Hamiltonians for neutron densities and lattice calculations

Matthias Heinz, ORNL

INT Program:"Nuclear Hamiltonians for Advancing Nuclear Physics and Beyond"
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Hamiltonians for many-body physics

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

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- ***I will not discuss many-body methods***
- Many approaches at our disposal
- **Exact diagonalization** = exact computation of $|\Psi\rangle$, limited mass range
- **Hartree Fock** = Slater-determinant approximation of $|\Psi\rangle$, provides variational bounds on ground-state energy E
- **IMSRG, CC,** (SCGF) = improved correlated approximation of $|\Psi\rangle$, quantitative predictions of ground-state properties

Challenges for Hamiltonians

- **#1: Chiral effective field theory is (often) not very precise**
- #2: Accurate Hamiltonians exist, but are "fine-tuned"
- #3: Accurate Hamiltonians lack uncertainties or are untested
- #4: No "full UQ" accounting for cutoff scheme & scale, order, fit to data

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- Uncertainties for low-resolution Hamiltonians
  Plies, **MH**, Schwenk, arxiv:2509.24671
- Ab initio analysis of parity-violating electron scattering
  Noël, **MH**, Hoferichter, Miyagi, Schwenk, in prep.
- Testing lattice Hamiltonians with variational methods
  Rothman, Hagen, **MH**, Papenbrock, in prep.

Uncertainties for low-resolution Hamiltonians

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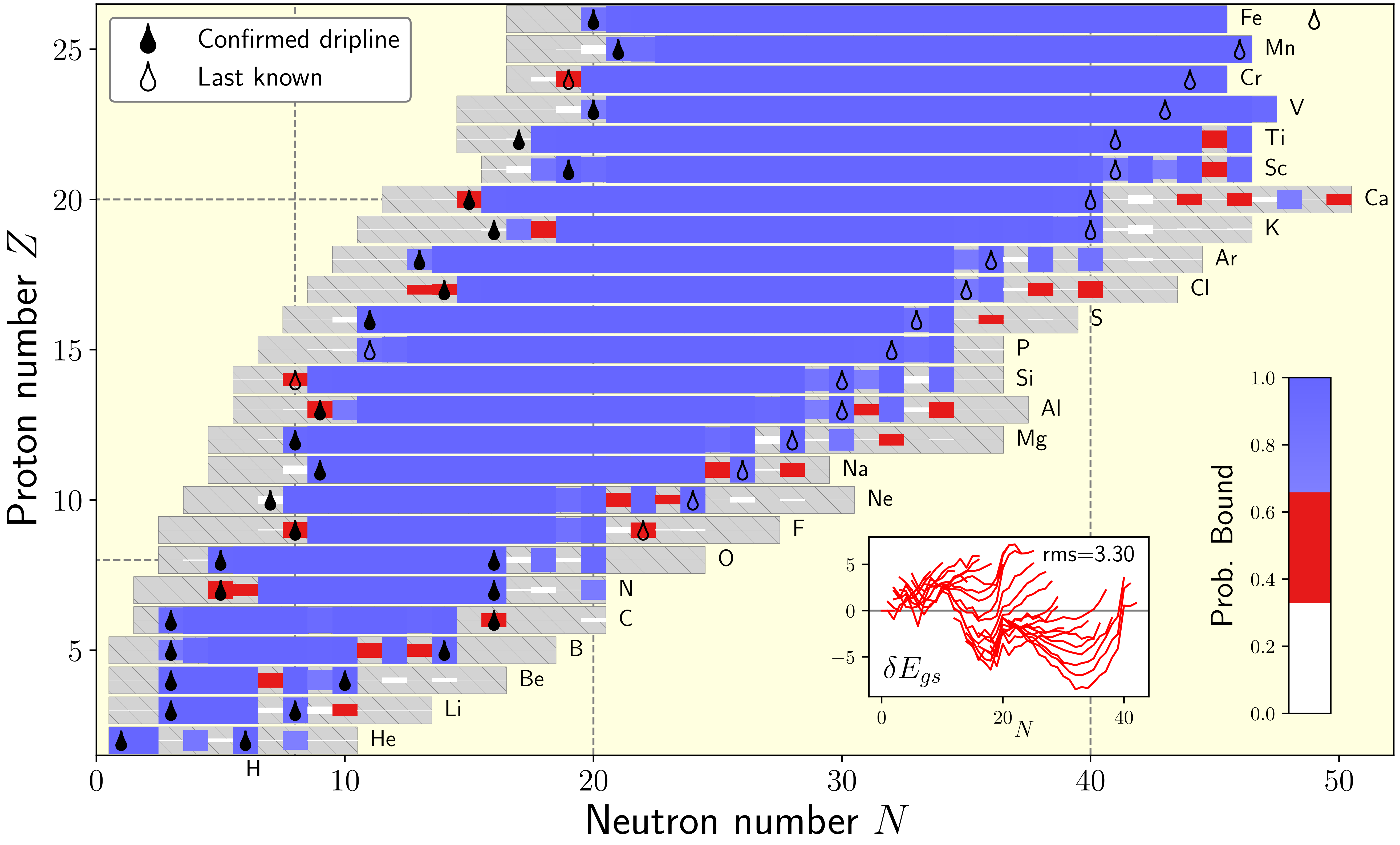
Some Hamiltonians are accurate



Stroberg et al., PRL (2021)

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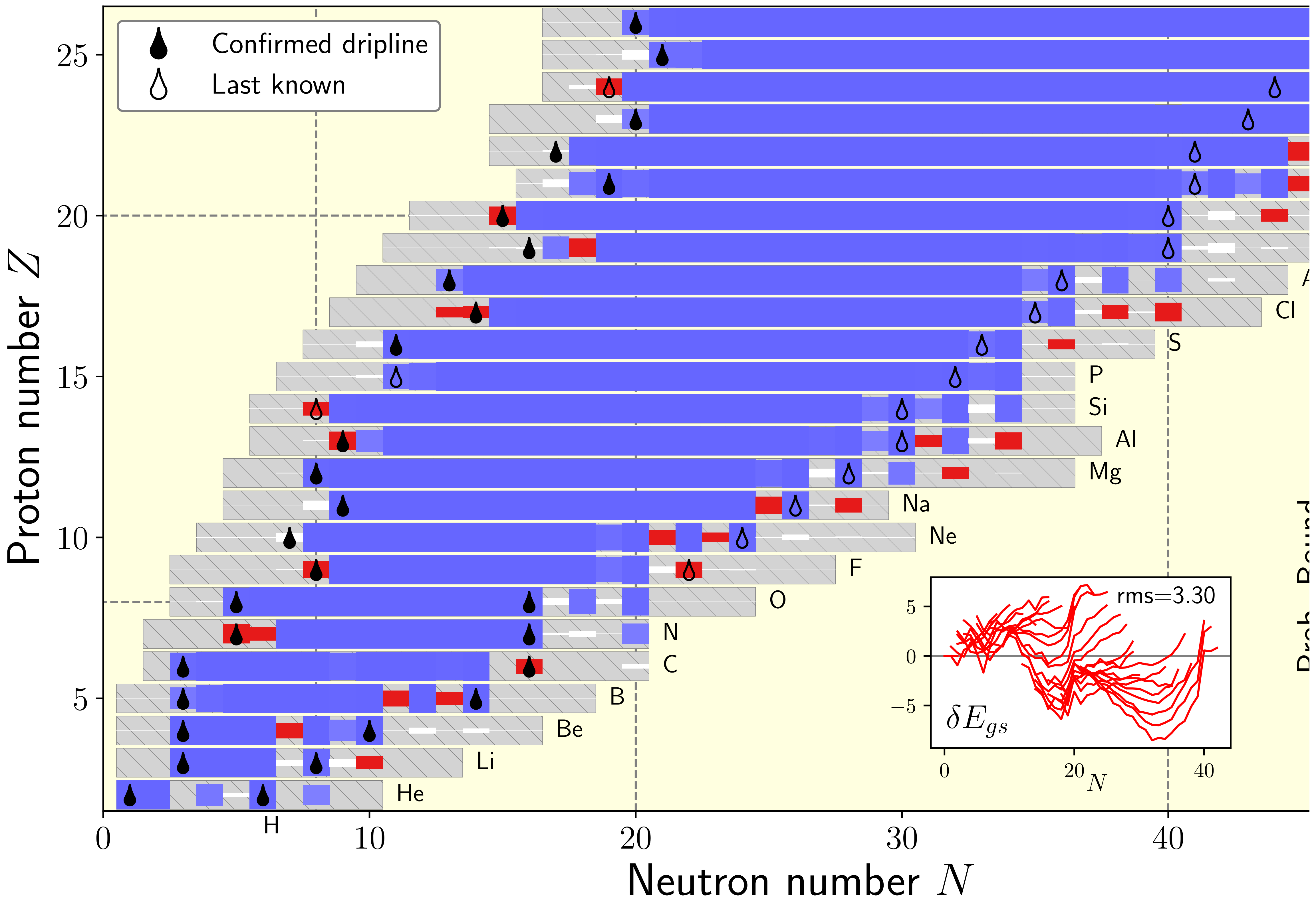

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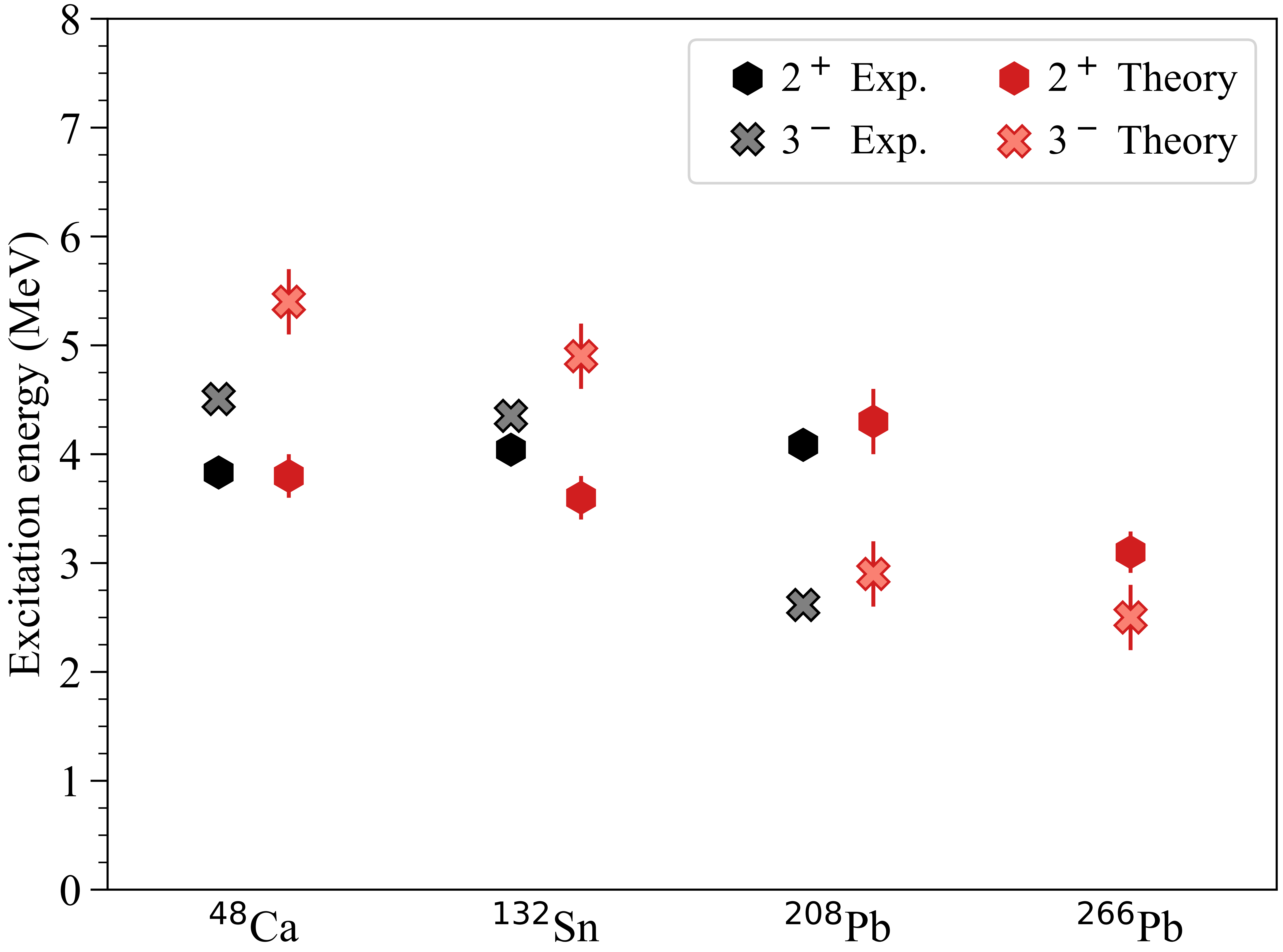

Bonaiti et al., arxiv:2508.14217

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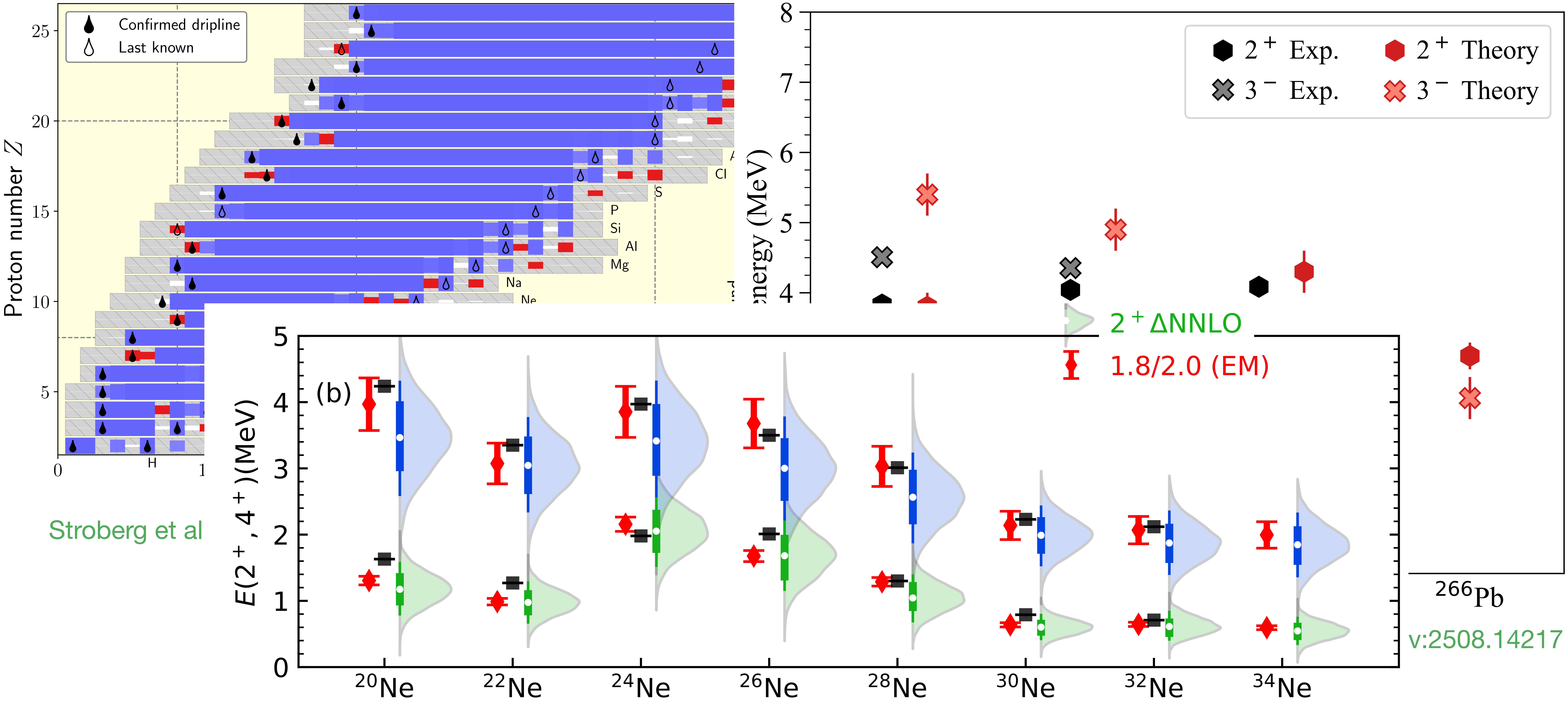


Stroberg et al

v:2508.14217

Sun et al., PRX (2025)

1.8/2.0 (EM)

- **NN:** $\mathrm{N^3LO}$ potential with cutoff $\Lambda = 500\ \mathrm{MeV}$ by Entem, Machleidt
  Optimized to NN scattering data
  SRG evolution to $\lambda = 1.8\ \mathrm{fm}^{-1}$
- **3N:** $\mathrm{N^2LO}$ potential with low cutoff $\Lambda = 2.0\ \mathrm{fm}^{-1} = 394\ \mathrm{MeV}$
  c_i from NN potential, c_D, c_E fit to $^3\mathrm{H}$, $^4\mathrm{He}$
- Accurate ground-state energies and spectra, differential charge radii, etc.
- But many conceptual problems (esp. from a purist perspective)
- **How do we quantify the Hamiltonian uncertainty here?**

1.8/2.0 (EM): Strategy for UQ

uncertainty quantification

1. Recover parametric form of Hamiltonian (operator basis + free parameters/LECs)

$$H = \sum_i s_i O_i$$

2. Perform Bayesian inference of free parameters

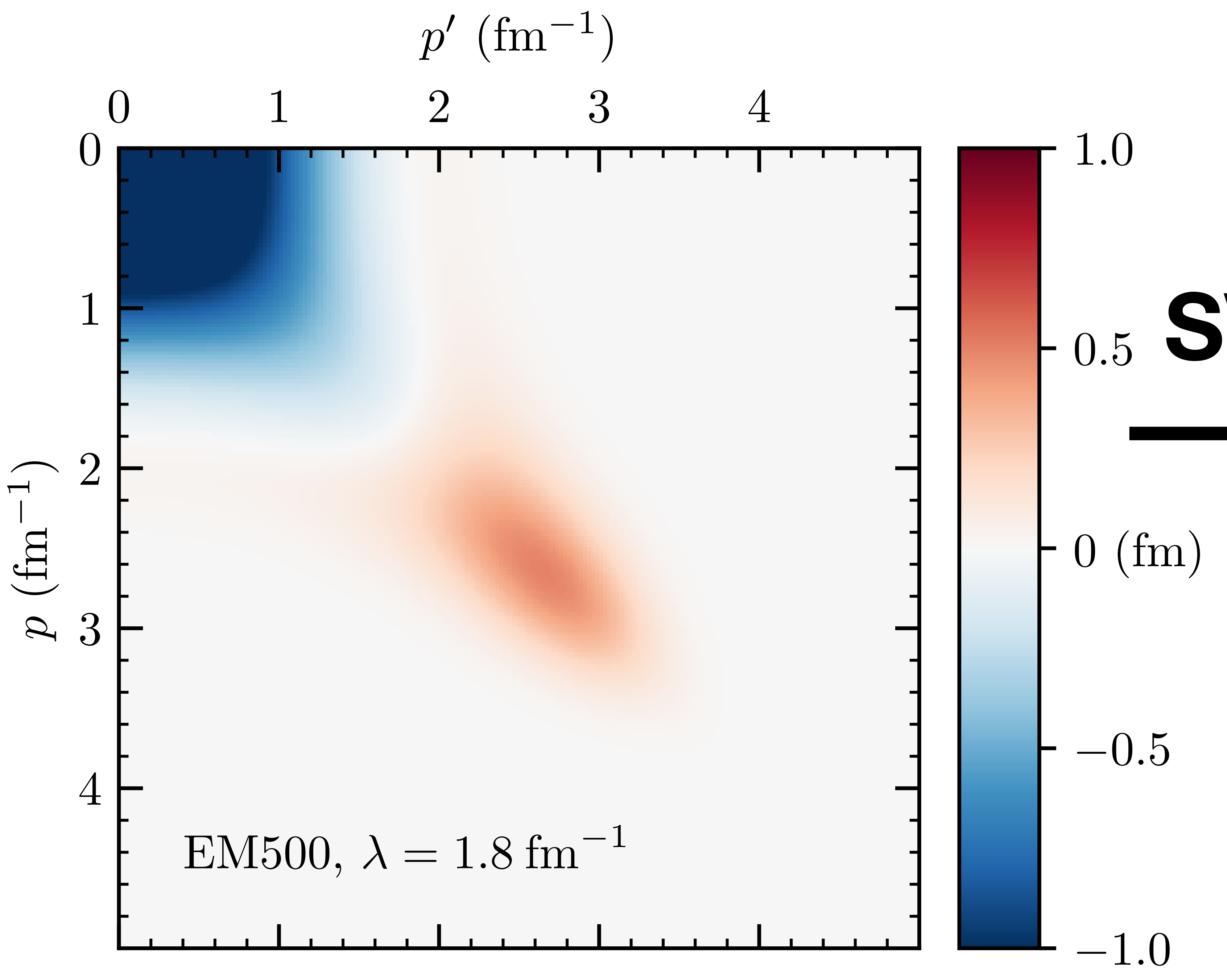
$$\mathrm{pr}(s_i, c_D, c_E \,|\, \mathcal{D}, I)$$

3. Check model with posterior predictive distribution
4. Predict medium-mass nuclei with posterior predictive distribution

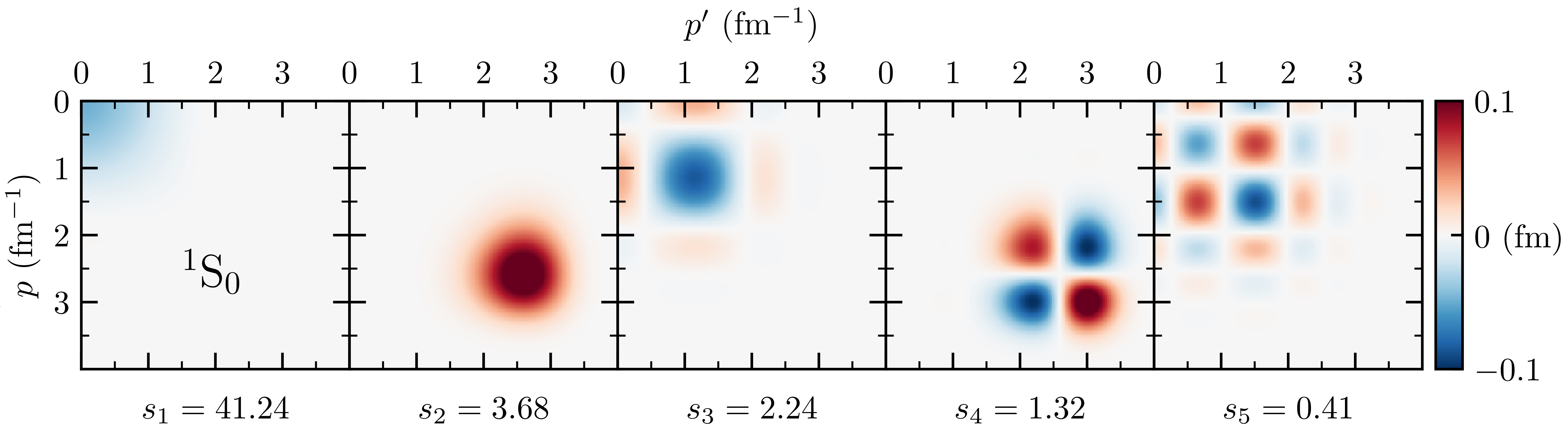
Tom Plies @ TU Darmstadt

SVD of NN potential

singular value decomposition



SVD →

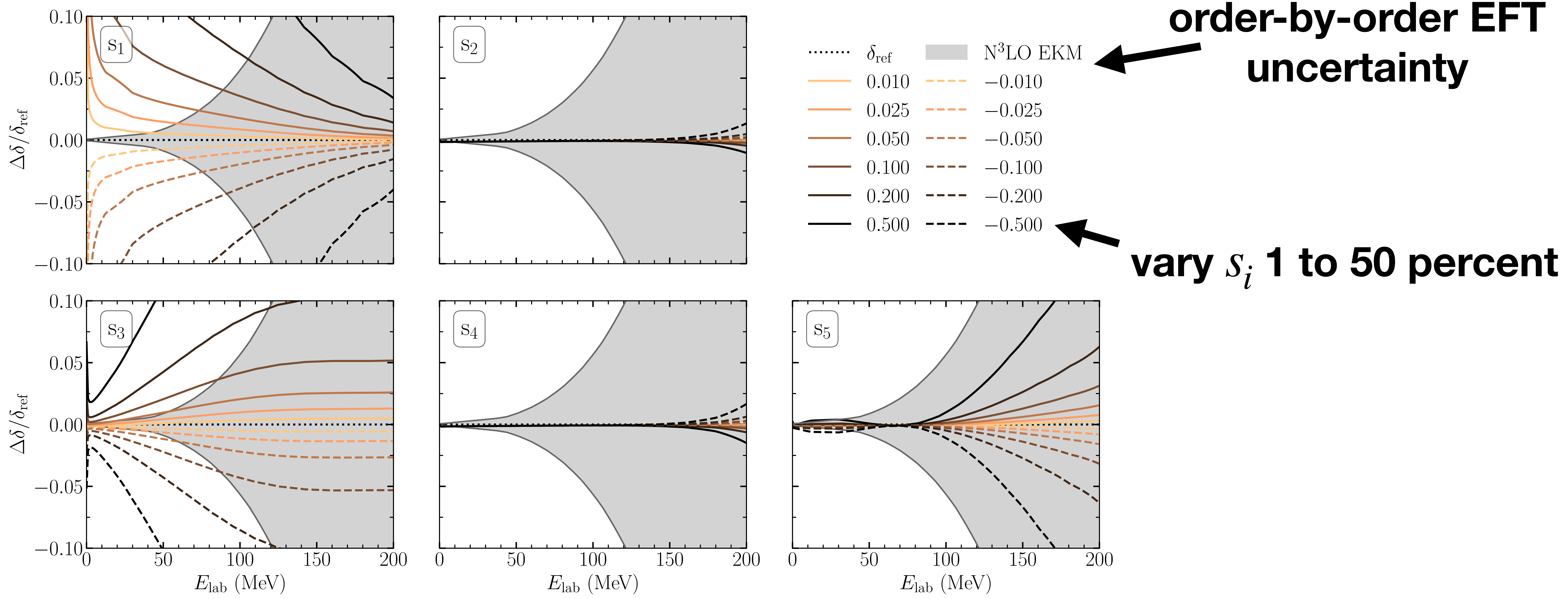


- SVD in plane-wave partial-wave basis:

$$V = \sum_i s_i \,|\, l_i \rangle \langle r_i \,| = \sum_i s_i O_i$$

- SVD recovers "affine" structure of Hamiltonian
- **Idea:** Treat singular values s_i as **uncertain free parameters** (like LECs)

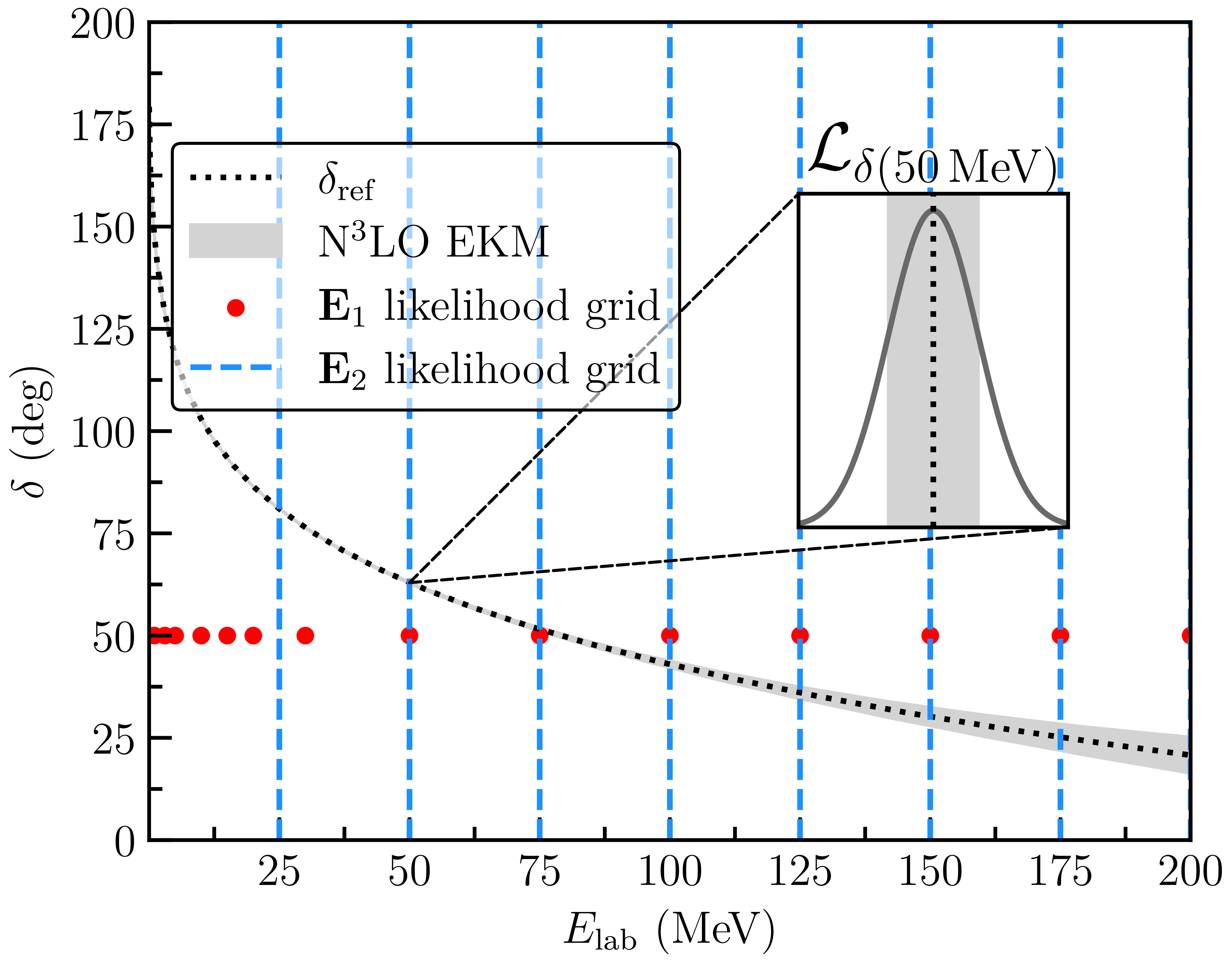
Impact of singular values



- Only some s_i are relevant at low E_{lab} (s_1, s_3, s_5) → leave others fixed

Bayesian inference of s_i, c_D, c_E

- NN: s_i in S- and P-waves
  - Isospin charge independence approx.
  - Higher partial waves included exactly
- 3N: c_D, c_E
- MCMC sampling using likelihood with
  - NN phase shifts ($\mathrm{N^3LO}$)
    $\mathbf{E}_1$: emphasis on low-E_{lab} phase shifts
    $\mathbf{E}_2$: even grid, more conservative
  - $^3\mathrm{H}$ ground-state energy and half life ($\mathrm{N^2LO}$)



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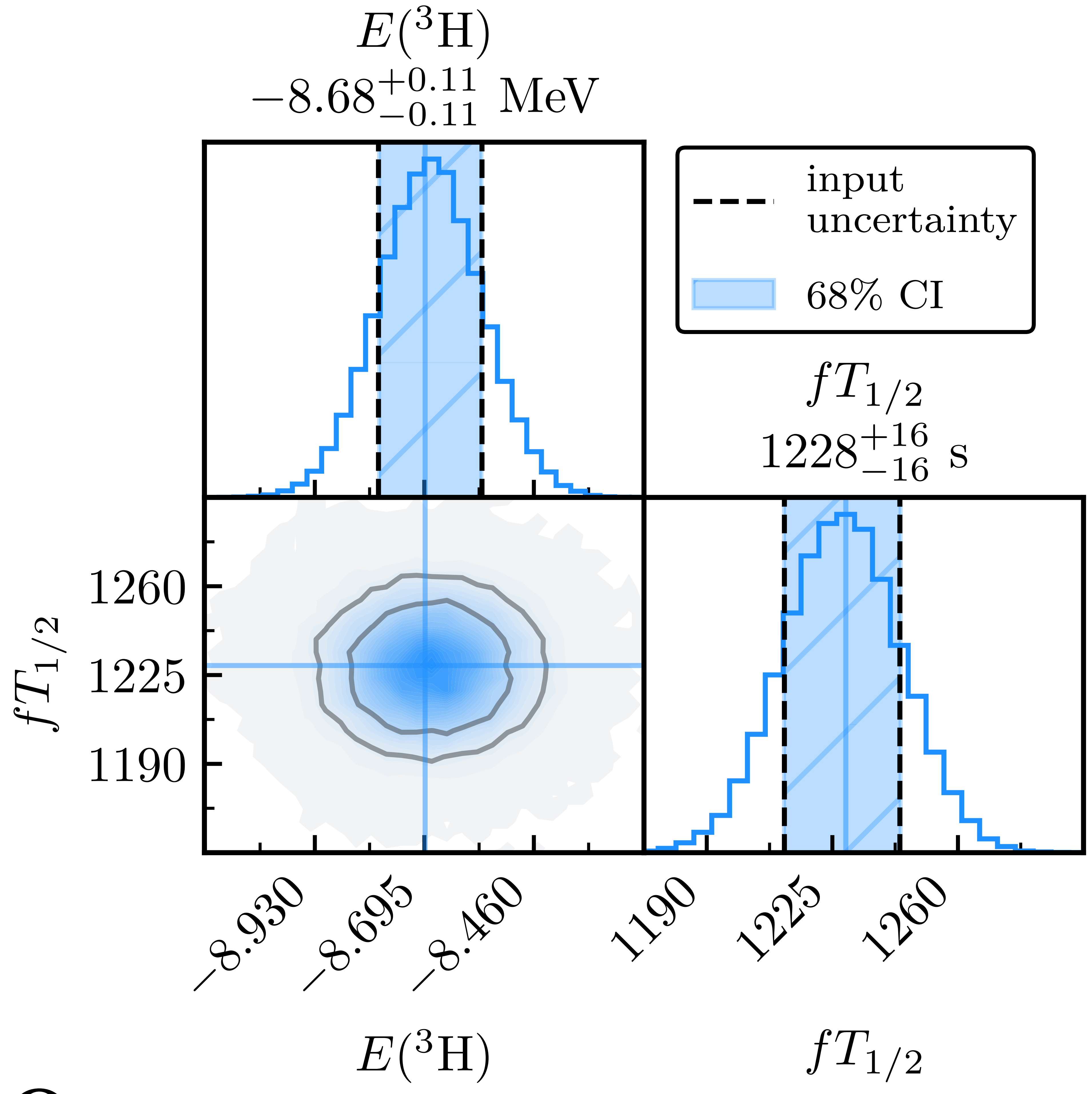
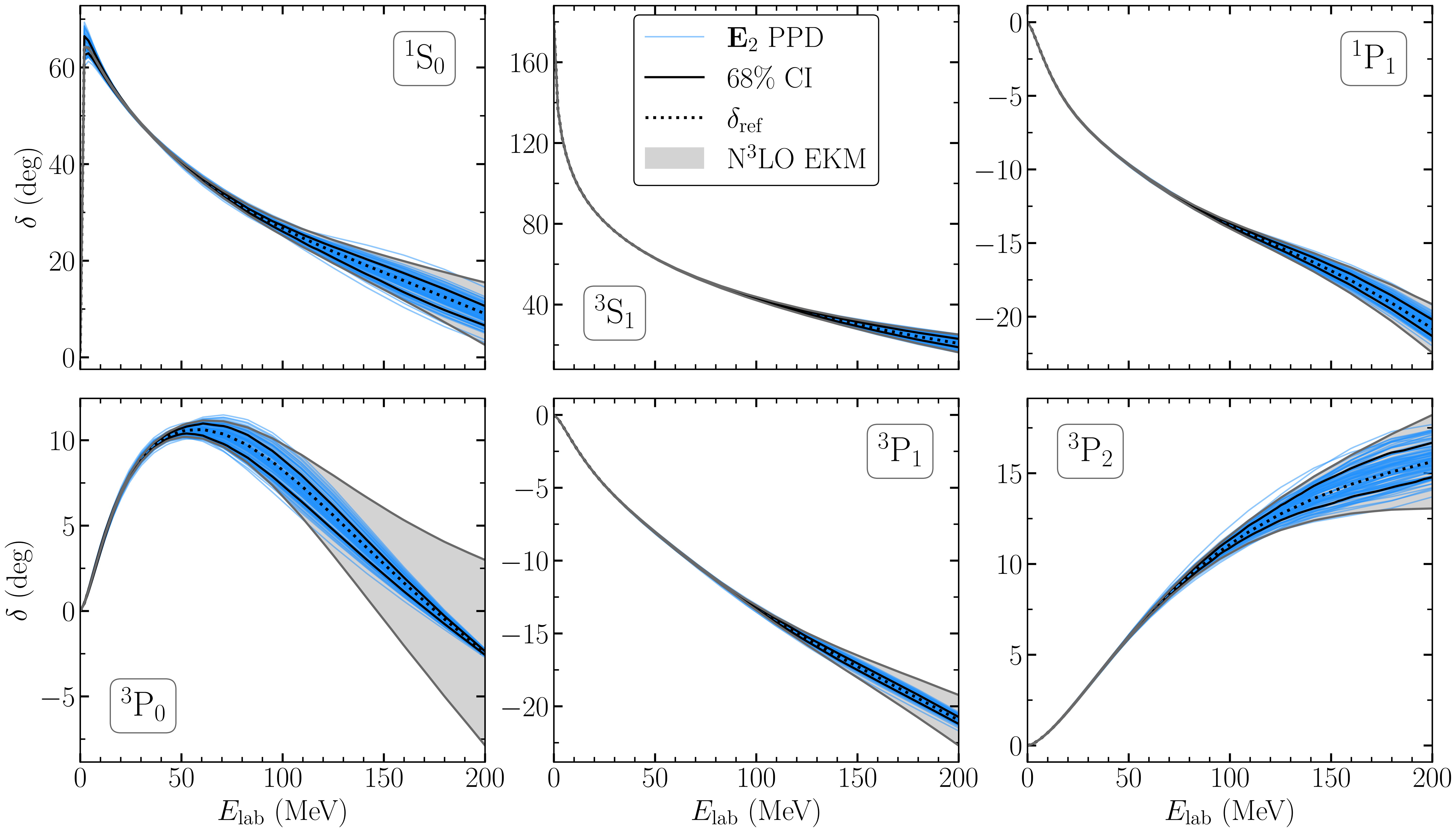


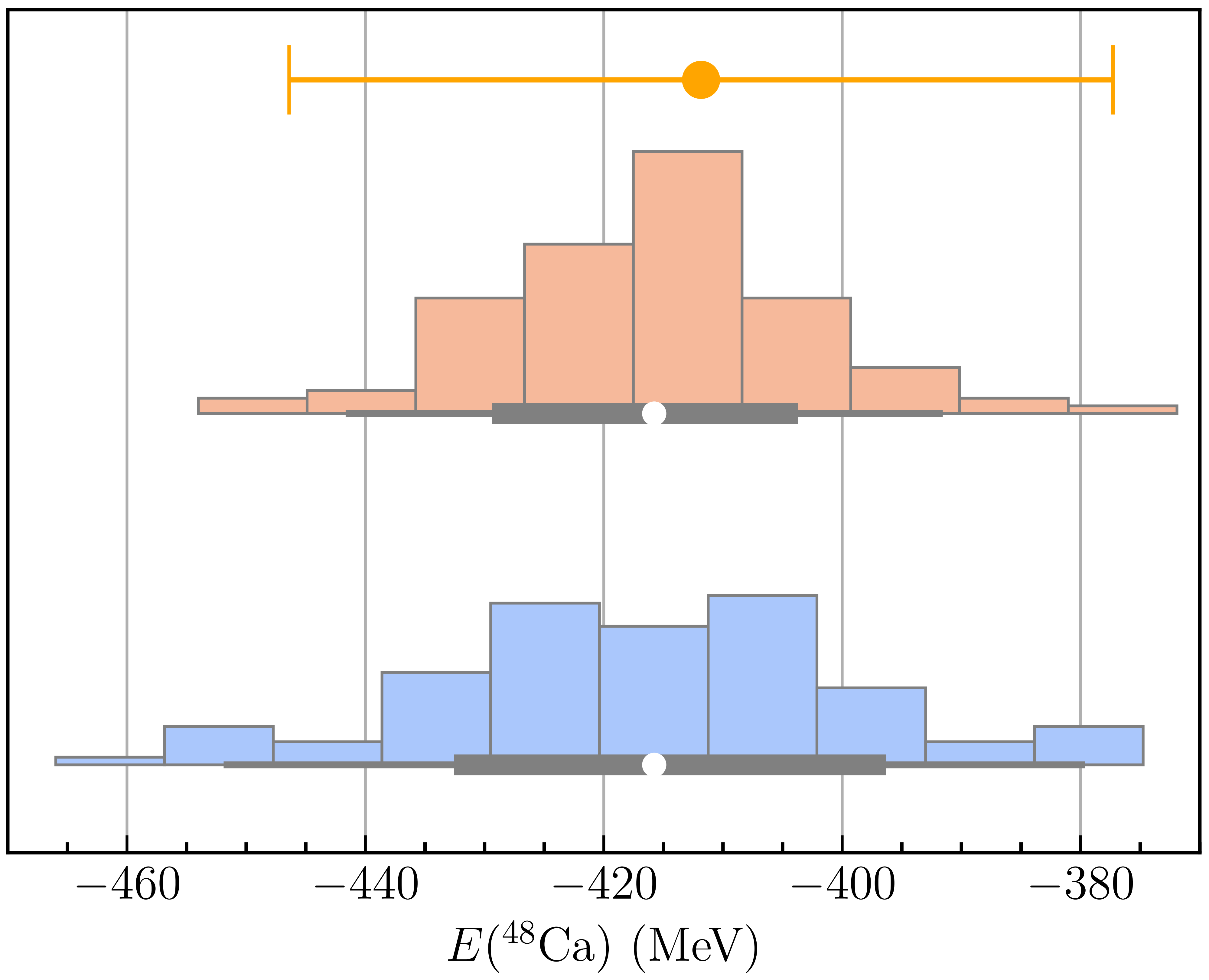
Results of model checking

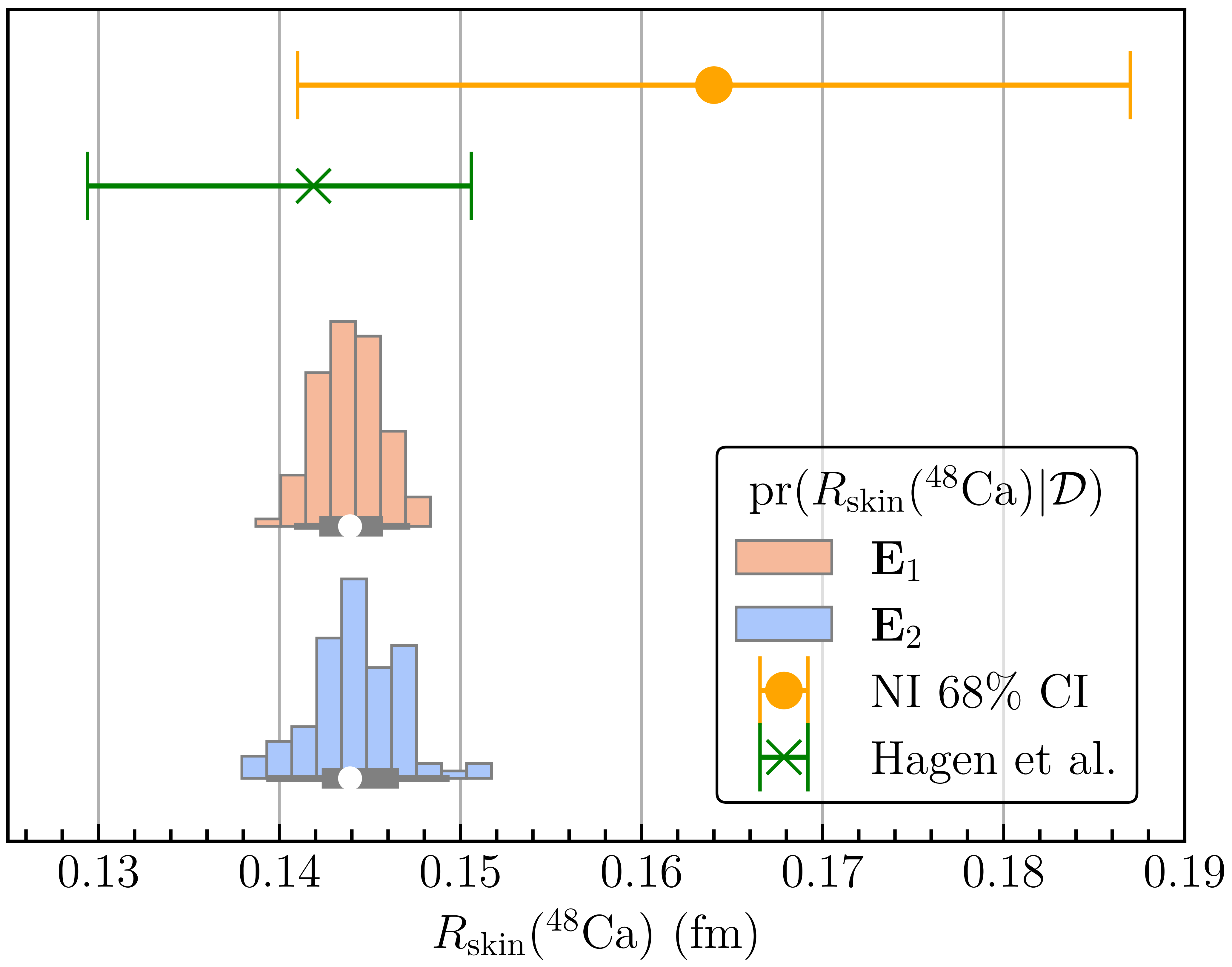
- 3N input likelihoods excellently reproduced
- For phase shifts
    - Overestimate unc. at low $E_{\text{lab}} \leq 10$ MeV *(not part of likelihood)*
    - Well reproduced for $20 - 75$ MeV
    - Underestimated at $E_{\text{lab}} \geq 100$ MeV



PPDs for ^{48}Ca

posterior predictive distributions





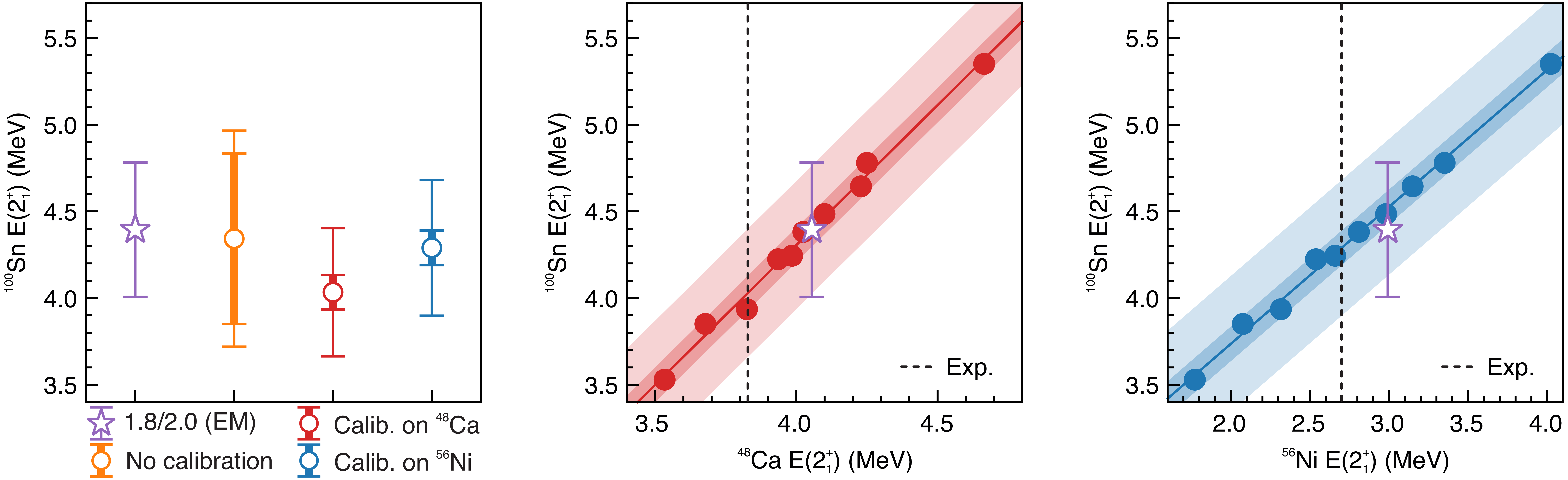
- Posterior predictive distributions with 100 samples

Success! But some limitations...

- **Model checking in NN phase shifts not completely satisfactory**
  - Uncorrelated likelihood
  - EKM uncertainties are small at low E_{lab}
  - Operator pool limits freedom at high E_{lab}
- **3N calibration uses triton half life** (anomalous convergence pattern)
- **Charge independence approximation required adjustment**
  - Mean shift of distribution (original approach)
  - **New and improved:** explicit charge independence breaking included, but no decomposition

2^+ of ^{100}Sn

- Reproduce 1.8/2.0 (EM) value, but with Hamiltonian uncertainty
- Correlation analysis allows us to reduce Hamiltonian uncertainty



Ab initio analysis of parity-violating electron scattering

Noël, **MH**, Hoferichter, Miyagi, Schwenk, in prep.

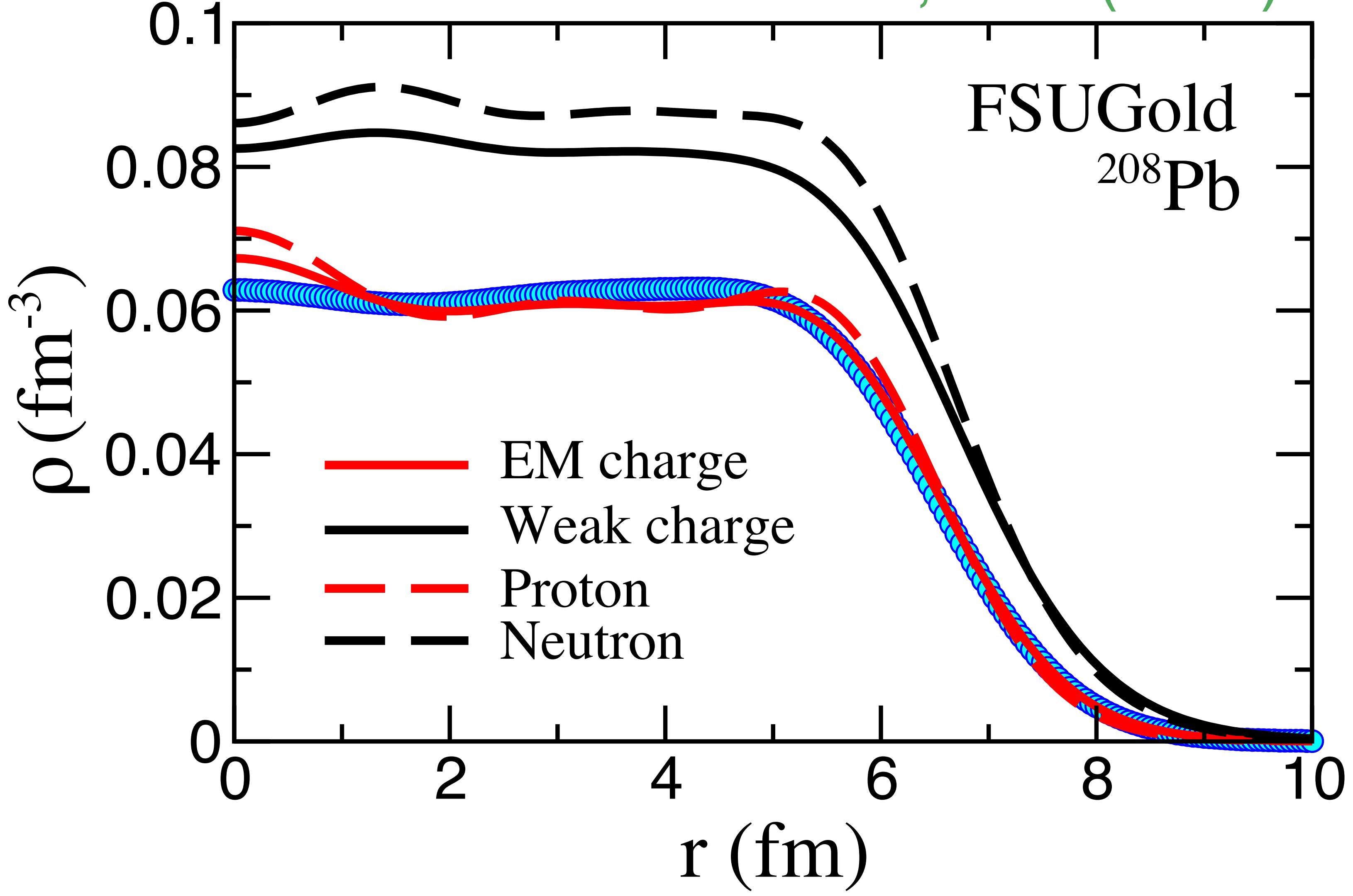
PVES motivation

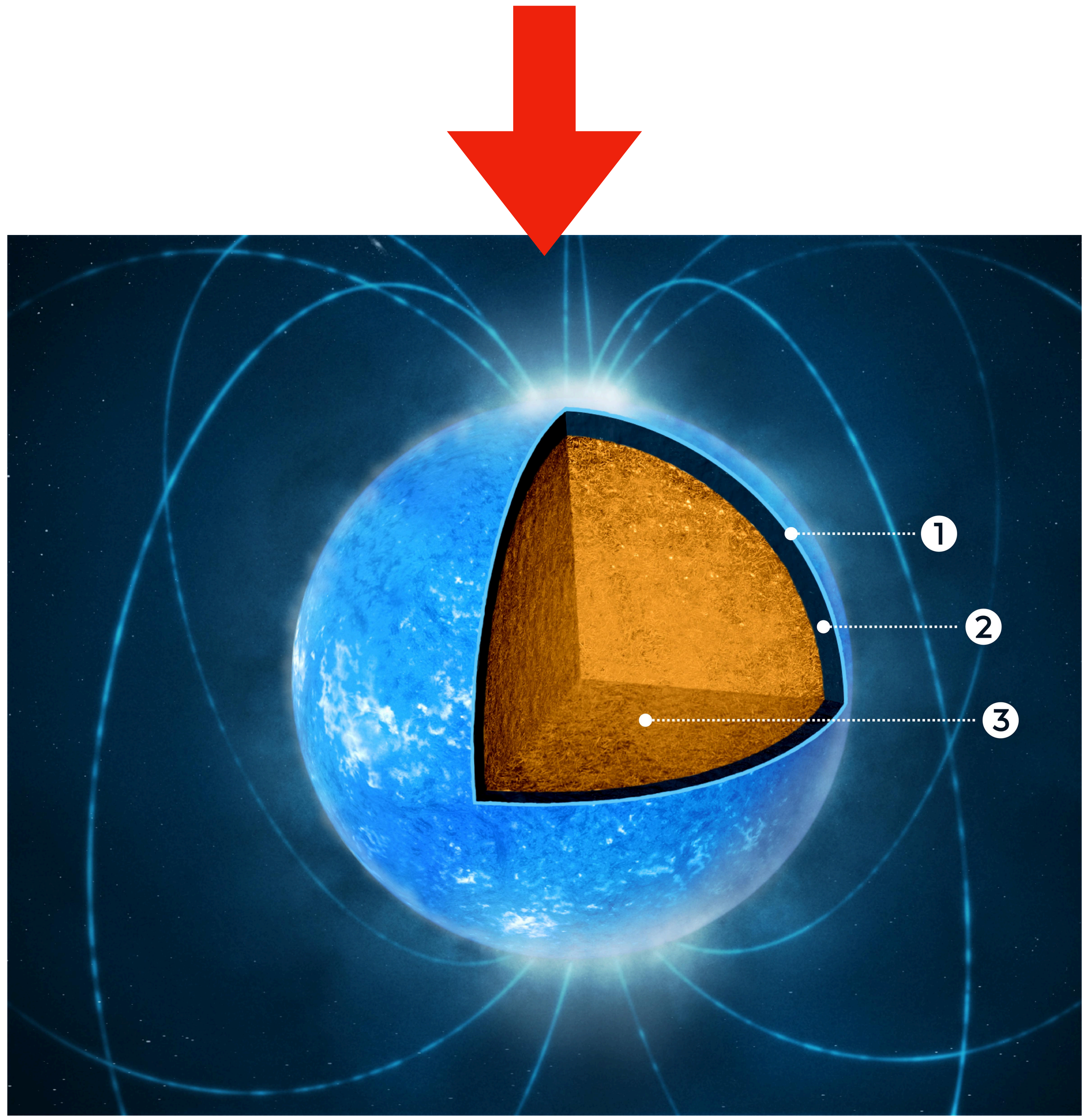
parity-violating electron scattering

$$R_{\text{skin}} = R_n - R_p$$

- Neutron skins give insight into nuclear interactions in neutron-rich environments, neutron stars
- PVES measures A_{PV}, infers neutron radius & skin
  - PREX: Larger skin in ^{208}Pb
  - CREX: Smaller skin in ^{48}Ca
  - Q_{weak}: $R_{\text{skin}} \approx 0$ in ^{27}Al
- **Nuclear theory so far unable to consistently explain CREX and PREX**

Thiel et al., JPG (2019)





Watts et al., RMP (2016)

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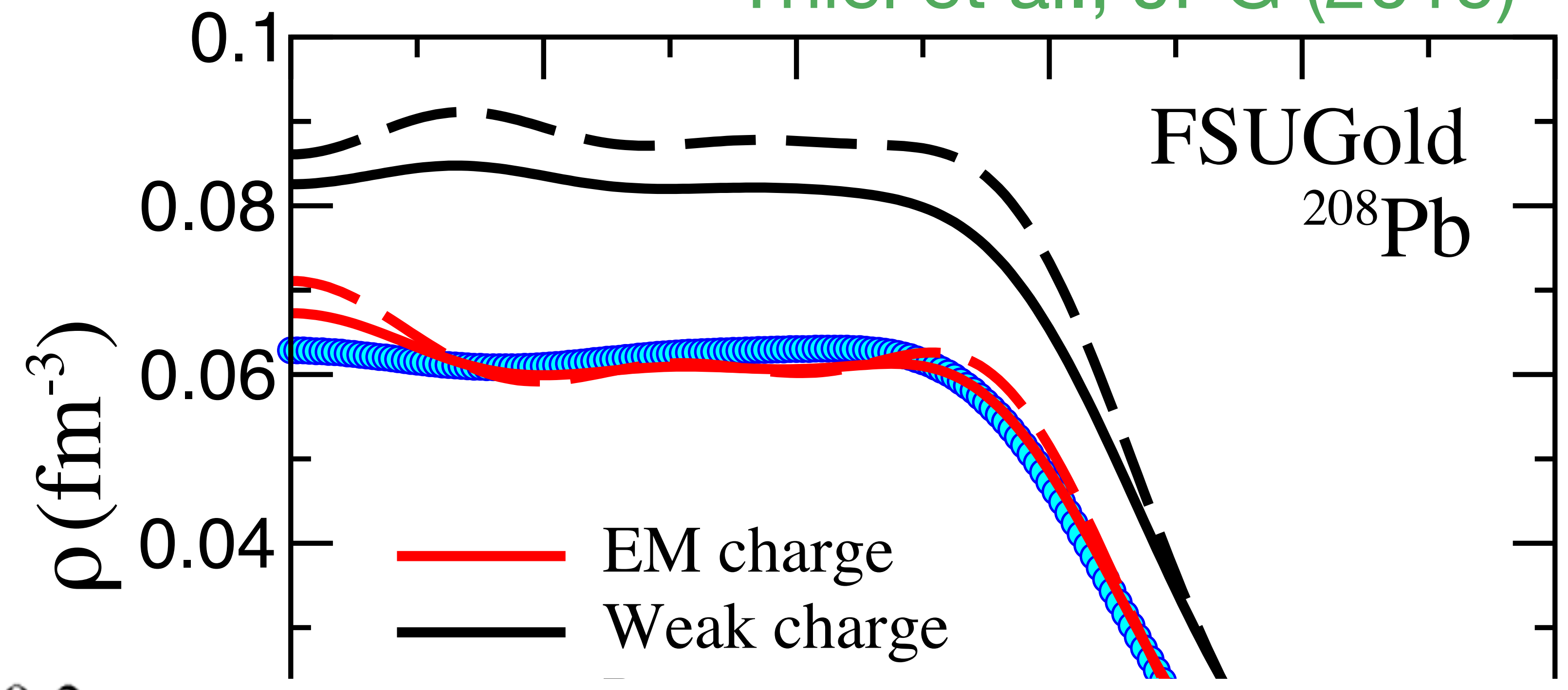

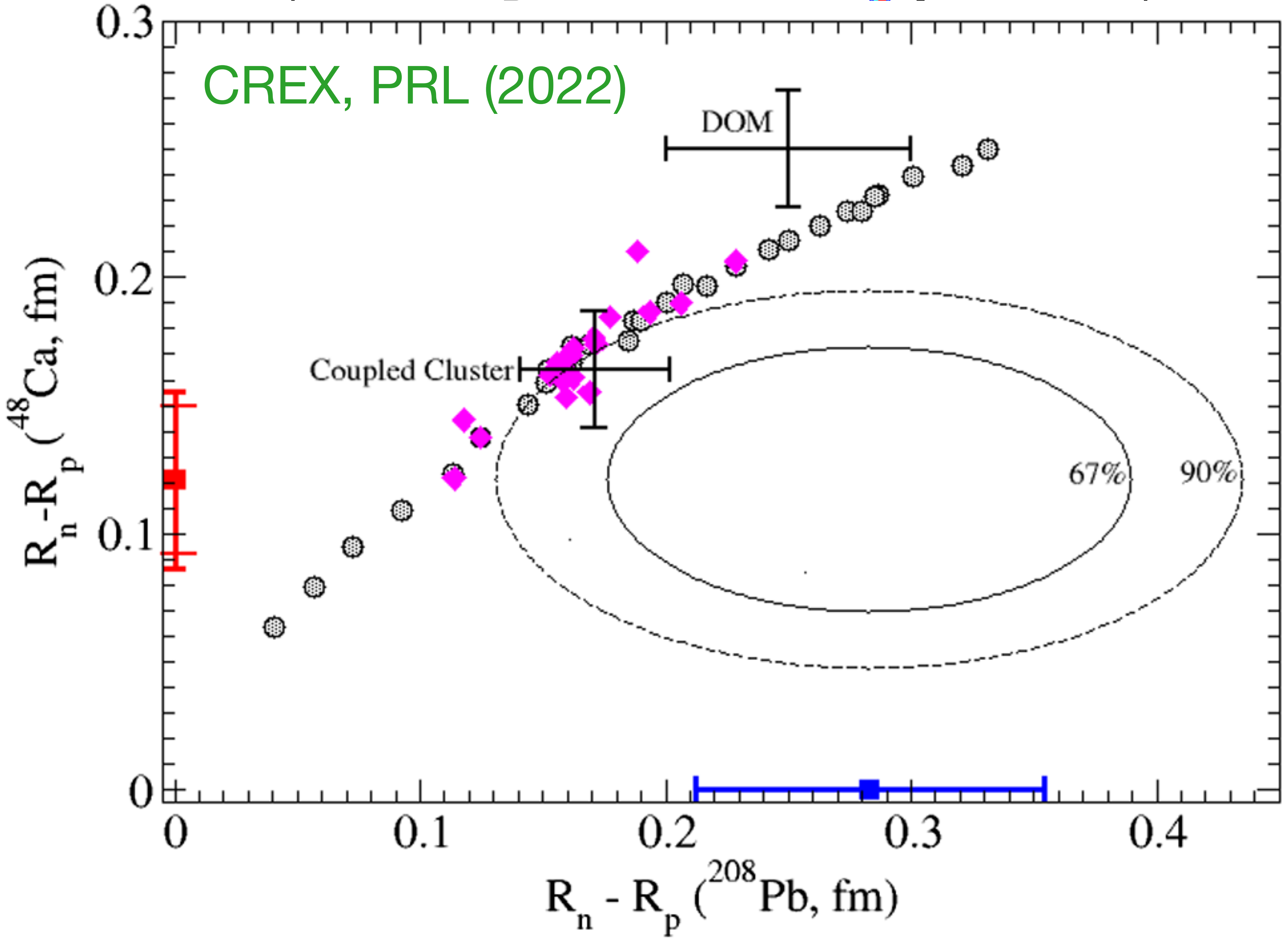

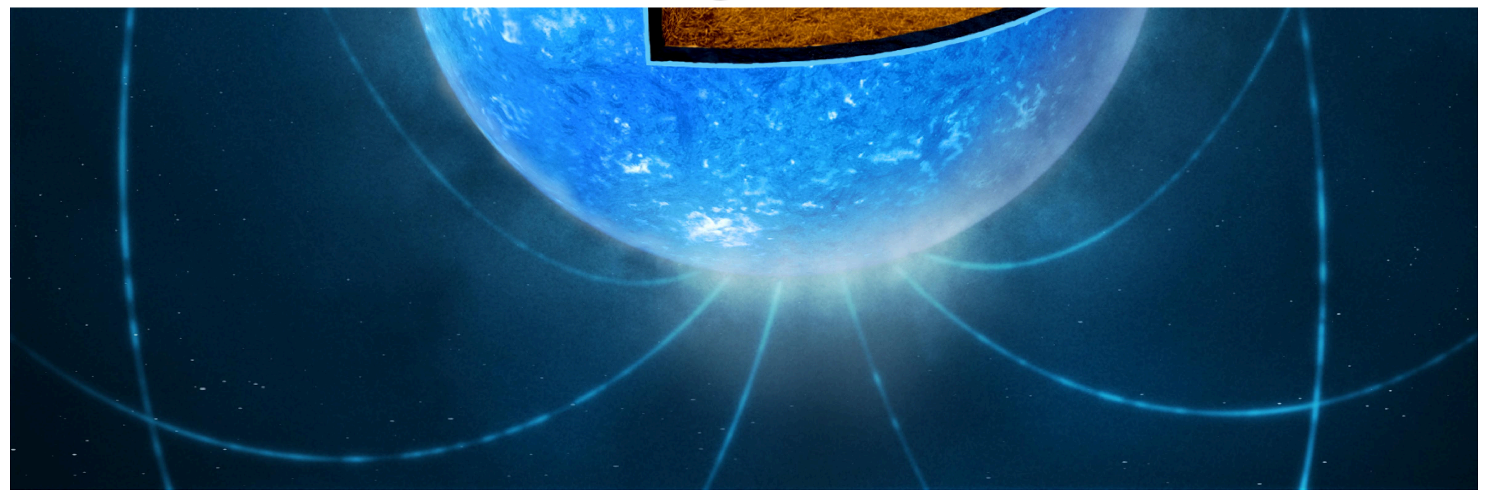

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Ab initio PVES

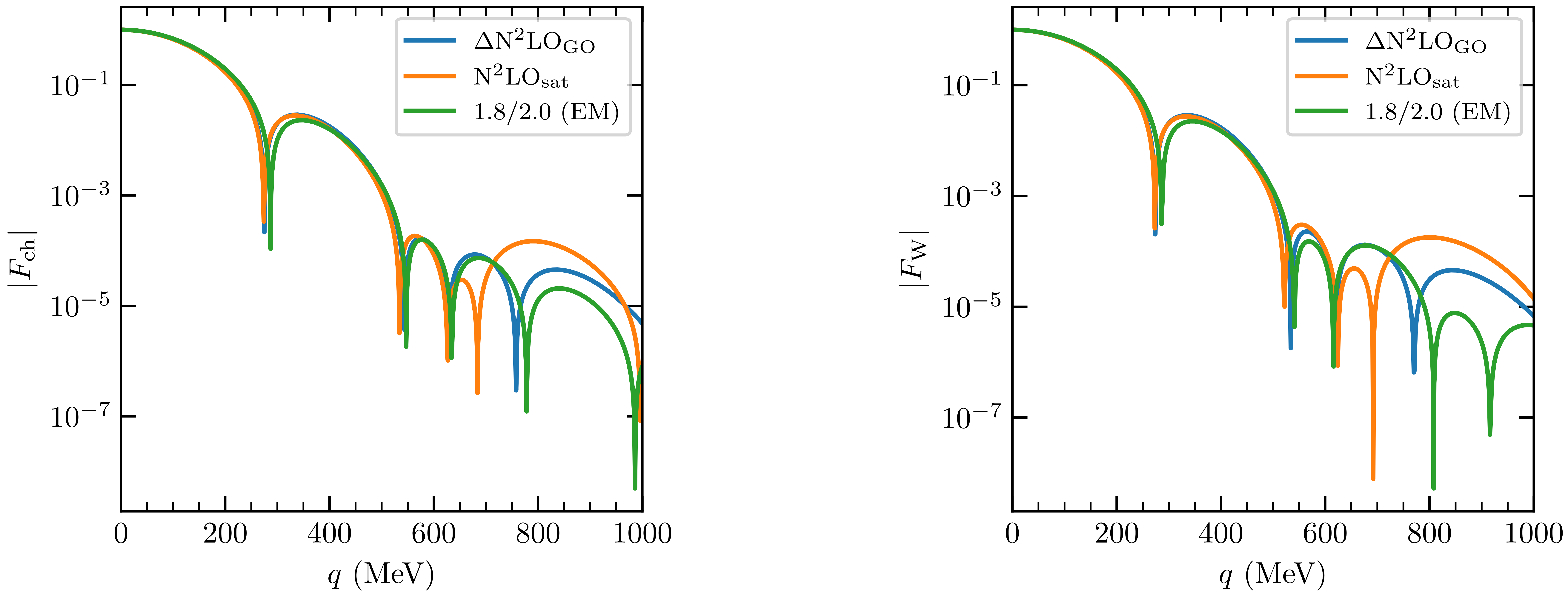
parity-violating electron scattering

- Computations based on EDFs are routine
- **But now we can compute this using ab initio methods!**
- Approach:
  - Start from given nuclear Hamiltonian
  - Compute charge and weak densities $\rightarrow V_{\mathrm{ch}}, V_{\mathrm{W}}$
  - Compute $d\sigma/d\Omega$ with Coulomb corrections

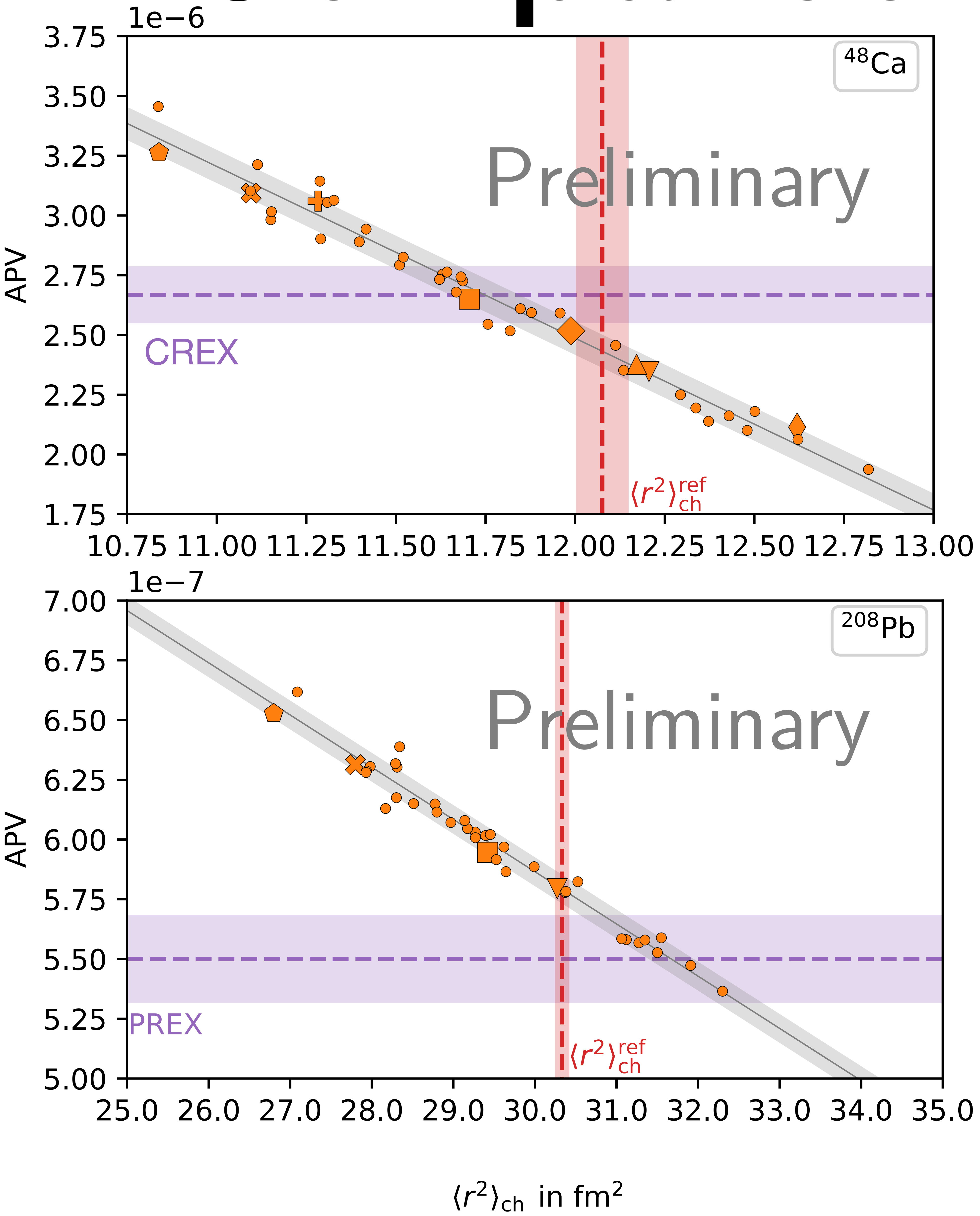
    https://pypi.org/project/phasr/ (Frederic Noël)
  - $A_{\mathrm{PV}} \sim \frac{d\sigma}{d\Omega}\left(V_{\mathrm{ch}} + V_{\mathrm{W}}\right) - \frac{d\sigma}{d\Omega}\left(V_{\mathrm{ch}} - V_{\mathrm{W}}\right)$

Taming uncertainties with correlations

- Predicted charge and weak densities are correlated (also with R_{ch})
- Same for any observable related to nuclear densities (like A_{PV})
- **Strategy: Study correlation with R_{ch} and calibrate on expt. value**



Comparison with CREX & PREX



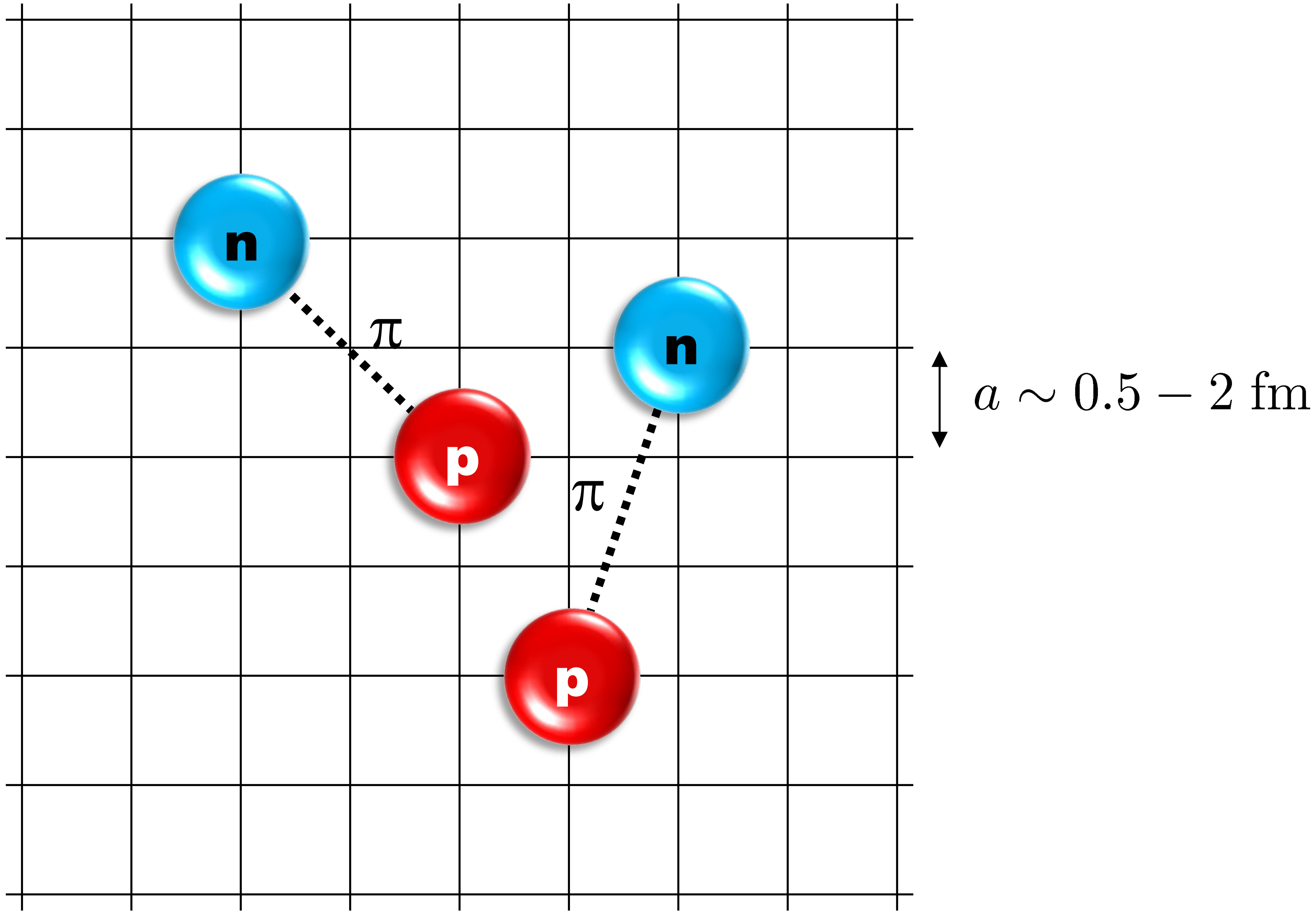
- Fiducial Hamiltonians, e.g., $\mathrm{NNLO}_{\mathrm{sat}}$, $\Delta\mathrm{NNLO}_{\mathrm{GO}}$, 1.8/2.0 (EM), 1.8/2.0 (EM7.5)
- 34 nonimplausible samples (no weights)
- **Point by point calculation of A_{PV}**
- Only weak tension found with both expts.
- Open questions:
  - Charge radius of $^{208}\mathrm{Pb}$ from μ atoms?
    Sun, Beyer, Mandrykina, Valuev, Keitel, Oreshkina, PRL (2025)
  - Model dependences in analyses of PREX and CREX?

Testing lattice Hamiltonians with variational methods

Rothman, Hagen, **MH**, Papenbrock, in prep.

Nuclei on a lattice

- Nuclear forces are finite-ranged
- On a spatial lattice,
  Hamiltonians are very sparse
- Interactions only in finite range r_{int}
- Volume of interactions small compared to total volume
- **This can drastically simplify computations!**

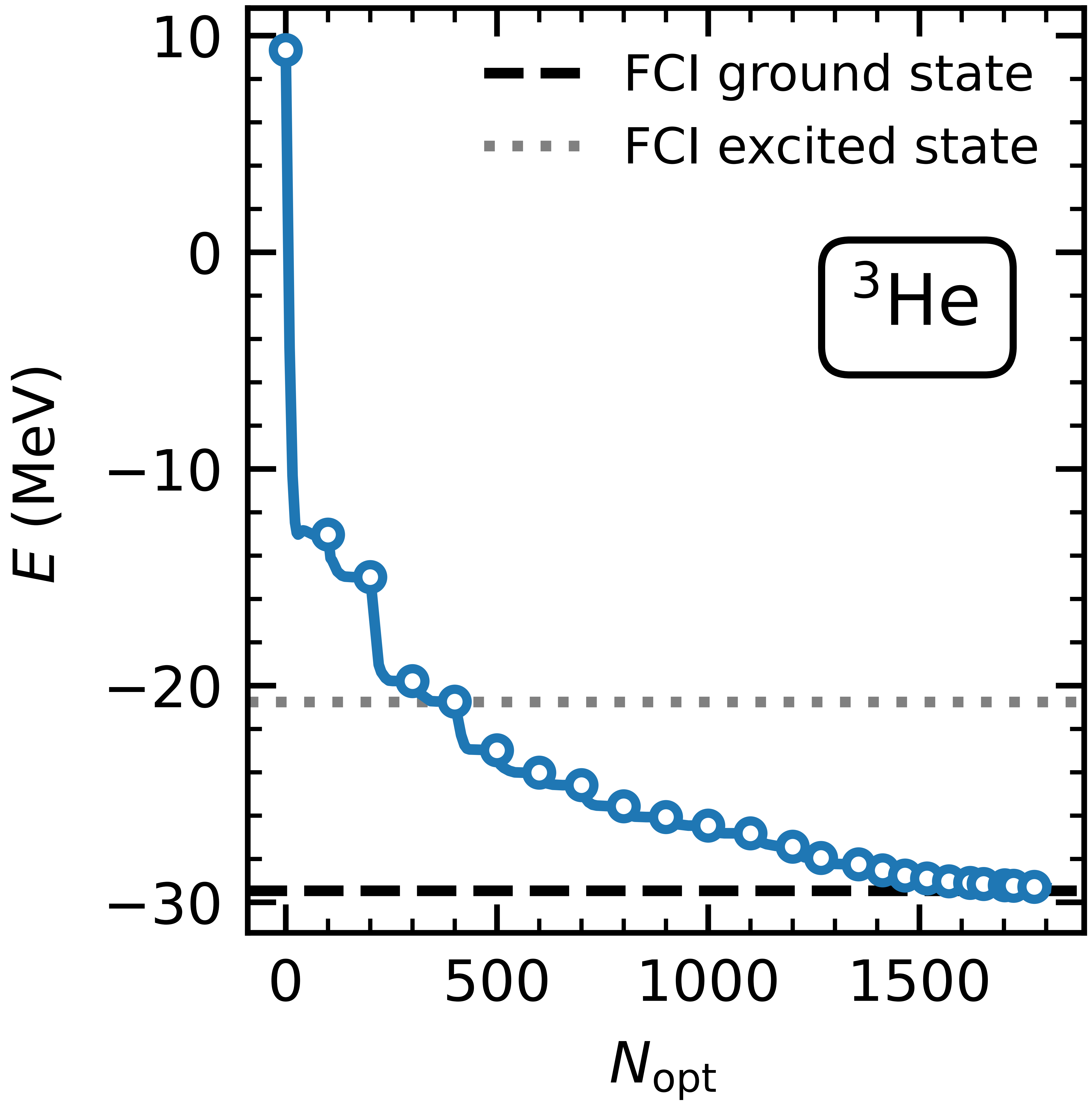


Lee, PPNP (2009)

Gu, **MH**, Kiss, Papenbrock, PRC (2026)

Quantum computing

- **Sparse Hamiltonian reduces number of 2-qubit gates**
- 2- and 3-body forces
- Simulations of 2- and 3-body systems
- Exact benchmarks met
- **Mild scaling of computational resources suggests this approach is scalable**



Rothman, Johnson-Toth, et al., PRC (2025)
Rothman, Johnson-Toth, et al., EPJA (2026)

NuLattice

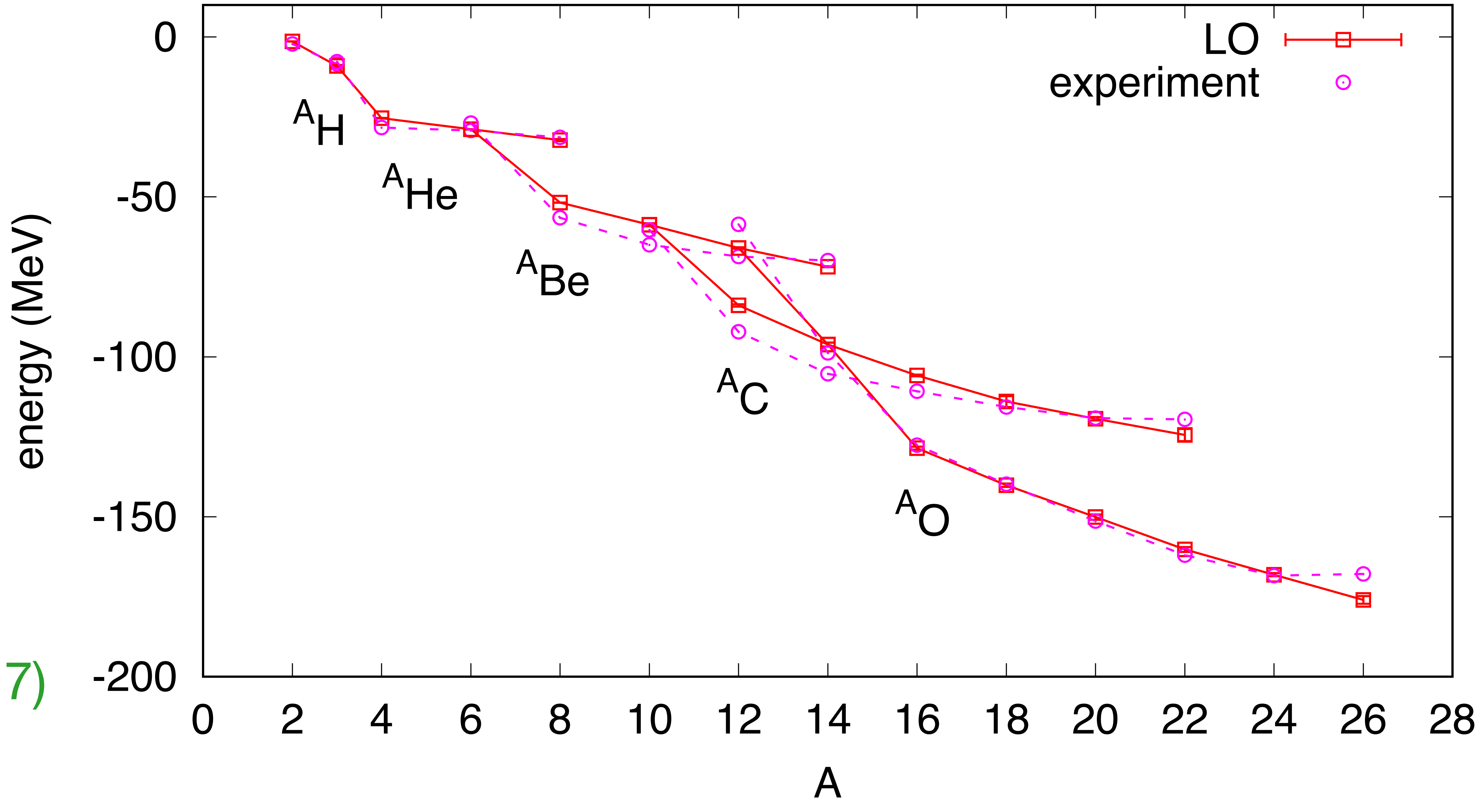
- Python computations of nuclei on spatial lattices
- https://github.com/NuLattice
- Many quantum many-body methods implemented
- Educational tool
- But also new science insights:
    - Validation of standard approximation for 3-body forces
    - Hartree Fock is pretty good for short-ranged forces

Maxwell Rothman @ UTK

Ben Johnson-Toth @ UTK

How simple is too simple?

- First studies used LO pionless EFT Hamiltonian
  - Purely on-site, attractive NN, repulsive 3N
  - Does not bind nuclei beyond α particle
- But simple NLEFT Hamiltonians propose to be successful in describing nuclei
- 2017: Only attractive NN interaction + OPE
  Elhatisari, Epelbaum, Krebs, Lähde, Lee, Li, Lu, Meißner, Rupak, PRL (2017)
- 2018: Attractive NN and attractive 3N interactions + OPE
  Lu, Li, Elhatisari, Lee, Epelbaum, Meißner, PLB (2018)
- **How does this work?**



Elhatisari et al., PRL (2017)

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Variational bounds on Hamiltonians

- Hartree-Fock computations of nuclei and nuclear matter
- 2017 Hamiltonian (NN-only) saturates only at high density (dense packing)
  Elhatisari, Epelbaum, Krebs, Lähde, Lee, Li, Lu, Meißner, Rupak, PRL (2017)

Nucleus	$L = 5$	$L = 6$	NLEFT	Exp.
^{4}He	-20.054	-19.797	-25.4	-28.3
^{8}Be	-63.31	-63.13	-51.9	-56.5
^{12}C	-137.75	-137.22	-83.8	-92.2
^{16}O	-214.07	-213.300	-128.2	-127.6

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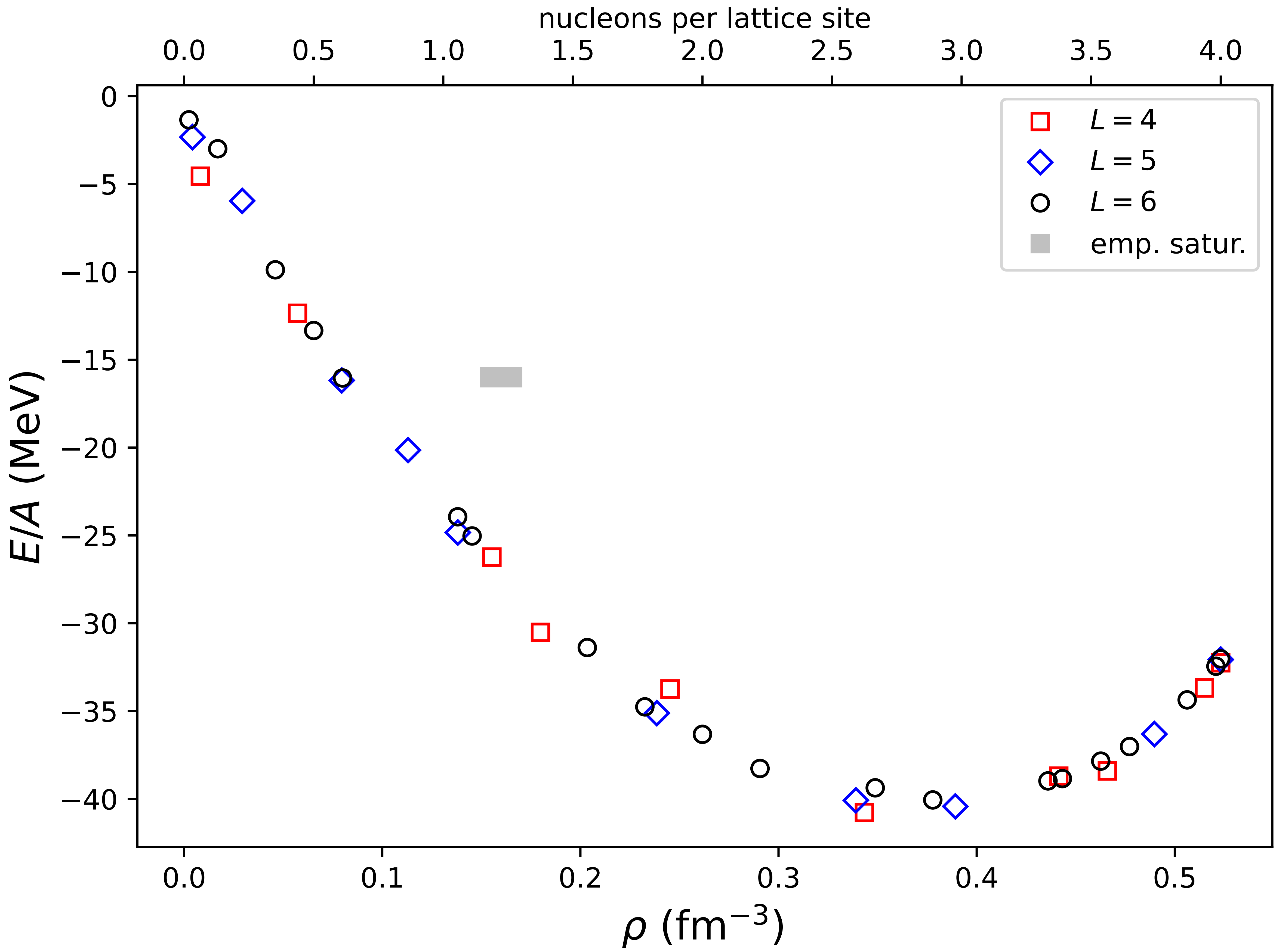

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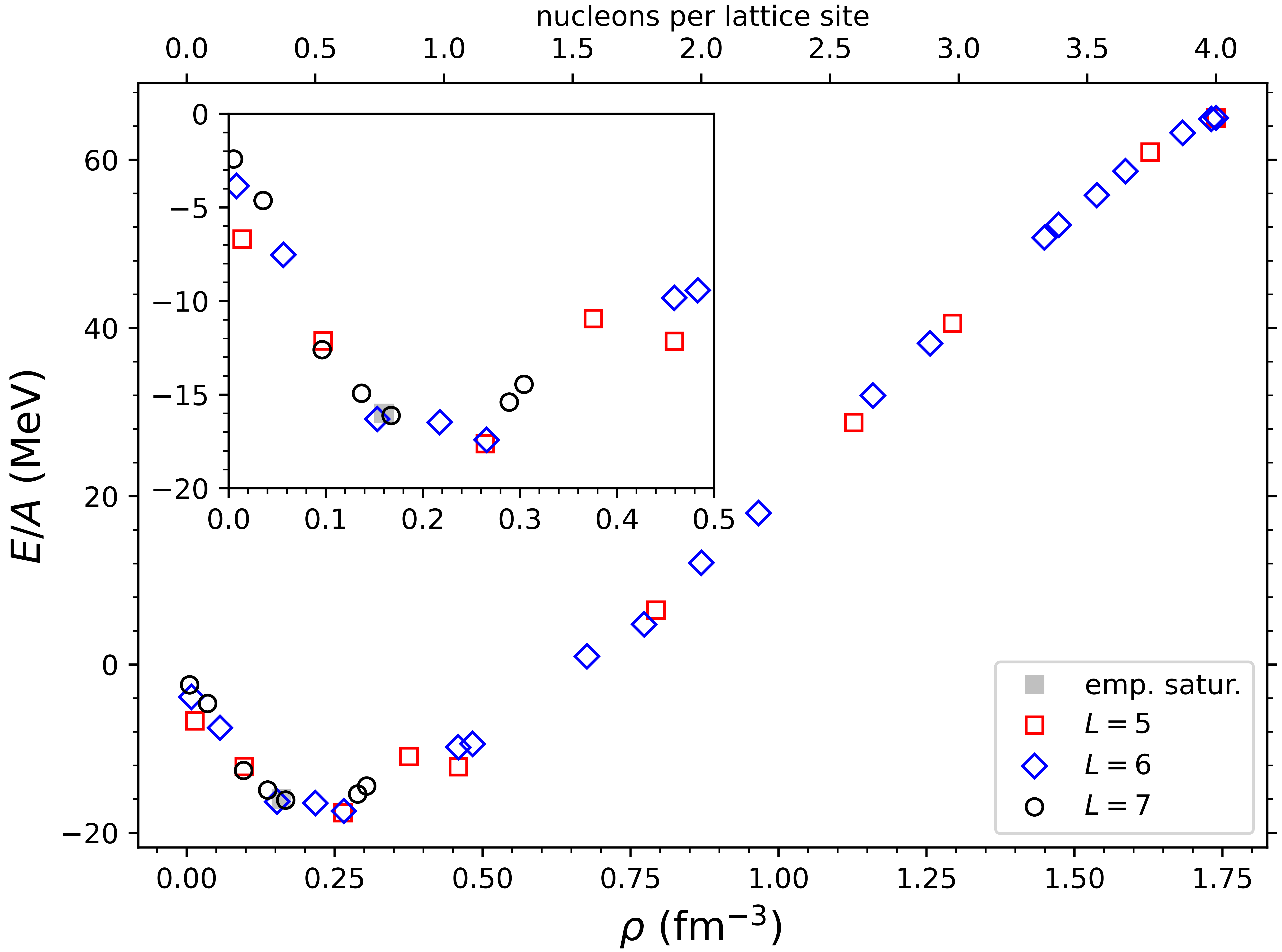

- 2018 Hamiltonian (NN+3N, both attractive) shows realistic saturation
  Lu, Li, Elhatisari, Lee, Epelbaum, Meißner, PLB (2018)
- Saturation driven by
  - More repulsive kinetic energy (smaller lattice spacing)
  - Strong nonlocal smearing
  - Pauli principle and lattice spacing
- See talk by Thomas Papenbrock for details and analysis

Challenges for this Program

- How should we think about uncertainties for accurate (fine-tuned) Hamiltonians?
- What about exploring optimization to properties of open-shell medium-mass nuclei?
- How do we explore/improve lattice Hamiltonians and connect understanding of nuclear systems on the lattice and in continuous bases?

Acknowledgments:

Low-res. Hamiltonians: **Tom Plies**, Achim Schwenk

PVES: **Frederic Noël**, Martin Hoferichter, Takayuki Miyagi, Achim Schwenk

Lattice: **Maxwell Rothman**, **Ben Johnson-Toth**, **Francesca Bonaiti**,
Gaute Hagen, Thomas Papenbrock