

# First-principles nuclear structure theory and implications for fundamental physics

Matthias Heinz, ORNL

*ESNT Workshop: "Theoretical and experimental developments for  
symmetry-violating nuclear properties"  
Saclay, France, June 26, 2025*

Work supported by:



This research used resources of the Oak Ridge Leadership Computing Facility located at Oak Ridge National Laboratory, which is supported by the Office of Science of the Department of Energy under contract No. DE-AC05-00OR22725.

# Progress in first-principles calculations

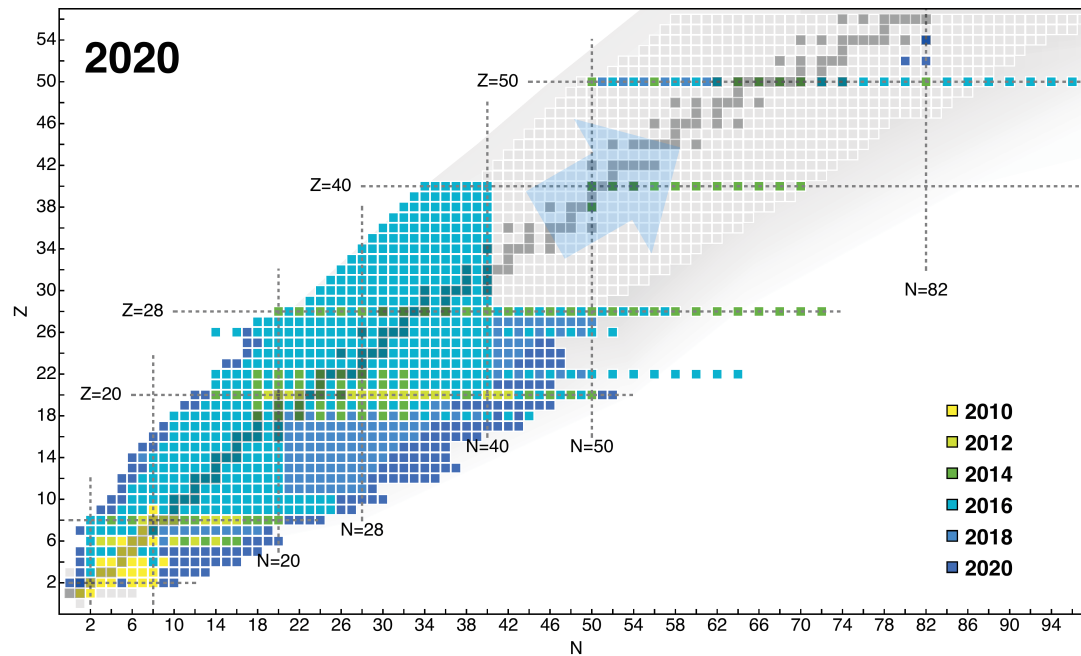
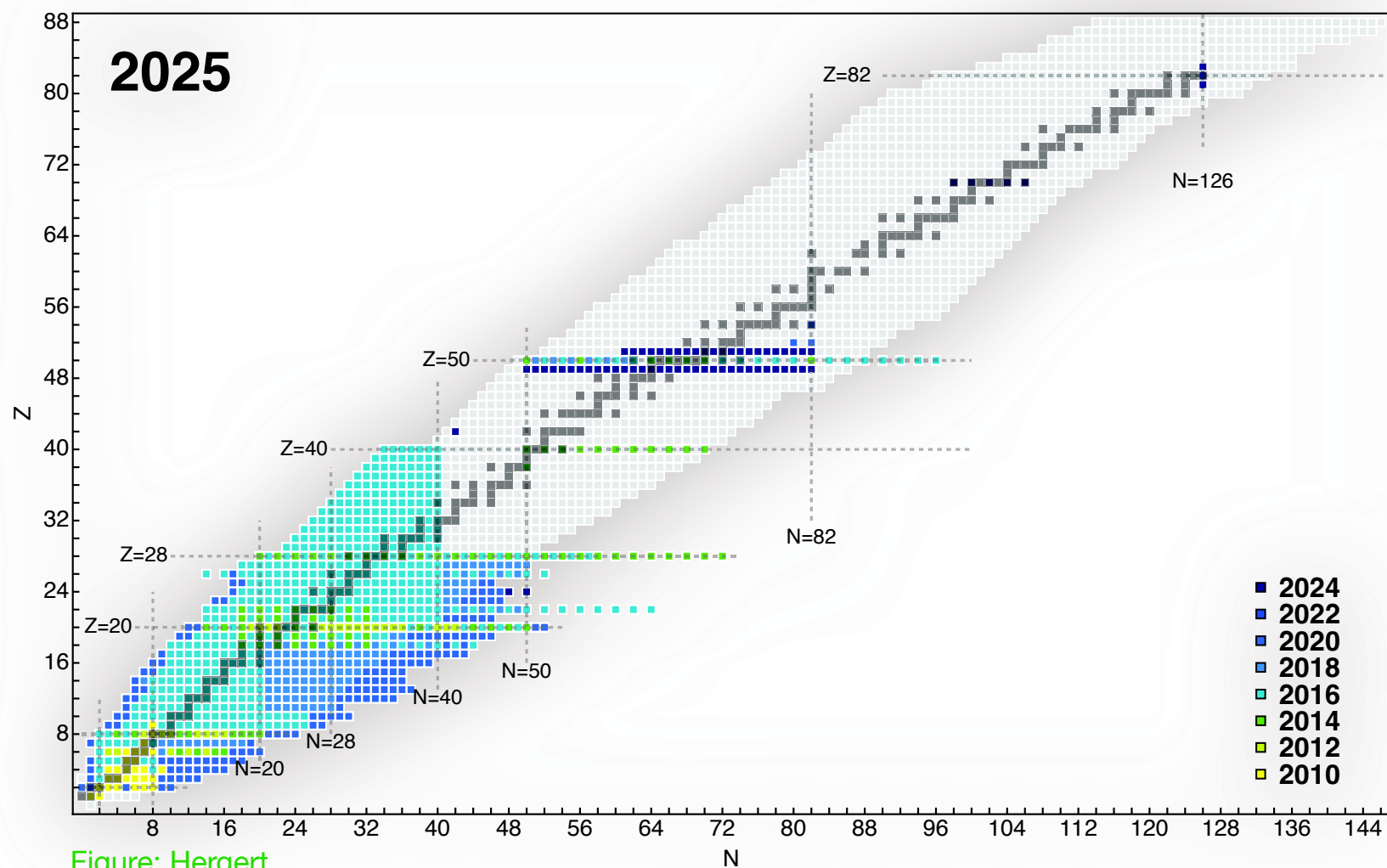


Figure: Hergert

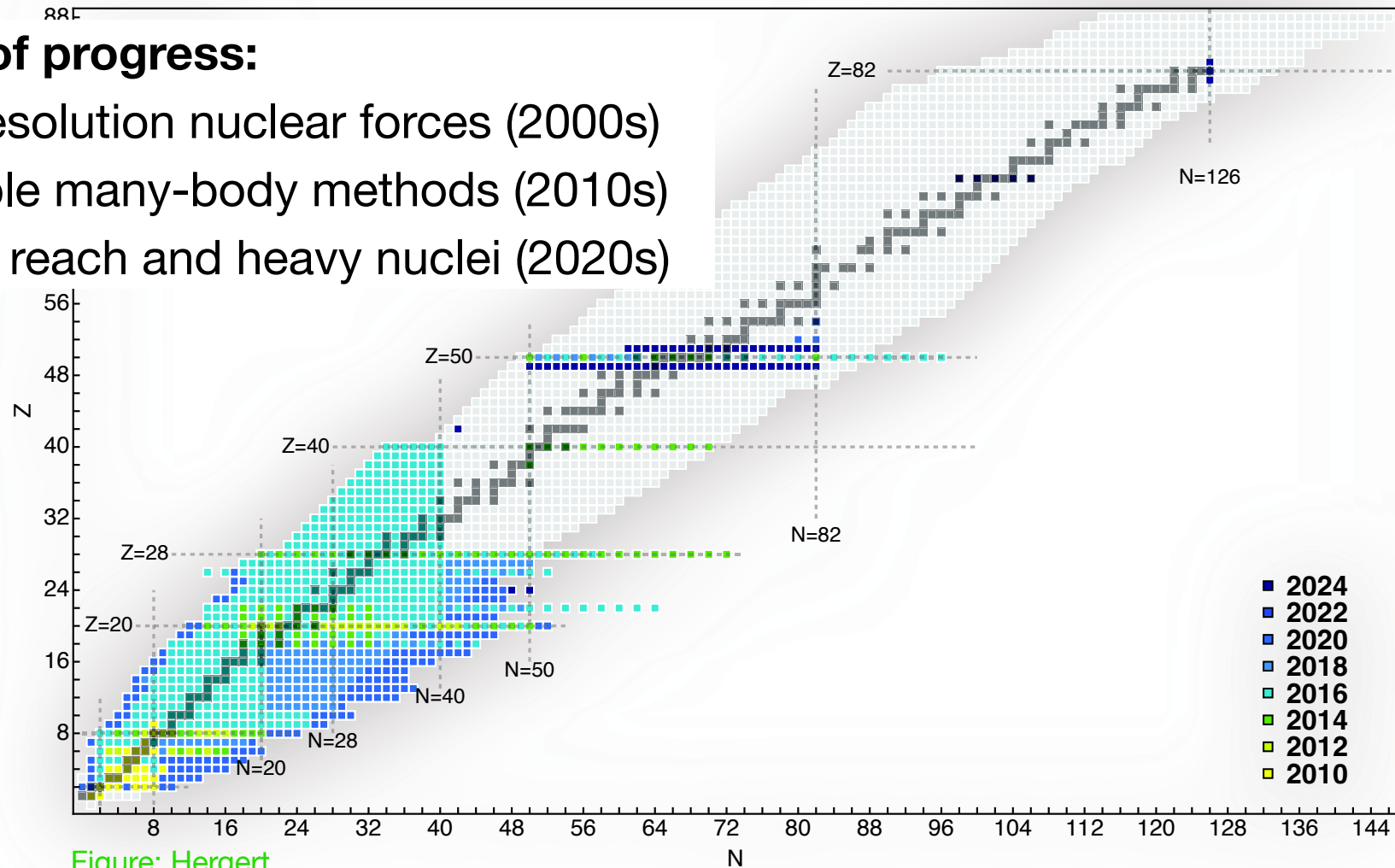
# Progress in first-principles calculations



# Progress in first-principles calculations

## Drivers of progress:

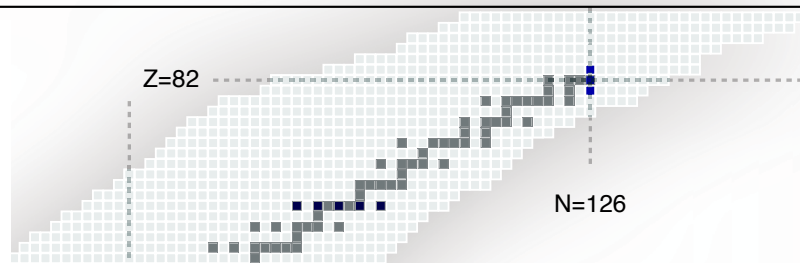
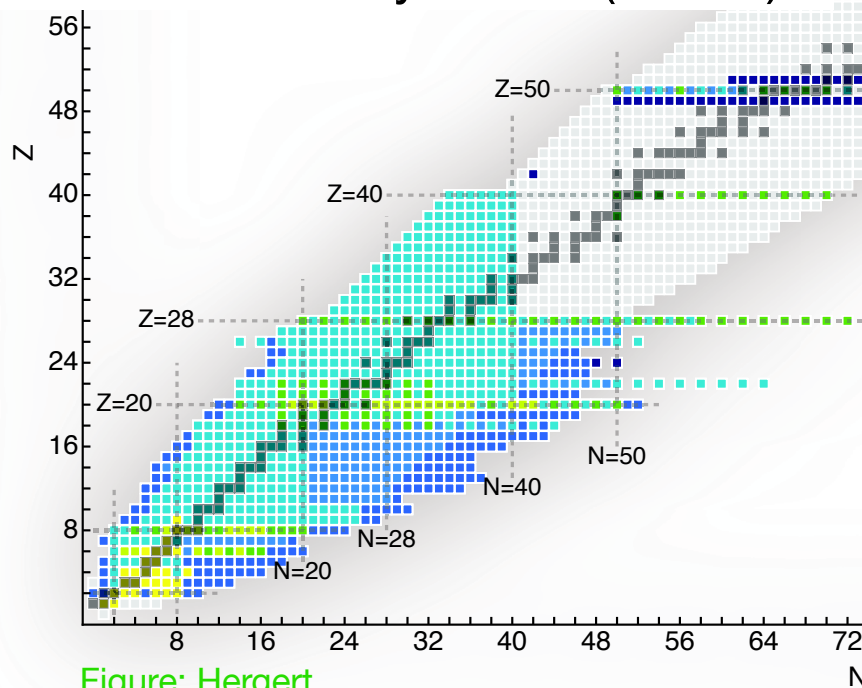
- Low-resolution nuclear forces (2000s)
- Scalable many-body methods (2010s)
- Global reach and heavy nuclei (2020s)



# Progress in first-principles calculations

## Drivers of progress:

- Low-resolution nuclear forces (2000s)
- Scalable many-body methods (2010s)
- Global reach and heavy nuclei (2020s)



## New frontiers for applications:

- Neutrinoless double-beta decay  
Novario et al., PRL (2021), Belley et al. PRL (2021), PRL (2024)
- Neutron skin and structure of  $^{208}\text{Pb}$   
Hu et al., Nat. Phys. (2022), Hebeler et al., PRC (2023)
- Magnetic moments also in heavy nuclei  
Miyagi et al., PRL (2024)
- Calibration of RMF models to ab initio  
Reed et al., arXiv:2505.00828
- Polarizability and constraints for EOS  
Fearick et al., PR Res. (2023), Bonaiti (2024)
- Much more to come!

# Progress in first-principles calculations

## Outline:

### Drivers of progress:

- Low-resolution nuclear forces (2000s)
- Scalable many-body methods (2010s)
- Global reach and heavy nuclei (2020s)

- Brief intro

- Improved nuclear structure of calcium isotopes

MH et al., PRC (2021, 2025)

- Exploring nuclear structure (and new physics) with ytterbium isotope shifts

Door, Yeh, MH, et al., PRL (2025)

- Improving predictions with experimental data

MH et al., arXiv:2412.04545

- Perspectives for the future

### New frontiers for applications:

• Neutrinoless double-beta decay

Novario et al., PRL (2021), Bailey et al. PRL (2021), PRL (2024)

• Neutron skin and structure of  $^{208}\text{Pb}$

Hu et al., Nat. Phys. (2022), Hebeler et al., PRC (2023)

• Magnetic moments also in heavy nuclei

Miyagi et al., PRL (2024)

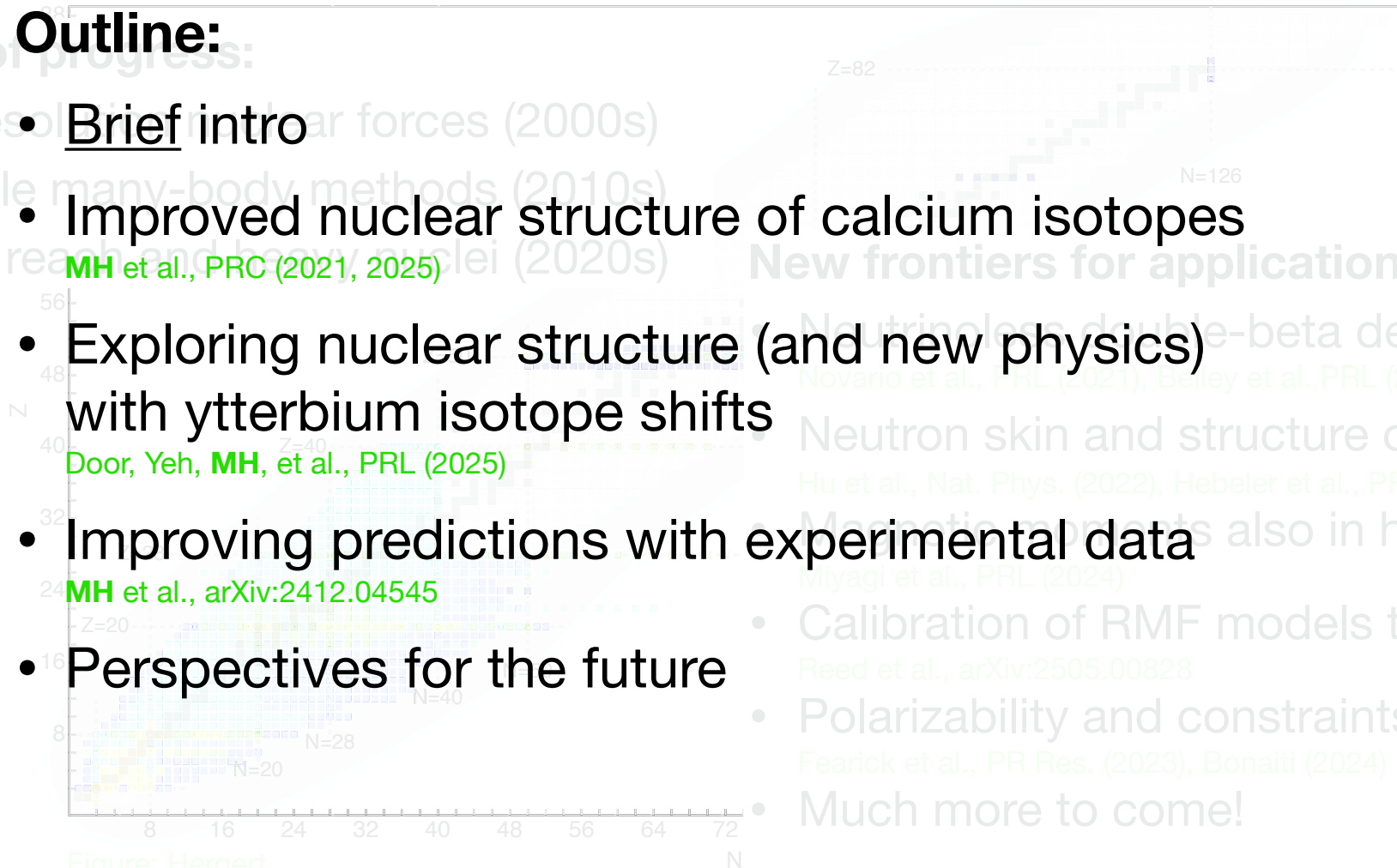
• Calibration of RMF models to ab initio

Reed et al., arXiv:2505.00828

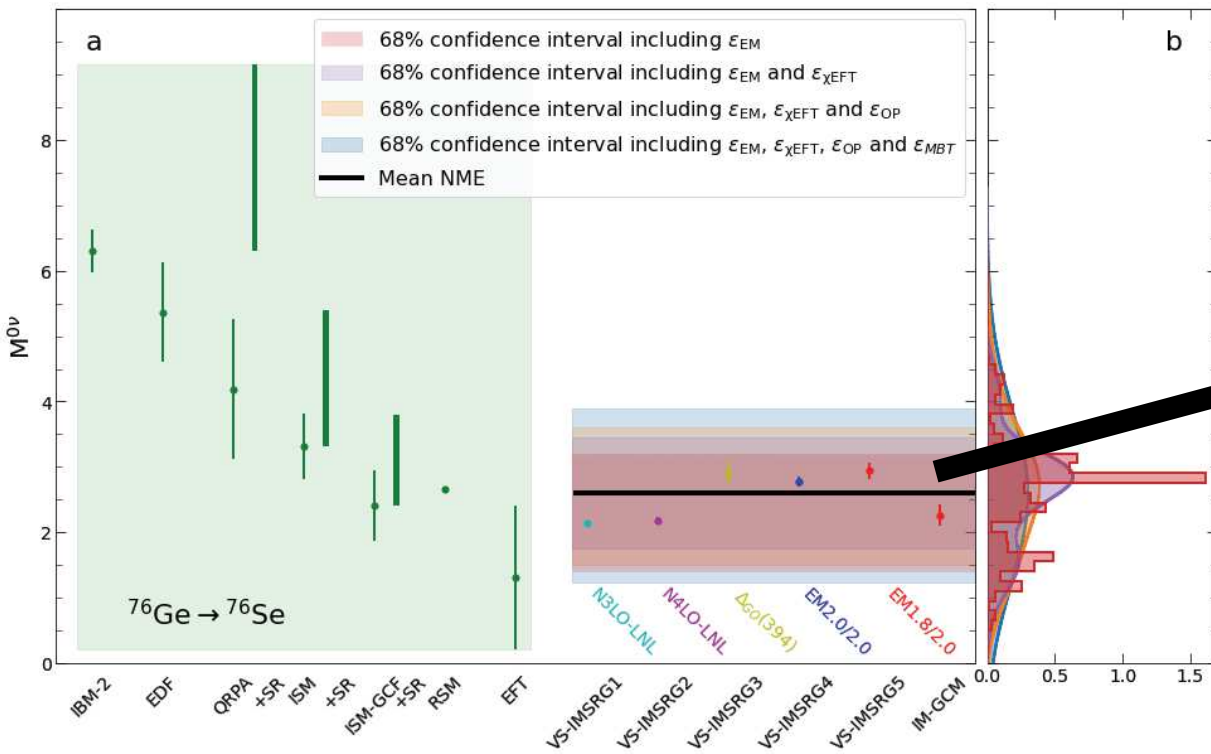
• Polarizability and constraints for EOS

Fearick et al., PR Res. (2023), Bonaiti (2024)

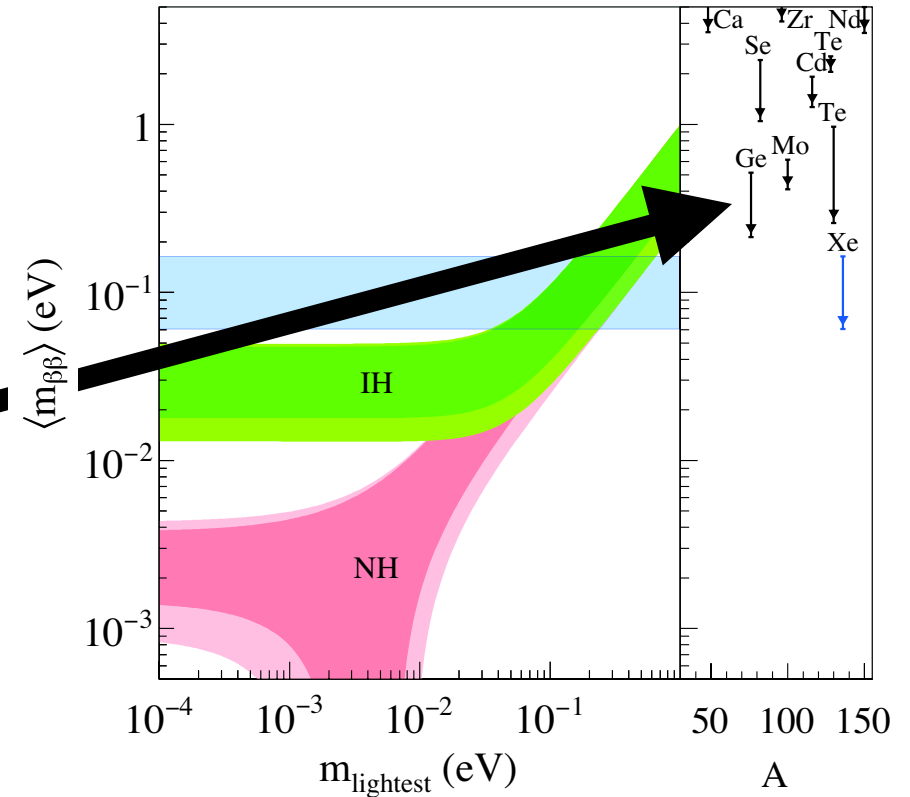
• Much more to come!



# New physics in nuclei requires nuclear theory



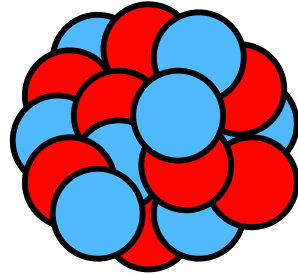
Belley et al., PRL (2024)



Engel, Menéndez, RPP (2016)

# First-principles nuclear structure



●  $N$  neutrons  
●  $Z$  protons  
 $A$  nucleons

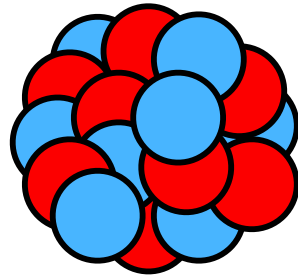


$$H|\Psi\rangle = E|\Psi\rangle$$














# First-principles nuclear structure

  $N$  neutrons  
  $Z$  protons  
 $A$  nucleons



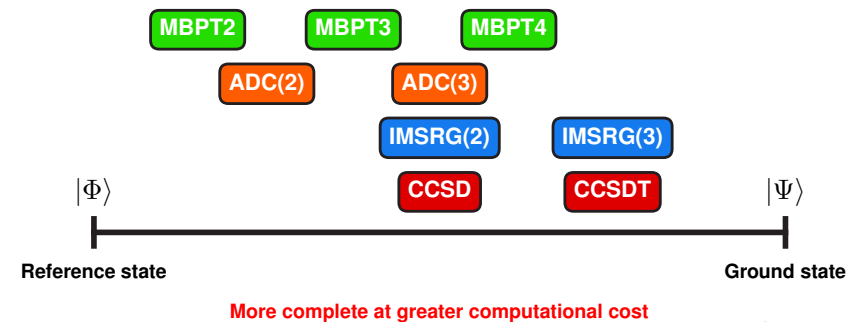
$$H|\Psi\rangle = E|\Psi\rangle$$

## Nuclear forces

	NN	3N	4N
LO $\mathcal{O}(Q^0/\Lambda^0)$	 1990 [2]	—	—
NLO $\mathcal{O}(Q^2/\Lambda^2)$	 1992 [7]	 1992, 1994	—
$N^2$ LO $\mathcal{O}(Q^3/\Lambda^3)$	 1992 [0]	 1994 [2]	—
$N^3$ LO $\mathcal{O}(Q^4/\Lambda^4)$	 2000–2002 [12]	 2008–2011 [0]	 2006 [0]
$N^4$ LO $\mathcal{O}(Q^5/\Lambda^5)$	 2015 [0]	 2011– [?]	 [?]

Hebeler, Phys. Rep. 890 (2021)

## Many-body methods



# First-principles nuclear structure

  $N$  neutrons

  $Z$  protons

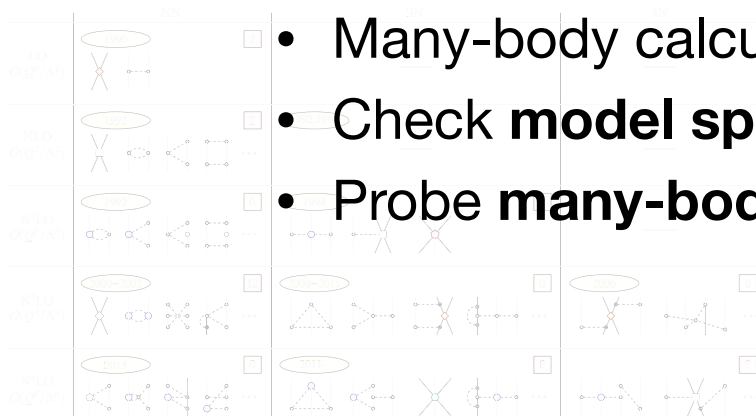
$A$  nucleons

## Uncertainties in our calculations:

- Nuclear Hamiltonians are **uncertain**
- **Hamiltonian variation** to probe uncertainty

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

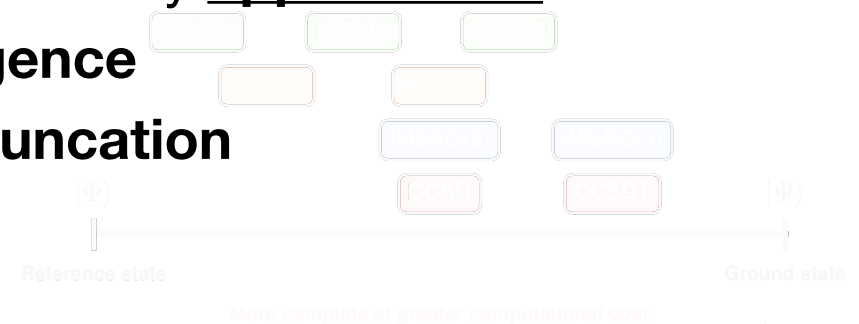
## Nuclear forces



Hebeler, Phys. Rep. 890 (2021)

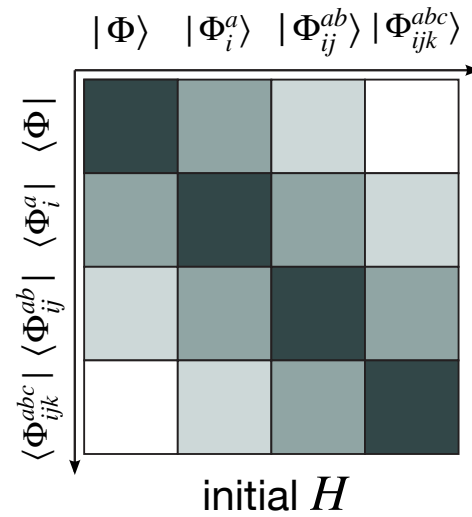
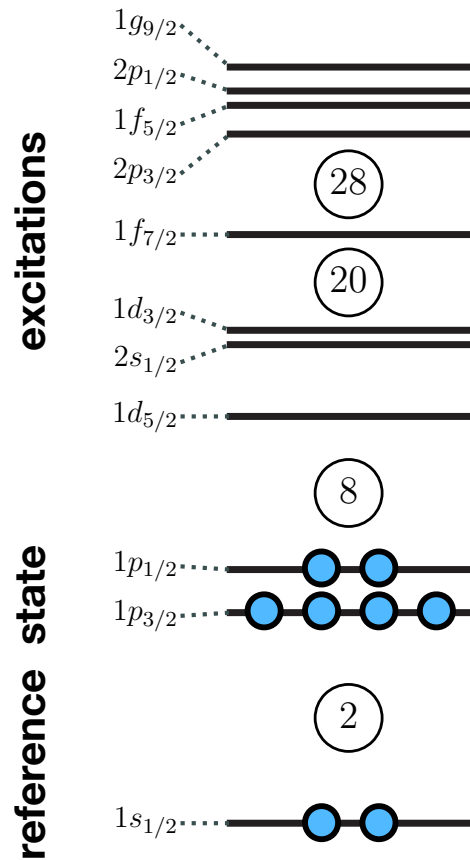
- Many-body calculations are generally **approximate**
- Check **model space convergence**
- Probe **many-body method truncation**

## Many-body methods



# The IMSRG

in-medium similarity renormalization group

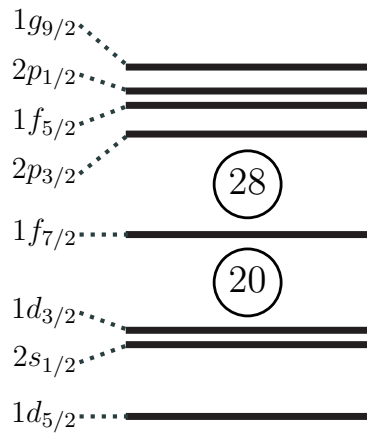


Tsukiyama et al., PRL (2011)  
Hergert et al., Phys. Rep. (2016)

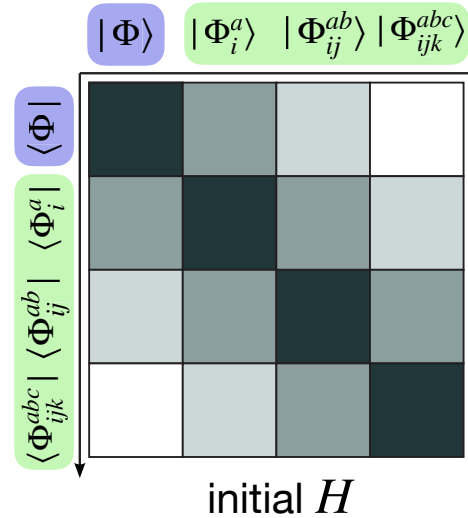
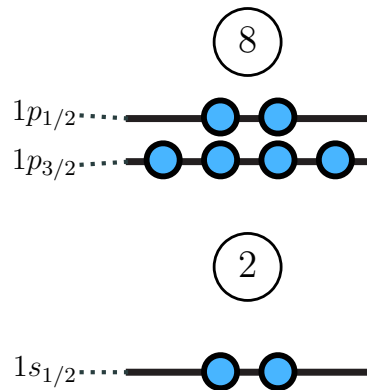
# The IMSRG

in-medium similarity renormalization group

excitations



reference state

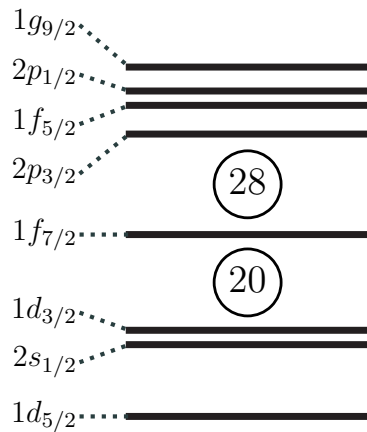


Tsukiyama et al., PRL (2011)  
Hergert et al., Phys. Rep. (2016)

# The IMSRG

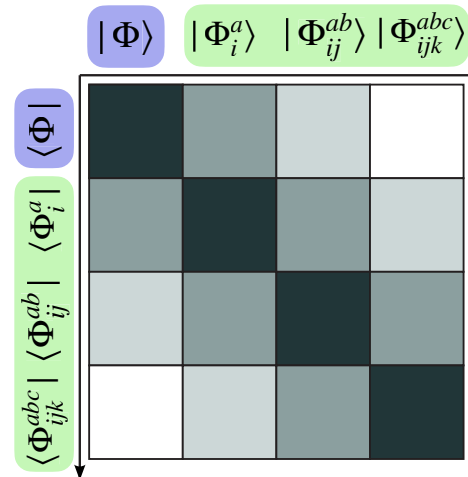
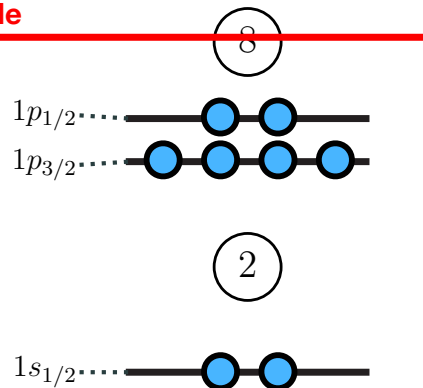
in-medium similarity renormalization group

excitations



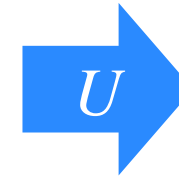
decouple

reference state

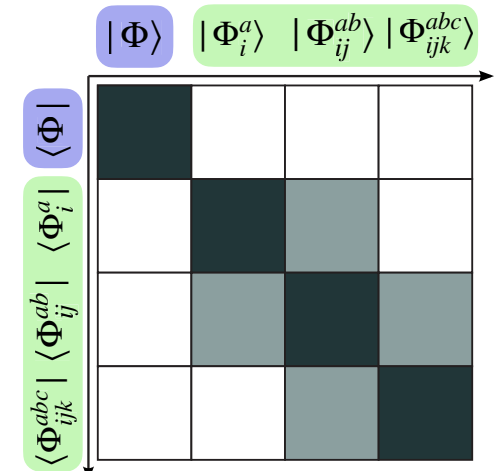


initial  $H$

IMSRG



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



transformed  $H$

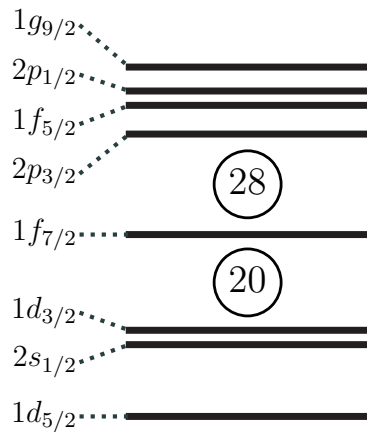
Hergert et al., Phys. Rep. (2016)

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

# The IMSRG

in-medium similarity renormalization group

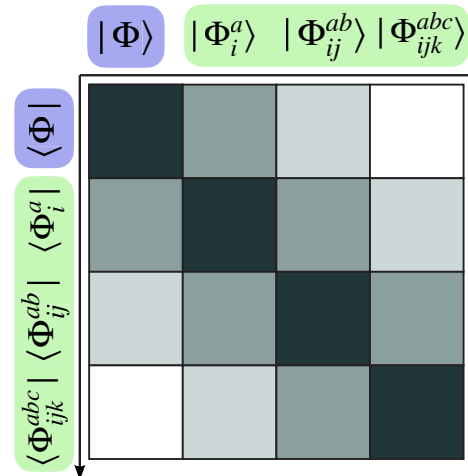
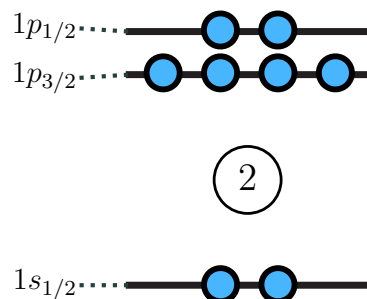
excitations



decouple

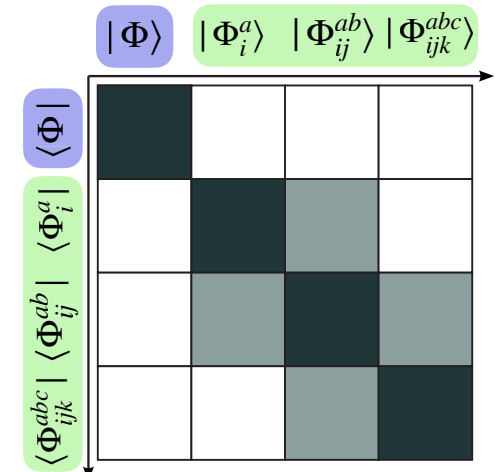
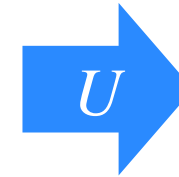
8

reference state



initial  $H$

IMSRG



transformed  $H$

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

Tsukiyama et al., PRL (2011)  
Hergert et al., Phys. Rep. (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 (2021, 2025)  
Stroberg, He, PRC (2024)

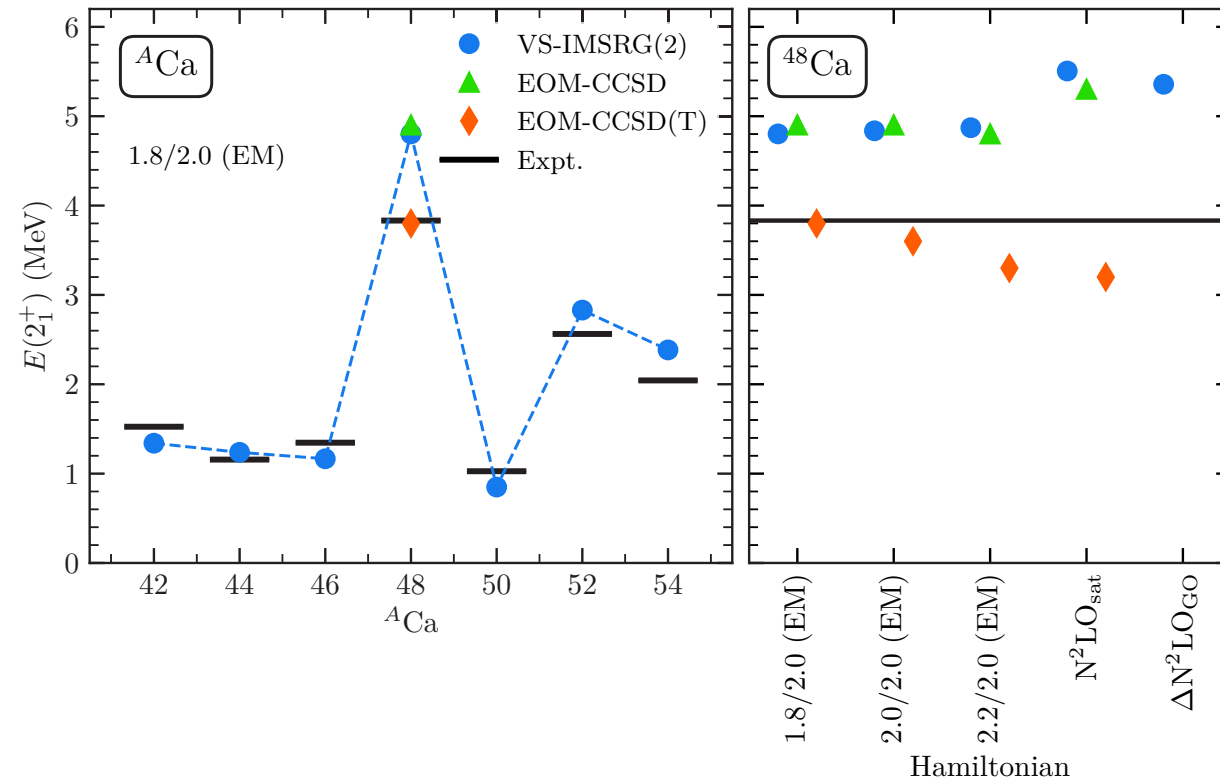
- **IMSRG(3)** for precision and uncertainty quantification

# Improved (?) nuclear structure of calcium isotopes

MH et al., PRC (2021, 2025)

# IMSRG(2) challenges in calcium

- IMSRG(2) predictions for  $2^+$  excitation energy in calcium follow experimental trends...
- ... **except at  $^{48}\text{Ca}$**
- Overprediction resolved by **3-body contributions** [e.g., CC with triples, IMSRG(3)]

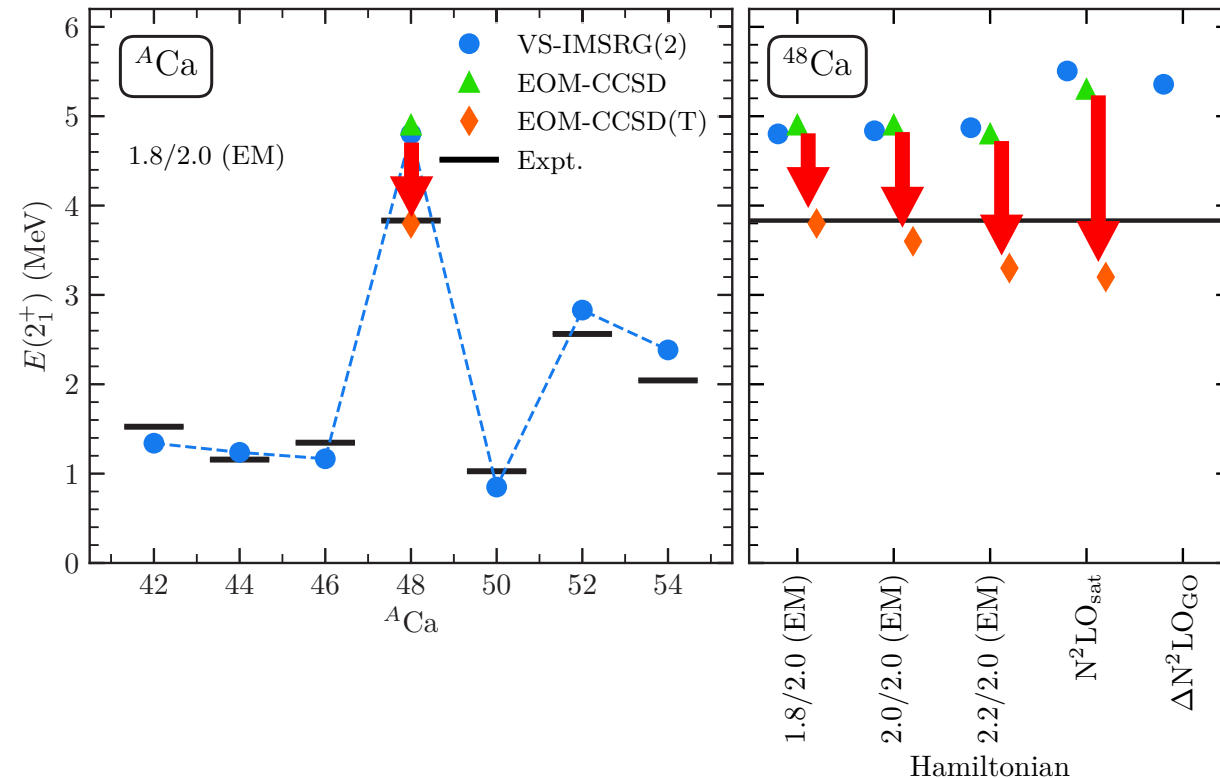


Hagen et al., PRL (2016)  
Simonis et al., PRC (2017)



# IMSRG(2) challenges in calcium

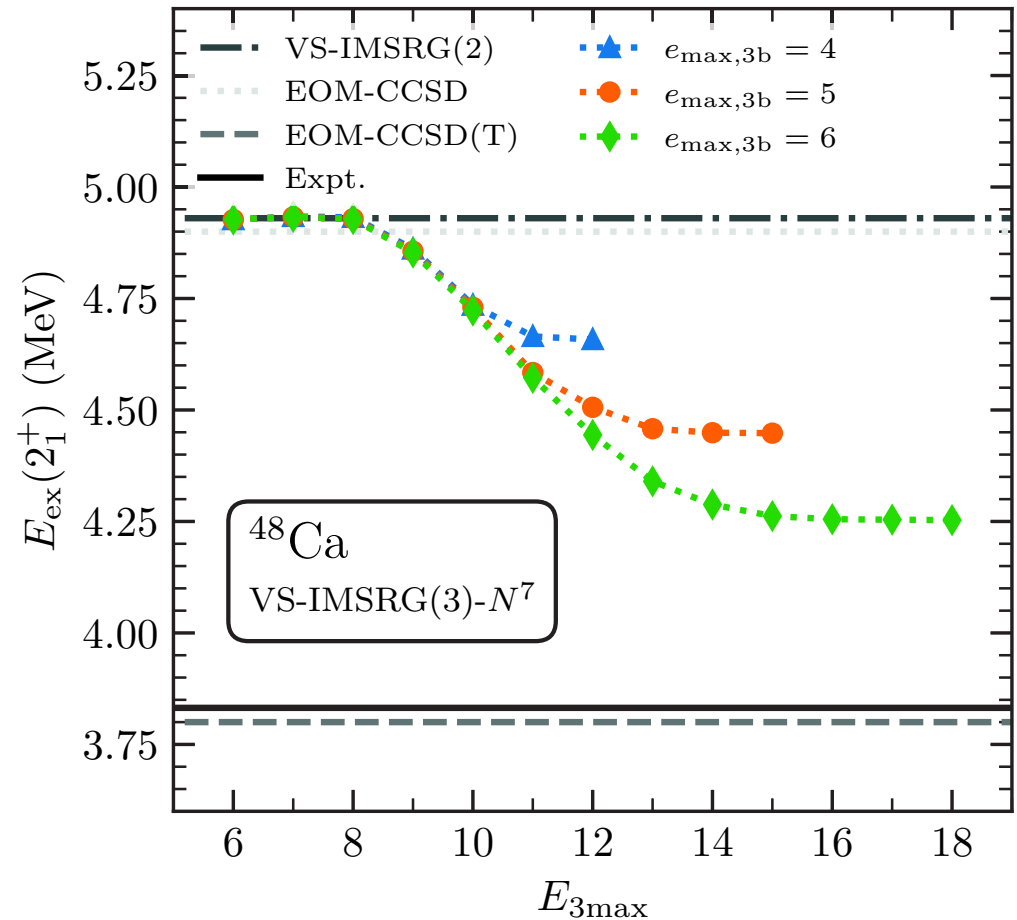
- IMSRG(2) predictions for  $2^+$  excitation energy in calcium follow experimental trends...
- ... **except at  $^{48}\text{Ca}$**
- Overprediction resolved by **3-body contributions** [e.g., CC with triples, IMSRG(3)]



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

# IMSRG(2) challenges in calcium

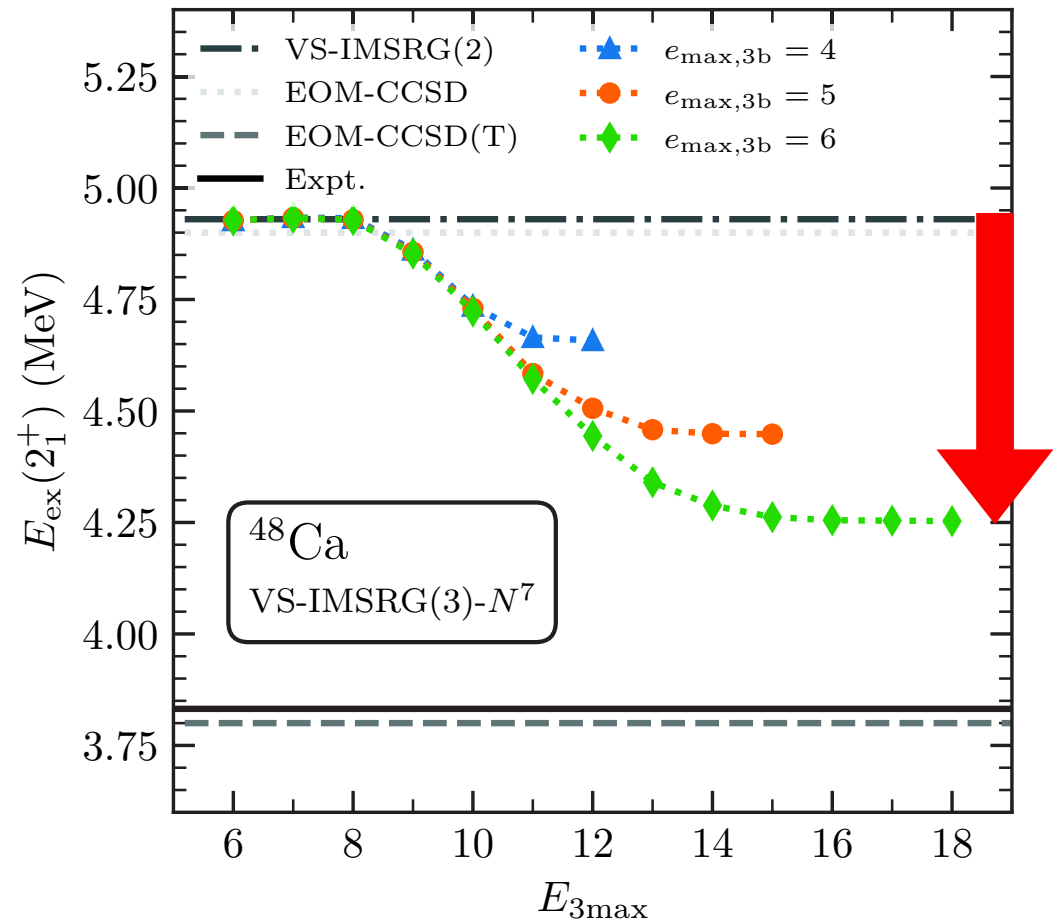
- IMSRG(2) predictions for  $2^+$  excitation energy in calcium follow experimental trends...
- ... **except at  $^{48}\text{Ca}$**
- Overprediction resolved by **3-body contributions** [e.g., CC with triples, IMSRG(3)]



MH, et al., PRC (2025)

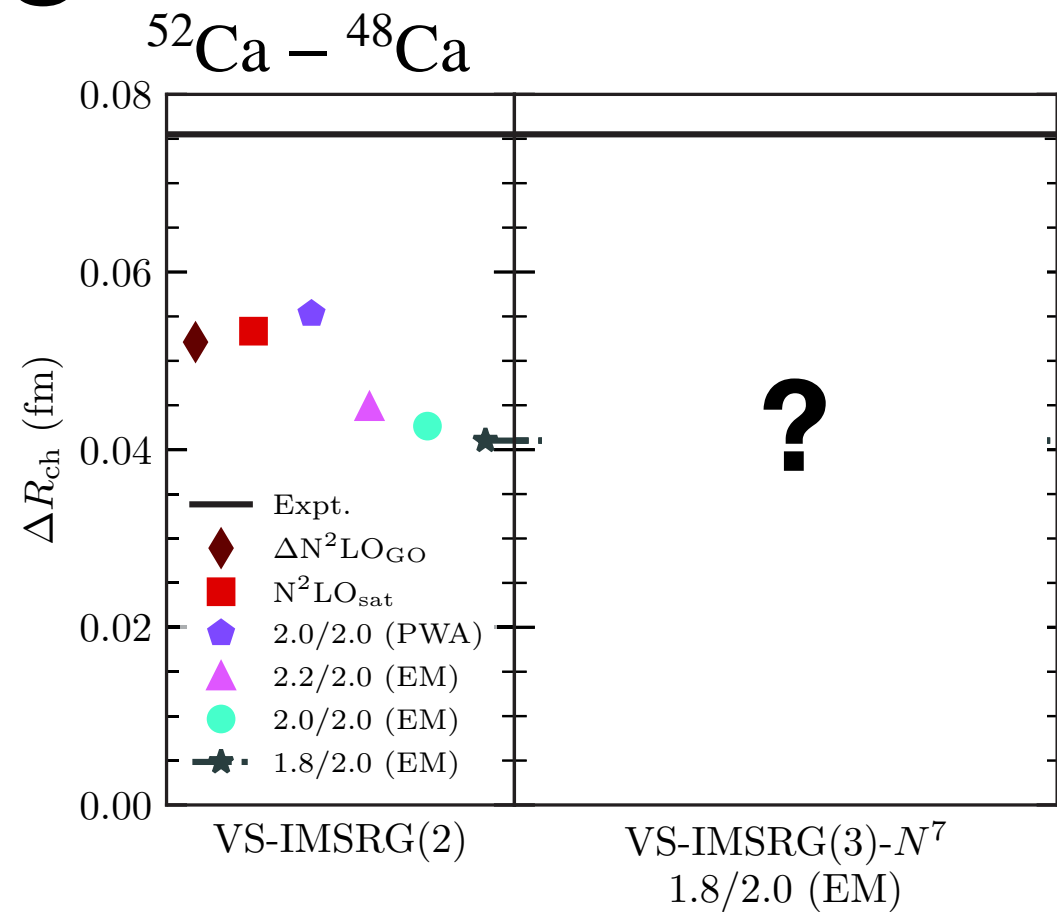
# IMSRG(2) challenges in calcium

- IMSRG(2) predictions for  $2^+$  excitation energy in calcium follow experimental trends...
- ... **except at  $^{48}\text{Ca}$**
- Overprediction resolved by **3-body contributions** [e.g., CC with triples, IMSRG(3)]



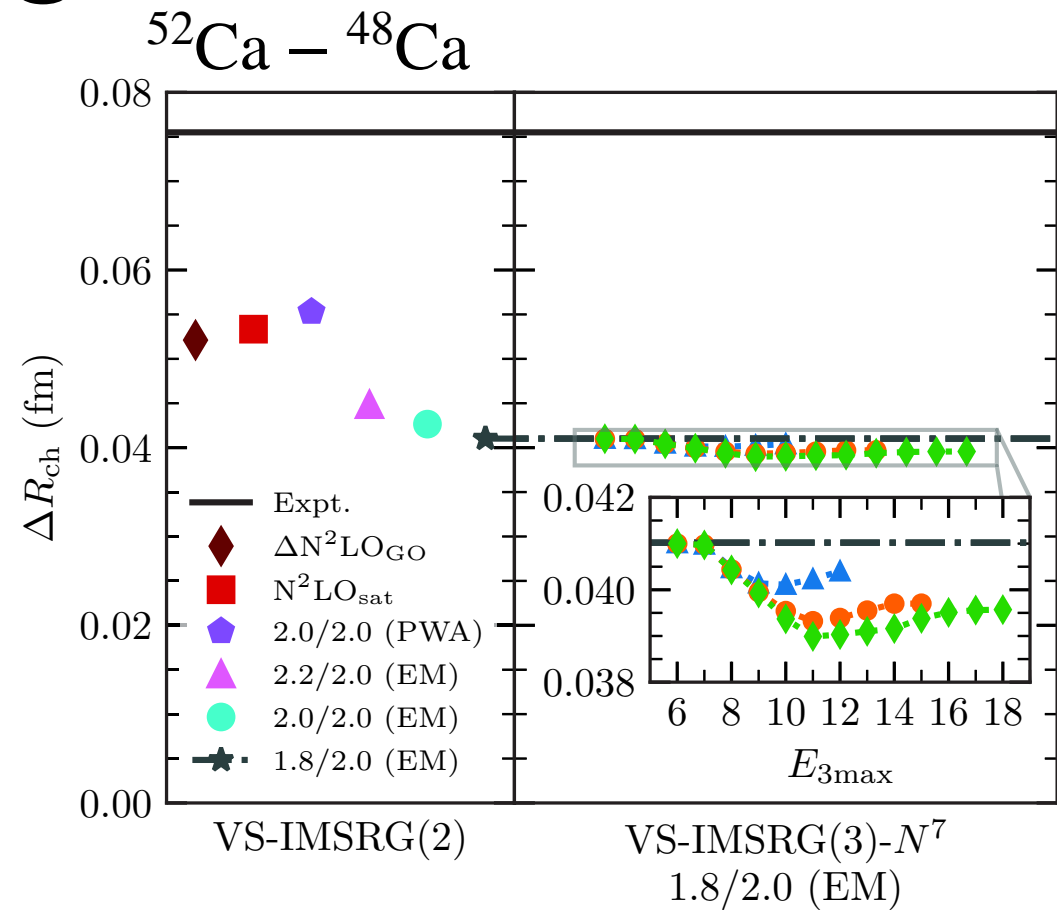
MH, et al., PRC (2025)

# Calcium charge radii



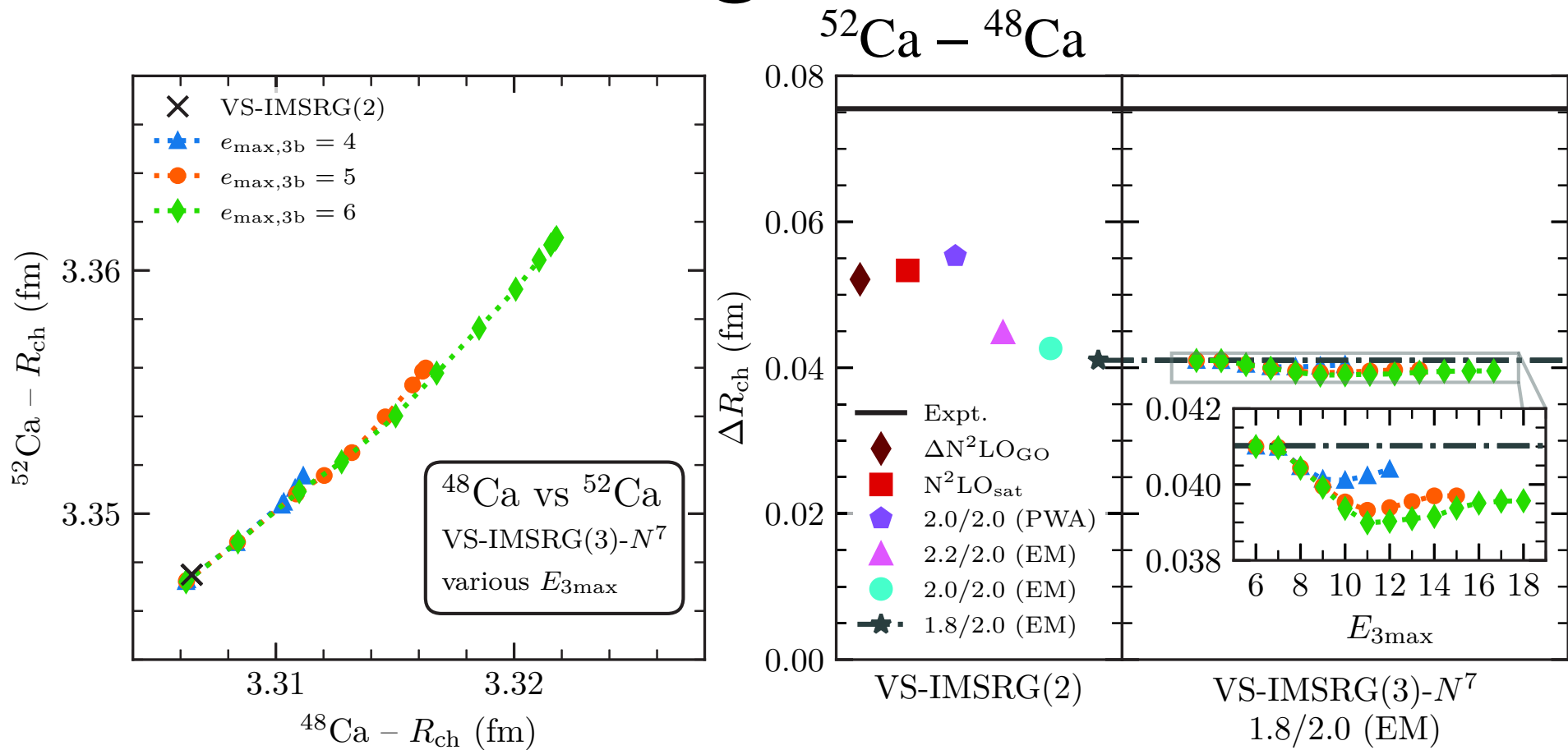
MH et al., PRC (2025)

# Calcium charge radii



MH et al., PRC (2025)

# Calcium charge radii



MH et al., PRC (2025)

# Nuclear structure and new physics in ytterbium isotope shifts

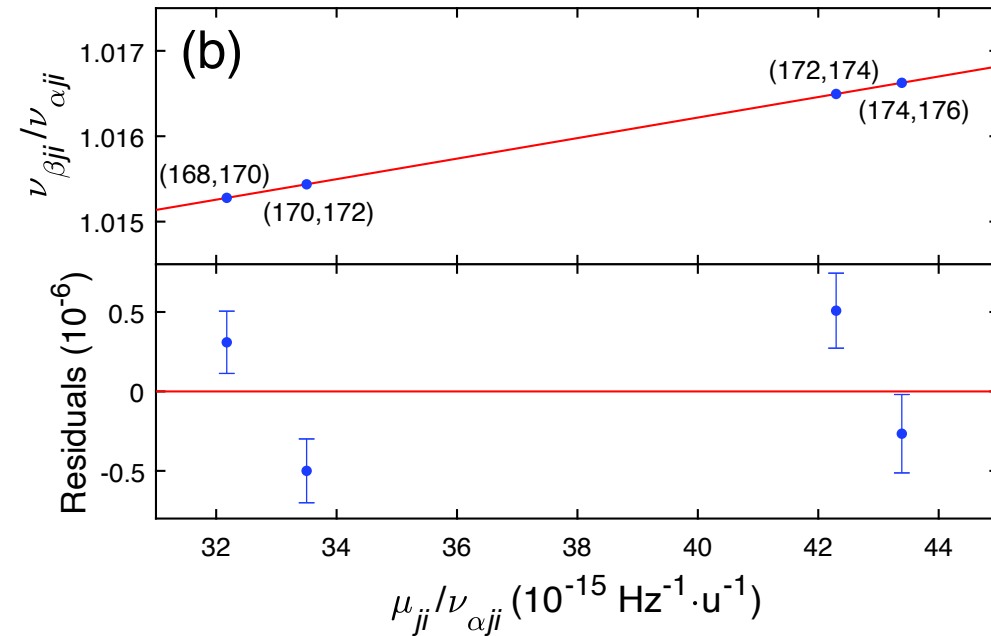
Door, Yeh, **MH**, et al., PRL (2025)

# Nonlinear King plot in ytterbium

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

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

- Leads to **linear King plot**



Counts et al., PRL (2020)

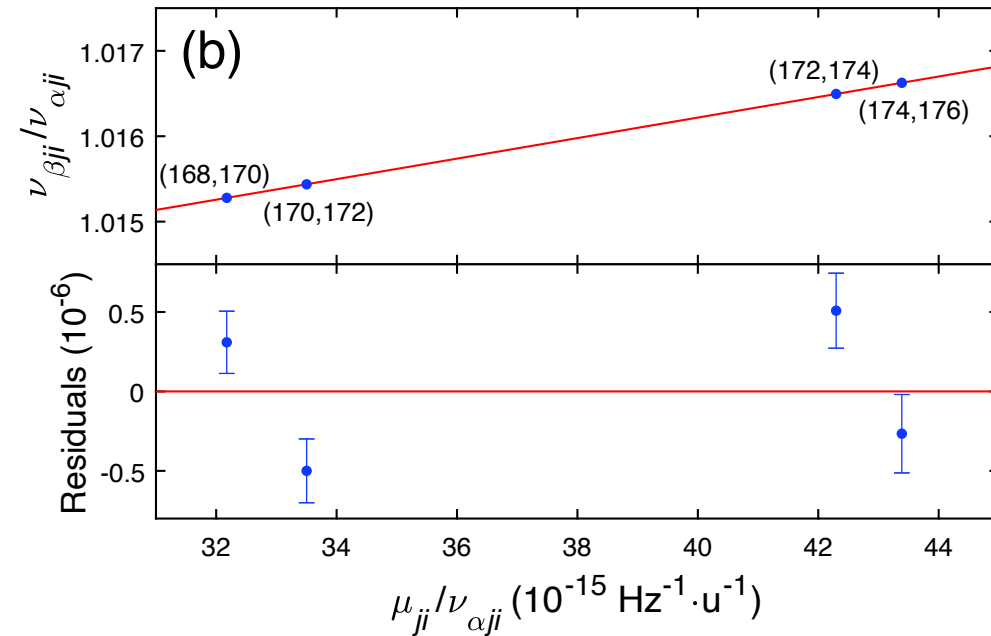


# Nonlinear King plot in ytterbium

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

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

- Leads to **linear King plot**



Counts et al., PRL (2020)

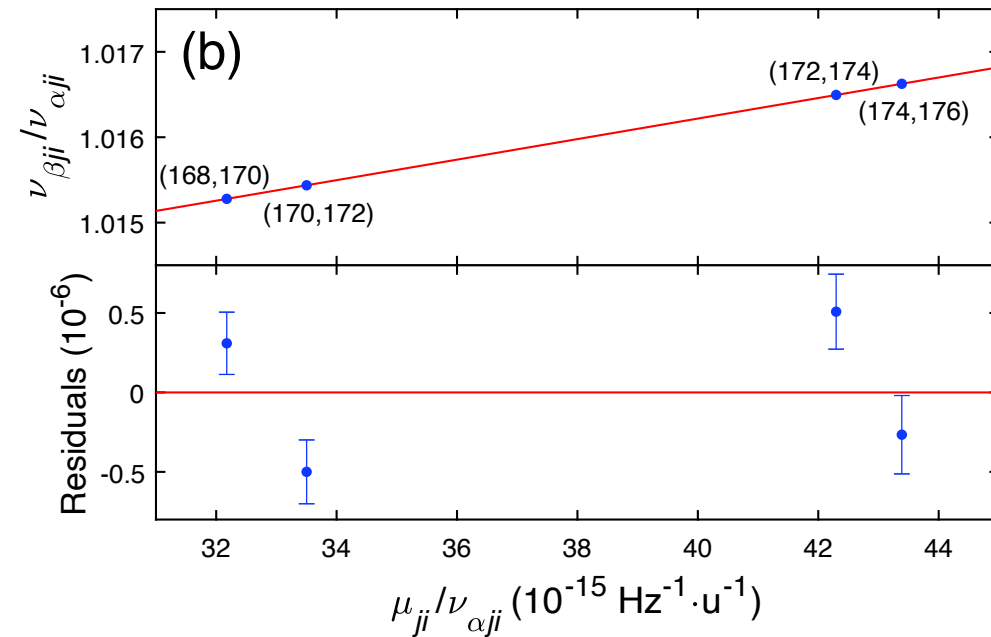
# Nonlinear King plot in ytterbium

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

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

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

$$\nu_{\tau,\text{nonlin.}}^{A,A'} = \underbrace{G_{\tau}^{(2)} (\delta \langle r^2 \rangle^2)^{A,A'} + G_{\tau}^{(4)} \delta \langle r^4 \rangle^{A,A'}}_{\text{higher-order nuclear structure}} + \underbrace{\frac{\alpha_{\text{NP}}}{\alpha_{\text{EM}}} D_{\tau} h^{A,A'}}_{\text{possible new boson}} + \dots$$



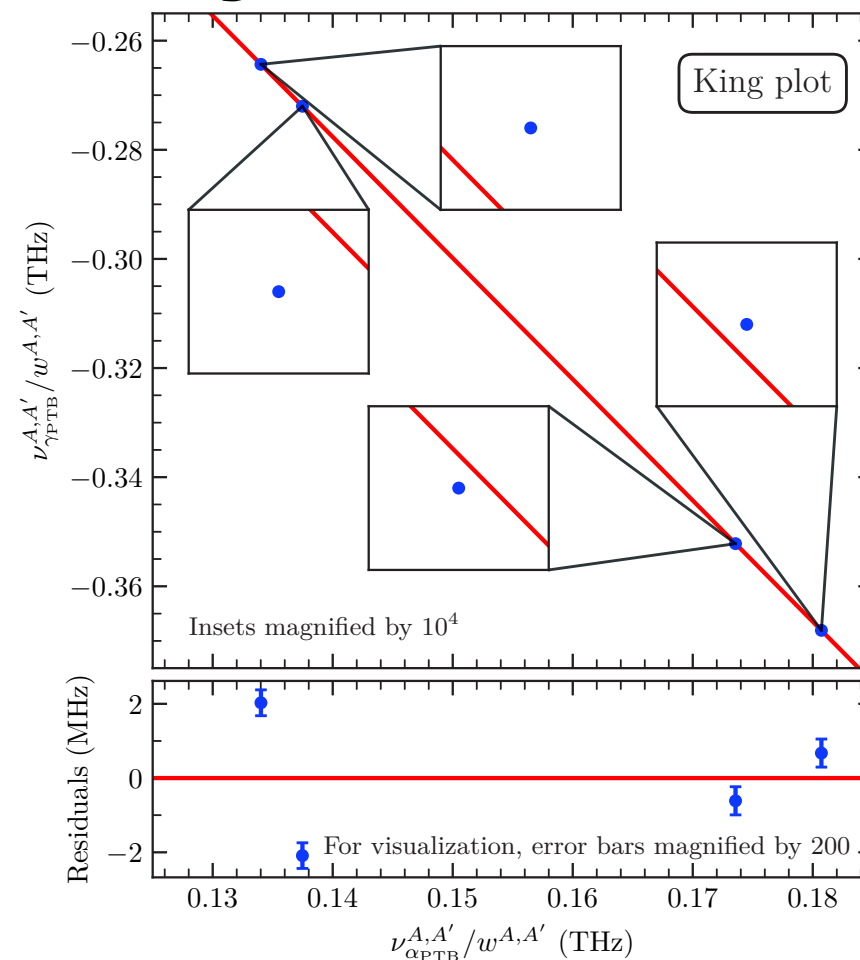
Counts et al., PRL (2020)

# Nonlinear King plot in ytterbium

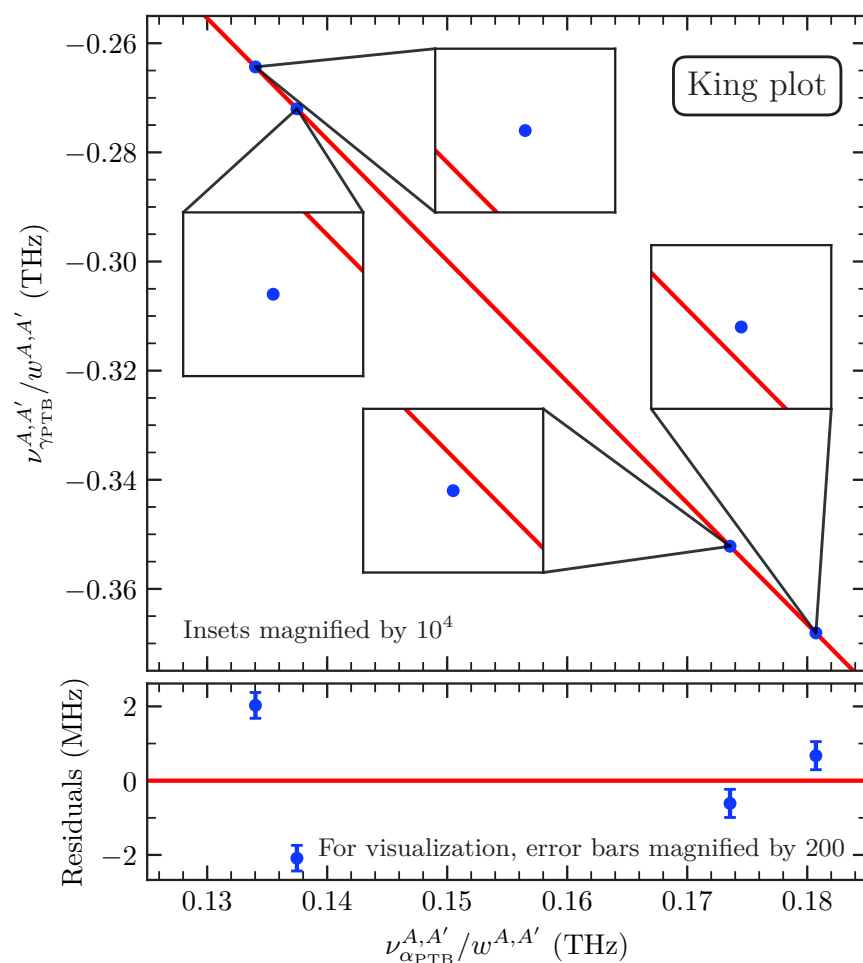
## New data:

- $^{168,170,172,174,176}\text{Yb}$  (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?**



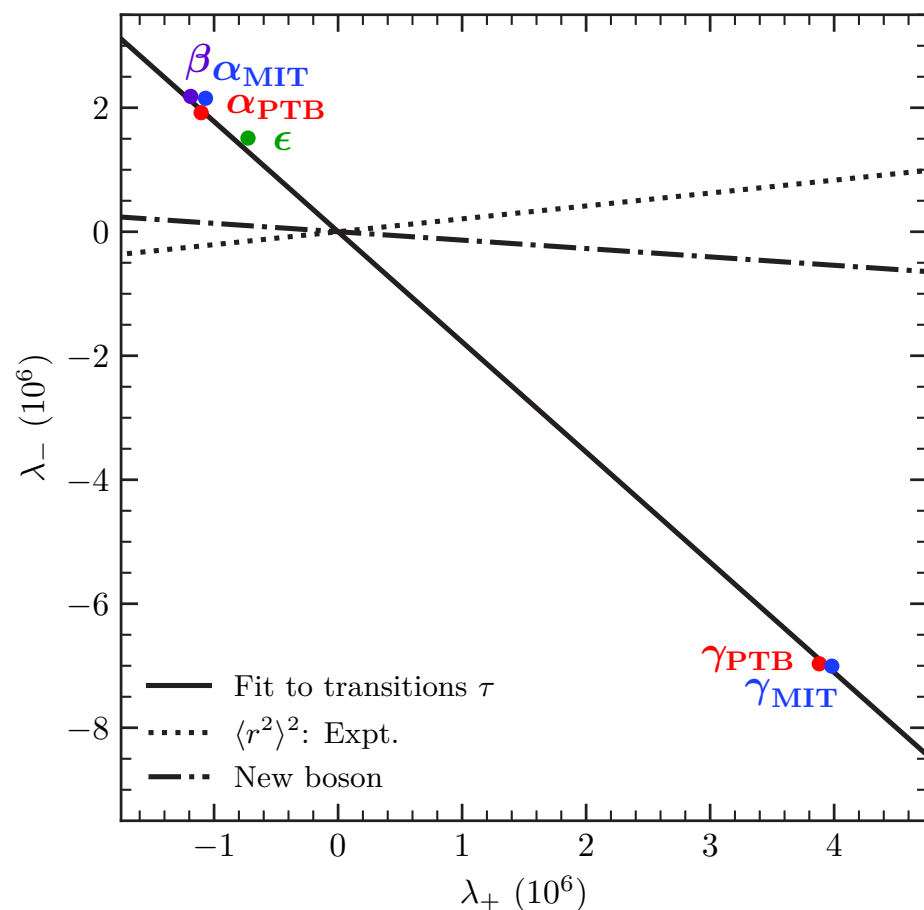
# Analyzing the nonlinearity



Door, Yeh, MH, et al., PRL (2025)

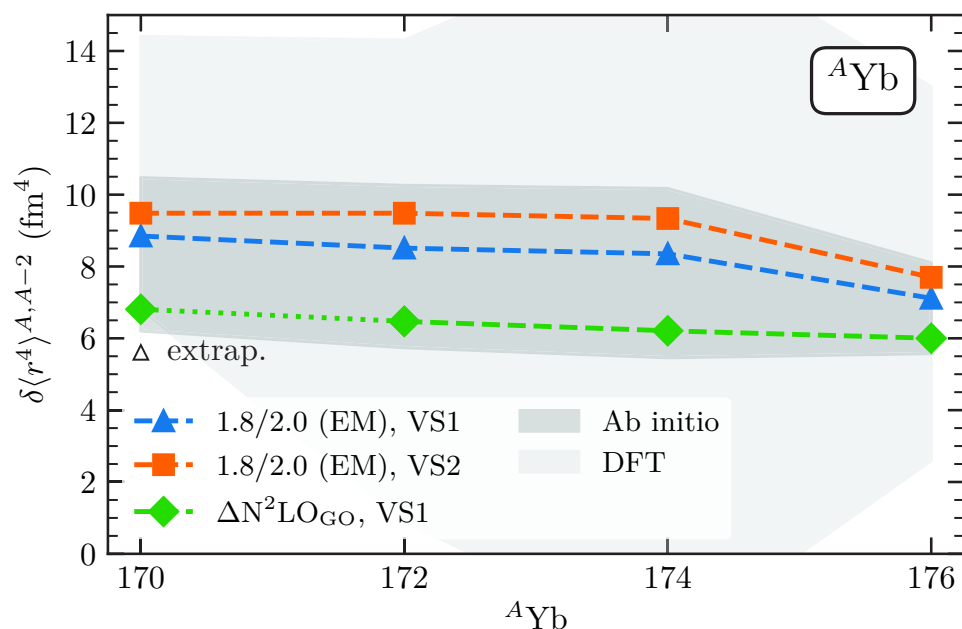
- Describe 4 data points as vector:  $\tilde{\mathbf{x}}$
- Decompose in basis of 4 vectors
 
$$\tilde{\mathbf{x}} = \underbrace{K \mathbf{1} + F \tilde{\mathbf{v}}_\tau}_{\text{linear part}} + \underbrace{\lambda_+ \Lambda_+ + \lambda_- \Lambda_-}_{\text{nonlinear part}}$$
- Nonlinear contribution described by coefficients  $\lambda_+, \lambda_-$
- Assuming **1 dominant nonlinearity**, slope  $\lambda_-/\lambda_+$  is same for all transitions  
 → **same underlying nuclear-structure effect responsible for nonlinearity**

# Impact of nuclear structure effects

Door, Yeh, **MH**, et al., PRL (2025)

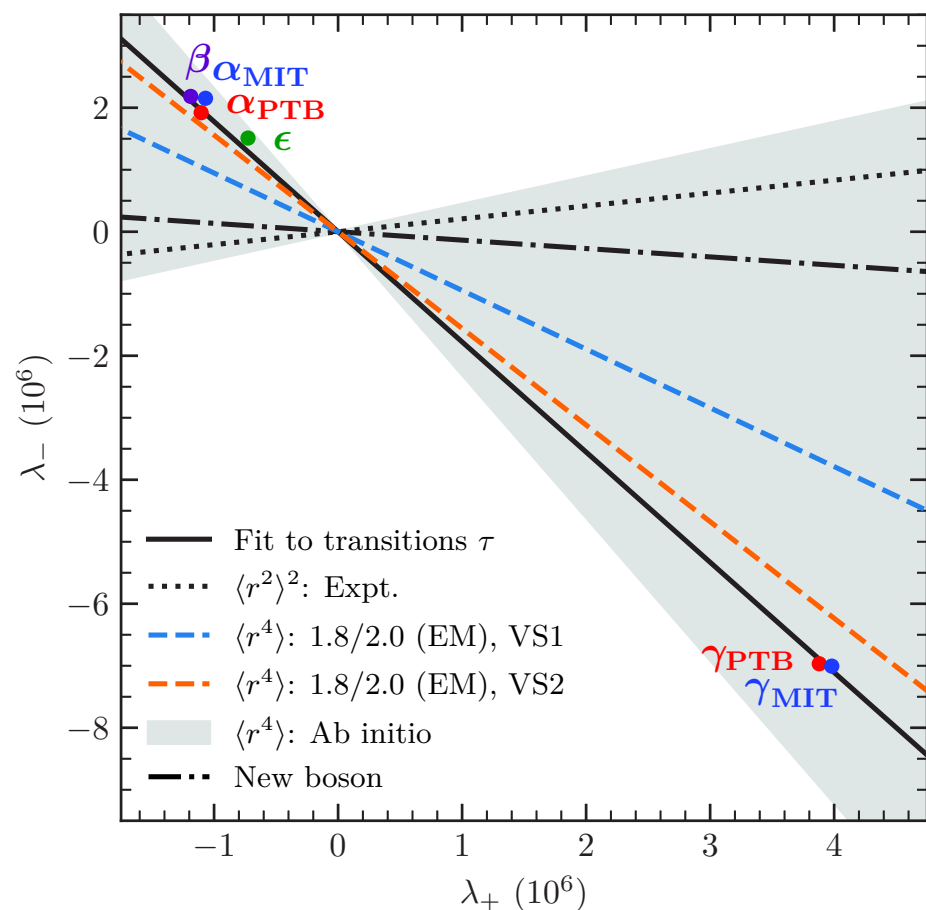
- Nonlinearity analysis suggests **single dominant higher-order term**
- $\langle r^2 \rangle^2$  and new boson **incompatible** with observed nonlinearity
- **Theory predictions for  $\langle r^4 \rangle$  required!**

# Impact of nuclear structure effects

Door, Yeh, **MH**, et al., PRL (2025)

- 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!**
- **Our input:** ab initio calculations of Yb
- Two Hamiltonians, two model spaces
- Comprehensive uncertainty estimate

# Impact of nuclear structure effects

Door, Yeh, **MH**, et al., PRL (2025)

- 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!**
- **Our input:** ab initio calculations of Yb
- Two Hamiltonians, two model spaces
- Comprehensive uncertainty estimate

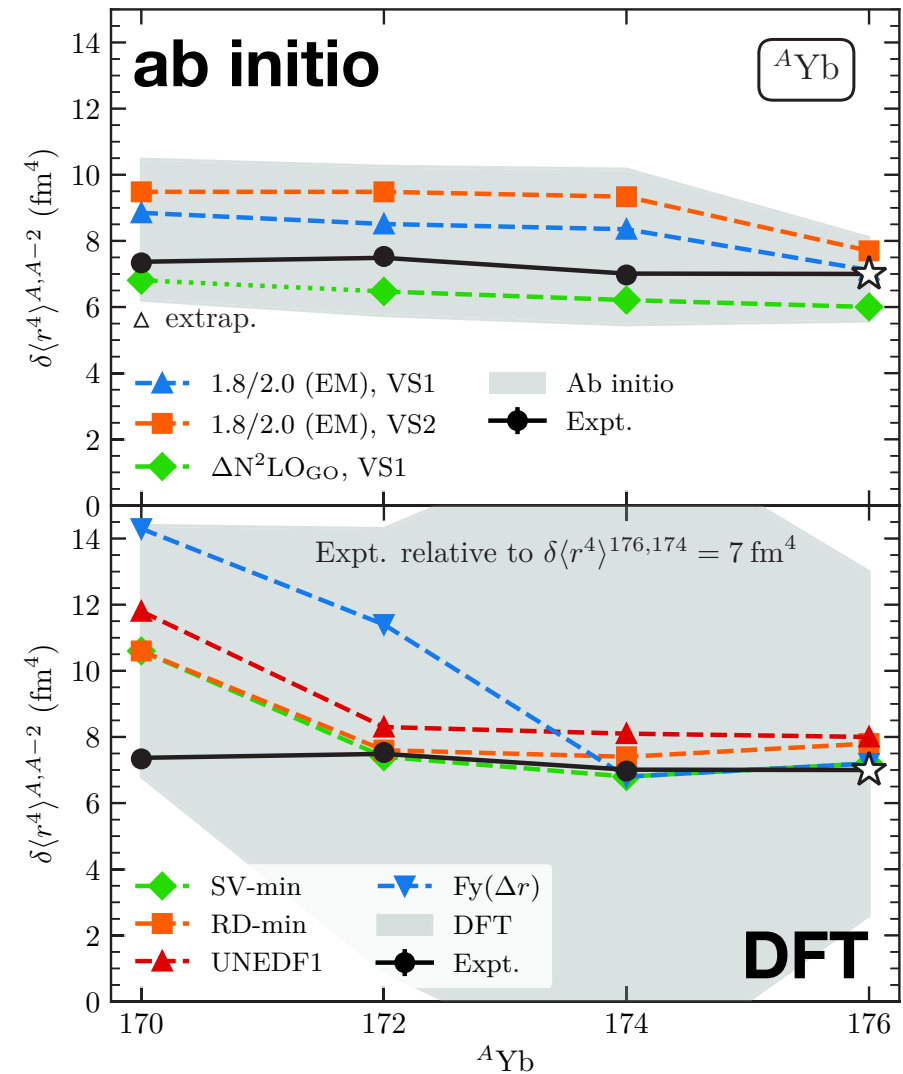
**Nuclear theory:  $\langle r^4 \rangle$ , not new boson, is leading source of nonlinearity!**

# 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  
→ Extraction only sensitive to relative changes in  $\delta\langle r^4 \rangle^{A,A'}$
- **Newly accessible observable related to deformation**

**Precision isotope shift spectroscopy to study higher-order nuclear structure!**

Door, Yeh, **MH**, et al., PRL (2025)



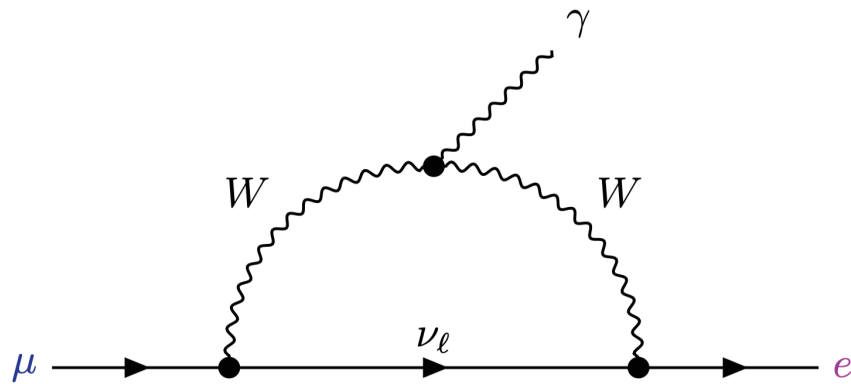
Door, Yeh, **MH**, et al., PRL (2025)



# Improving predictions with experimental data

MH et al., arXiv:2412.04545

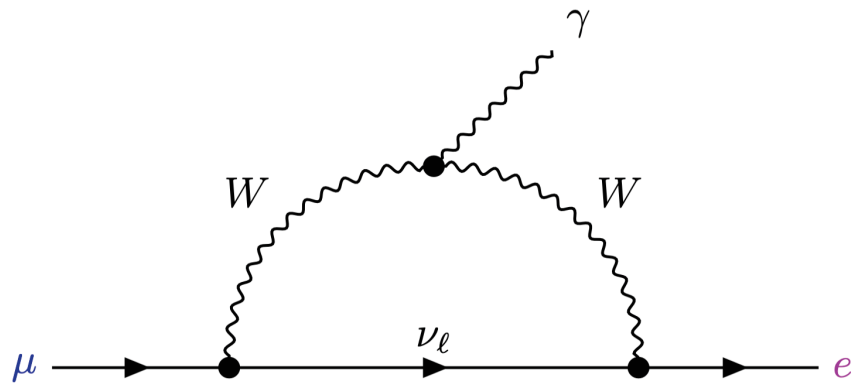
# Muon to electron conversion



Figures: F. Noël

- Lepton flavor violation in the standard model suppressed by  $(\Delta m_\nu / m_W)^4 \sim 10^{-50}$
- Searches for  $\mu \rightarrow e$  conversion constrain new lepton flavor violating interactions
- Complementary channels:  $\mu \rightarrow e\gamma$ ;  $\mu \rightarrow 3e$ ;  $\mu \rightarrow e$  [nucl.]

# Muon to electron conversion



Figures: F. Noël

- Lepton flavor violation in the standard model suppressed by  $(\Delta m_\nu / m_W)^4 \sim 10^{-50}$
- Searches for  $\mu \rightarrow e$  conversion constrain new lepton flavor violating interactions
- Complementary channels:  $\mu \rightarrow e\gamma$ ;  $\mu \rightarrow 3e$ ;  $\mu \rightarrow e$  [nucl.]

**Our focus:**  $^{27}\text{Al}$ ,  $^{48}\text{Ti}$

# Nuclear structure effects in $\mu \rightarrow e$

$$\mu \rightarrow e \text{ decay rate} \sim \sum_i \left| \bar{C}^{I_i} \times I_i \right|^2$$

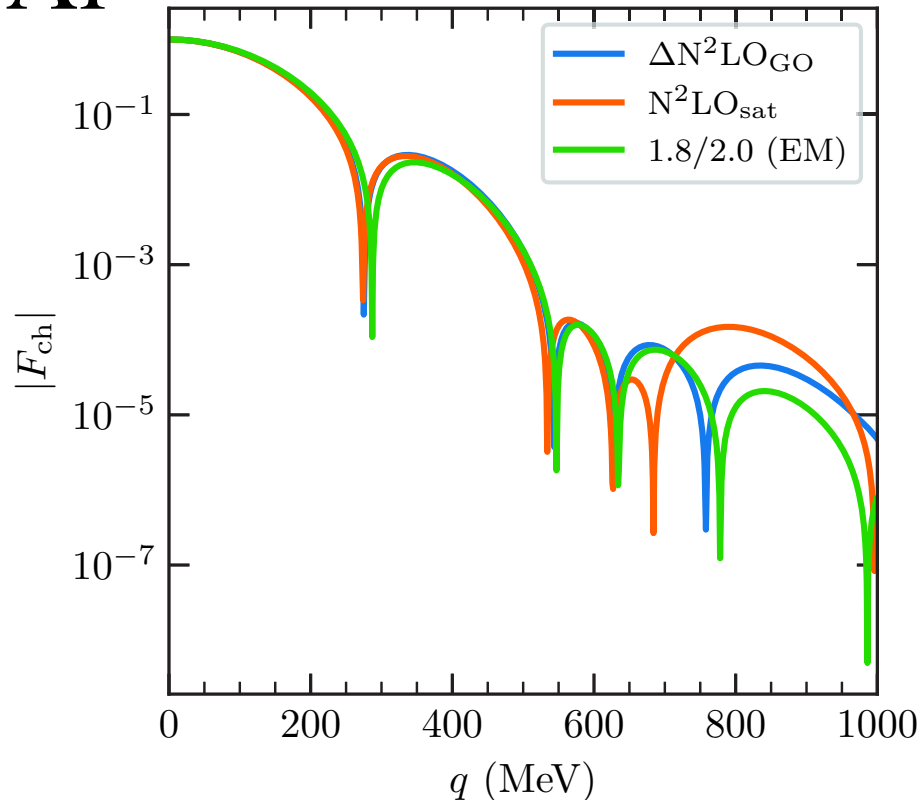
- Knowing **overlap integrals** constrains **Wilson coeffs** of underlying theories
- Overlap integrals combine nuclear densities and lepton wave functions

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

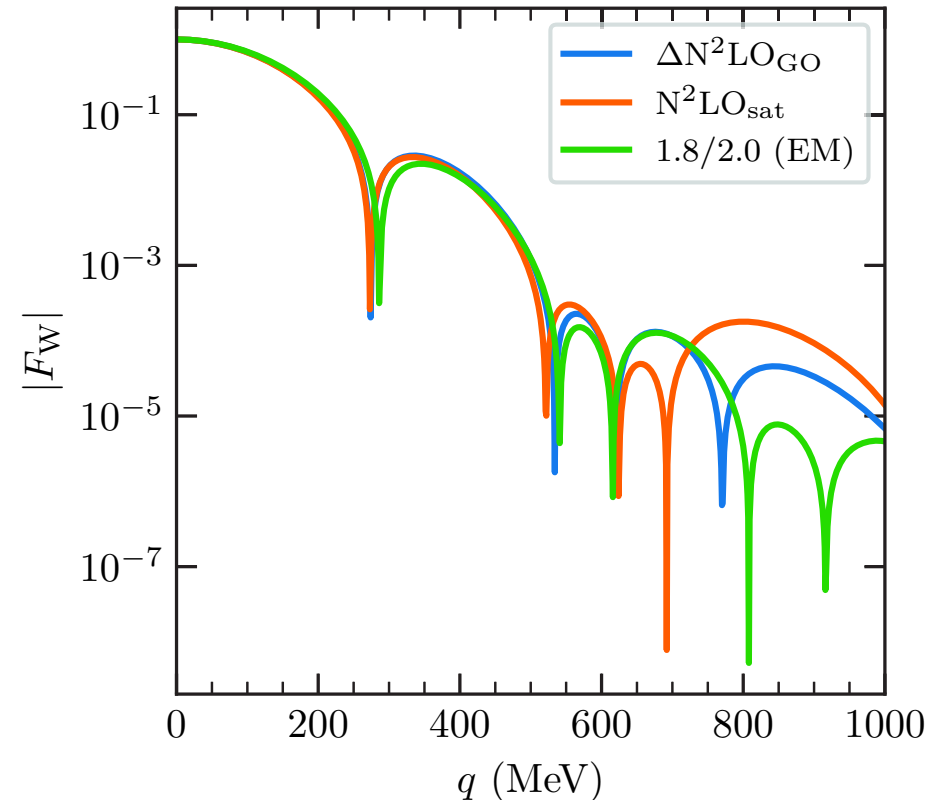
- Full set for spin-independent formalism:  $D$ ,  $S^{(p)}$ ,  $V^{(p)}$ ,  $S^{(n)}$ ,  $V^{(n)}$
- Charge, **point-proton**, and **point-neutron** densities required

# Charge and weak responses are correlated

$^{27}\text{Al}$  charge = easy to measure



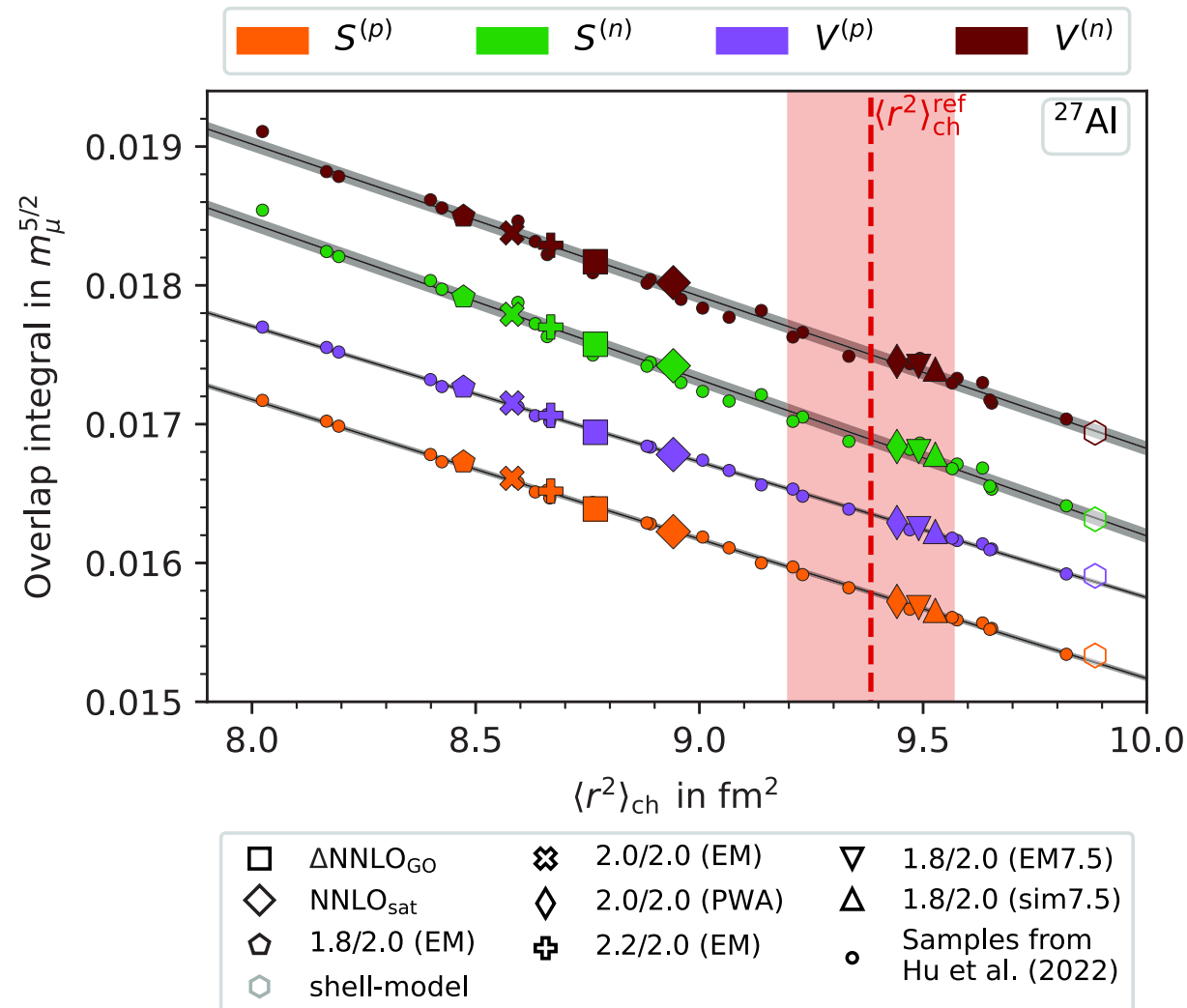
weak = hard to measure



- **Approach:** Correlations between  $\rho_{\text{ch}}(r)$ ,  $\rho_n(r)$ ,  $\rho_p(r)$  constrain overlap integrals

# Application to overlap integrals

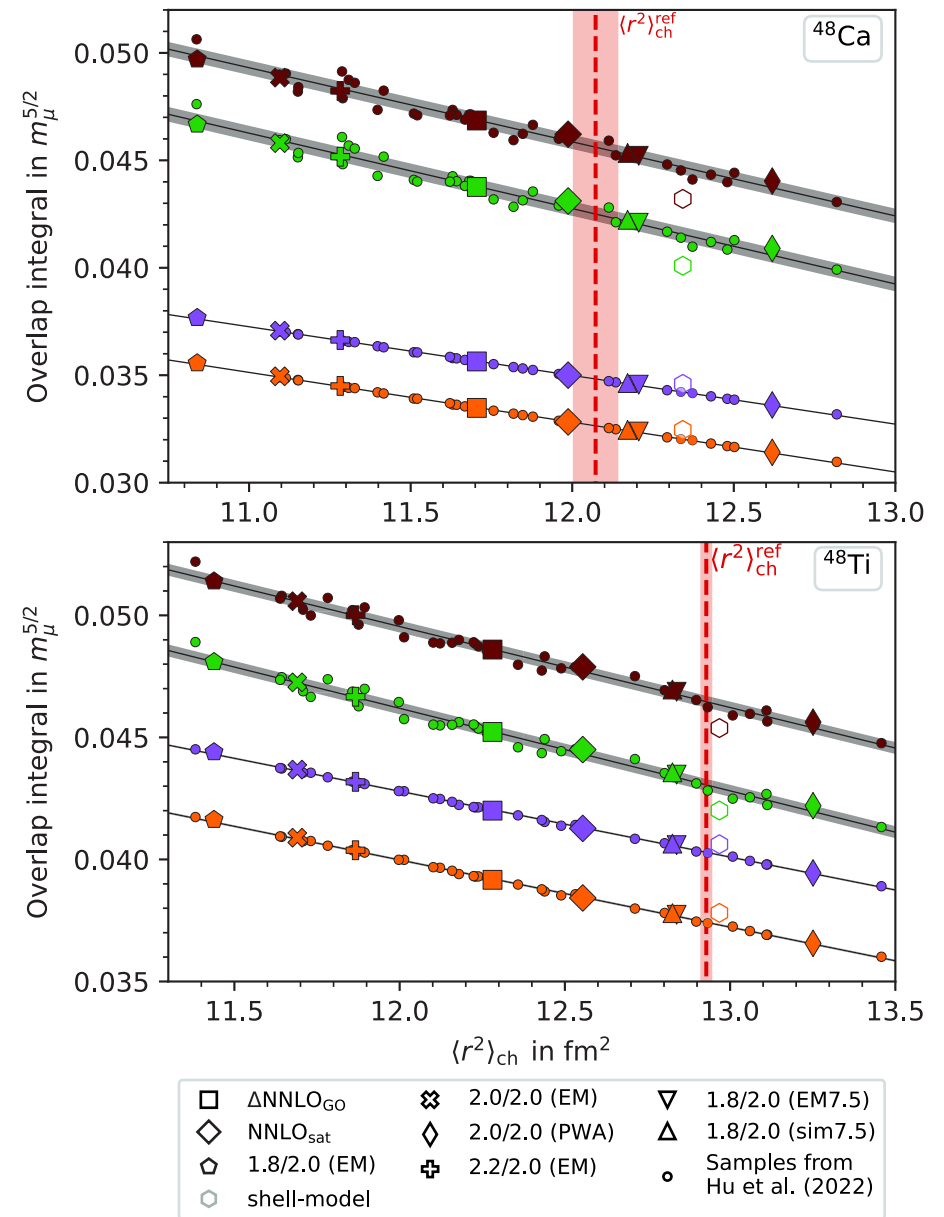
- Predictions for 42 Hamiltonians
- Each gives **different charge radius, charge and weak densities**
- Strong correlations observed:
  - $S^{(p)} \leftrightarrow \rho_p \leftrightarrow R_{\text{ch}}^2$ : unsurprising
  - $S^{(n)} \leftrightarrow \rho_n \leftrightarrow R_{\text{ch}}^2$ : **prediction**
- **Constraints on BSM input with exp. data!**



MH et al., arXiv:2412.04545

# Application to overlap integrals

- Predictions for 42 Hamiltonians
- Each gives **different charge radius, charge and weak densities**
- Strong correlations observed:
  - $S^{(p)} \leftrightarrow \rho_p \leftrightarrow R_{\text{ch}}^2$ : unsurprising
  - $S^{(n)} \leftrightarrow \rho_n \leftrightarrow R_{\text{ch}}^2$ : **prediction**
- **Constraints on BSM input with exp. data!**



**Perspectives for the future**



# Role of theory

- Theory connects what we know with **what we want to know**
- "**Ab initio**" = **first-principles** (no experimental input needed?)
- But **plenty is known** about systems of interest → how to leverage this?
- Key challenges:
  - Octupole deformation
  - Heavy mass
  - Small energy differences
- Theory to guide experiment can be coarser,  
precise predictions to interpret results can come later

# No answers, only questions

- Octupole deformation:
  - How quantitative does description of deformation have to be?
  - What are the best observables to guide prediction of deformation?
  - Fine nuclear structure may not be as important [see P. Navratil's talk for a different view](#)
- What else can we learn about nuclei from these precision studies?
- Major obstacles:
  - How do we handle 3N forces in strongly deformed heavy nuclei?
  - How do we quantify (and ultimately reduce) uncertainties?  
(interactions, 3N potentials, deformation, many-body calculations)

# Acknowledgments

## Coauthors and collaborators:

@TU Darmstadt: Kai Hebel, Jan Hoppe, Achim Schwenk, Alex Tichai

@Univ. Notre Dame: Ragnar Stroberg

@MPIK: **Menno Door**, **Chunhai Lyu**, Klaus Blaum, Zoltán Harman

@PTB: **Indy Yeh**, Tanja Mehlstäubler

@LU Hannover: **Fiona Kirk**, Elina Fuchs

@UNSW: Julian Berengut

@Univ. Tsukuba: **Takayuki Miyagi**, Noritaka Shimizu

@Univ. Bern: **Frederic Noël**, Martin Hoferichter

@TAMU: **Baishan Hu**

@ORNL/UTK: Gaute Hagen, Thomas Papenbrock

@Chalmers: **Alberto Scalesi**, Christian Forssén, Andreas Ekström

## Thank you for your attention!

