Uncertainties with low-resolution nuclear forces

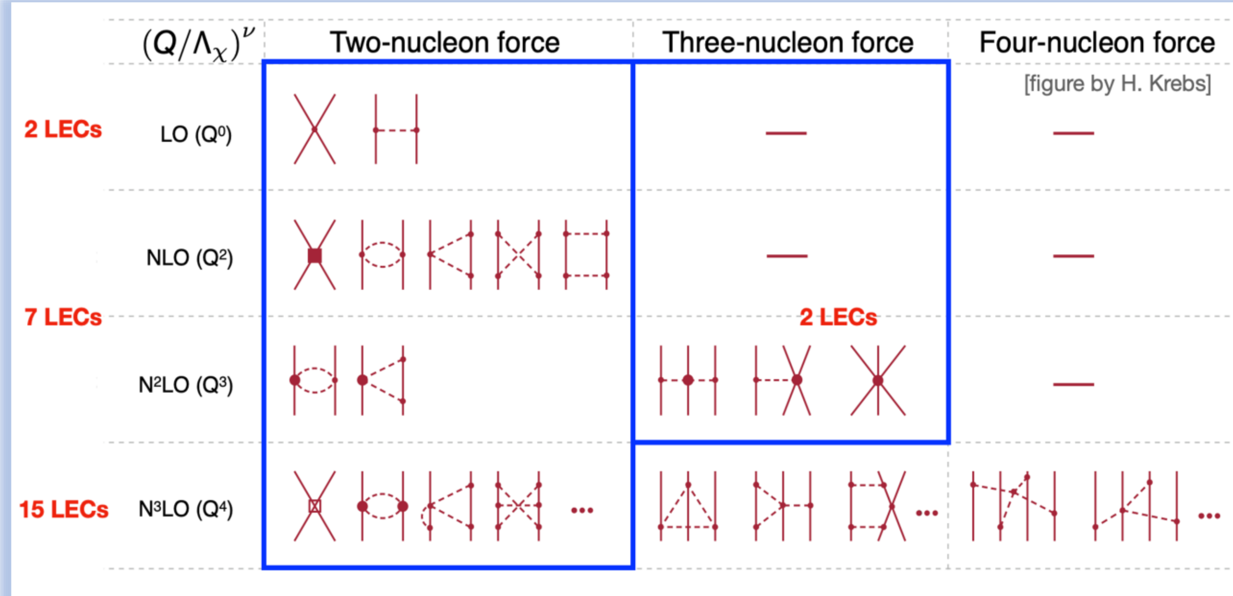
Journal club, Chenrong Ding

Nov. 26, 2025, SYSU

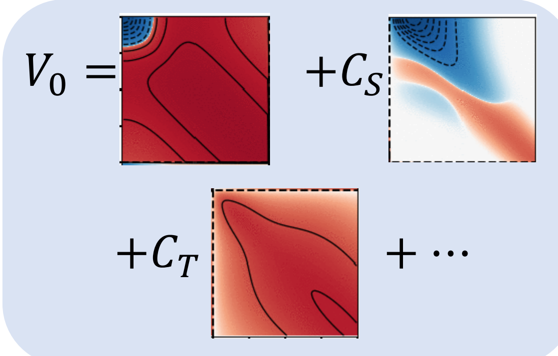
T. Plies et al., arXiv:2509.24671(2025)

Introduction

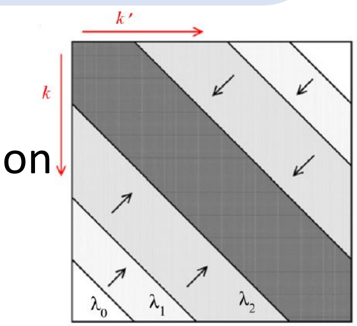
- Low-resolution nuclear Hamiltonians, obtained from chiral effective field theory (EFT) and softened using renormalization group techniques, have been very successful in nuclear structure theory.
- The associated statistical uncertainty and EFT truncation uncertainty for these potentials is difficult to quantify.



NN+3N (EM): R. Machleidt, D. R. Entem, Phys. Rep. 503, 1 (2011)



Similarity renormalization group (SRG)



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

Methods: decomposition of the potential

- **The singular value decomposition (SVD)** $\boldsymbol{V = LSR^\dagger}$
  - V is represented in the relative-momentum space
  - $L, R^\dagger$ are unitary matrix, $S = diag(s_i)$ is the nonnegative singular value matrix.

We note that $VV^\dagger = LSR^\dagger(LSR^\dagger)^\dagger = LSS^\dagger L^\dagger$, $V^\dagger V = (LSR^\dagger)^\dagger LSR^\dagger = RS^\dagger SR^\dagger$.
Thus, L and R are the eigenmatrices of $VV^\dagger$ and $V^\dagger V$, respectively.

- Rewrite the matrix V as **a linear operator structure** with the coefficients s_i and the associated operators constructed as outer products of left and right vectors $|L_i\rangle\langle R_i|$

$$\boldsymbol{V = \sum_i s_i\, |L_i\rangle\langle R_i|.}$$

This is this linear operator structure that we leverage in this work!

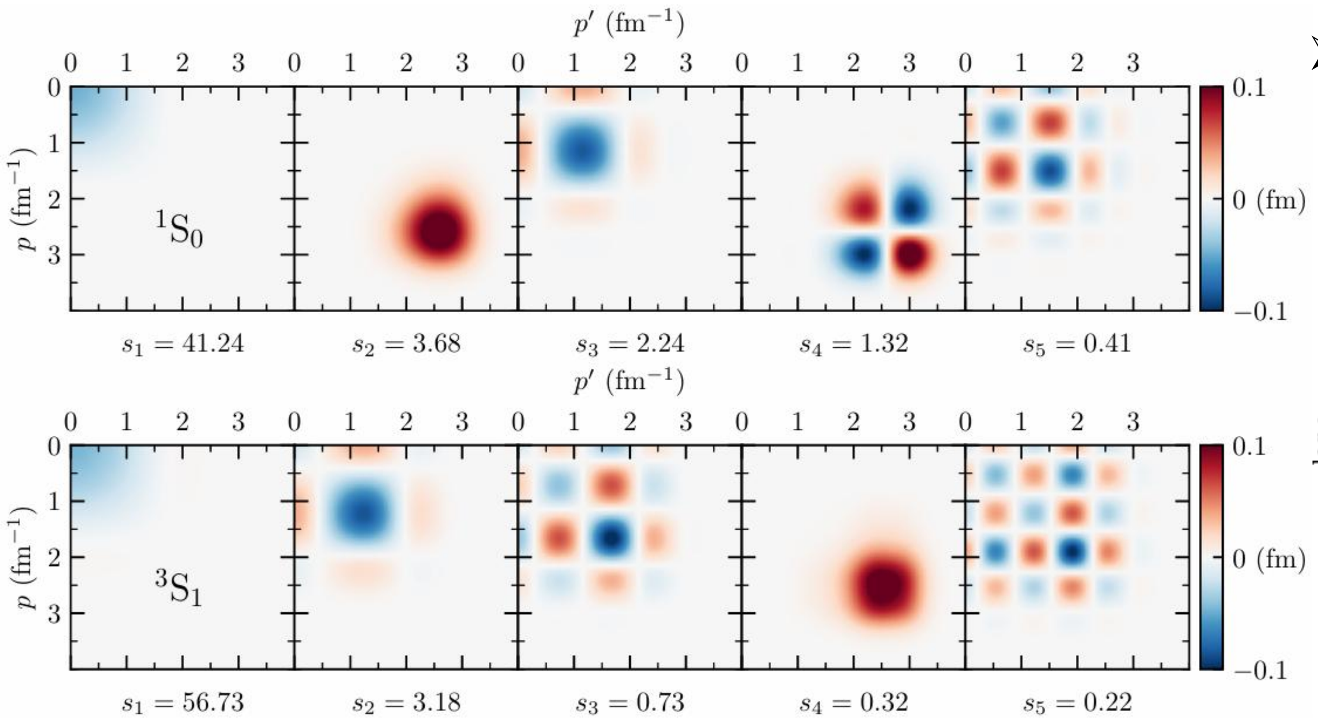
Methods: decomposition of the potential

- Decompose NN potentials in a momentum-space partial-wave basis

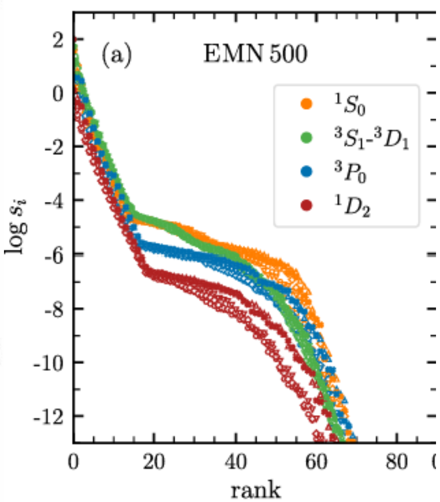
$$V(p,p') = \langle p\,(lS)JTM_T|V_{\mathrm{NN}}|p'\,(l'S)JTM_T\rangle$$

The matrix $V(p,p')$ is decomposed in each partial wave.

- First five SVD operators for N3LO EM500 $\lambda = 1.8\ \mathrm{fm}^{-1}$ potential in two partial waves.



- Singular values of EMN 500 potential as a function of SVD rank.



A. Tichai et al., Phys.Lett.B 821(2021)136623

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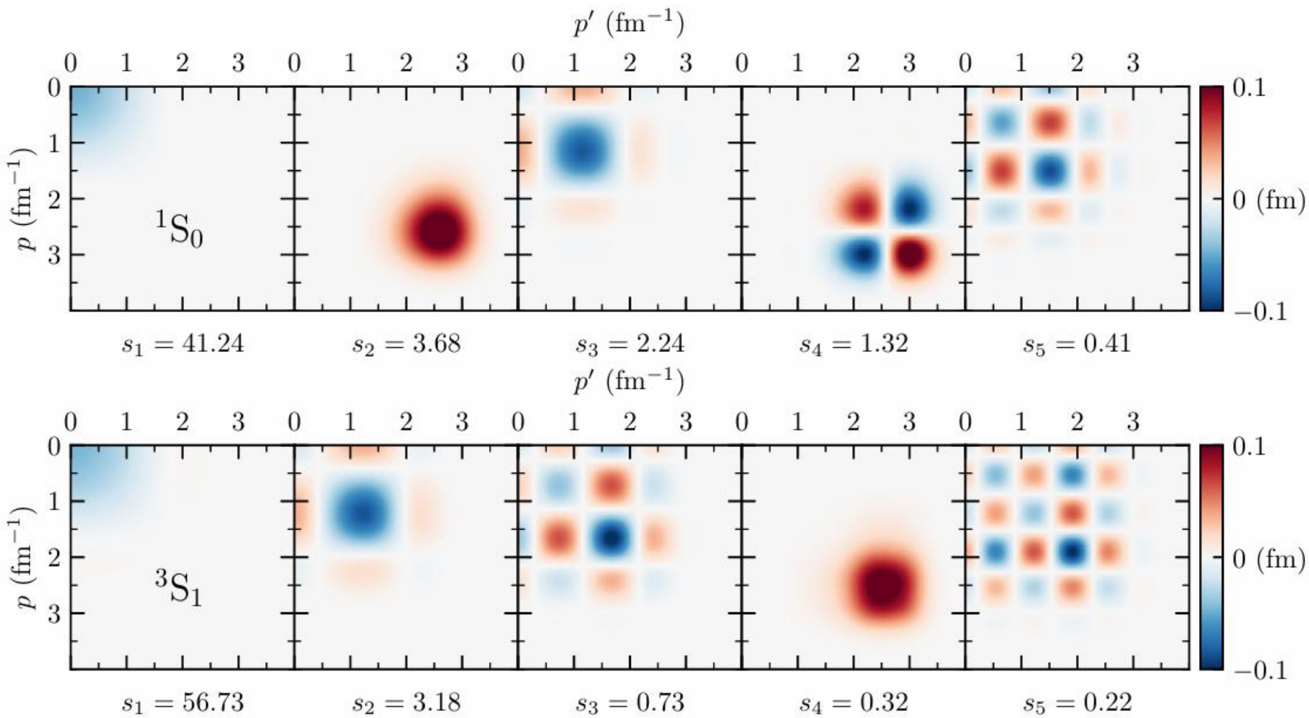


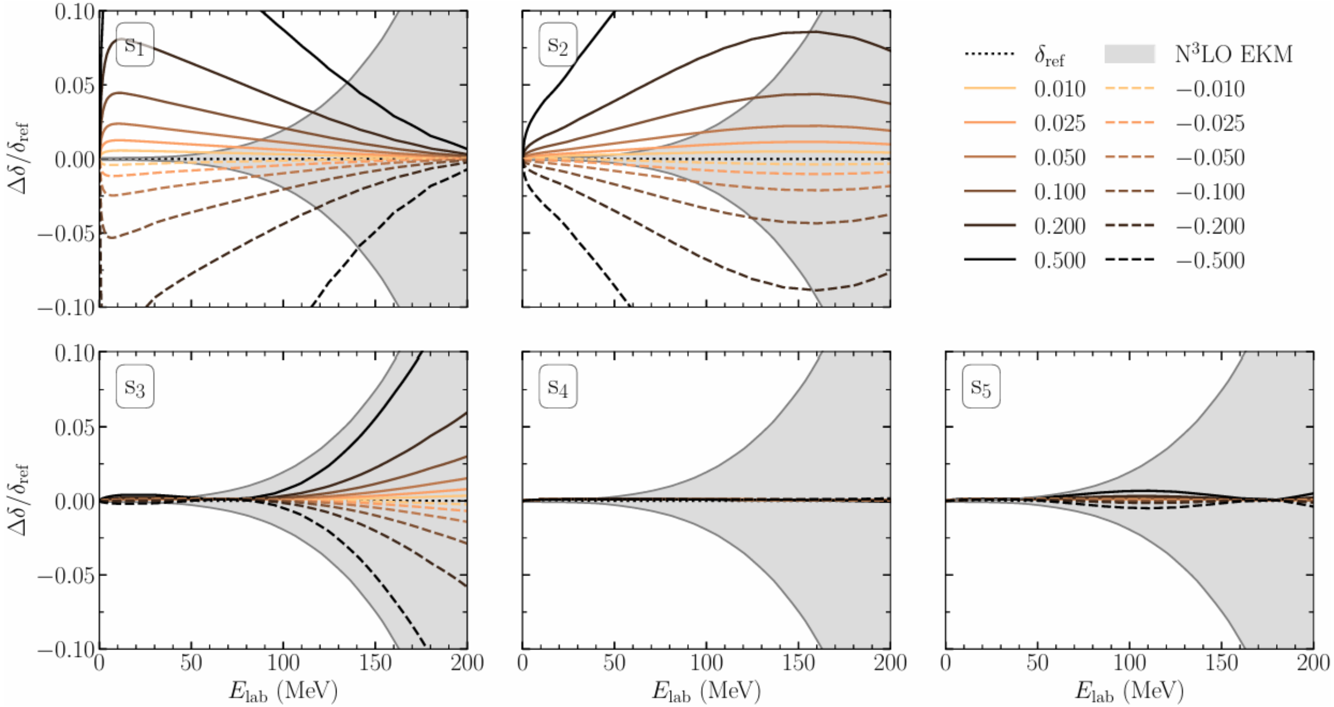
For all partial waves, the hierarchy of singular values allows us to use SVD-decomposed potentials truncated at rank five

$$\tilde{V} = \sum_{i=1}^{R_{\mathrm{SVD}}=5} s_i\,|L_i\rangle\langle R_i|$$

Treat the parameters s_i as uncertain and perform Bayesian inference for their values.

Methods: decomposition of the potential

- Vary the singular values in an interval of $[0.5s_i, 1.5s_i]$ and compute the $^3S_1$ phase shift.



- The fourth and fifth operators of this potential have negligible impact on phase shifts at energies below 200MeV.
- Still keep these operators in the potential, but keep their respective singular values fixed.

	$^1S_0$	$^3S_1$	$^1P_1$	$^3P_0$	$^3P_1$	$^3P_2$
s_1	x	x	x	x	x	x
s_2	–	x	x	–	–	x
s_3	x	x	x	–	x	x
s_4	–	–	–	x	x	–
s_5	x	–	–	–	–	–

Methods: EFT truncation uncertainty

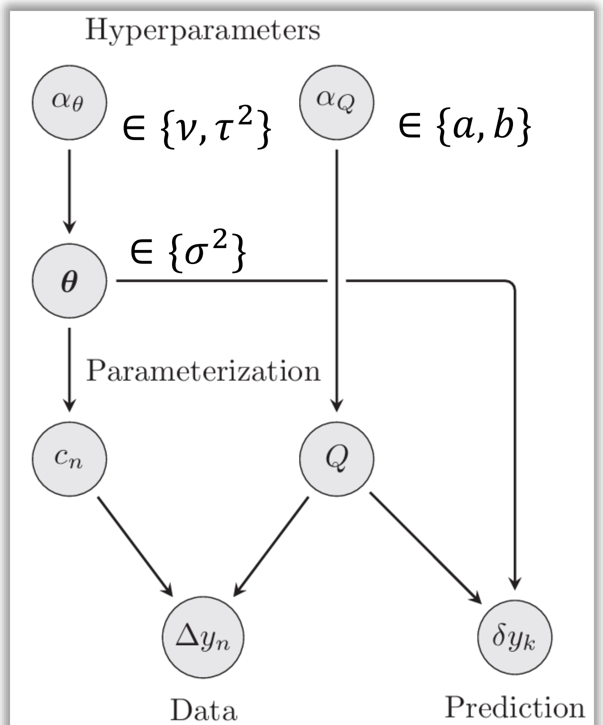
➢ How to quantify EFT uncertainties for observables? –Assume a power expansion:

$$y = y_{\rm ref} \sum_{n=0}^{\infty} c_n \left(\frac{Q}{\Lambda_b}\right)^n$$

- c_n are the dimensionless coefficients with natural size.
- Q/Λ_b is the expansion parameter.

Assume we truncate the EFT at finite order k, how to predict error $\Delta y_k \equiv y_{\rm ref} \sum_{n=k+1}^{\infty} c_n \left(\frac{Q}{\Lambda_b}\right)^n$

☐ Method 1: Bayesian inference



$$P(A|B) \propto P(B|A)P(A)$$

posterior likelihood prior

J. A. Melendez et al., Phys.Rev.C 100.044001(2019)

$\theta|\alpha_\theta \sim \chi^{-2}(\nu_0, \tau_0^2)$

Conjugate prior

$c_\theta|\theta \sim N(0, \sigma^2)$

$Q|\alpha_Q \sim Beta(a, b)$

$\Delta y_n | c_n, Q = y_{ref} c_n Q^n / \Lambda_b^n$

$$\theta|\vec{c}_k \sim \chi^{-2}(\nu, \tau^2), \nu = \nu_0 + n_k, \nu\tau^2 = \nu_0\tau_0^2 + \vec{c}_k^{\,2}$$

$$P(y_\infty|\vec{y}_k) = t_\nu\left(y_k, y_{ref}^2 \frac{Q^{2k+2}}{1-Q}\tau^2\right).$$

Here we simplify $Q/\Lambda_b \to Q$.

Methods: EFT truncation uncertainty

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Assume we truncate the EFT at finite order k, how to predict error $\Delta y_k \equiv y_{\mathrm{ref}} \sum_{n=k+1}^{\infty} c_n \left(\frac{Q}{\Lambda_b}\right)^n$

Method 2: Prescription of Epelbaum, Krebs, and Meißner(EKM)

Assume the coefficients c_n to be of natural size. The resulting uncertainty at N3LO is then given by

$$\Delta y_{\mathrm{EKM}}^{\mathrm{N^3LO}} = \max\left(\left(\frac{Q}{\Lambda_b}\right)^5 |y^{\mathrm{LO}}|,\ \left(\frac{Q}{\Lambda_b}\right)^3 |y^{\mathrm{LO}} - y^{\mathrm{NLO}}|,\right.$$
$$\left(\frac{Q}{\Lambda_b}\right)^2 |y^{\mathrm{NLO}} - y^{\mathrm{N^2LO}}|,$$
$$\left.\left(\frac{Q}{\Lambda_b}\right) |y^{\mathrm{N^2LO}} - y^{\mathrm{N^3LO}}|\right). \qquad (10)$$

- Note that we need order-by-order results to assess uncertainties this way. However, the EM interaction is only available at N3LO.

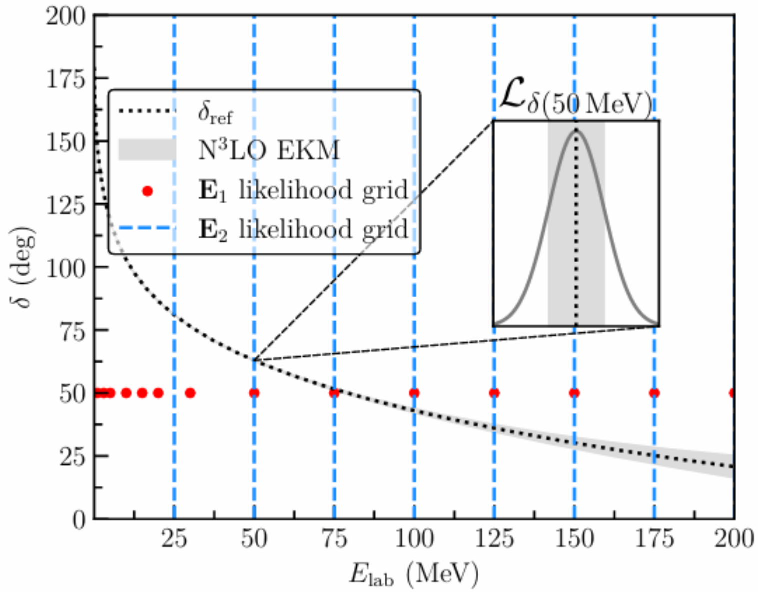
- We evolve EMN interactions to $\lambda = 2.0\mathrm{fm}^{-1}$. The EMN interactions have the same cutoff of 500MeV and the same regularization scheme, making them appropriate for estimating EFT uncertainties for the N3LO EM interaction.

Methods: Bayesian inference

- Bayes' theorem: $\mathrm{pr}(\boldsymbol{\alpha}|\mathcal{D}) \propto \mathcal{L}(\boldsymbol{\alpha})\mathrm{pr}(\boldsymbol{\alpha}) = \mathrm{pr}(\mathcal{D}|\boldsymbol{\alpha})\mathrm{pr}(\boldsymbol{\alpha})$
  - D are the observables, which are phase shifts in NN part of potential.
  - $\boldsymbol{\alpha}$ are the three (two) singular values that parametrize NN potential in a partial wave.
- Prior: uniform prior. Likelihood: Gaussian likelihood:

$$f(\boldsymbol{\alpha}, E) = \frac{1}{\Delta\delta_{\mathrm{EKM}}(E)\sqrt{2\pi}} \exp\left(-\frac{(\delta_{\boldsymbol{\alpha}}(E) - \delta_{\mathrm{ref}}(E))^2}{2[\Delta\delta_{\mathrm{EKM}}(E)]^2}\right)$$

As phase shifts are given as a function of energy, we construct a multivariate Gaussian for n different energies in the range between 0 MeV and 200 MeV.



$$\mathcal{L}(\boldsymbol{\alpha}) = \frac{1}{\sqrt{(2\pi)^n \det(\Sigma)}} \times$$

$$\exp\left(-\frac{1}{2}\left[\boldsymbol{\delta}_{\boldsymbol{\alpha}}(E) - \boldsymbol{\delta}_{\mathrm{ref}}(E)\right]^T \Sigma^{-1}\left[\boldsymbol{\delta}_{\boldsymbol{\alpha}}(E) - \boldsymbol{\delta}_{\mathrm{ref}}(E)\right]\right)$$

The definition of the covariance matrix $\sum$: **dragonized**, there is zero correlation between the phase shifts at different energies

$$\mathcal{L}_{\mathrm{NN}}(\boldsymbol{\alpha}_{\mathrm{NN}}) = \mathcal{L}_{^1\mathrm{S}_0}(\boldsymbol{\alpha}_{^1\mathrm{S}_0})\mathcal{L}_{^3\mathrm{S}_1}(\boldsymbol{\alpha}_{^3\mathrm{S}_1})\mathcal{L}_{^1\mathrm{P}_1}(\boldsymbol{\alpha}_{^1\mathrm{P}_1}) \times \mathcal{L}_{^3\mathrm{P}_0}(\boldsymbol{\alpha}_{^3\mathrm{P}_0})\mathcal{L}_{^3\mathrm{P}_1}(\boldsymbol{\alpha}_{^3\mathrm{P}_1})\mathcal{L}_{^3\mathrm{P}_2}(\boldsymbol{\alpha}_{^3\mathrm{P}_2})$$

Methods: Bayesian inference

- For the 3N part, we limit ourselves to varying the two short-range LECs c_D and c_E and leave the long-range LECs unchanged.

- 3N Likelihood: Gaussian likelihood and the covariance matrix $(\Sigma)_{ij} = \left[\frac{(y_{\mathrm{EM}}\bar{c}(\frac{Q}{\Lambda_b})^{k+1})^2}{1-(\frac{Q}{\Lambda_b})^2}\right]\delta_{ij}$

$$\mathcal{L}_{3\mathrm{N}}(c_D, c_E, \boldsymbol{\alpha}_{\mathrm{NN}}) = \mathcal{N}(\boldsymbol{y}_{\mathrm{ref}}, \Sigma)\,, \quad \boldsymbol{y}_{\mathrm{ref}} = (E(^3\mathrm{H})_{\mathrm{ref}}, fT_{1/2_{\mathrm{ref}}})$$

	y_{ref}	y_{EM}	σ	Experiment
$E(^3\mathrm{H})$ (MeV)	-8.69	-8.48	0.11	-8.48 [48]
$fT_{1/2}$ (s)	1228.76	1227.72 [46]	16.09	1129.6 [49]

Follow the Bayes' theorem,

$$\mathrm{pr}(c_D, c_E, \boldsymbol{\alpha}_{\mathrm{NN}} | E(^3\mathrm{H}), fT_{1/2}) \propto \mathrm{pr}(E(^3\mathrm{H}), fT_{1/2} | c_D, c_E, \boldsymbol{\alpha}_{\mathrm{NN}})\, \mathrm{pr}(c_D, c_E, \boldsymbol{\alpha}_{\mathrm{NN}})$$

- Combine the likelihoods of NN and 3N interaction: $\mathcal{L}(c_D, c_E, \boldsymbol{\alpha}_{\mathrm{NN}}) = \mathcal{L}_{\mathrm{NN}}(\boldsymbol{\alpha}_{\mathrm{NN}})\mathcal{L}_{3\mathrm{N}}(c_D, c_E, \boldsymbol{\alpha}_{\mathrm{NN}})\,.$

  Select 2 sets of energy grids about the phase shifts:

$$\mathbf{E}_1 = (1, 3, 5, 10, 15, 20, 30, 50, 75, 100, 125, 150, 175, 200)\ \mathrm{MeV}\,, \qquad \mathbf{E}_2 = (25, 50, 75, 100, 125, 150, 175, 200)\ \mathrm{MeV}\,.$$

  Use MCMC to obtain 500,000 samples, and subsample $N = 100$ samples.

Model checking: Posterior predictive distributions

Using the sampled values for the parameters $\tilde{\alpha}$, compute the PPDs $= \{\mathbf{y}(\tilde{\alpha}) : \tilde{\alpha} \sim \mathrm{pr}(\tilde{\alpha}|\mathcal{D})\}$

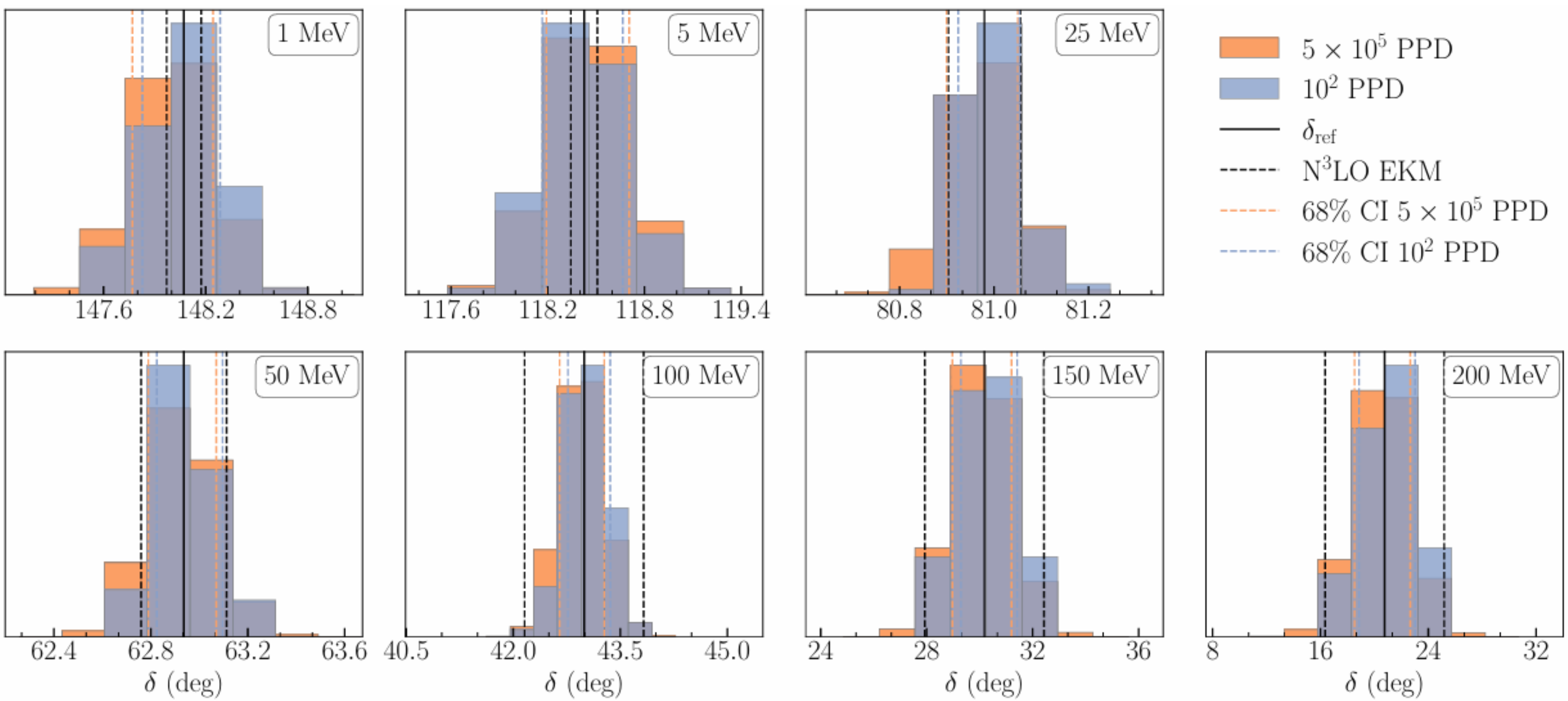


FIG. 5. Comparison of phase shifts PPDs in the $^3S_1$ partial wave for all 5×10^5 samples (red) and for the resampled 10^2 samples (blue) at different energies. Results were obtained using the $\mathbf{E}_2$ likelihood. The red and blue dashed lines show the corresponding 68% confidence intervals. The solid black line represents the reference phase shifts obtained by using the SVD-decomposed N^{3}LO EM 500 $\lambda = 1.8\,\mathrm{fm}^{-1}$ interaction at rank five. The black dashed lines represent the EKM uncertainty at N^{3}LO.

The results from 500,000 samples and 100 samples are similar, This validates our approximation to use only a fraction of the initial samples.

Model checking: Posterior predictive distributions

Using the sampled values for the parameters $\widetilde{\boldsymbol{\alpha}}$, compute the PPDs $= \{\mathbf{y}(\tilde{\boldsymbol{\alpha}}) : \tilde{\boldsymbol{\alpha}} \sim \mathrm{pr}(\tilde{\boldsymbol{\alpha}}|\mathcal{D})\}$

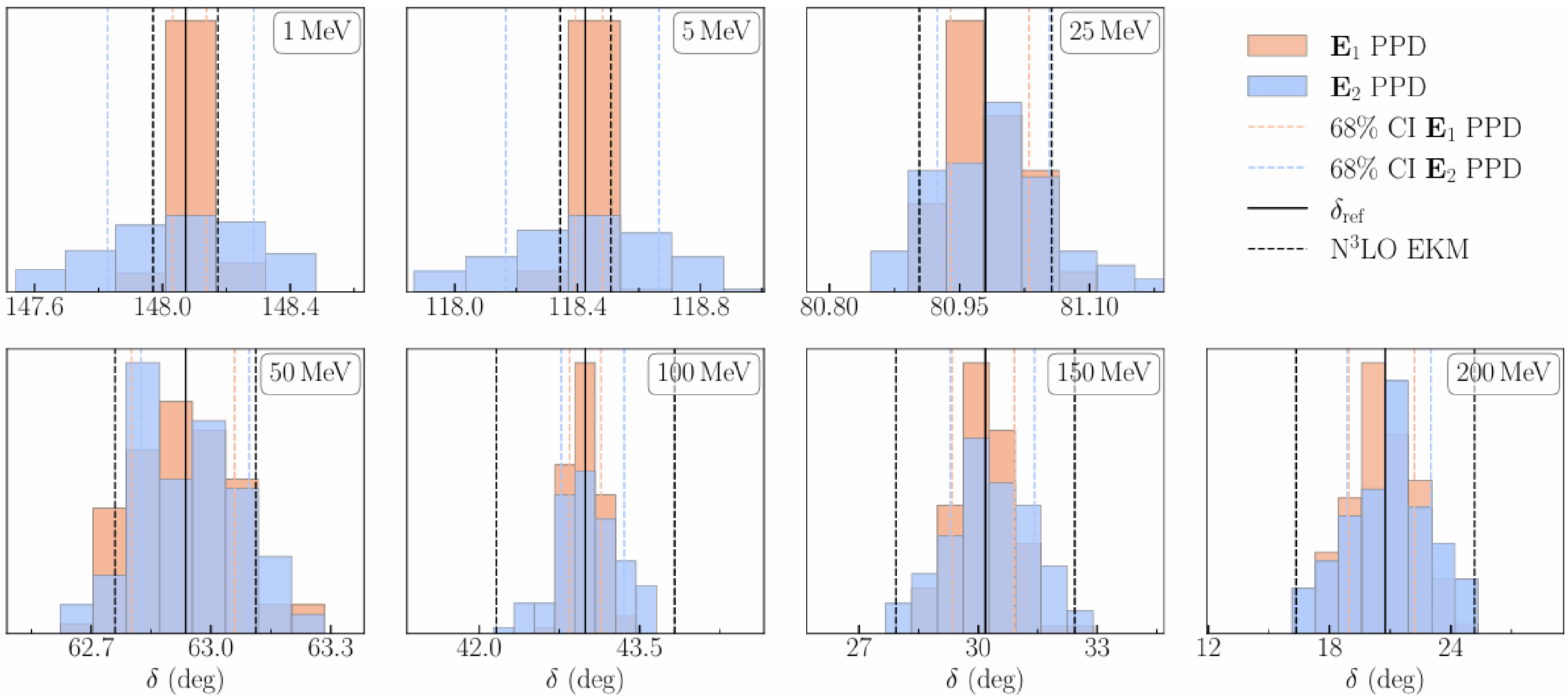


FIG. 6. Comparison of phase shifts PPDs in the $^3S_1$ partial wave using the $\mathbf{E}_1$ likelihood (orange) and the $\mathbf{E}_2$ likelihood (blue) at different energies. Shown are the 100 subsamples. The orange and blue dashed lines show the corresponding 68% confidence intervals. The solid black line represents the reference phase shifts obtained by using the EM 500 $\lambda = 1.8\,\mathrm{fm}^{-1}$ interaction at N^{3}LO in SVD decomposition up to rank five. The black dashed lines represent the EKM uncertainty at N^{3}LO.

At energies below 25MeV, the E_2 results overpredict the EKM uncertainty while E_1 distributions underpredict, and both underpredict EFT uncertainties at energies above 25MeV.

Stronger constraints on low-energy phase shifts result in stronger constraints at higher energies.

Application: Medium mass nuclei

➢ Examine the impact of the two hypotheses on the computed results of the observables.

SVD: limit $R_{SVD} = 5$

CII: charge-independence assumption $V_{nn} \approx V_{np} \approx V_{pp} - V_C$

Observable	Configuration	^{24}O Value	^{24}O Δ	^{28}O Value	^{28}O Δ	^{48}Ca Value	^{48}Ca 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

Uncertainties caused by the SVD truncation are always below 1%. The charge-independence assumption causes deviations of up to 3% for energies.

Since we are more concerned with uncertainty estimates than reproducing the exact values for observables, this accuracy is sufficient.

Application: Medium mass nuclei

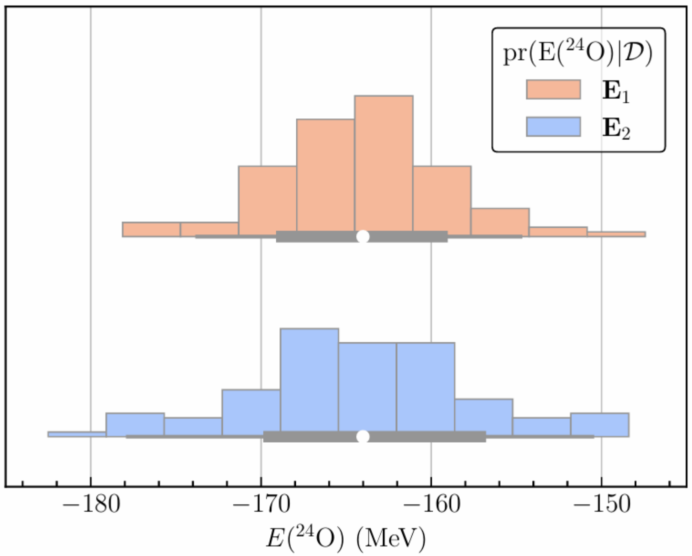


FIG. 11. PPDs for the ground-state energy of ^{24}O from the $\mathbf{E}_1$ and $\mathbf{E}_2$ likelihoods. The white dot shows the median while the thick and thin gray bars represent the 68% and 95% confidence intervals respectively. Note that the medians were shifted to reproduce the 1.8/2.0 (EM) interaction predictions.

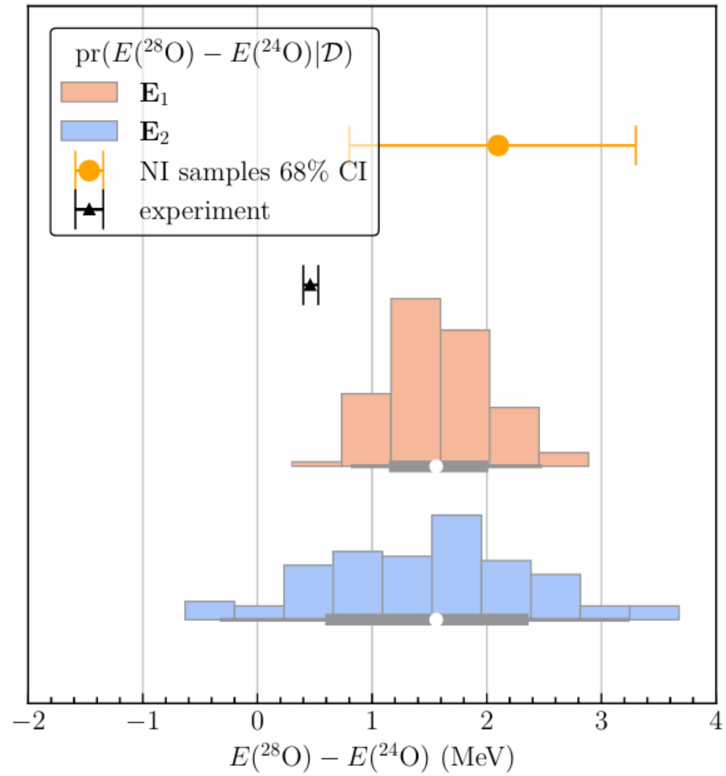
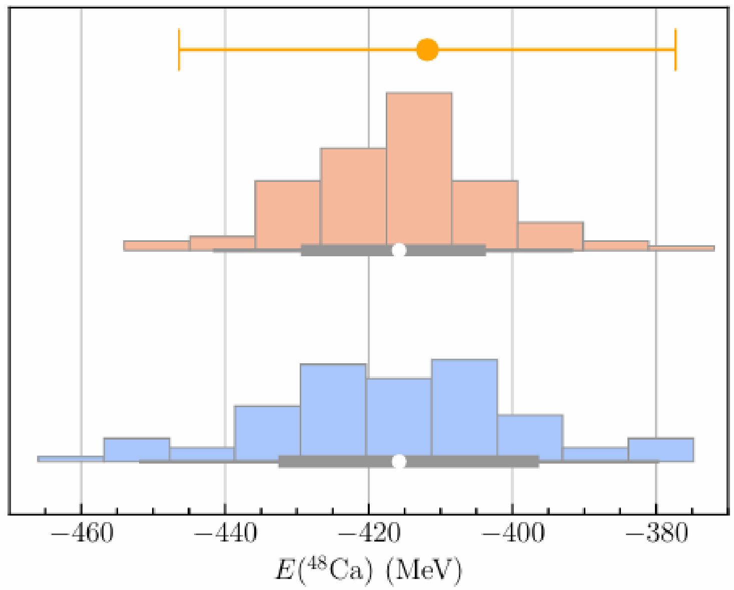
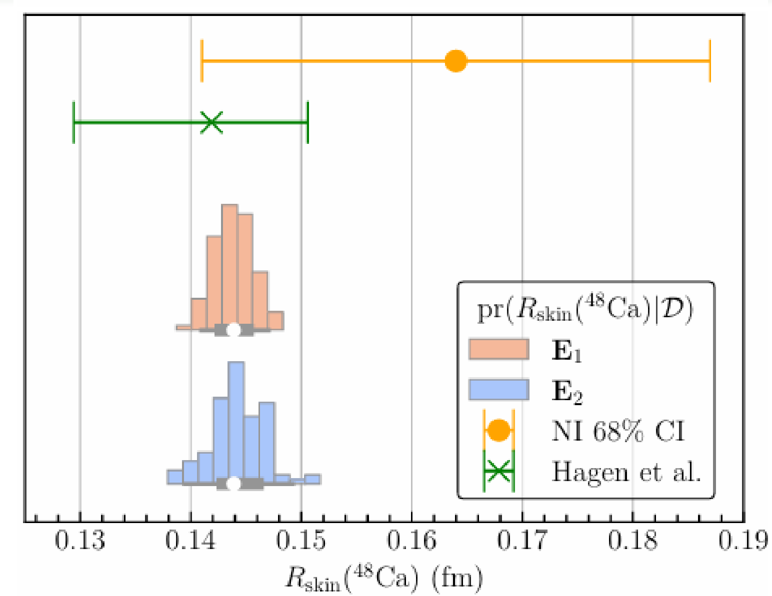


FIG. 12. PPDs for the difference between the ground-state energies of ^{28}O and ^{24}O from the $\mathbf{E}_1$ and $\mathbf{E}_2$ likelihoods. The white dot shows the median while the thick and thin gray bars represent the 68% and 95% confidence intervals respectively. Note that the medians were shifted to reproduce the 1.8/2.0 (EM) interaction predictions. The black triangle is experiment [11], and the orange dot and error bar represent the median and 68% confidence interval of the 121 nonimplausible samples from [11].

- O28 is a slightly unbound system.
- For the 4-neutron separation energy, the difference between E_1 and E_2 is even more significant. So shift the median values to the EM1.8-2.0 prediction.

Application: Medium mass nuclei





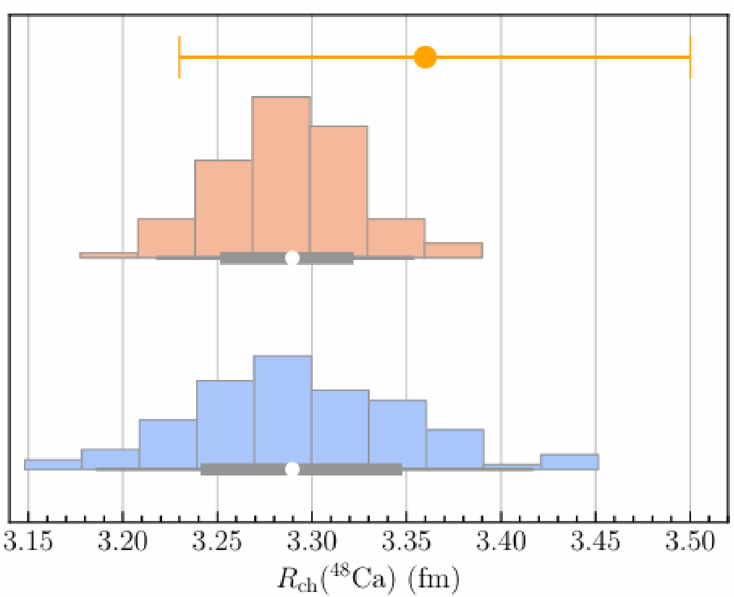


TABLE V. Uncertainty quantified predictions for ^{24}O, ^{28}O, and ^{48}Ca observables. The results are summarized by the medians and the 68% confidence intervals. In this table, results are not shifted to the median of the unchanged 1.8/2.0 (EM) Hamiltonian.

Nucleus	Observable	$\mathbf{E}_1$	$\mathbf{E}_2$
^{24}O	E (MeV)	$-167.83^{+4.98}_{-5.09}$	$-166.87^{+7.22}_{-5.85}$
^{28}O	E (MeV)	$-166.84^{+4.43}_{-4.71}$	$-165.76^{+5.89}_{-5.65}$
$^{28}\mathrm{O} - {}^{24}\mathrm{O}$	ΔE (MeV)	$1.06^{+0.45}_{-0.41}$	$1.13^{+0.81}_{-0.97}$
^{48}Ca	E (MeV)	$-424.45^{+12.07}_{-13.61}$	$-421.61^{+19.43}_{-16.78}$
	R_{skin} (fm)	$0.1455^{+0.0018}_{-0.0017}$	$0.1449^{+0.0027}_{-0.0016}$
	R_{ch} (fm)	$3.288^{+0.032}_{-0.038}$	$3.288^{+0.058}_{-0.048}$

Summary and outlook

Develop a framework to **quantify EFT truncation uncertainties** for **low-resolution interactions.**

- Obtain a linear operator structure for SRG-evolved NN interactions through singular value decompositions.

- Perform Bayesian inference for the underlying singular values.
  - Construct the likelihood for the inference from predictions for NN scattering phase shifts in S- and P-waves and for the triton energy and comparative half life.
  - For NN phase shifts, consider two likelihoods E_1 and E_2, both using phase shifts at energies up to 200MeV.

The NN phase shifts did not exactly reproduce the likelihood. The **limited amount of independent operators** in each partial wave and **untreated correlations in phase shifts** are responsible for this.

- For full uncertainty quantification in nuclear structure calculations, **the parametric uncertainty** must be augmented with **additional EFT truncation and many-body method uncertainties**.

- A key challenge here is that these three uncertainties are all **correlated**, but this correlation is challenging to study quantitatively.

Thank you for your attention!