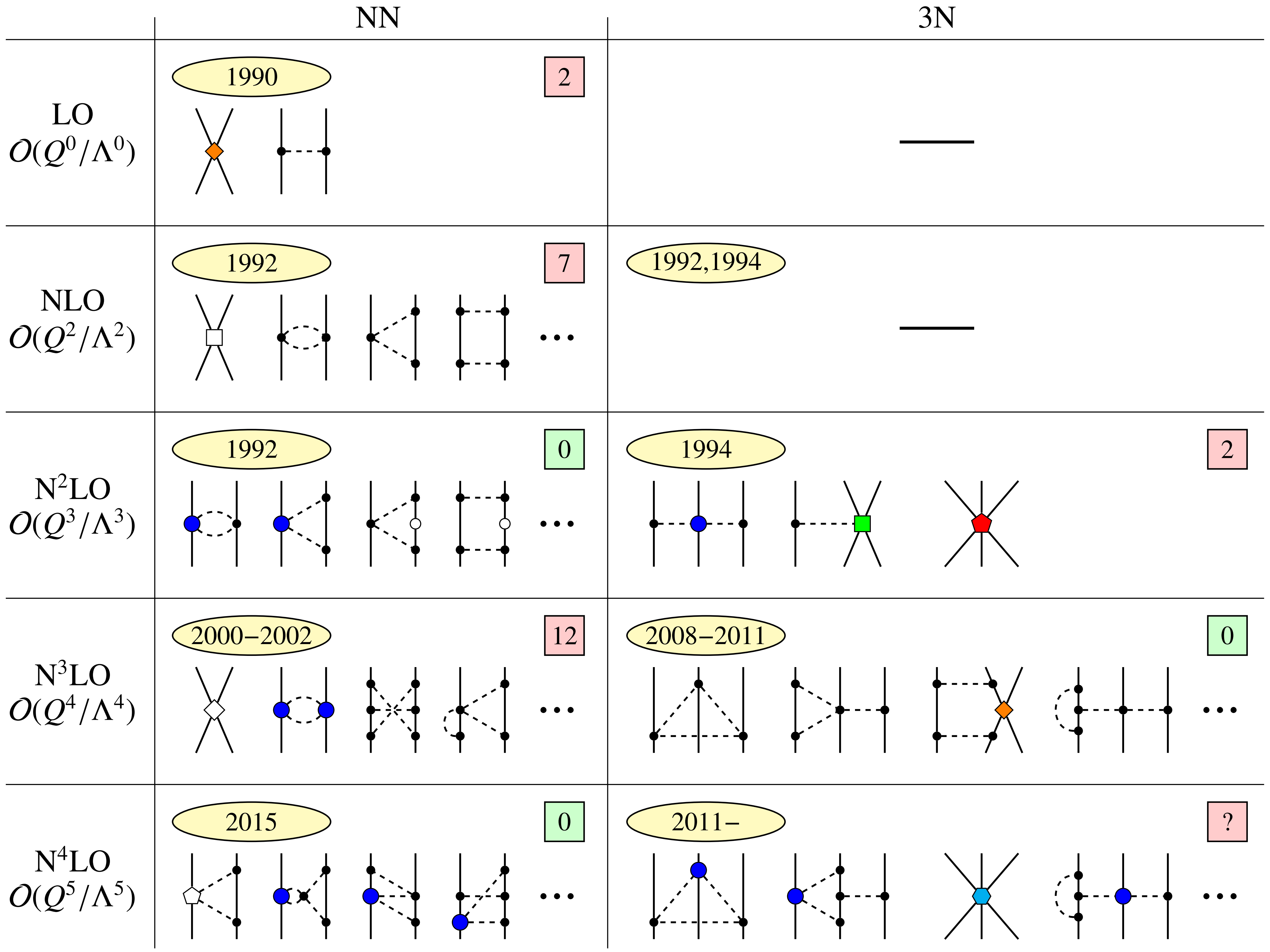
$|\Phi\rangle$ $|\Psi\rangle$

Reference state **Ground state**

More complete at greater computational cost

Chiral EFT for nuclear forces

effective field theory



Hebeler, Phys. Rep. **890** (2021)

- **Nuclear forces are uncertain**
- Chiral EFT:
  Low-energy expansion of QCD
- Free couplings to fit to data
- **Systematically improvable**
- **Uncertainty quantifiable**

Many-body expansion methods

$|\Phi\rangle$

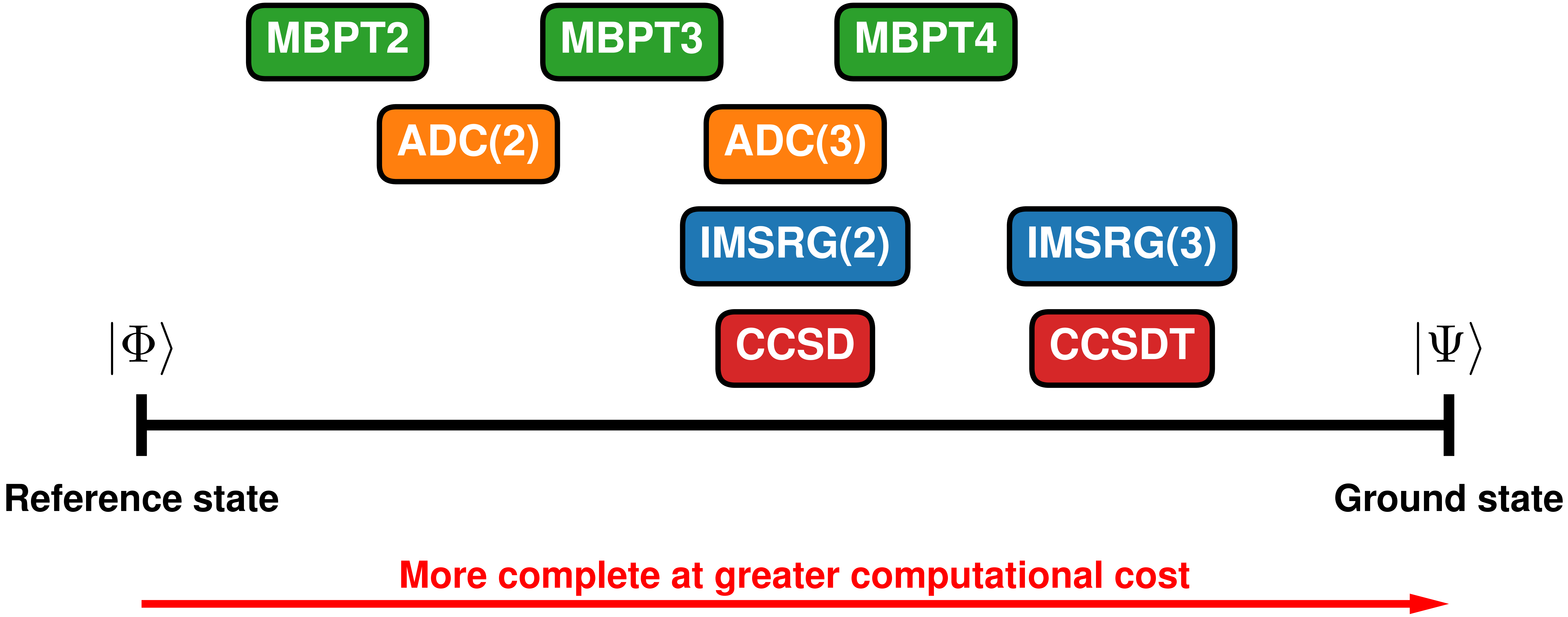
$|\Psi\rangle$

Reference state

Ground state

More complete at greater computational cost

Many-body expansion methods

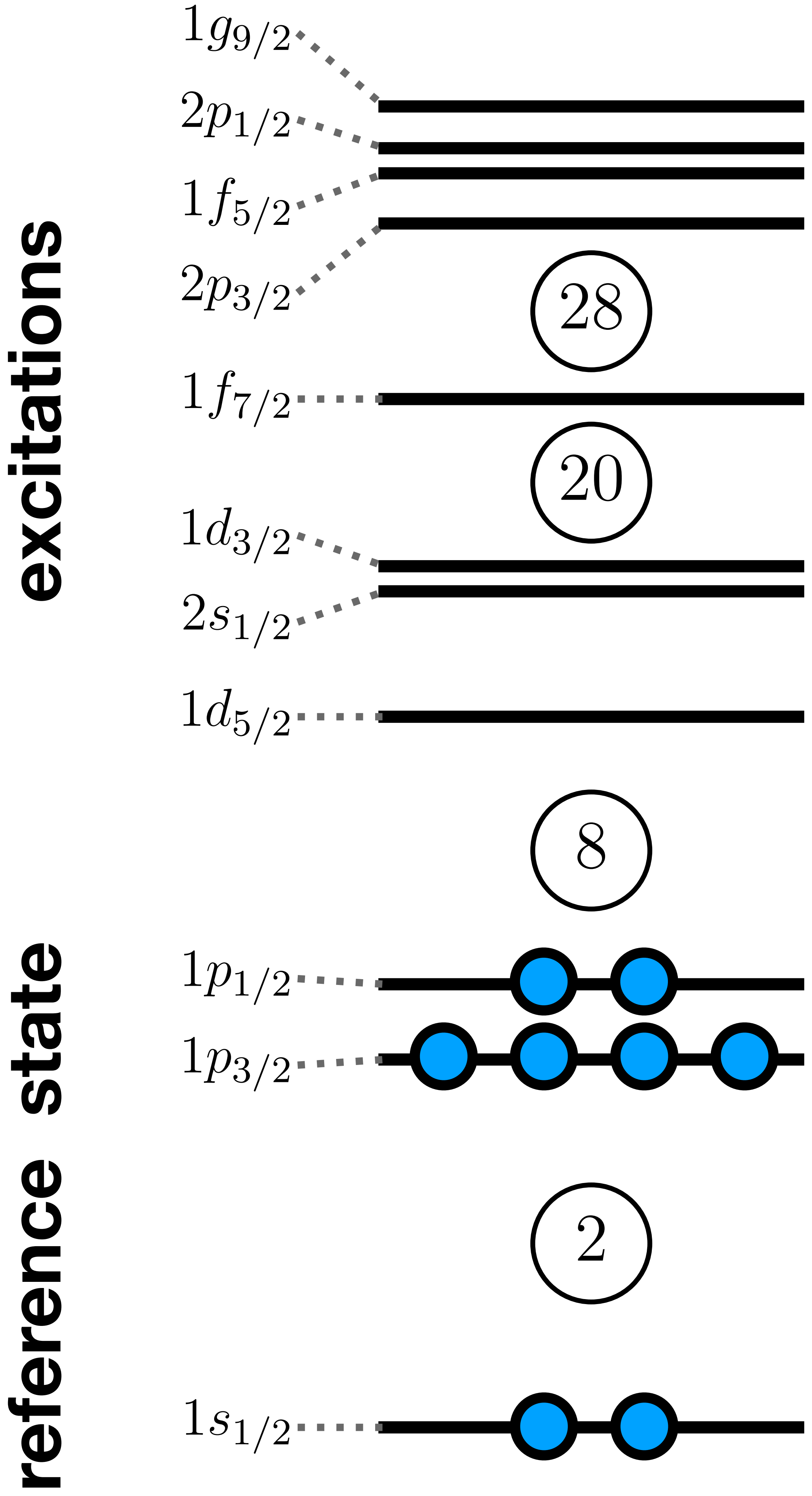


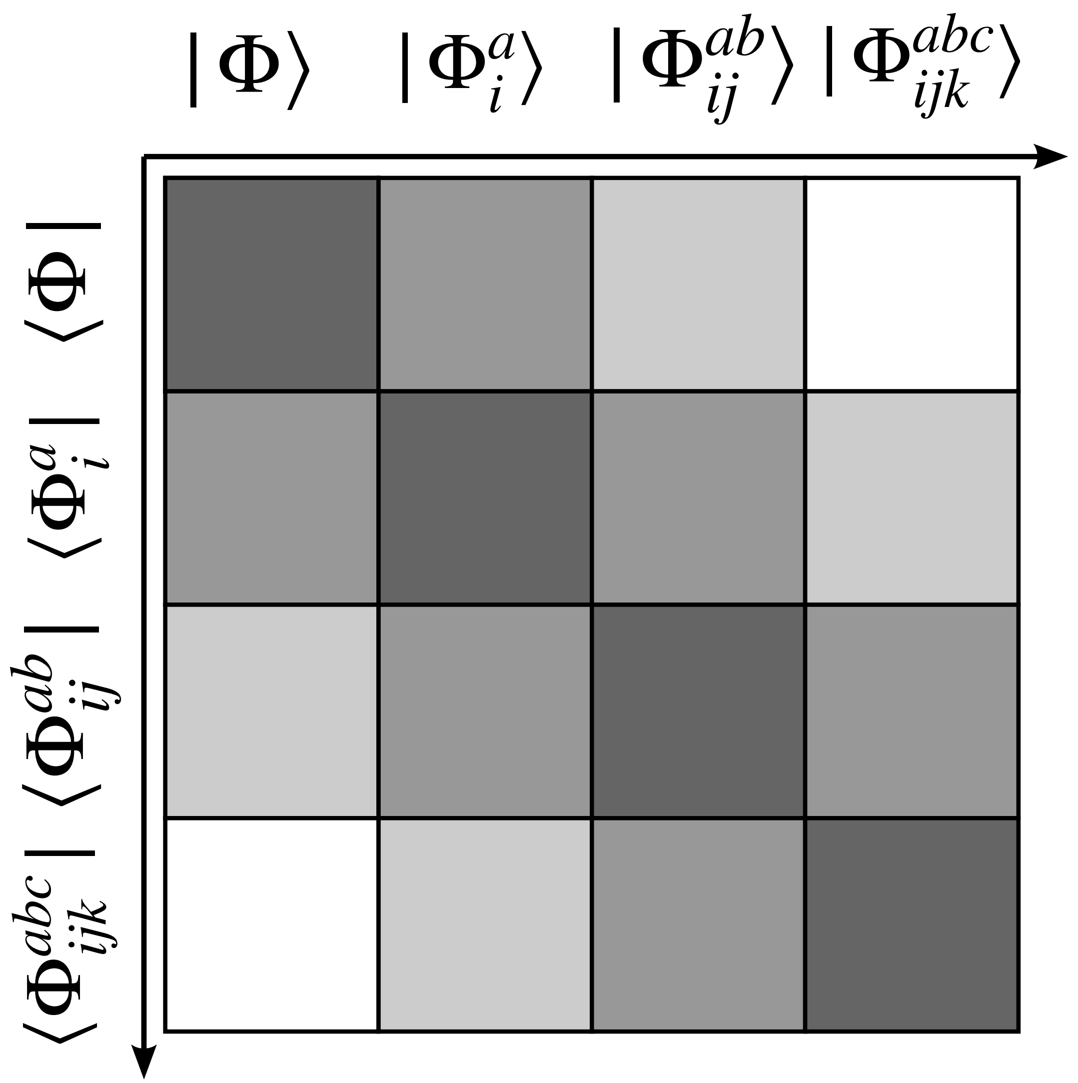
- **Systematically improvable expansion** around reference state $|\Phi\rangle$
- **Tractable computational cost** in larger nuclei
- Approximate many-body solution with **quantifiable uncertainty**

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

The IMSRG

in-medium similarity renormalization group





initial H

Tsukiyama et al., PRL **106** (2011)
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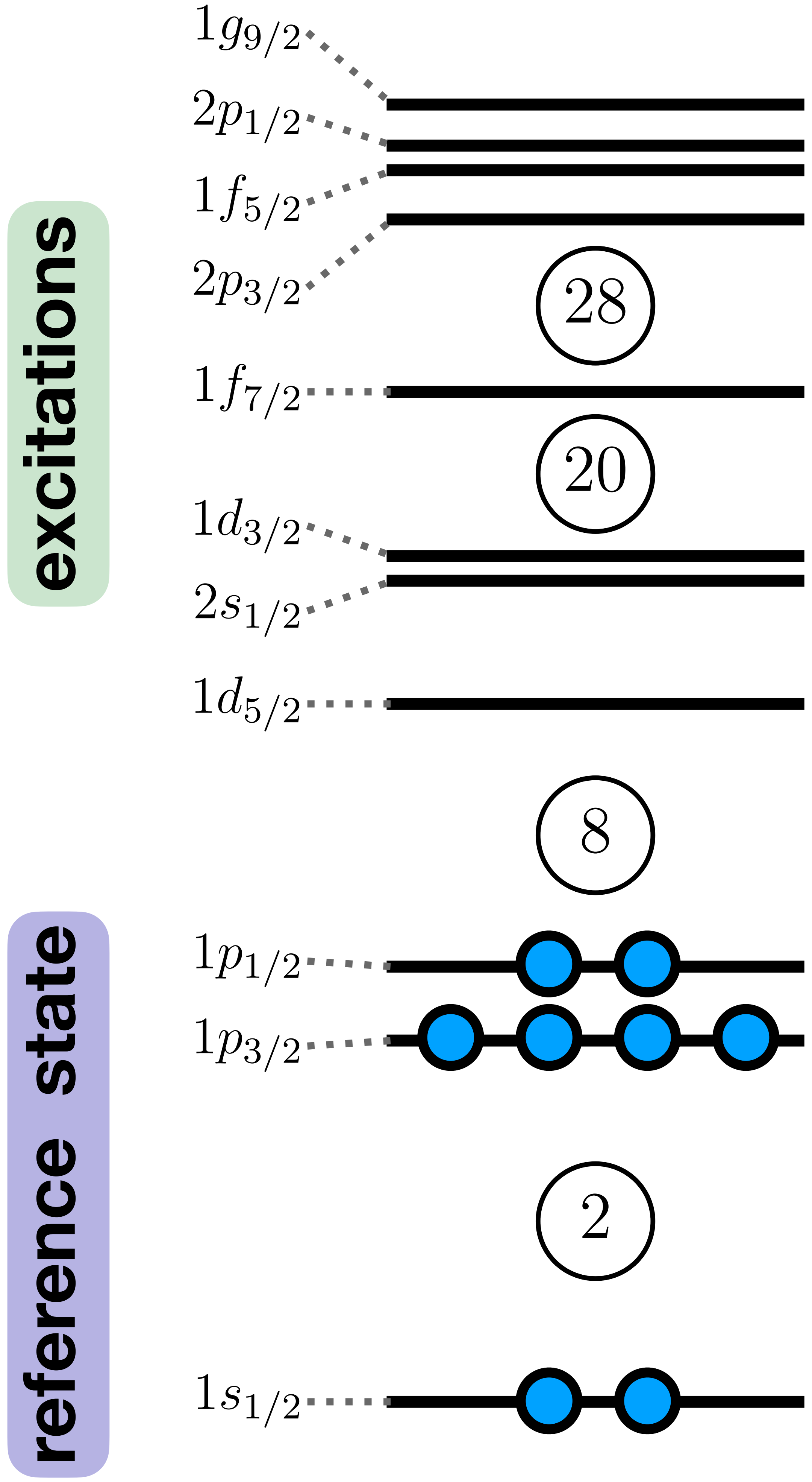

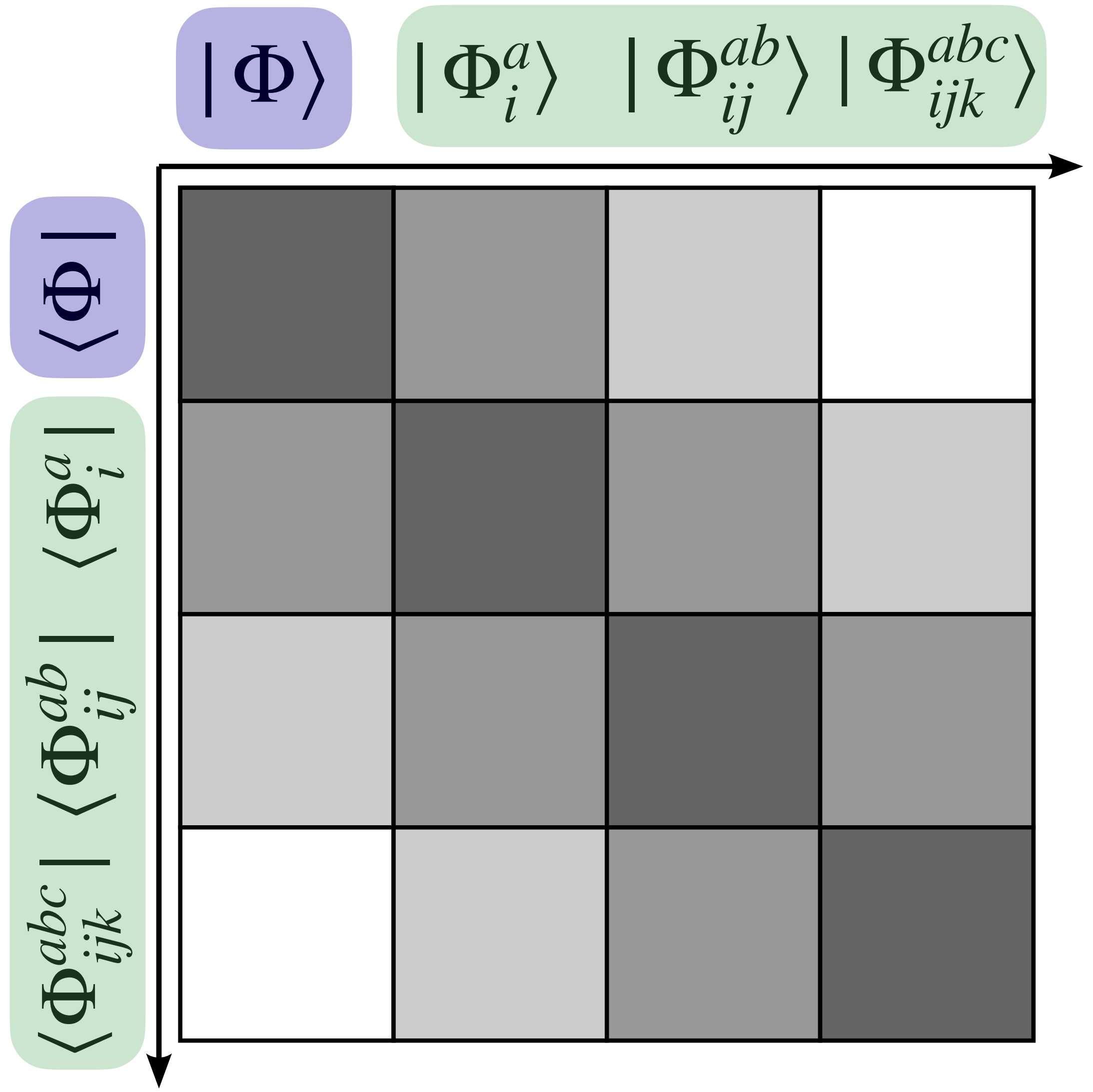

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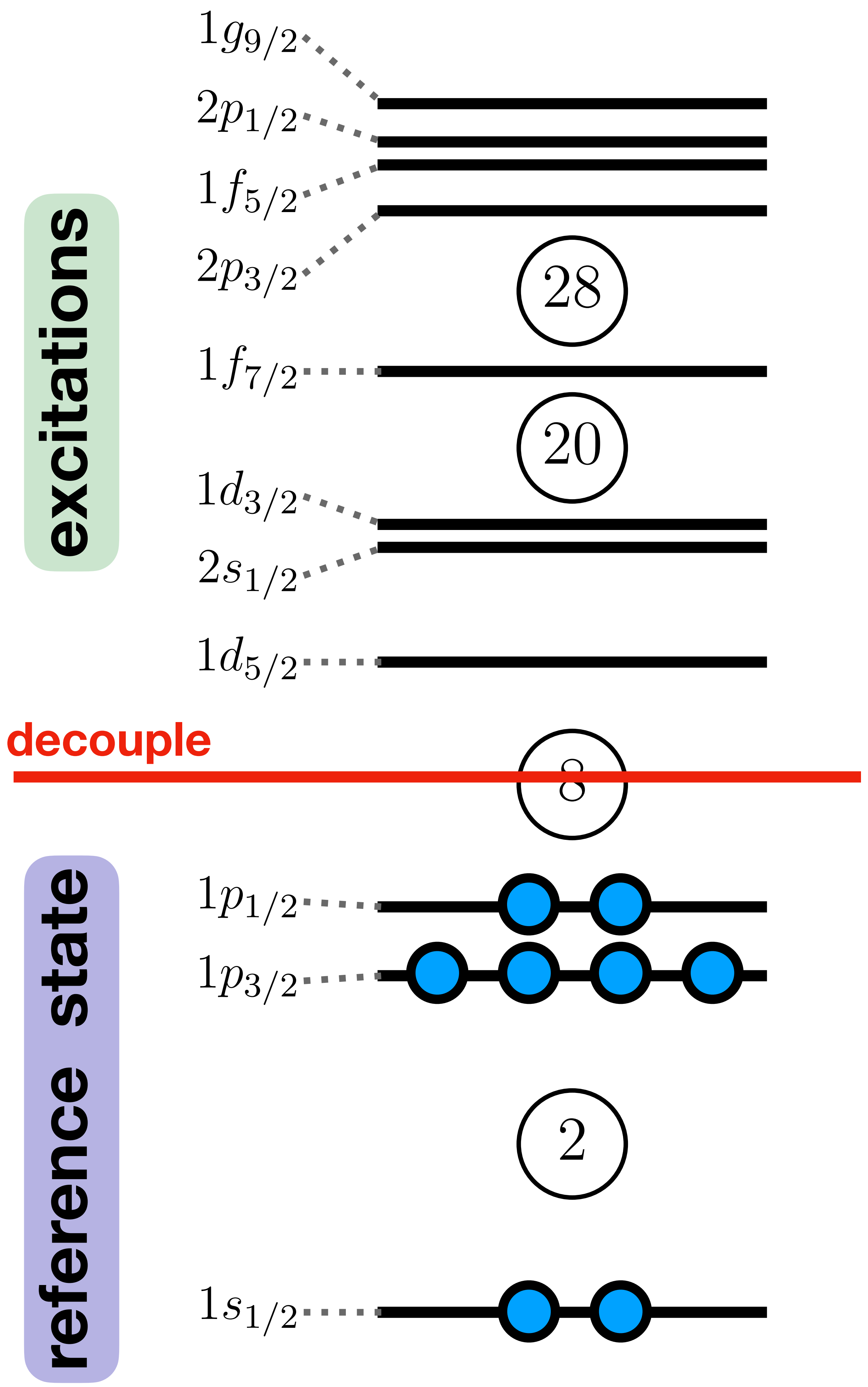

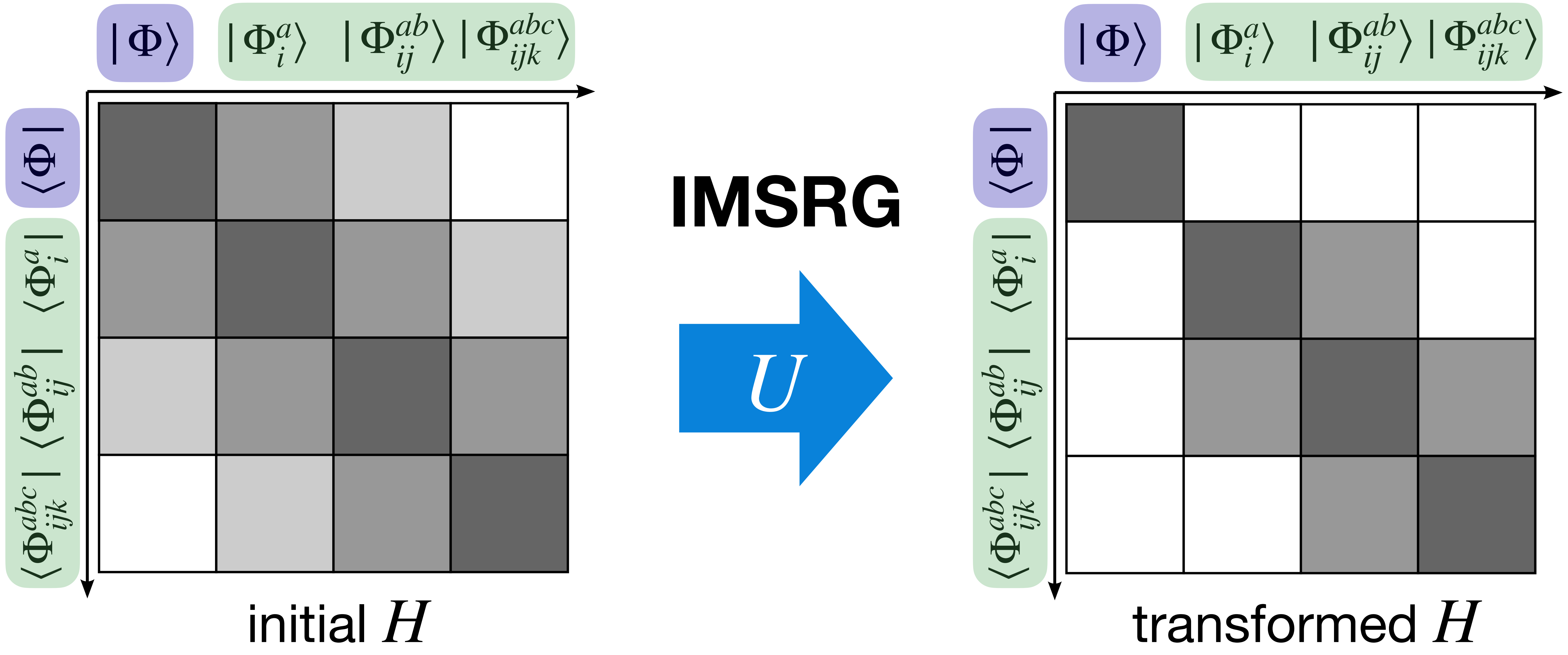

Hergert et al., Phys. Rep. **621** (2016)

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

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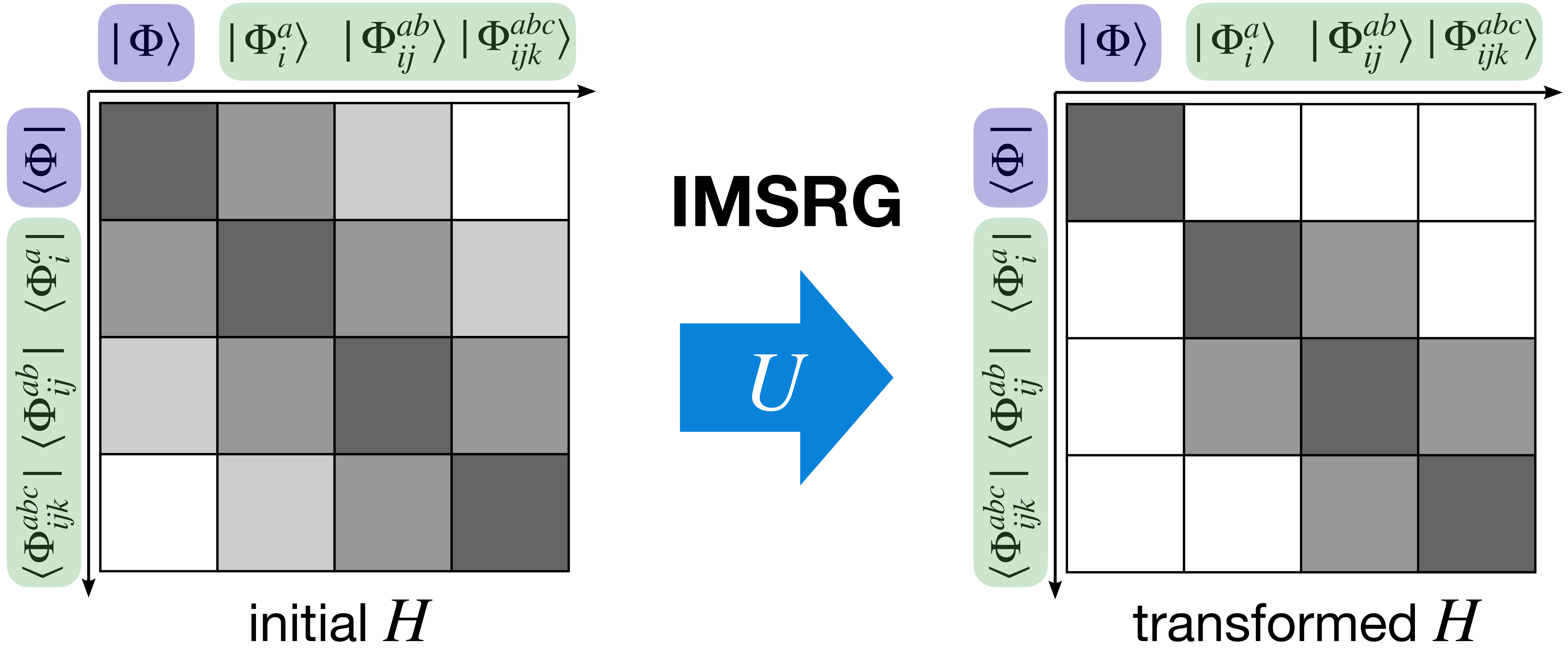

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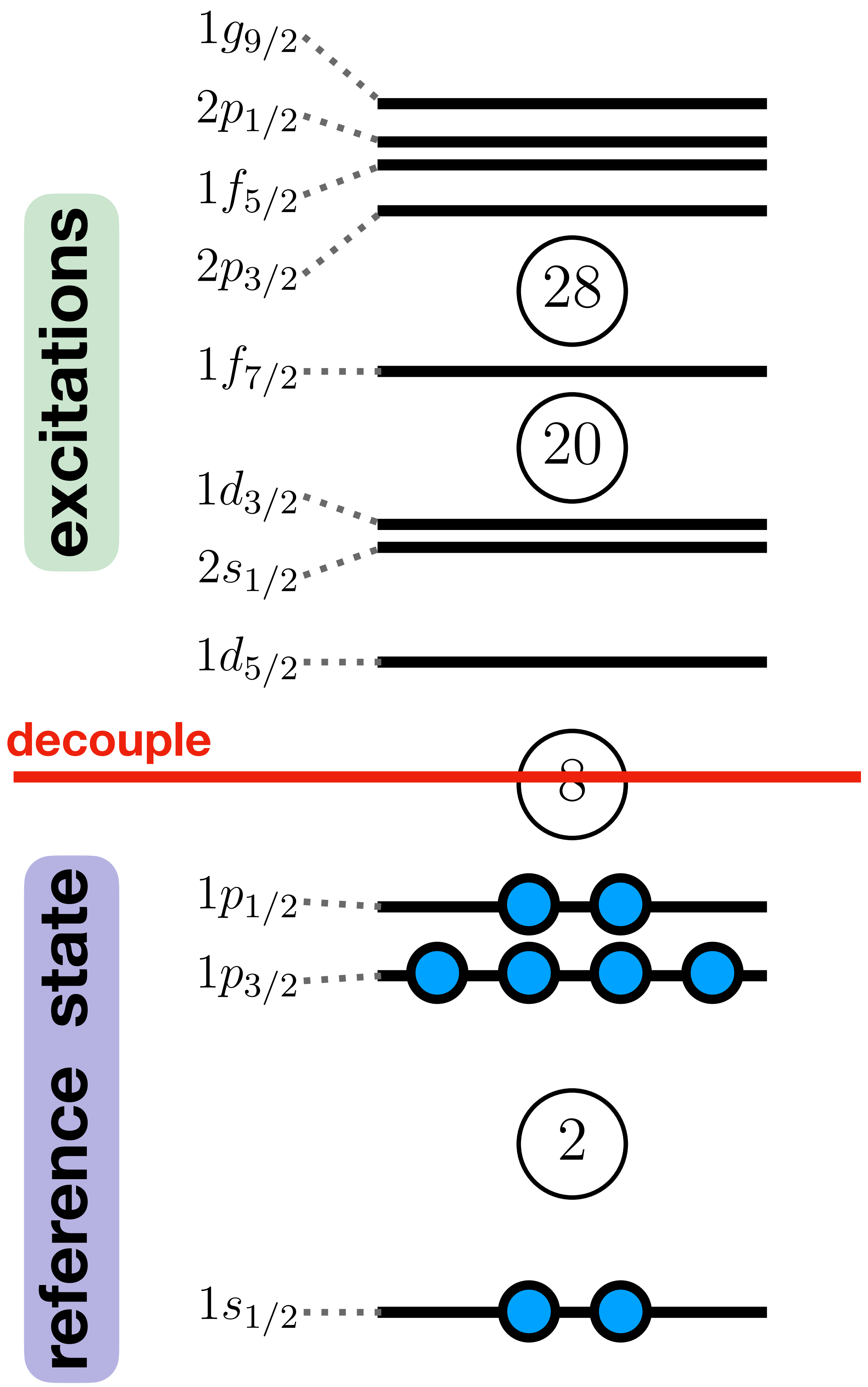


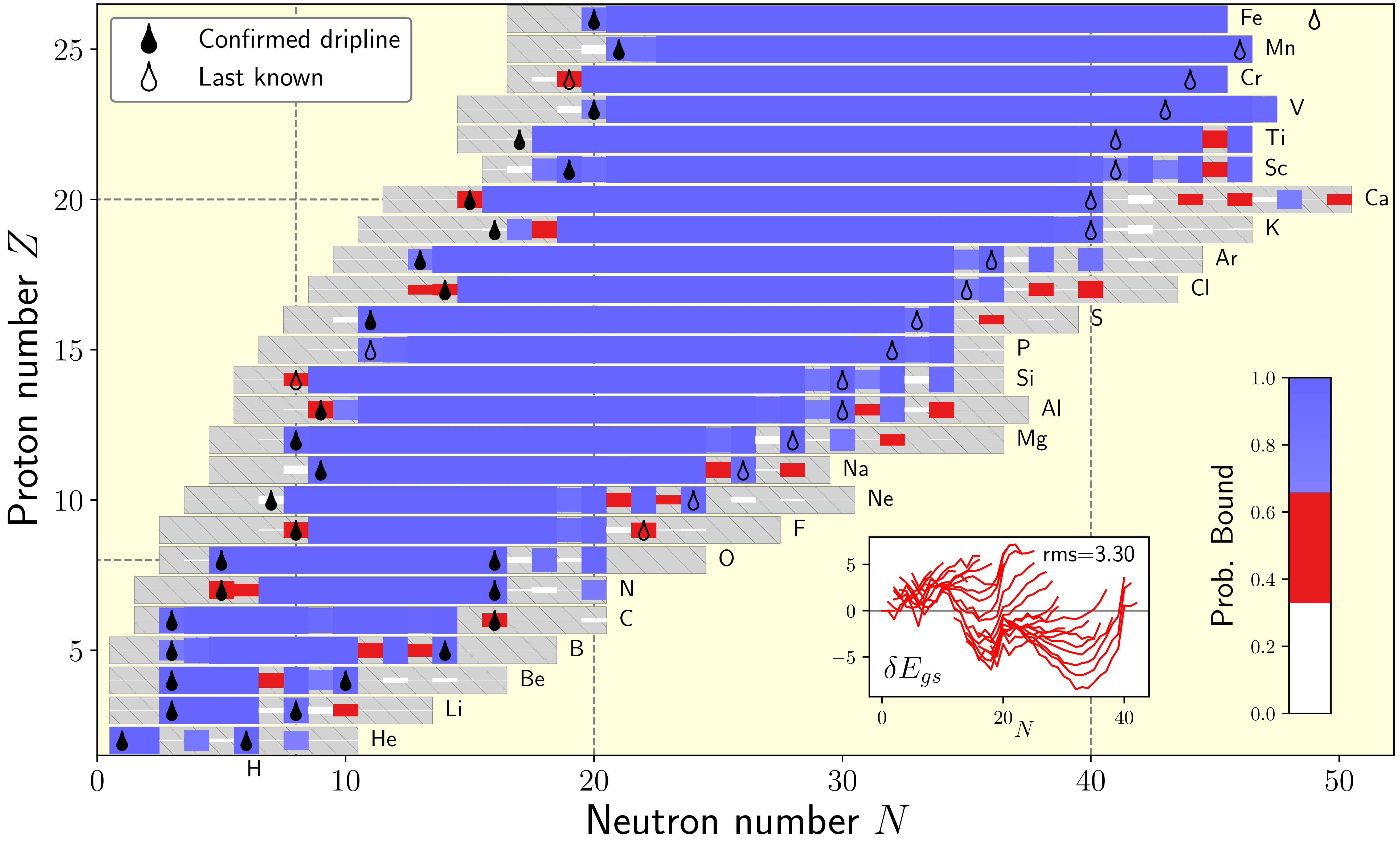
- **IMSRG**: Unitary transformation $U = e^{\Omega}$ to decouple reference state from excitations
- Expansion and truncation in **many-body operators**

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

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

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

Global description of lightest nuclei



- Ab initio prediction of separation energies based on single Hamiltonian
- Study of systematic and statistical errors to **predict limits of stability**

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

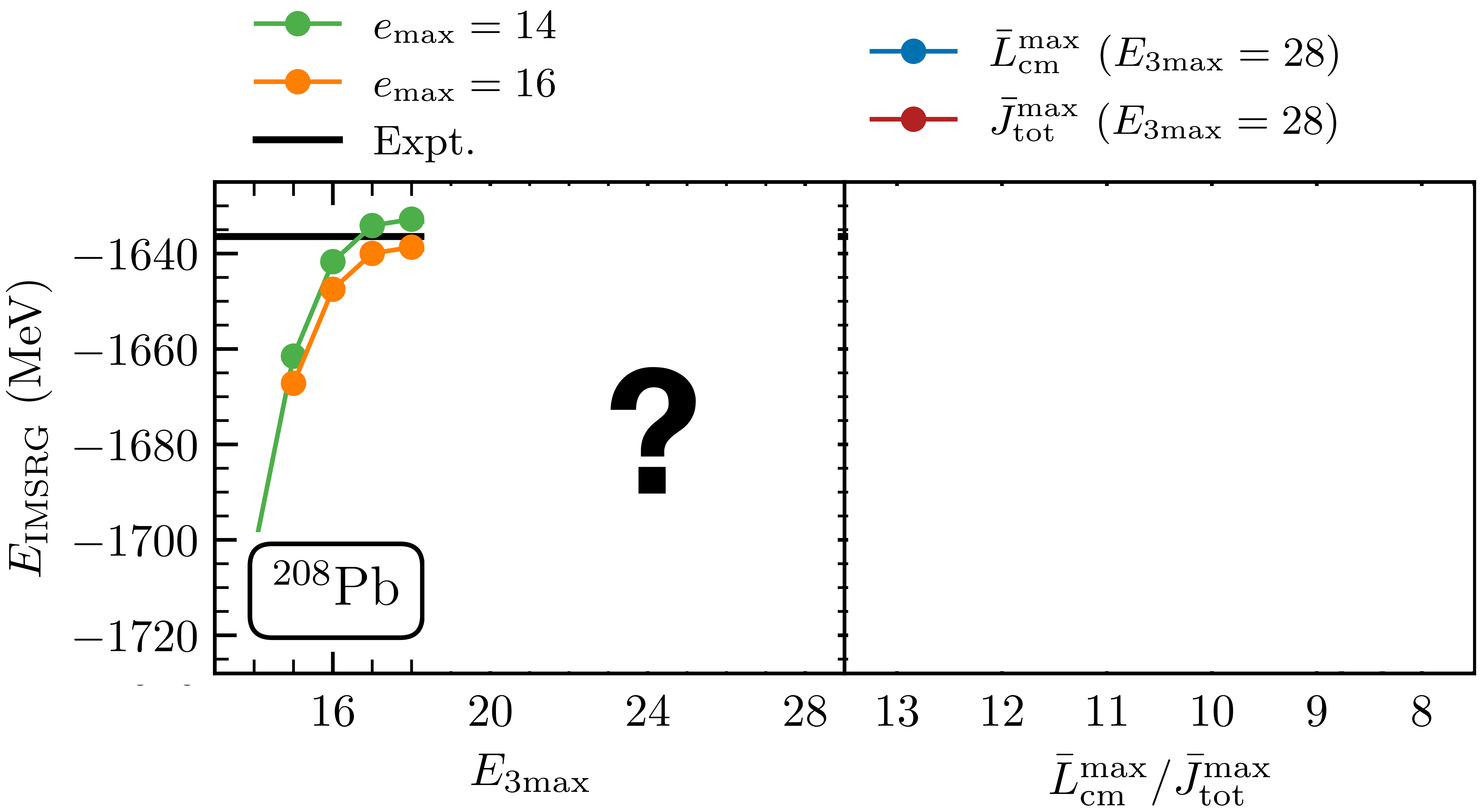
Global description of nuclear structure of lightest 700 isotopes!

Frontiers

Miyagi et al., PRC **105** (2022)
Hebeler, **MH**, et al., PRC **107** (2023)

Converged description of heavy nuclei

- Treatment of 3N interactions **limiting in heavy nuclei**
- **New developments** to relax necessary truncations
- **Converged ground-state results for lead-208**



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

New frontier of heavy nuclei unlocked!

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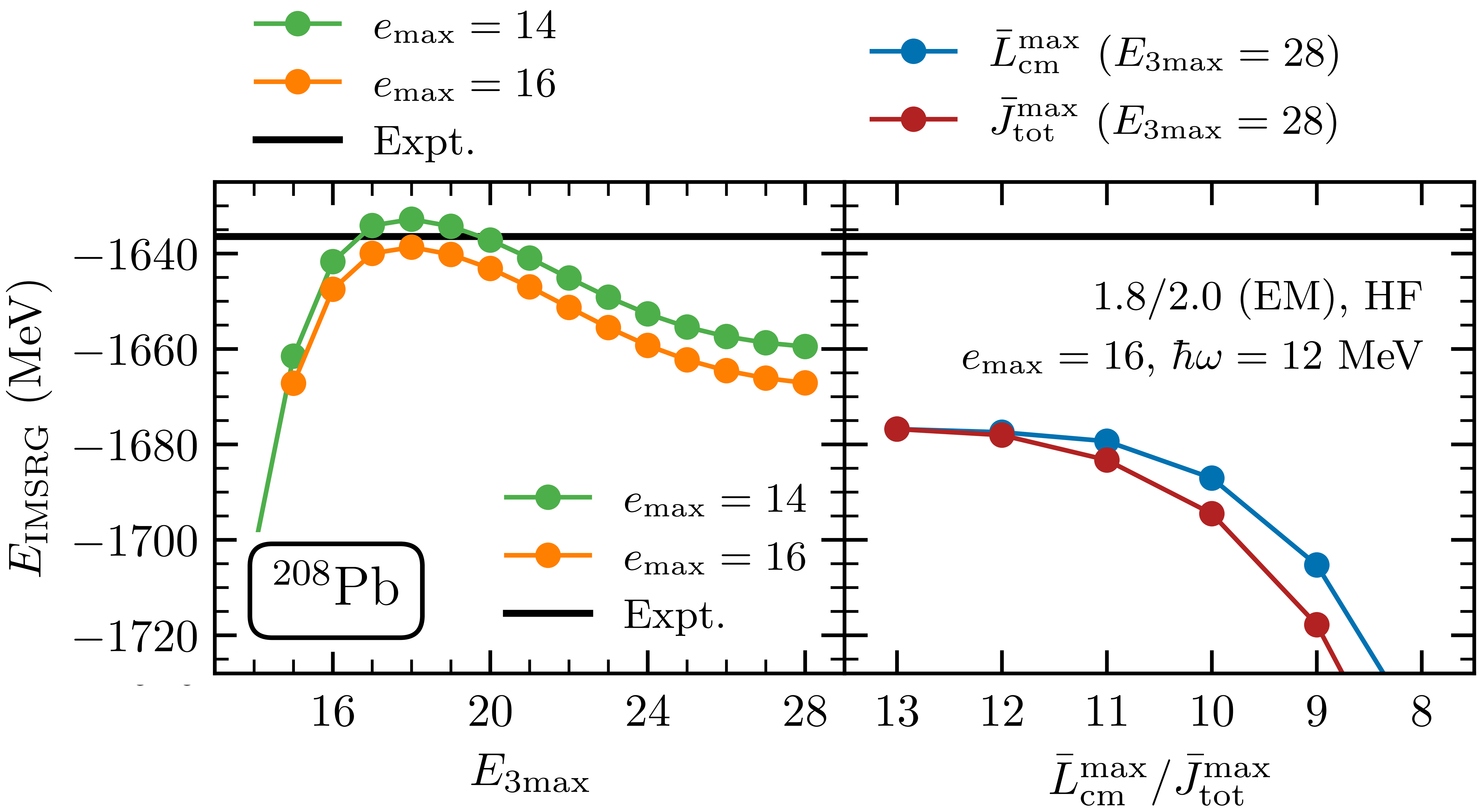

Hebeler, **MH**, et al., PRC **107** (2023)

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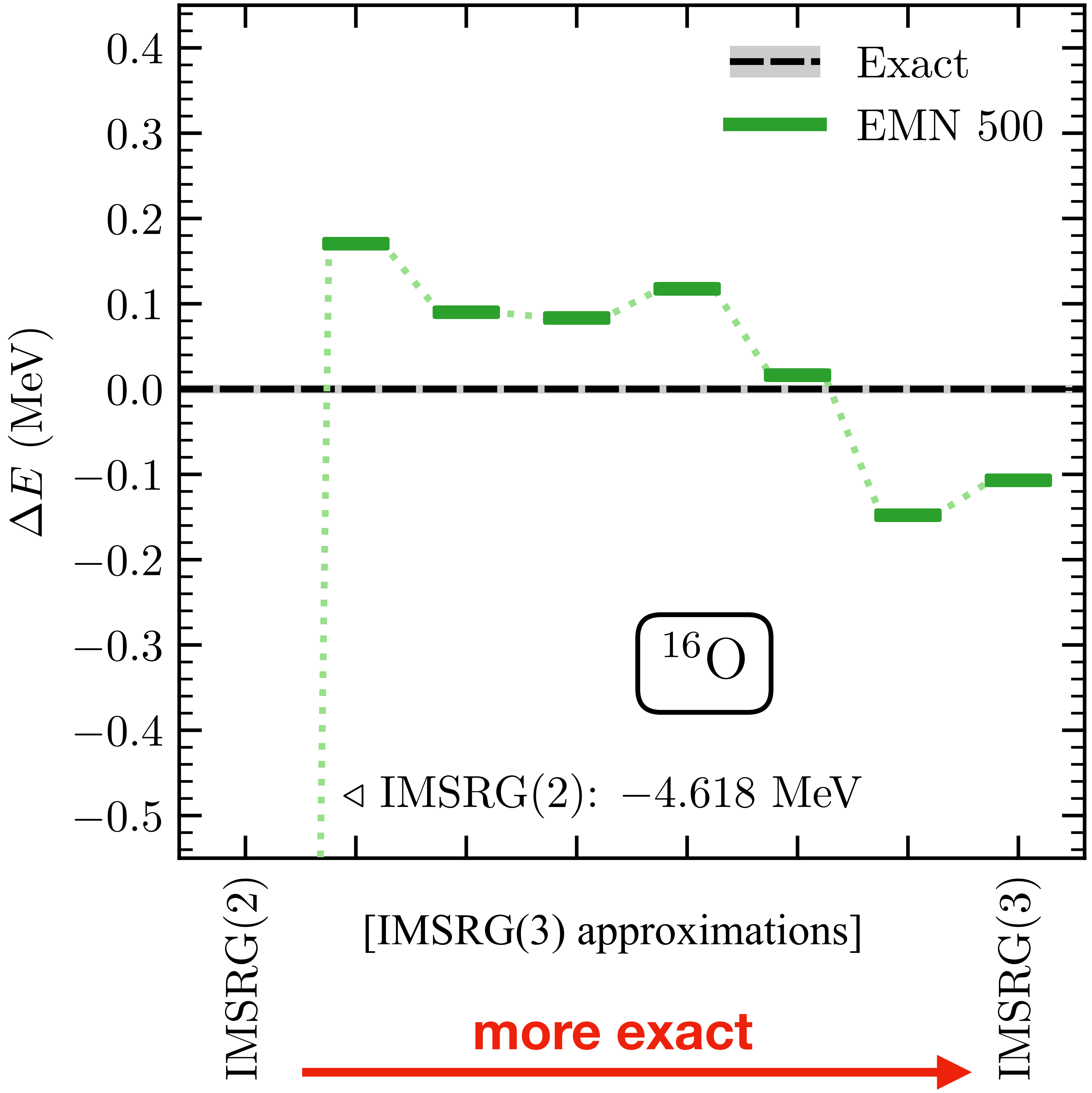
MH et al., PRC **103** (2021)

Precision with IMSRG(3)



more exact

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

- IMSRG(2) → IMSRG(3)
- **Systematic improvement** towards exact results
- Benefit greatest for very nonperturbative problems
- **Excellent precision** (0.5-1%) on ground-state energies

IMSRG(3) calculations now available for uncertainty quantification and precision!

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

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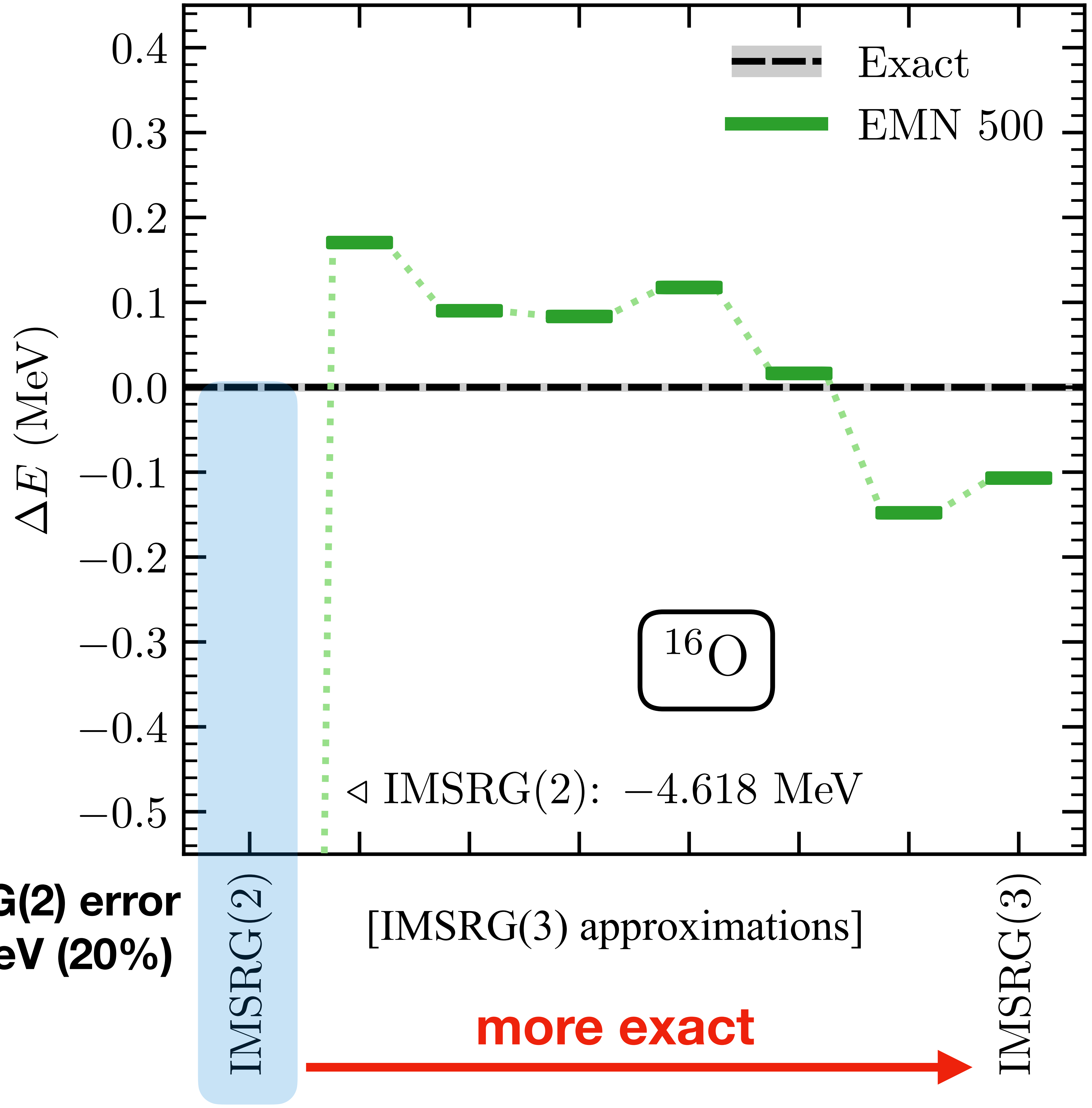

IMSRG(2) error 4.6 MeV (20%)

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

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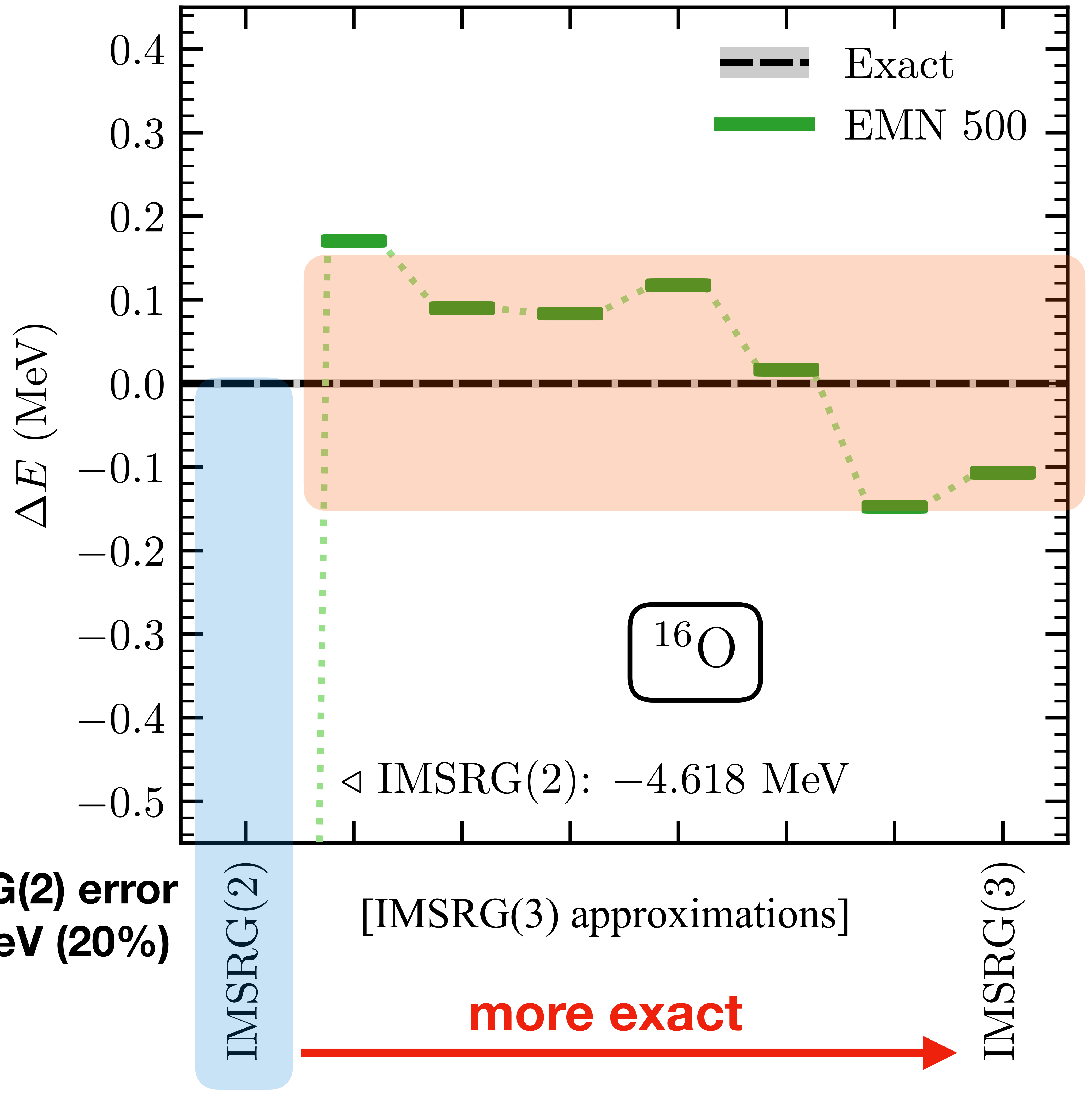
MH et al., PRC **103** (2021)

Precision with IMSRG(3)



IMSRG(2) error 4.6 MeV (20%)

IMSRG(3) error ~150 keV (1%)

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

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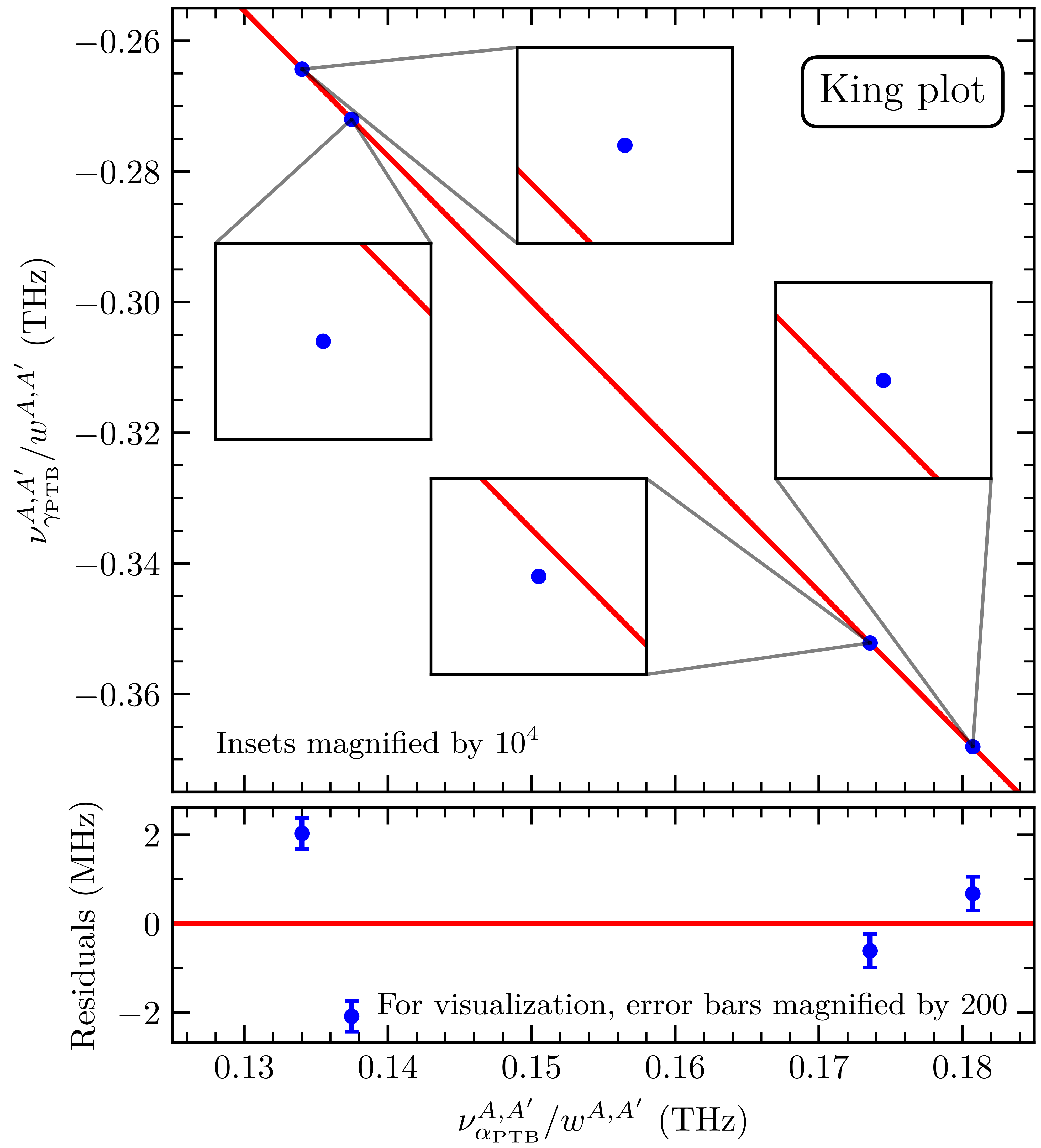
Understanding the nonlinearity with ab initio nuclear structure

Analyzing the nonlinearity



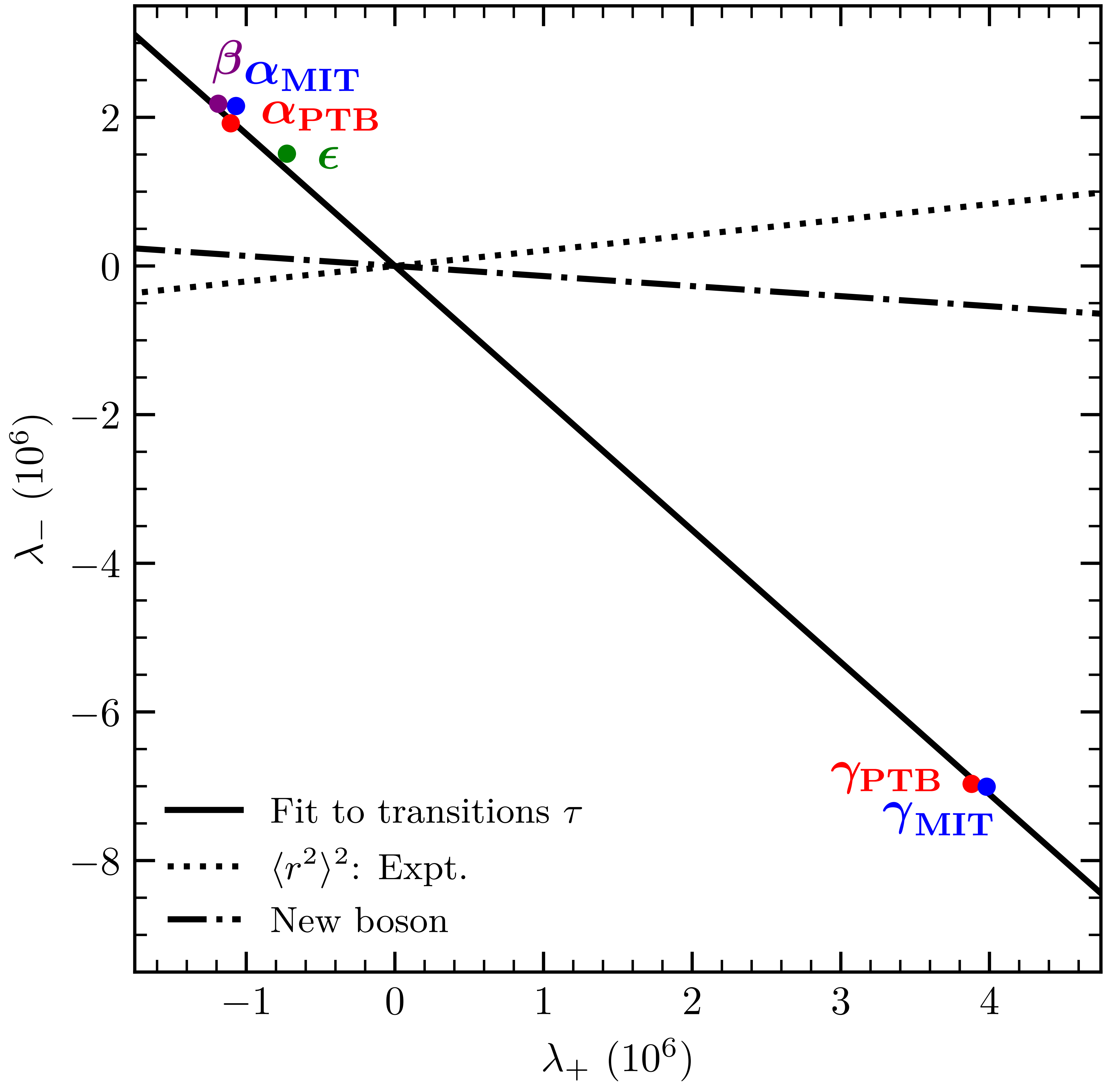
- Describe 4 data points as vector: $\tilde{\boldsymbol{x}}$
- Decompose in basis of 4 vectors: $\mathbf{1}$, $\tilde{\boldsymbol{\nu}}_\tau$, $\boldsymbol{\Lambda}_+$, $\boldsymbol{\Lambda}_-$

$$\tilde{\boldsymbol{x}} = \underbrace{K\mathbf{1} + F\tilde{\boldsymbol{\nu}}_\tau}_{\text{linear part}} + \underbrace{\lambda_+\boldsymbol{\Lambda}_+ + \lambda_-\boldsymbol{\Lambda}_-}_{\text{nonlinear part}}$$

- Nonlinear contribution described by coefficients λ_+, λ_-
- Assuming **1 dominant nonlinearity**, slope λ_-/λ_+ is same for all transitions → **same underlying nuclear-structure effect responsible for nonlinearity**

Door, Yeh, **MH**, et al., arXiv:2403.07792

Impact of nuclear structure effects



Door, Yeh, **MH**, et al., arXiv:2403.07792

- Nonlinearity analysis suggests **single dominant higher-order term**
- $\langle r^2\rangle^2$ and new boson **incompatible** with observed nonlinearity
- **Theory predictions for $\langle r^4\rangle$ required!**

Door, Yeh, **MH**, et al., arXiv:2403.07792

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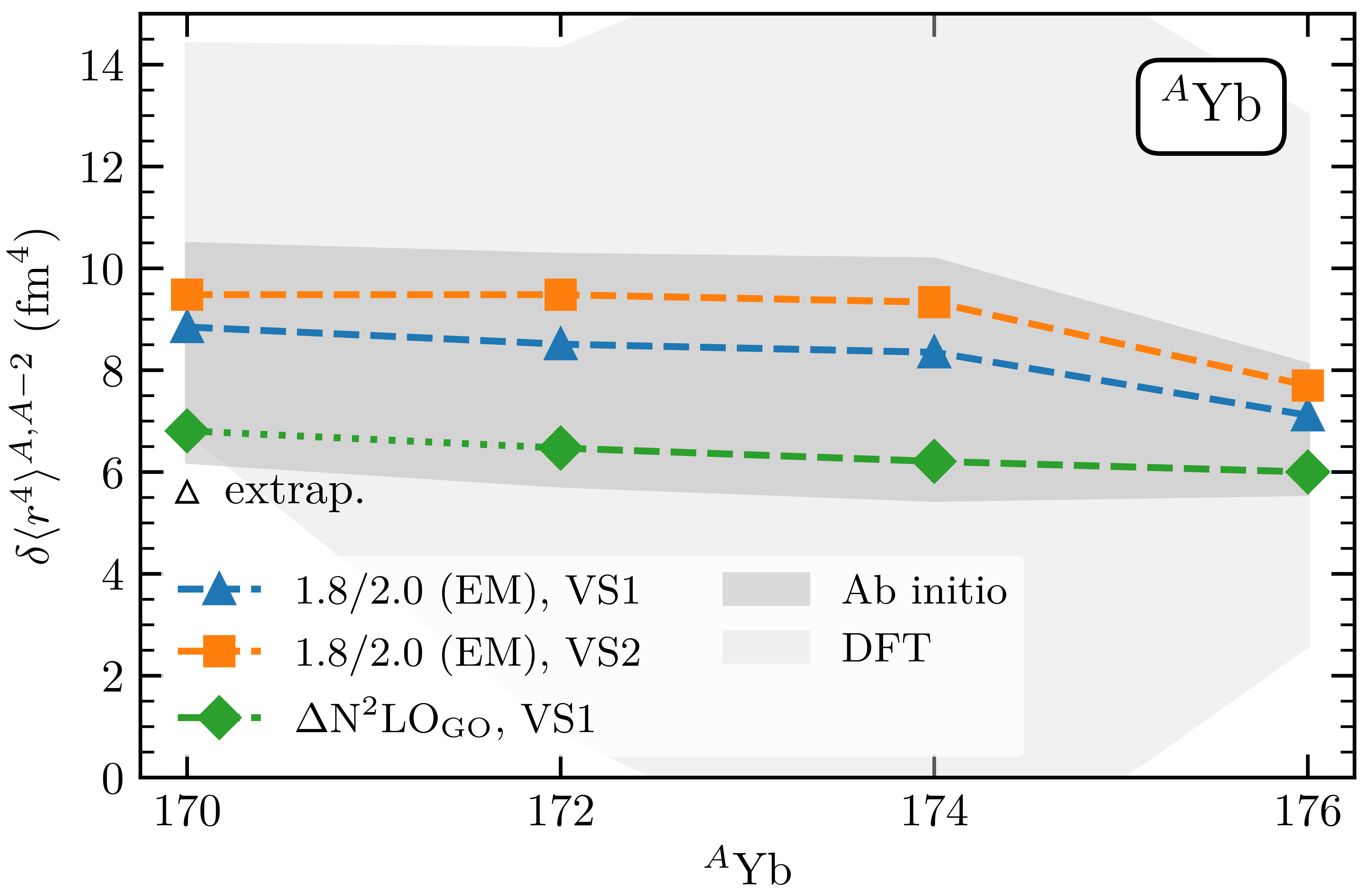

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- **Our input**: VS-IMSRG calculations of Yb
- Two Hamiltonians, two valence spaces
- IMSRG(3) to probe many-body uncertainty

Door, Yeh, **MH**, et al., arXiv:2403.07792

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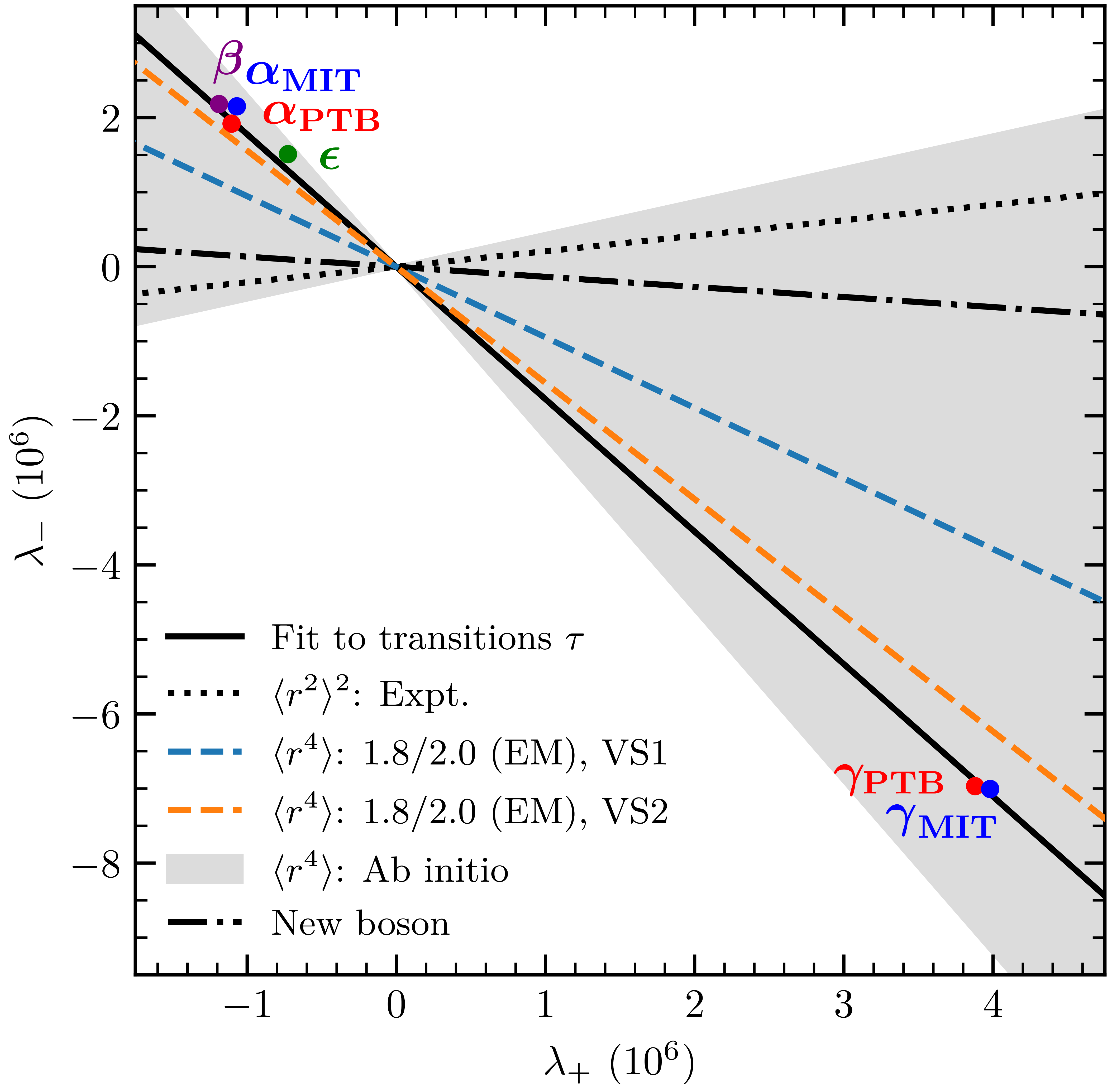

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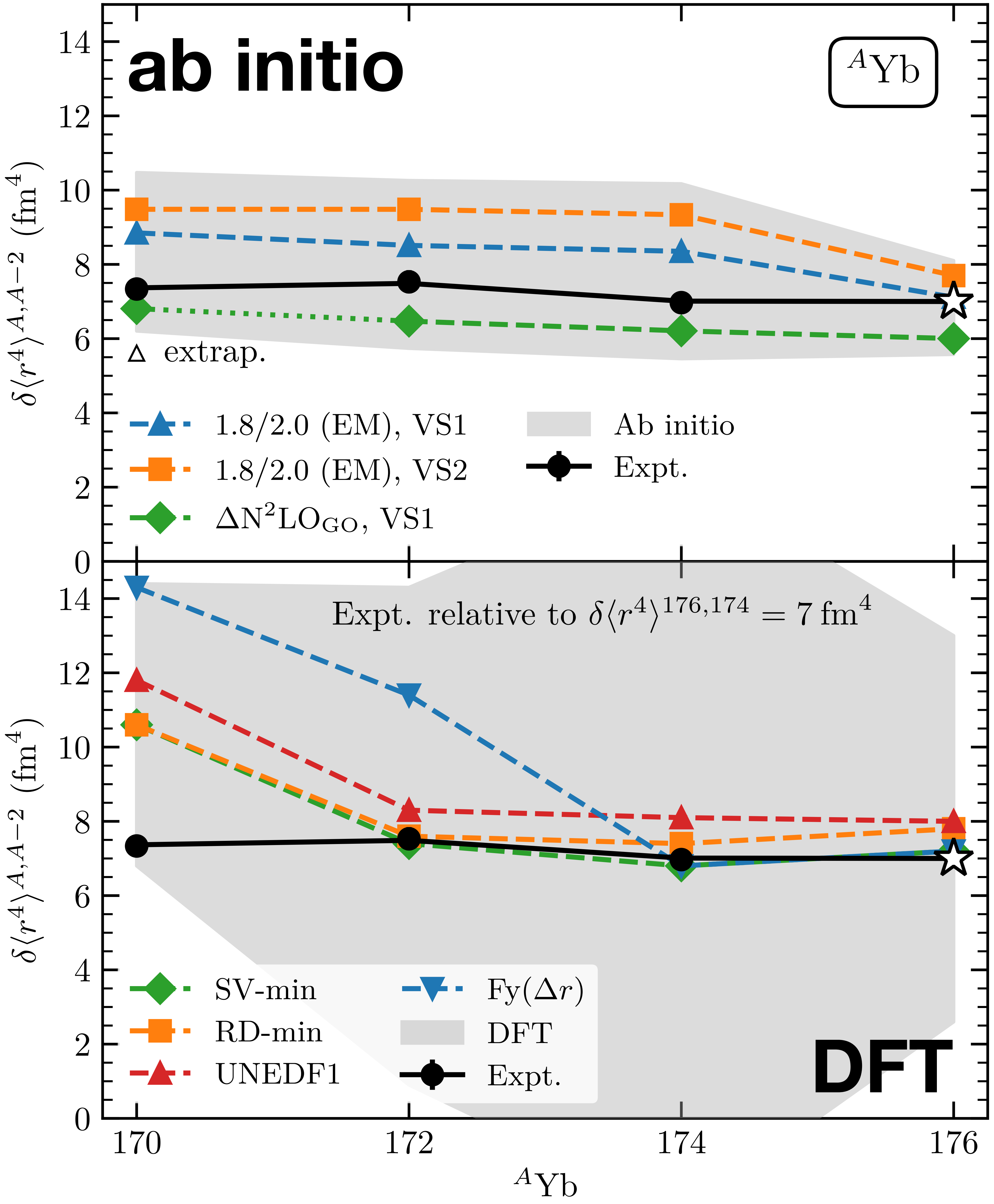
Nuclear theory: $\langle r^4\rangle$, not new boson, is leading source of nonlinearity!

Door, Yeh, **MH**, et al., arXiv:2403.07792

New insights into nuclear structure

- Assume nonlinearity due to $\langle r^4 \rangle$
- Extract information on $\langle r^4 \rangle$ from experimental data
- Subtlety: Only sensitive to nonlinearity
  $\rightarrow$ Extraction only sensitive to
  relative changes in $\delta\langle r^4 \rangle^{A,A'}$
- **New observable related to deformation**

Trends more consistent with ab initio than DFT

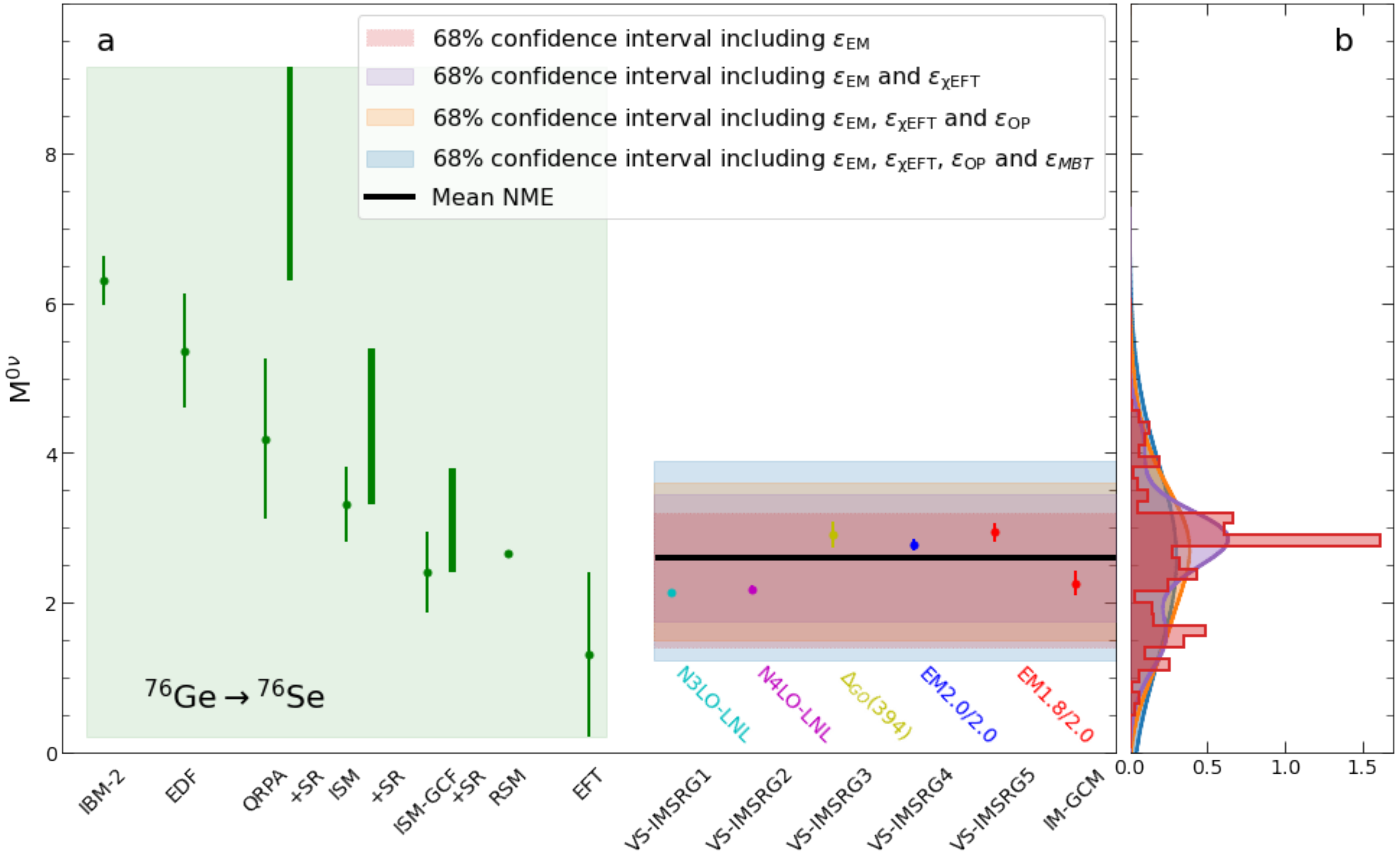


Door, Yeh, **MH**, et al., arXiv:2403.07792

Improved NMEs for $0\nu\beta\beta$

nuclear matrix elements

- **Fully uncertainty quantified** NMEs
- Largest uncertainty: **IMSRG(2)**
- Comparable uncertainty:
  chiral EFT at **NNLO**
- Need IMSRG(3) for **uncertainty quantification, precision**



Belley, et al., PRL **132** (2024)

Improved NMEs require improved many-body calculations & Hamiltonians!

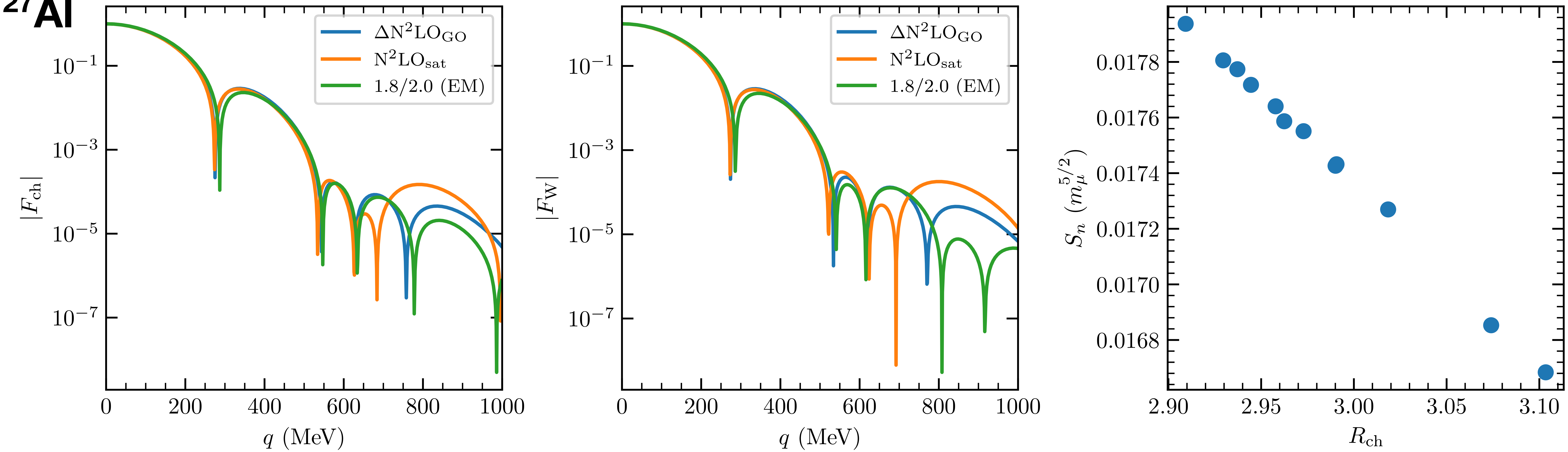
MH, Noël, Hoferichter, et al., preliminary

Neutron densities for new physics

See talk by Martin Hoferichter, Tuesday

- Coupling to **neutron densities** important for searches for new interactions
- **Nuclear theory** can connect neutron density to measurable charge density

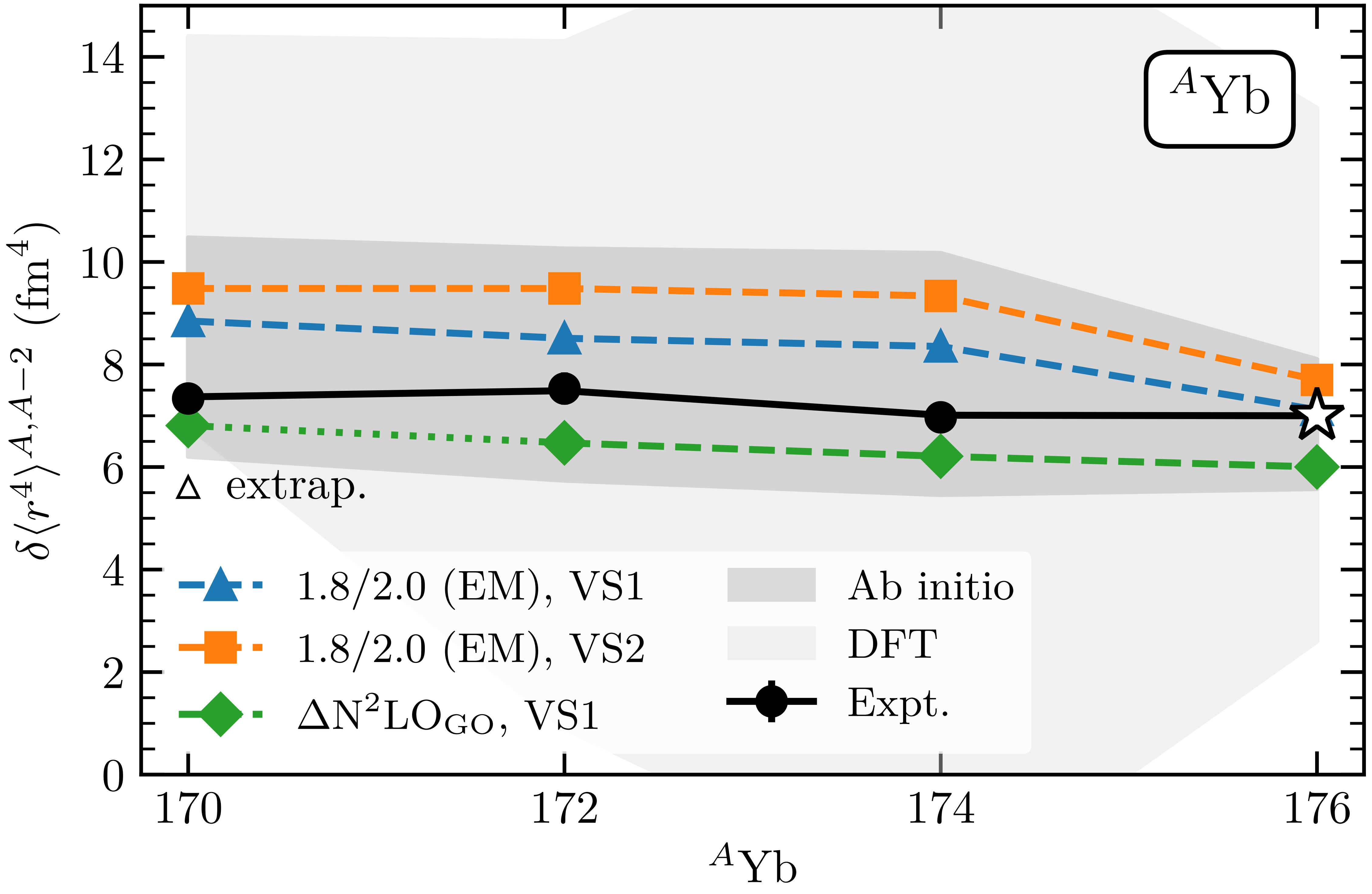
^{27}Al



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

Conclusion and outlook

- **Significant progress** on **reach, precision**, and **applications** of ab initio nuclear structure calculations
- Nuclear structure input with **quantified uncertainties essential** to understand Yb King plot
- Leading signal due to **nuclear structure, not new physics**
- Remarkable reach to provide input for **new physics searches** in heavy nuclei



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Acknowledgments

Coauthors:

- **TU Darmstadt**: **Jan Hoppe**, **Takayuki Miyagi**, **Alex Tichai**, Kai Hebeler, Achim Schwenk
- **MPIK**: **Menno Door**, **Chunhai Lyu**, Klaus Blaum, Zoltán Harman
- **PTB Braunschweig**: **Indy Yeh**, Tanja Mehlstäubler
- **Leibniz University Hannover**: **Fiona Kirk**, Elina Fuchs
- **UNSW**: Julian Berengut
- **University of Tsukuba**: Noritaka Shimizu
- **Uni Bern**: **Frederic Noël**, Martin Hoferichter

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SFB 1245

Thank you for your attention!

$0\nu\beta\beta$ details

Belley, et al., PRL **132** (2024)

TABLE I. **The recommended value for the total NME of $0\nu\beta\beta$ decay in ^{76}Ge, together with the uncertainties from different sources.**

$M^{0\nu}$	ϵ_{LEC}	$\epsilon_{\chi\mathrm{EFT}}$	ϵ_{MBT}	ϵ_{OP}	ϵ_{EM}
$2.60^{+1.28}_{-1.36}$	0.75	0.3	0.88	0.47	<0.06