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UNCERTAINTY QUANTIFICATION WITH LOW-RESOLUTION NUCLEAR FORCES

Tom Plies

with Matthias Heinz[1] and Achim Schwenk

[1]Oak Ridge National Laboratory

arXiv:2509.24671

SFB 1245

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INTRODUCTION

- *Ab initio* description of nuclei

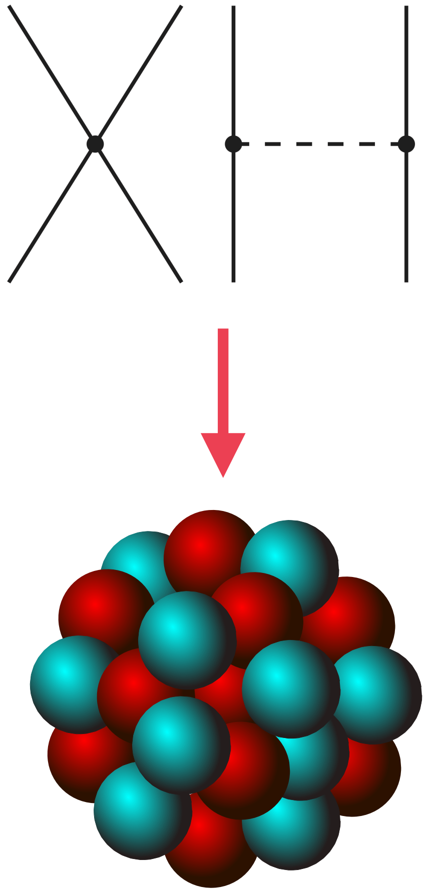
1. Interactions from chiral effective field theory

2. Similarity renormalization group

3. Many-body method: In-medium similarity renormalization group (IMSRG)

→ Observables

Machleidt, Entem, Phys. Rep. **503** (2011)



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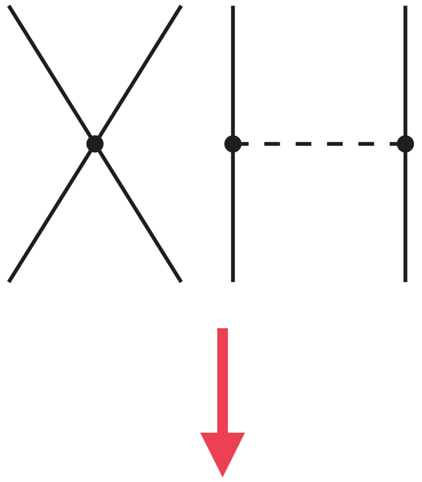

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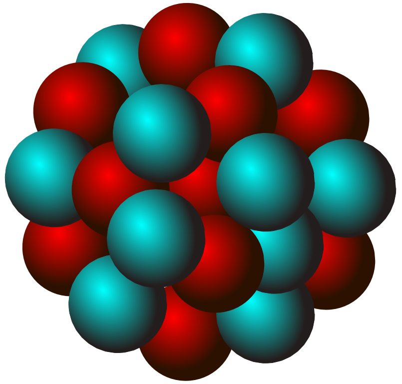

Observables

- All steps induce uncertainties
- Focus on EFT uncertainties

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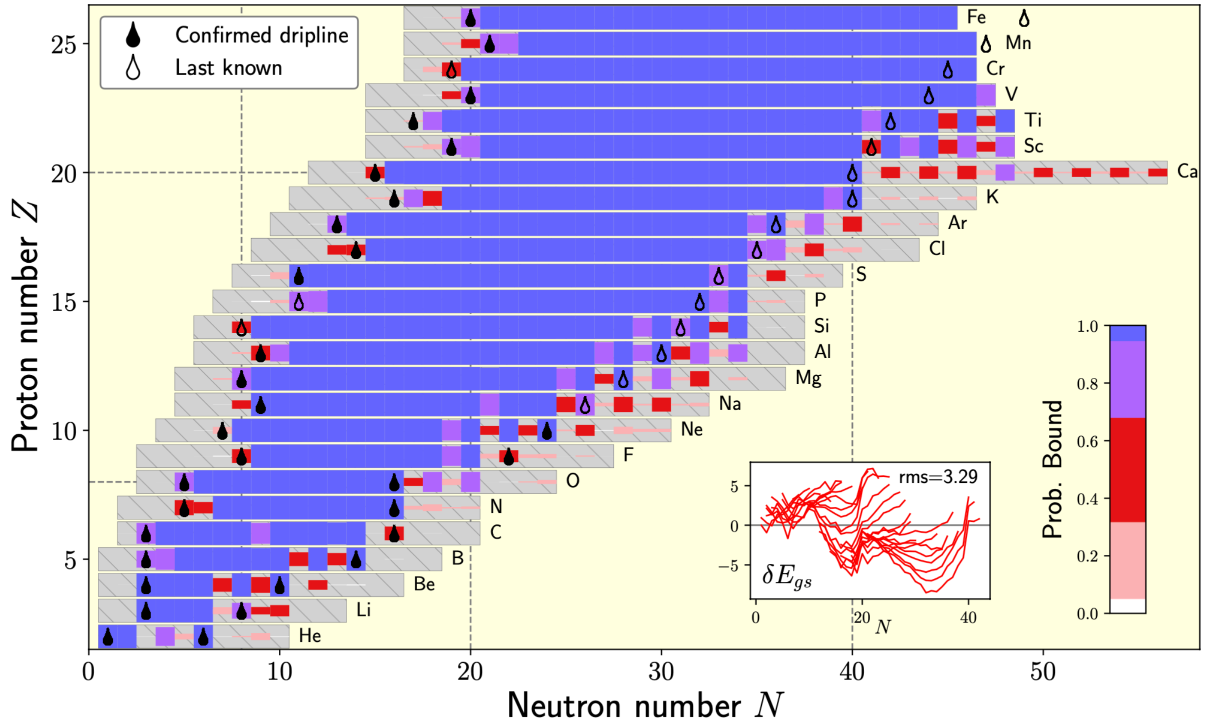
MOTIVATION

- Many successful applications with 1.8/2.0 (EM) interaction
- Uncertainty quantification (UQ) for this interaction challenging



Hebeler et al., PRC **83** (2011)
Stroberg et al., PRL **126** (2021)

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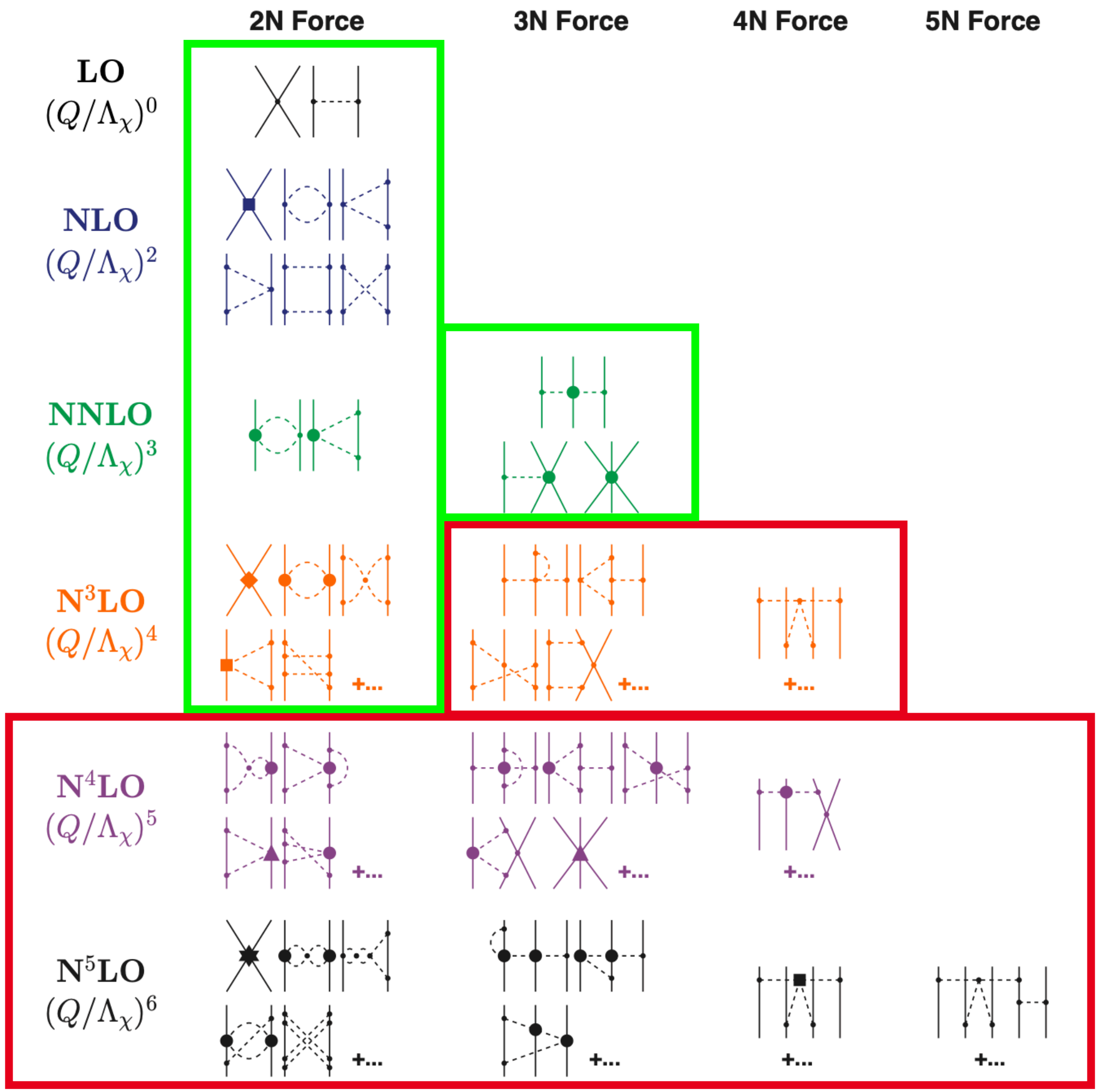
NUCLEAR FORCES FROM CHIRAL EFT

- Chiral EFT provides systematic expansion
- Fit to experiment (uncertainties reside in LECs)
- Uncertainties from missing higher-order contributions
- Including truncation uncertainties when fitting to avoid overfitting
- **Truncation uncertainties also reside in parametric uncertainty**



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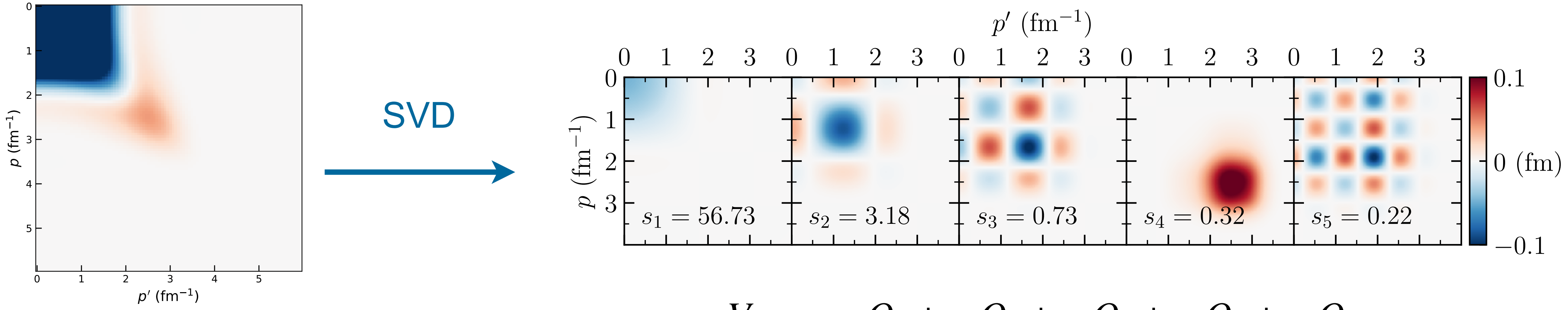
LINEAR OPERATOR STRUCTURE

- Chiral EFT potentials have linear operator structure: $V(c_i) \sim \sum_{i=1}^{N} c_i O_i$
- EC emulators largely benefit from such a structure
- Similarity-renormalization-group evolution of potentials destroys linear operator structure (non-linear mixing of terms)
- Want to numerically restore such a structure

SINGULAR VALUE DECOMPOSITION

Tichai et al., PLB **821** (2021)

- SVD to recover linear operator structure destroyed by SRG



$$V_{\text{NN}} \approx s_1 O_1 + s_2 O_2 + s_3 O_3 + s_4 O_4 + s_5 O_5$$

$$V_{\text{NN}} = L \Sigma R^\dagger = \sum_{i=1}^{N} s_i |L_i\rangle\langle R_i|$$

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SINGULAR VALUE DECOMPOSITION

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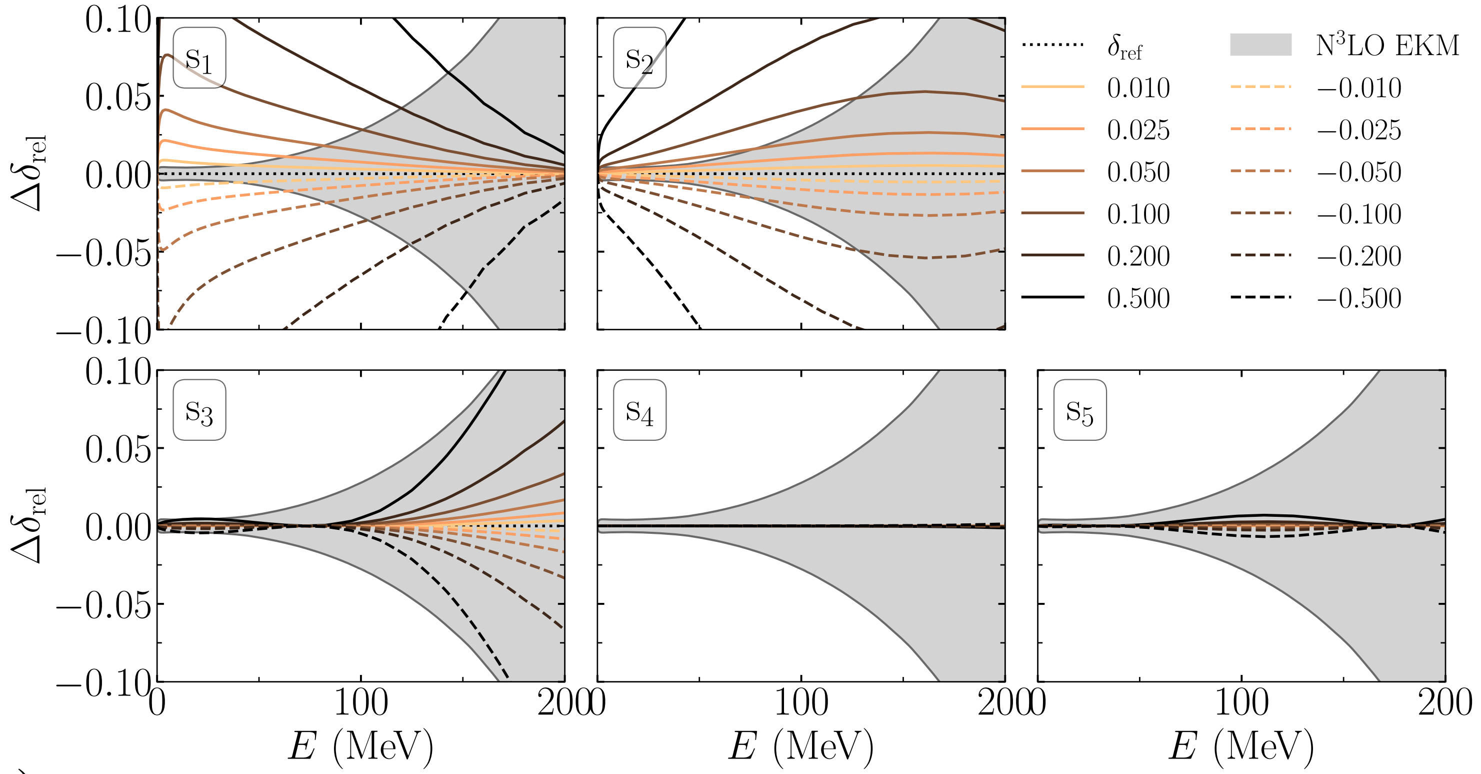
$$\Delta\delta_{\mathrm{rel}} = \frac{\delta - \delta_{\mathrm{ref}}}{\delta_{\mathrm{ref}}}$$

$$V_{\mathrm{NN}} = L\Sigma R^{\dagger} = \sum_{i=1}^{N} s_i \, |L_i\rangle\langle R_i|$$



- Singular values are the new "LECs" $V(s_1, s_2, s_3)$

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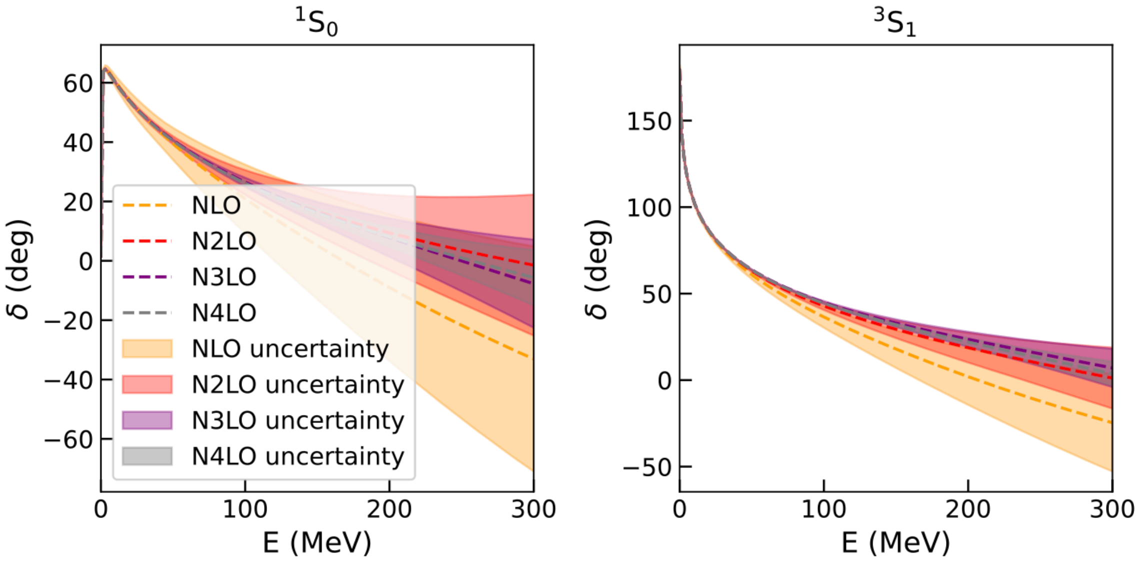
TRUNCATION UNCERTAINTIES

- Power series expansion for observables from chiral EFT expansion
- Each term corresponds to a different chiral order

$$y_k(x) = y_{\text{ref}}(x) \sum_{n=0}^{k} c_n(x) \left(\frac{Q(x)}{\Lambda_b} \right)^n \qquad \delta y_k(x) = y_{\text{ref}}(x) \sum_{n=k+1}^{\infty} c_n(x) \left(\frac{Q(x)}{\Lambda_b} \right)^n$$

EKM: $\delta y_k(x) \sim y_{\text{ref}}(x) \max\{c_n(x)\} \left(\frac{Q(x)}{\Lambda_b} \right)^{k+1}$

- Conservative estimate of $k+1$ contribution to an observable
- We assume the EKM uncertainty to be Gaussian



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TRUNCATION UNCERTAINTIES

Data:

- Phase shifts to constrain NN interactions
- Triton observables to constrain 3N interactions
- Bayes' theorem to propagate uncertainties in observables to parameter distributions

$$\mathrm{pr}(\boldsymbol{\alpha}\,|\,\mathscr{D}) = \mathscr{L}(\boldsymbol{\alpha})\mathrm{pr}(\boldsymbol{\alpha})$$

→ Distribution of Hamiltonians $H(\boldsymbol{\alpha})$

- Posterior predictive distributions for any nuclear structure observable

$$\mathrm{PPD} = \{\mathrm{y}(\boldsymbol{\alpha}) : \boldsymbol{\alpha} \sim \mathrm{pr}(\boldsymbol{\alpha}\,|\,\mathscr{D})\}$$

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$$\mathrm{pr}(\boldsymbol{\alpha}\,|\,\mathscr{D}) = \mathscr{L}(\boldsymbol{\alpha})\mathrm{pr}(\boldsymbol{\alpha})$$

→ Distribution of Hamiltonians $H(\boldsymbol{\alpha})$

→ **Goal:**

Construct likelihood $\mathscr{L}(\boldsymbol{\alpha})$ that allows us to capture NN and 3N truncation uncertainties within parameter distributions $\mathrm{pr}(\boldsymbol{\alpha}\,|\,\mathscr{D})$

- Posterior predictive distributions for any nuclear structure observable

$$\mathrm{PPD} = \{\mathrm{y}(\boldsymbol{\alpha}) : \boldsymbol{\alpha} \sim \mathrm{pr}(\boldsymbol{\alpha}\,|\,\mathscr{D})\}$$

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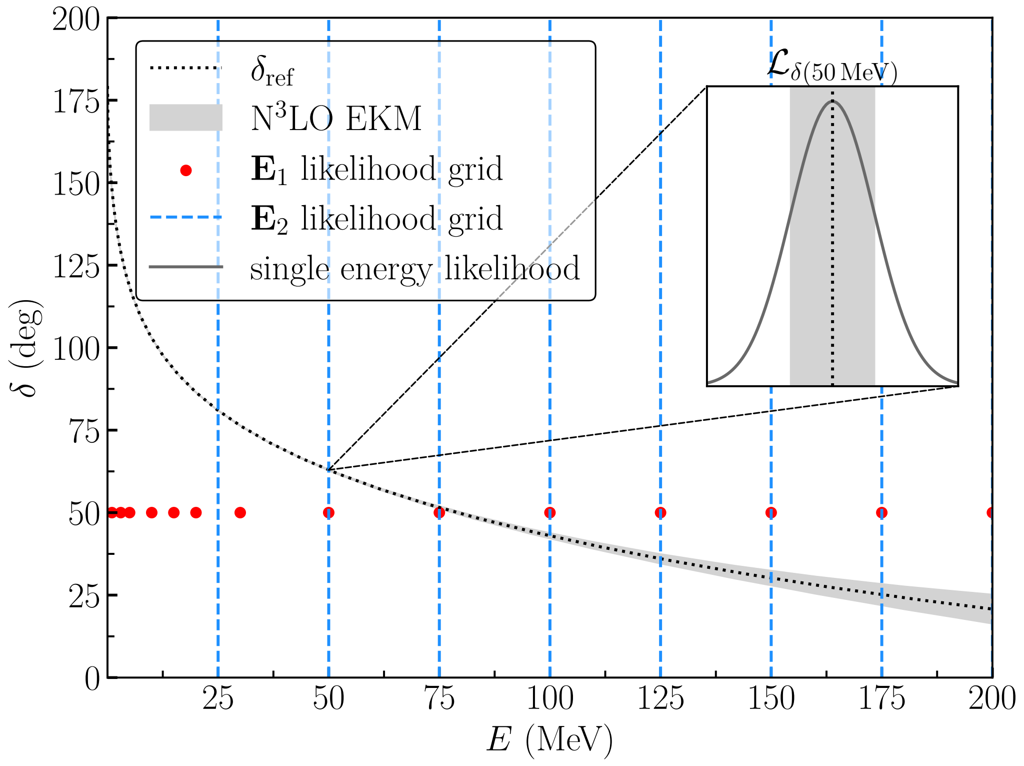
LIKELIHOODS

Goal: Construct likelihood to capture NN and 3N uncertainties

NN

- Use phase shifts to constrain NN interactions
- Construct Gaussian likelihood
- Two different likelihoods: $\mathbf{E}_1$, $\mathbf{E}_2$

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



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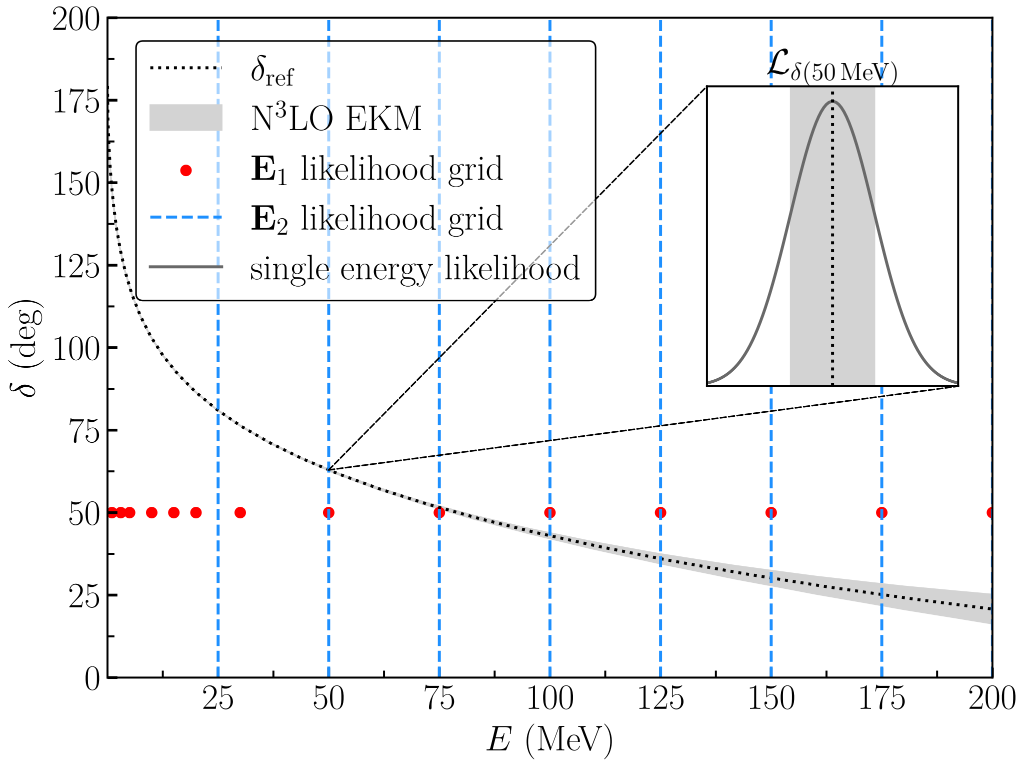

→ Future work: correlated treatment for NN observables

3N UNCERTAINTIES

- Vary only c_D and c_E, not c_i's
- Triton binding energy $E(^3\mathrm{H})$ and comparative half-life $fT_{1/2}$ as calibration
- EC Emulators for efficient calculation Thanks to Takayuki Miyagi

$$\mathcal{L}_{3\mathrm{N}}(c_D, c_E, \boldsymbol{\alpha}_{\mathrm{NN}}) = \mathcal{N}(\mathbf{y}_{\mathrm{th}}, \Sigma), \qquad (\Sigma)_{ij} = \left[\frac{(y_{\mathrm{ref}} \bar{c} (\frac{Q}{\Lambda_b})^{k+1})^2}{1 - (\frac{Q}{\Lambda_b})^2} \right] \delta_{ij}$$

- $\bar{c}$ and Q/Λ_b from order-by-order triton and helium observables Wesolowski et al., PRC **104** (2021)

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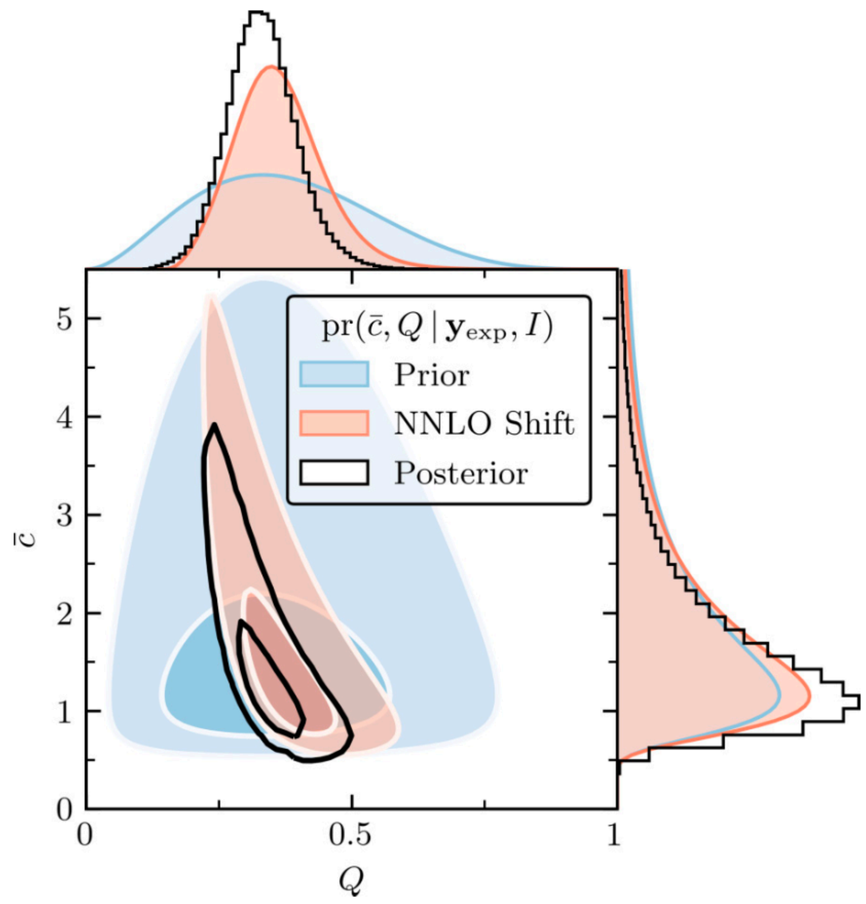

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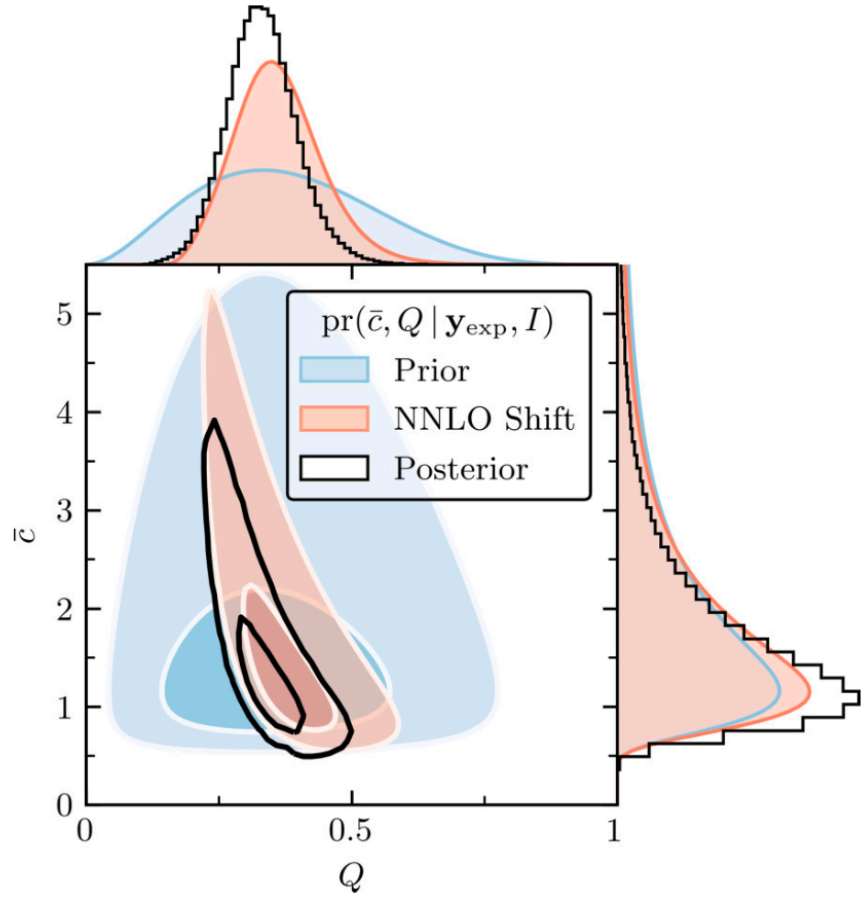
Full likelihood: $\mathscr{L}(\boldsymbol{\alpha}_{\mathrm{NN}}, c_D, c_E) = \mathscr{L}_{\mathrm{NN}}(\boldsymbol{\alpha}_{\mathrm{NN}})\mathscr{L}_{3\mathrm{N}}(\boldsymbol{\alpha}_{\mathrm{NN}}, c_D, c_E)$

Wesolowski et al., PRC **104** (2021)



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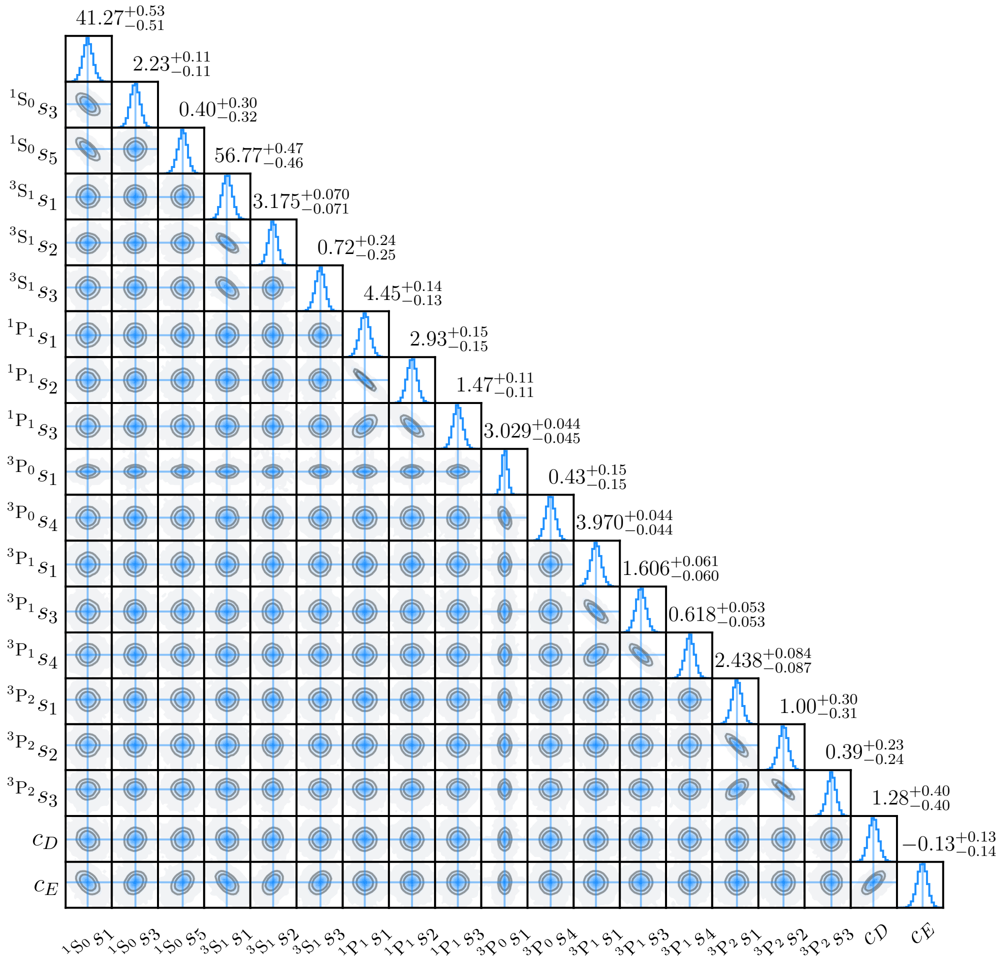
BAYESIAN INFERENCE

- Markov chain Monte Carlo sampling

$$\mathrm{pr}(\boldsymbol{\alpha} \,|\, \mathscr{D}) = \mathscr{L}(\boldsymbol{\alpha})\mathrm{pr}(\boldsymbol{\alpha})$$



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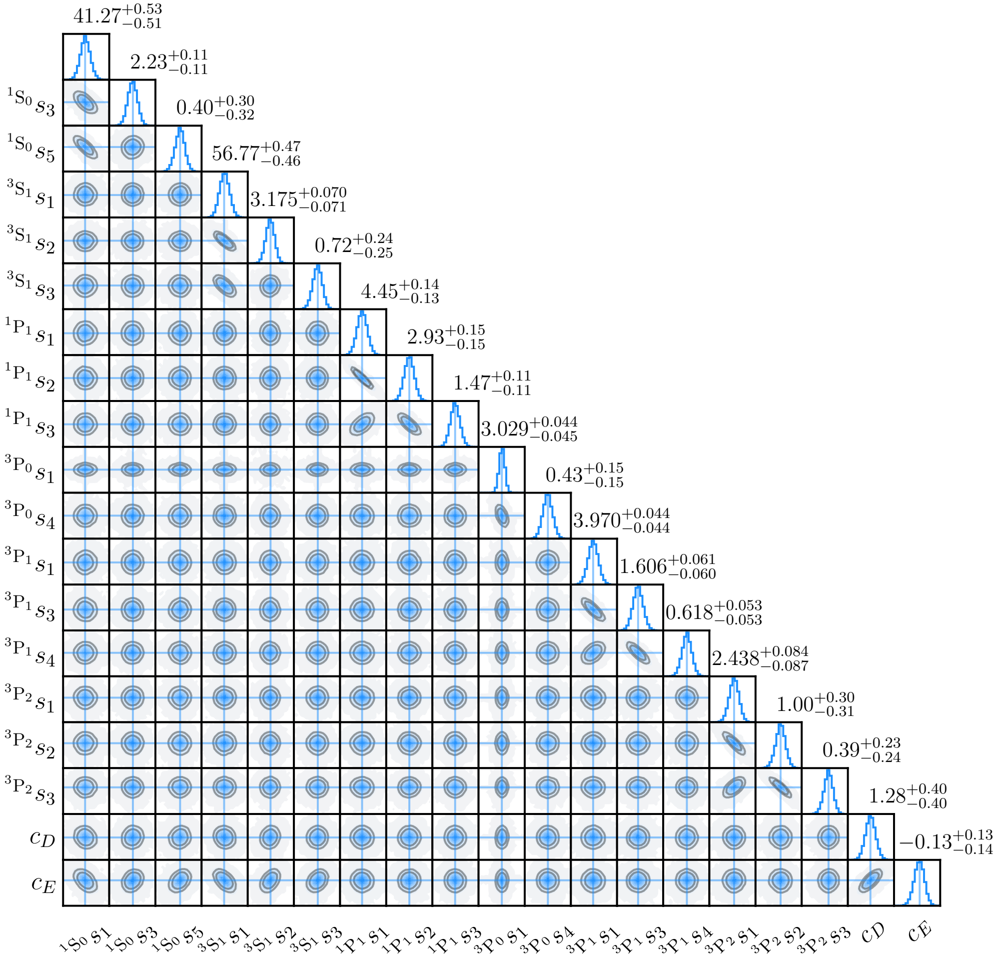

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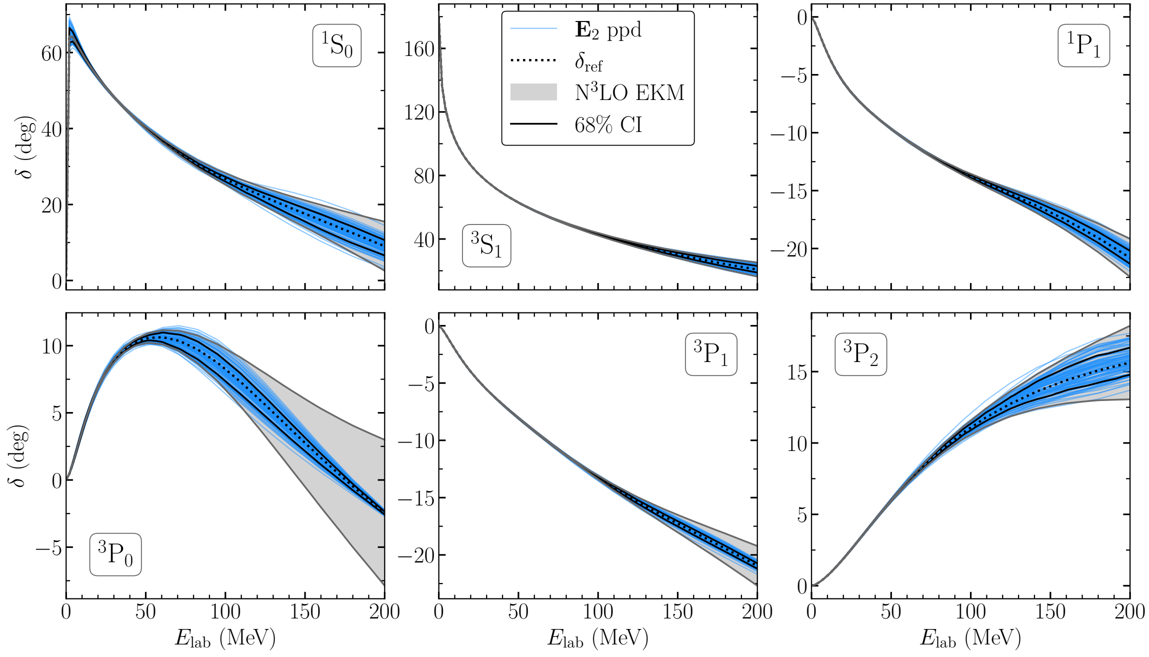
MODEL CHECKING

NN

- Phase shift posterior predictive distributions (PPDs) reproduce input EKM uncertainties
- Underestimated at high energies due to operator basis limitations



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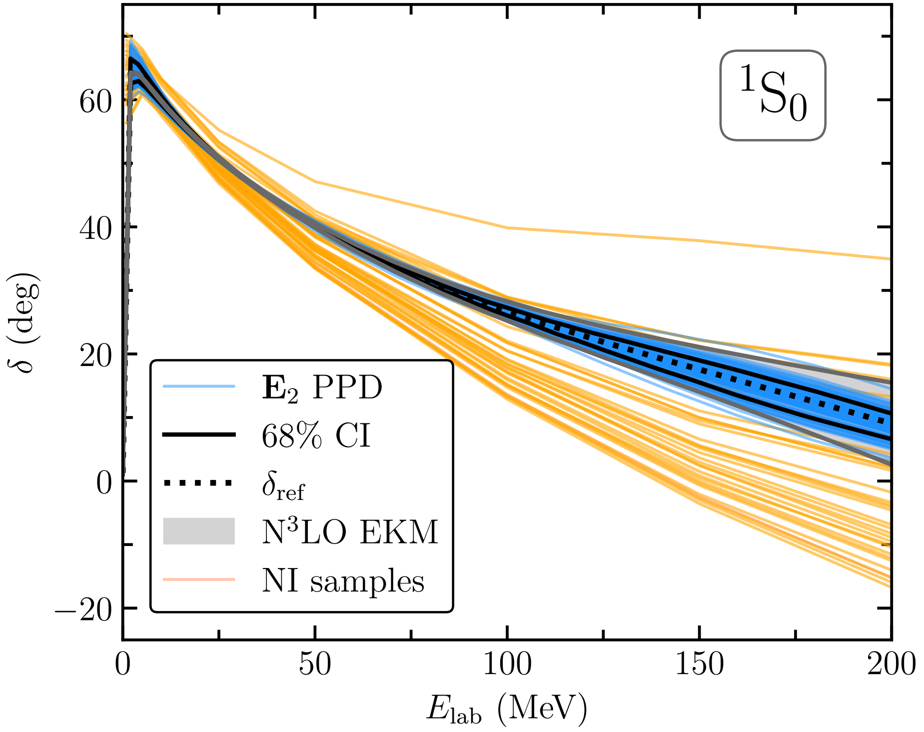
MODEL CHECKING

Hu et al., Nat. Phys. **18** (2022)

- History matching more conservative



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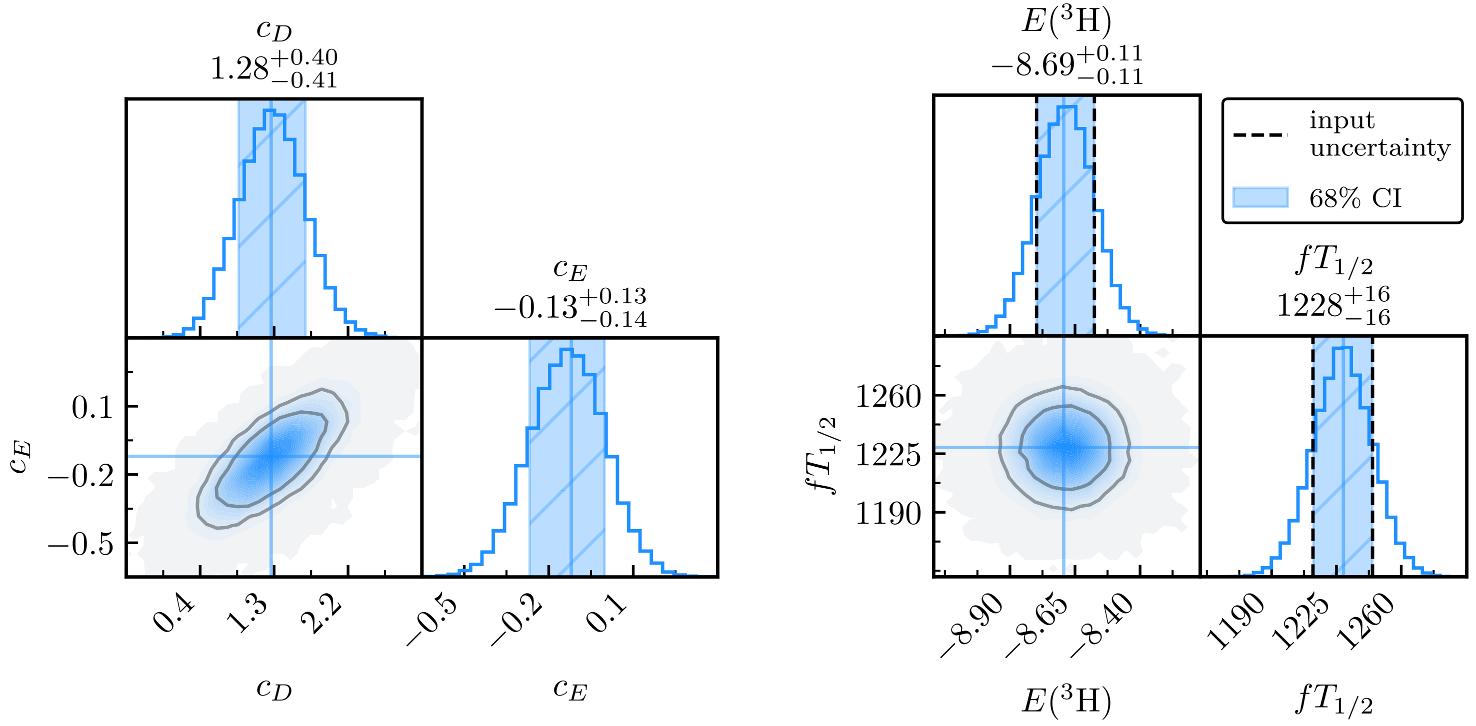

3N

- Triton PPDs excellently reproduce input uncertainties
- **We can capture truncation uncertainties within LEC distributions**

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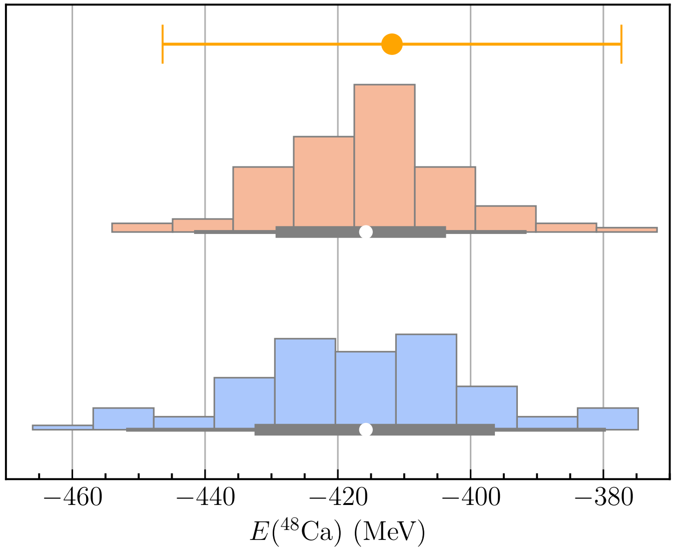
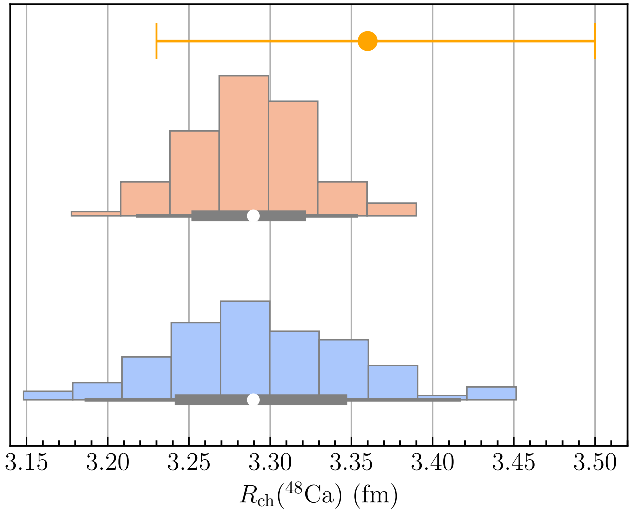
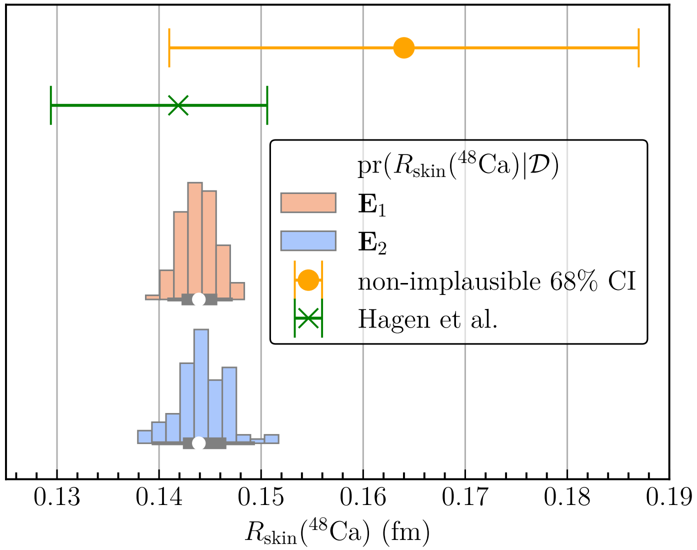
^{48}CA OBSERVABLES

- Resample from 10^6 to 100 representative samples
- IMSRG calculations
- PPDs for ground-state energy, charge radius, and neutron skin thickness
- **Distributed according to NN phase shift and triton observable truncation uncertainties**

History matching: $\delta y = \delta y_{\mathrm{param}} + \delta y_{\mathrm{trunc}}$







Hu et al., Nat. Phys. **18** (2022)
Hagen et al., Nat. Phys. **12** (2016)

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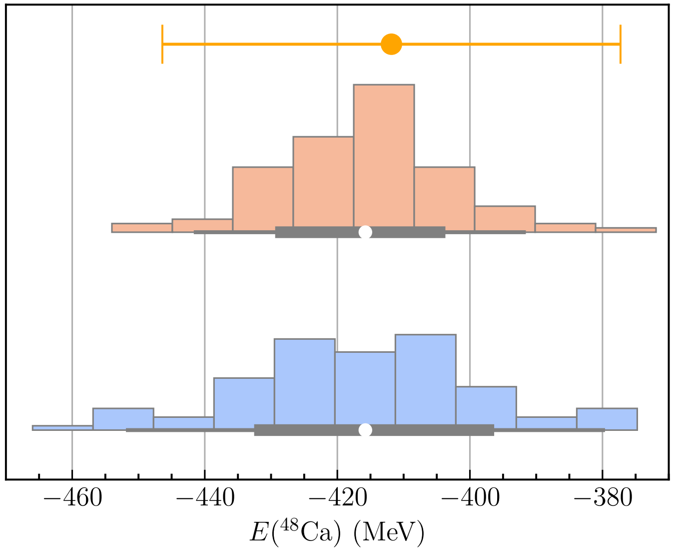

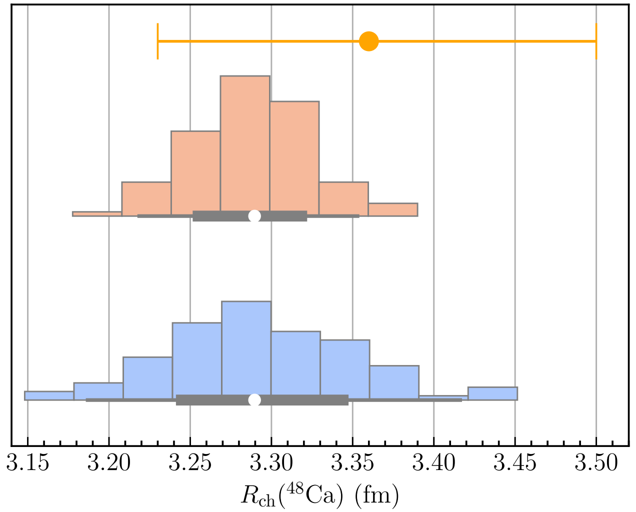

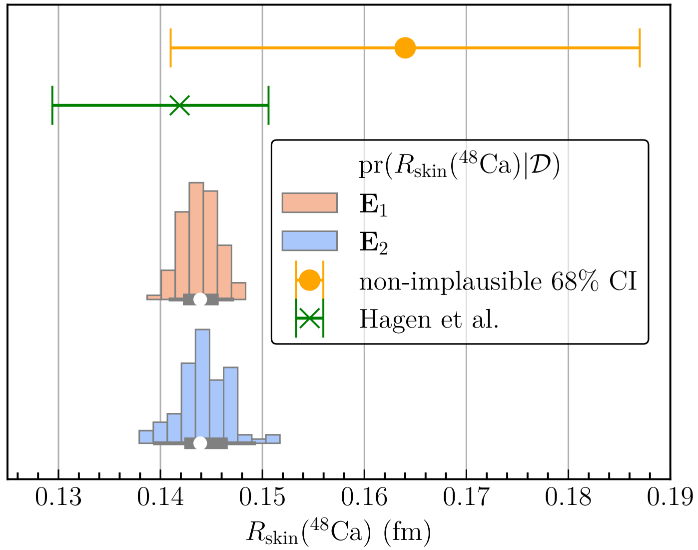

Hu et al., Nat. Phys. **18** (2022)
Hagen et al., Nat. Phys. **12** (2016)

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CORRELATED TRUNCATION UNCERTAINTIES

constraining observable: X **target observable:** Y

Assuming perfect correlation: $\mathrm{corr}(\delta X, \delta Y) = 1 \longrightarrow \delta y = \delta y_{\mathrm{param}}$

- Use observable X (and its truncation uncertainty) to infer distribution of parameters
- Parameter distribution should capture full truncation uncertainty of X
- Propagate parameter distribution to observable Y

Assuming no correlation: $\mathrm{corr}(\delta X, \delta Y) = 0 \longrightarrow \delta y = \delta y_{\mathrm{param}} + \delta y_{\mathrm{trunc}}$

- Use observable X (and its truncation uncertainty) to infer distribution of parameters
- Propagate parameter distribution to observable Y
- Calculate truncation uncertainty of observable Y
- Combine parametric uncertainty of X with truncation observable Y

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OPEN QUESTIONS

- How much missing higher-order physics can we actually capture within LEC distributions?
- What happens if we include Y in the inference of LEC distributions
- Do we still need an additional truncation uncertainty on top of the parametric uncertainty?
- What is the relation between parametric uncertainty and truncation uncertainty?

- How to learn/model the correlation between $\delta X, \delta Y$?
- $\mathrm{Corr}(X, Y) \to \mathrm{Corr}(\delta X, \delta Y)$?
- How does the correlation between $\delta X, \delta Y$ affect results?
- (How to correlate integrated observables?)

SUMMARY AND OUTLOOK

- Method to construct uncertainties for low-resolution interactions established
- Built ensemble of Hamiltonian based on MCMC
- Propagated distributions to nuclear structure observables

- Uncertainties for different observables: excitation energies, separation energies, etc.
- Sensitivity analysis to improve understanding of operator basis
- Study correlations in truncation uncertainties of different systems

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Thanks to Takayuki Miyagi, Isak Svensson,
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Thank you for your attention!

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SRG OPERATOR STRUCTURE

$$H_s = U_s H U_s^\dagger = T_{\text{rel}} + V_s$$

$$\frac{dH_s}{ds} = [\eta_s, H_s]$$

$$\eta_s = \frac{dU_s}{ds} U_s^\dagger$$

$$\eta_s = [G_s, H_s]$$

$$U_s = \mathcal{T}_s \exp\left(-\int_0^s \eta_{s'} \, ds' \right)$$

$$V_s = U_s H U_s^\dagger - T_{\text{rel}}$$

$$V_s = U_s T_{\text{rel}} U_s^\dagger + U_s V_{1\pi} U_s^\dagger + U_s V_{\text{ct}}^{(0)} U_s^\dagger \ldots - T_{\text{rel}}$$

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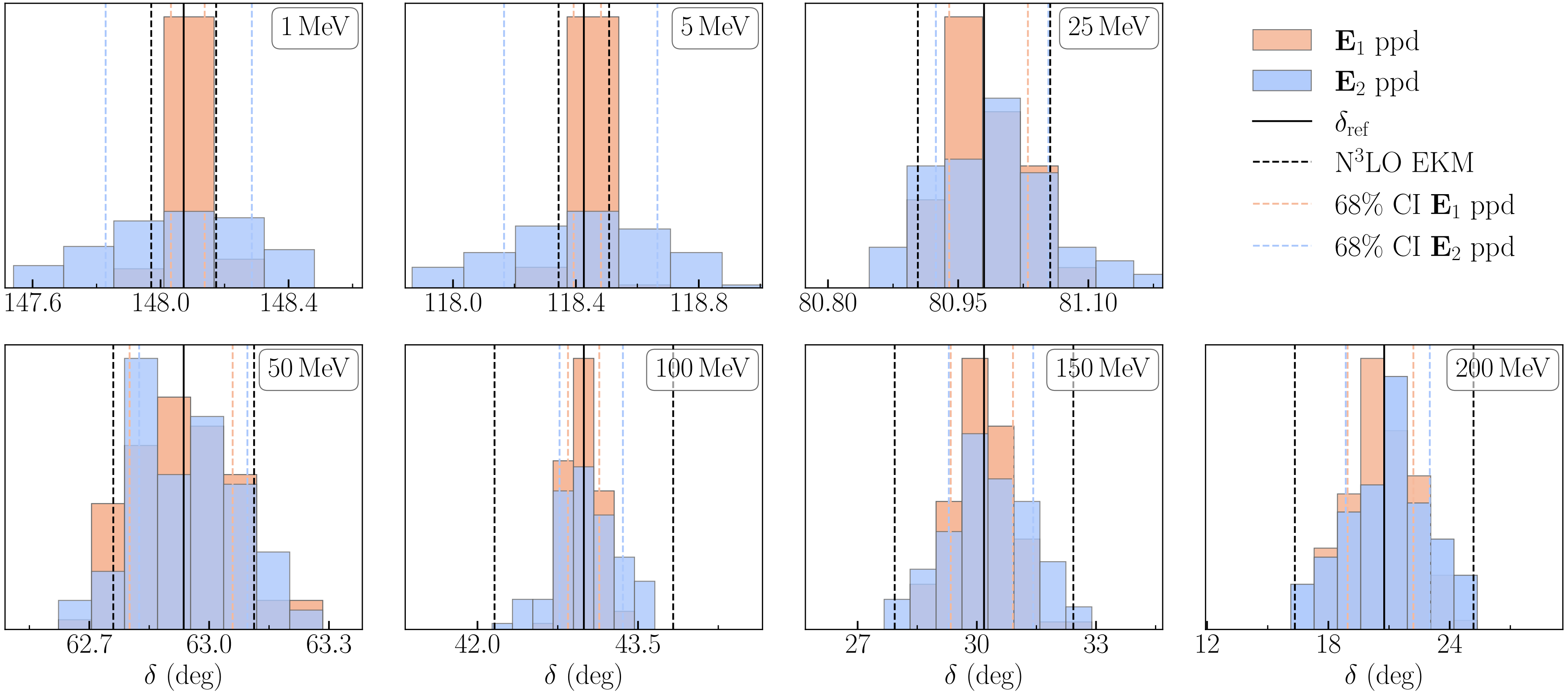
$^3S_1$ PHASE-SHIFT DISTRIBUTIONS



- EKM uncertainties should be reproduced
- $\mathbf{E}_1$ as lower bound; $\mathbf{E}_2$ as upper bound for uncertainties

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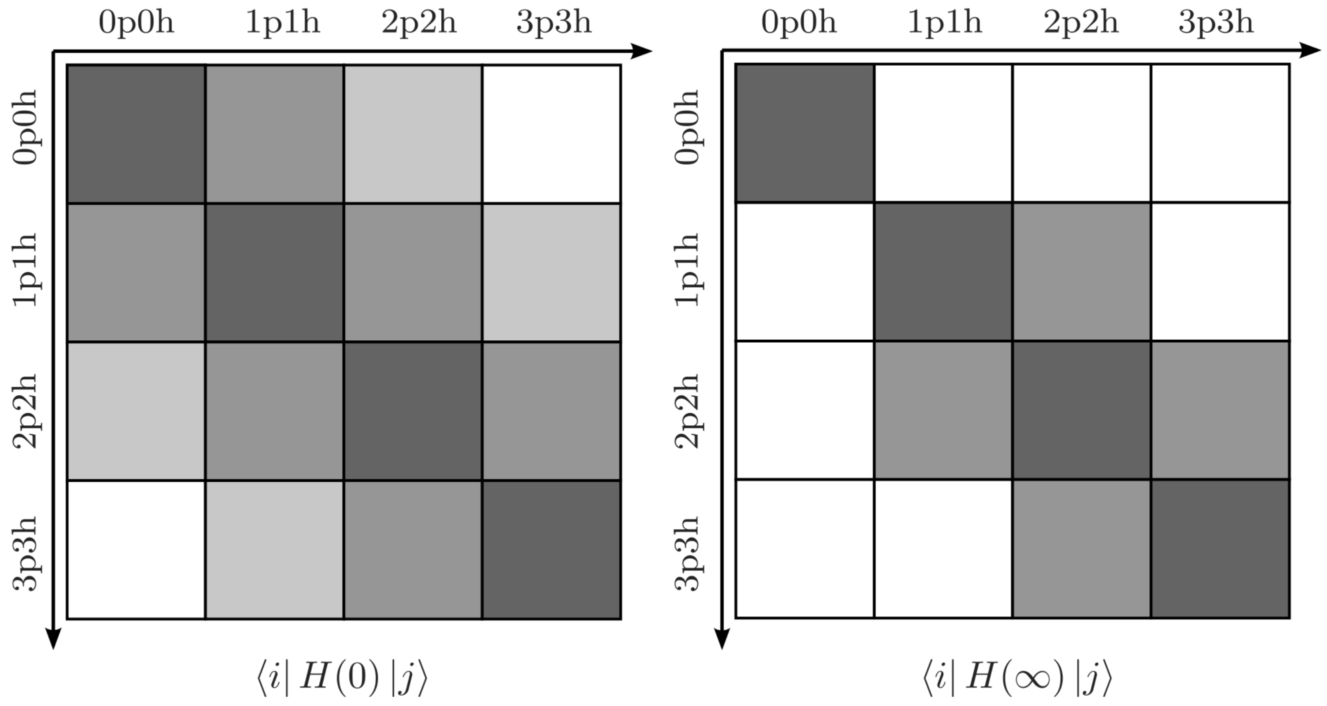
IN-MEDIUM SIMILARITY RENORMALIZATION GROUP

Tsukiyama, Bogner, Schwenk, PRL **106** (2011)

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

Goal: Efficiently extract ground-state properties from many-body Schrödinger equation

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



- Normal order with respect to reference state
- Particle-hole excitations of reference state
- Flow equation: $\dfrac{dH_s}{ds} = [\eta_s, H_s]$
- Decouple ground state from excitations

Output: Ground-state energy E_{gs}

For each set of singular values $\tilde{\boldsymbol{\alpha}} = (s_1, s_2, s_3, s_4, s_5, \ldots)$

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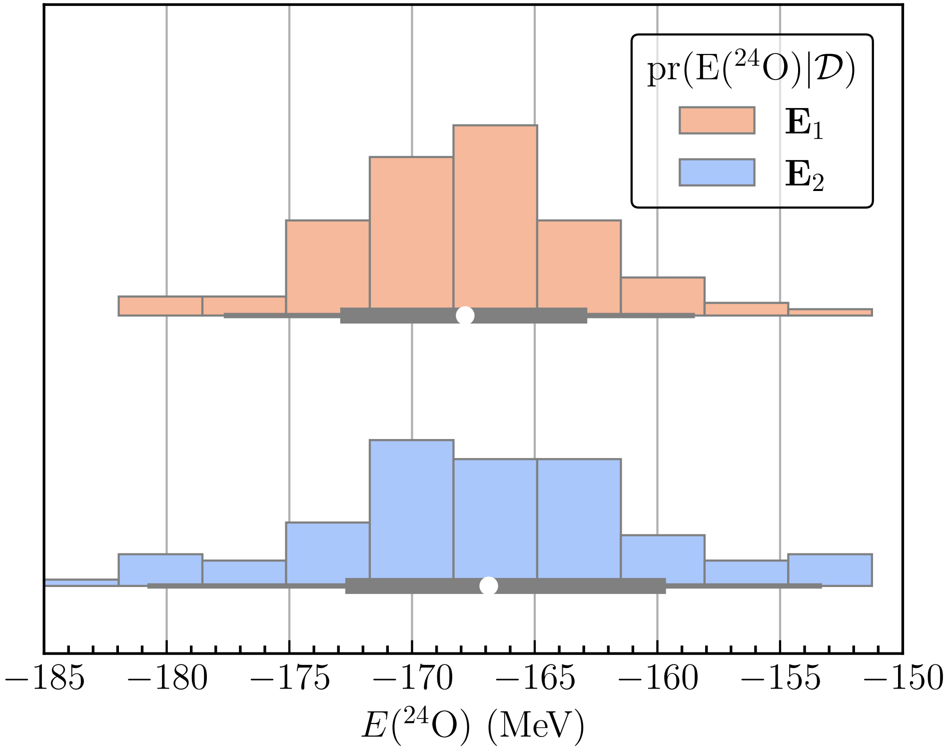
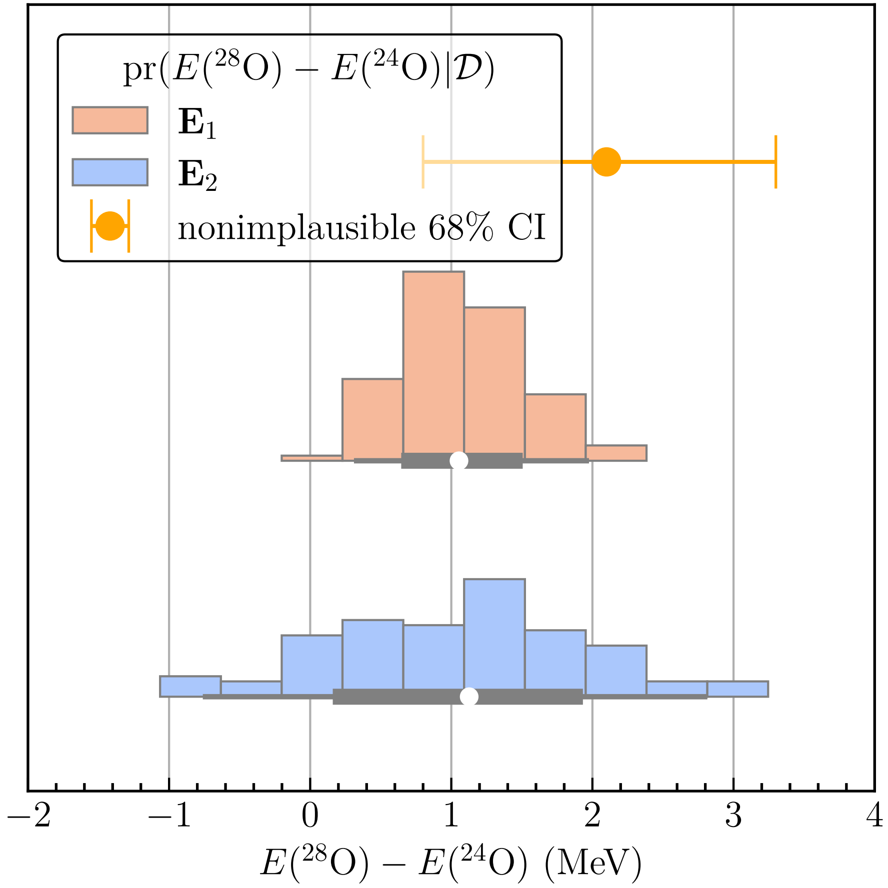
OXYGEN ISOTOPES





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COMBINING PARTIAL-WAVE DISTRIBUTIONS

- Gaussian likelihood in 6 partial waves separately: ${}^1\mathrm{S}_0, {}^3\mathrm{S}_1, {}^1\mathrm{P}_1, {}^3\mathrm{P}_0, {}^3\mathrm{P}_1, {}^3\mathrm{P}_2$ ⟶ 42 parameters
- Assume charge independence to reduce number of parameters

$$V_{nn} \approx V_{np} \approx V_{pp} - V_C$$

⟶ $6 \times 3 = 18$ different parameters (singular values) in total (3 for each partial wave)

- Combine partial wave likelihoods $\mathscr{L}_{\mathrm{NN}} = \mathscr{L}_{{}^1\mathrm{S}_0}\mathscr{L}_{{}^3\mathrm{S}_1}\mathscr{L}_{{}^1\mathrm{P}_1}\mathscr{L}_{{}^3\mathrm{P}_0}\mathscr{L}_{{}^3\mathrm{P}_1}\mathscr{L}_{{}^3\mathrm{P}_2}$

CHARGE INDEPENDENCE INFLUENCE

Observable	Configuration	^{24}O		^{28}O		^{48}Ca	
		Value	Δ	Value	Δ	Value	Δ
E (MeV)	Unchanged	−164.01	—	−162.45	—	−415.77	—
	SVD	−164.12	−0.11	−162.59	−0.14	−416.12	-0.35
	CII	−168.59	−4.58	−167.39	−4.94	−426.39	-10.62
	SVD & CII	−168.70	−4.69	−167.53	−5.08	−426.75	-10.98
R_{skin} (fm)	Unchanged	0.4764	—	0.6713	—	0.1439	—
	SVD	0.4762	−0.0002	0.6709	−0.0004	0.1439	0.0000
	CII	0.4730	−0.0034	0.6667	−0.0046	0.1444	0.0005
	SVD & CII	0.4728	−0.0035	0.6663	−0.0050	0.1444	0.0005
R_{ch} (fm)	Unchanged	2.611	—	2.765	—	3.290	—
	SVD	2.611	0.000	2.764	0.000	3.290	0.000
	CII	2.599	−0.012	2.753	−0.012	3.276	−0.013
	SVD & CII	2.599	−0.012	2.752	−0.012	3.277	−0.013

- SVD causes $< 1\,\%$ deviations
- Charge independence assumption causes $< 3\,\%$ deviation

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	CII	0.4730	−0.0034	0.6667	−0.0046	0.1444	0.0005
	SVD & CII	0.4728	−0.0035	0.6663	−0.0050	0.1444	0.0005
R_{ch} (fm)	Unchanged	2.611	—	2.765	—	3.290	—
	SVD	2.611	0.000	2.764	0.000	3.290	0.000
	CII	2.599	−0.012	2.753	−0.012	3.276	−0.013
	SVD & CII	2.599	−0.012	2.752	−0.012	3.277	−0.013

- SVD causes $< 1\,\%$ deviations $\longrightarrow$ Easy to fix
- Charge independence assumption causes $< 3\,\%$ deviation

CHARGE INDEPENDENCE INFLUENCE

Observable	Configuration	^{24}O		^{28}O		^{48}Ca	
		Value	Δ	Value	Δ	Value	Δ
E (MeV)	Unchanged	-164.01	—	-162.45	—	-415.77	—
	SVD	-164.12	-0.11	-162.59	-0.14	-416.12	-0.35
	CII	-168.59	-4.58	-167.39	-4.94	-426.39	-10.62
	SVD & CII	-168.70	-4.69	-167.53	-5.08	-426.75	-10.98
R_{skin} (fm)	Unchanged	0.4764	—	0.6713	—	0.1439	—
	SVD	0.4762	-0.0002	0.6709	-0.0004	0.1439	0.0000
	CII	0.4730	-0.0034	0.6667	-0.0046	0.1444	0.0005
	SVD & CII	0.4728	-0.0035	0.6663	-0.0050	0.1444	0.0005
R_{ch} (fm)	Unchanged	2.611	—	2.765	—	3.290	—
	SVD	2.611	0.000	2.764	0.000	3.290	0.000
	CII	2.599	-0.012	2.753	-0.012	3.276	-0.013
	SVD & CII	2.599	-0.012	2.752	-0.012	3.277	-0.013

- SVD causes $< 1\,\%$ deviations $\longrightarrow$ Easy to fix
- Charge independence assumption causes $< 3\,\%$ deviation $\longrightarrow$ Not so easy to fix