Emulating light hypernuclei for calibration of hypernuclear interactions

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Introduction

Introduction

Strangeness physics

- Interdisciplinary field connecting particle physics, nuclear physics, and astrophysics
- **One of its major goals is to understand the elusive interaction of hyperons with nucleons and the nuclear medium**

Theoretical analysis of hypernuclei

- Using **'effective'** *YN* interaction models & mean-field / shell-model approaches – successful but difficult to link with the underlying free-space *YN* interaction, limited predictive power
- Using **'realistic'** (free-space) *YN* interaction models ...

Constraining YN interactions

- **YN scattering** – 'pure' but very difficult to realize, sparse database with large uncertainties (J-PARC)
- **Final-state interactions** in hyperon photoproduction (CLAS)
- **Lattice QCD** (HAL QCD, NPLQCD)
- Heavy-ion collisions – **production and decays** of light hypernuclei, **correlation femtoscopy** (HADES, ALICE, STAR)
- **Hypernuclei** – precise spectroscopy of hypernuclear energy levels

Introduction

Theoretical analysis of hypernuclei using realistic YN interactions

- Combines modern developments of *YN* interactions based on χ**EFT** and **ab initio** few- and many-body approaches
- Computationally demanding $\rightarrow$ can reveal deficiencies of existing *YN* interaction models

Calibration of YN interaction models using hypernuclei?

- Quantify **method uncertainties** associated with the solution of the many-body problem
- Quantify **nuclear model uncertainties** associated with the choice of the nuclear interaction
- **Overcome the computational demands** – large number of evaluations
- **Sensitivity analysis** - hypernuclear spectra **might not be sensitive** to certain parameters (LECs) of the *YN* interaction models
- **Simultaneous fitting** of scattering observables is likely inevitable

Ab initio calculations of light hypernuclei

Ab initio calculations of light hypernuclei

- Ab initio methods aim to solve the (hyper)nuclear many-body problem starting from realistic (free-space) interactions exactly or with controlled approximations

No-core shell model

- Quasi-exact method to solve the few- and many-body Schrödinger equation

$$\left(\sum \frac{\hat{\mathbf{p}}_i^2}{2m_i} + \sum \hat{V}_{NN;ij} + \sum \hat{V}_{NNN;ijk} + \sum \hat{V}_{YN;ij} \right) \Psi = E\Psi$$

[Navrátil et al., JPG 36, 083101 (2009); DG et al., FBS 55, 857 (2014); Wirth et al., PRL 113, 192502 (2014); Le et al., EPJA 56, 301 (2020)]

- Wave function is expanded and Hamiltonian is diagonalized in a *finite* A-particle harmonic oscillator (HO) basis

$$\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_A) = \sum_{N \leq N_{max}} \Phi^{HO}_{N,\omega}(\mathbf{r}_1, \ldots, \mathbf{r}_A)$$

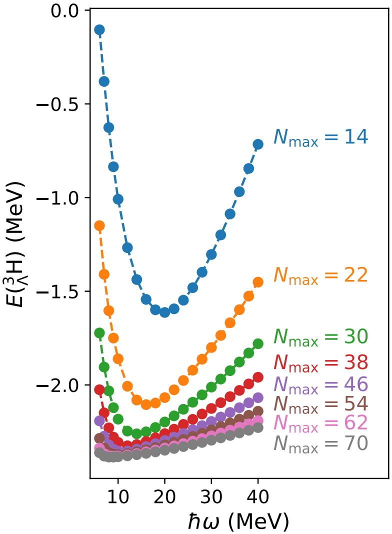
Converges to exact results for $N_{max} \to \infty$, independent of ω

- Input *NN*+*NNN* and *YN* interactions derived from χEFT

Method uncertainties

Method uncertainties

- Method uncertainties associated with convergence of the solution of the many-body problem



- NCSM-calculated energies typically exhibit undesired dependence on the HO basis frequency $\hbar\omega$ and truncation N_{max}
- Convergence properties of observables calculated in finite HO bases are rather well understood [Wendt et al., PRC 91, 061391 (2015)]
  - NCSM model-space parameters $(N_{max}, \hbar\omega)$ recast into infrared (IR) and ultraviolet (UV) scales (L_{IR}, Λ_{UV})
  - In a regime with negligible UV corrections, IR corrections are universal

$$E(L_{IR}) = E_\infty + a_0 \exp(-2\kappa_\infty L_{IR}) + \cdots$$

Ab initio calculations of light hypernuclei: method uncertainties

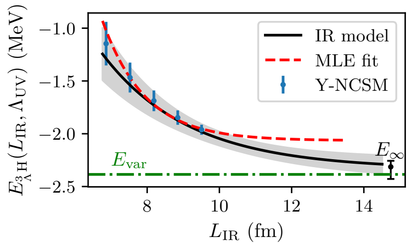
[DG, Htun, Forssén, PRC 106, 054001 (2022)]

- **Infrared extrapolation formulated as a Bayesian inference problem**

$$E(L_{\mathrm{IR}}) = E_\infty + \Delta E_{\mathrm{IR}} \exp(-2\kappa_\infty \Delta L_{\mathrm{IR}}) \times \left(1 + \frac{\epsilon_{\mathrm{NLO}}}{\kappa_\infty (L_{\mathrm{IR,\,max}} + \Delta L_{\mathrm{IR}})}\right),$$

with data $\mathcal{D} = \{E(L_{\mathrm{IR,i}})\}$ calculated in different model spaces and $\vec{\epsilon}_{\mathrm{NLO}} \sim N(0, \Sigma(\bar{\epsilon}, \rho))$ providing a stochastic model for the NLO energy correction

- Validation for ${}^3_\Lambda$H



- **Method uncertainty** quantified by 68 % credible interval for the extrapolated energy E_∞

	B_Λ^{Exp} (MeV)	B_Λ^{th} (MeV) median	68 % $\mathrm{CI}_{\mathrm{method}}$
${}^3_\Lambda$H	0.164(43)	0.166	$[-0.001, +0.001]$
${}^4_\Lambda$H	2.157(77)	2.78	$[-0.01, +0.01]$
${}^4_\Lambda$He	2.39(3)	2.76	$[-0.01, +0.01]$
${}^5_\Lambda$He	3.12(2)	6.03	$[-0.28, +0.18]$
${}^4_\Lambda$H; 1^+	1.067(80)	1.75	$[-0.12, +0.10]$
${}^4_\Lambda$He; 1^+	0.984(50)	1.71	$[-0.13, +0.10]$

Model uncertainties

Ab initio calculations of light hypernuclei: model uncertainties

- **Dominating source of uncertainty** of hypernuclear observables likely comes from the underlying *YN* interaction $\leftarrow \chi$EFT truncation, regulator artifacts, calibration data uncertainties
- Energy levels of light hypernuclei are also sensitive to details of the employed nuclear *NN*+*NNN* interactions
  - One can naively expect that calculated Λ separation energies should be insensitive to the choice of nuclear interaction, $B_\Lambda = E(^{A}Z) - E(^{A}_{\Lambda}Z)$
  - A rather weak residual dependence of B_Λ was found using a limited set of phenomenological [Nogga et al., PRL 88, 172501 (2002)] and χEFT [Le et al., EPJA 56, 301 (2020)] *NN* interactions

Ab initio calculations of light hypernuclei: model uncertainties

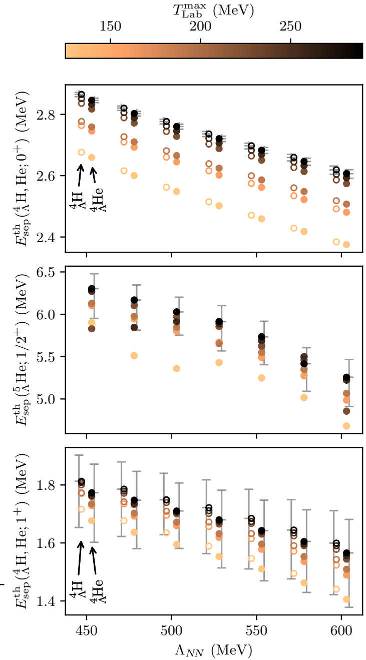
- To expose the magnitude of systematic **nuclear-model uncertainties** in B_Λ we employed the NNLO$_{\text{sim}}$ family of 42 different nuclear *NN*+*NNN* interactions [Carlsson et al., PRX 6, 011019 (2016)]

- **Uncertainty** connected to the choice of nuclear Hamiltonian quantified by variance, $\sigma^2(\text{NNLO}_{\text{sim}})$, of predictions for B_Λ

- For LO *YN*:

	$^{3}_{\Lambda}$H	$^{4}_{\Lambda}$H	$^{4}_{\Lambda}$He	$^{4}_{\Lambda}$H$_{1^+}$	$^{4}_{\Lambda}$He$_{1^+}$	$^{5}_{\Lambda}$He
σ_{model} (keV)	20	80	80	70	70	360

[DG, Htun, Forssén, PRC 106, 054001 (2022)]

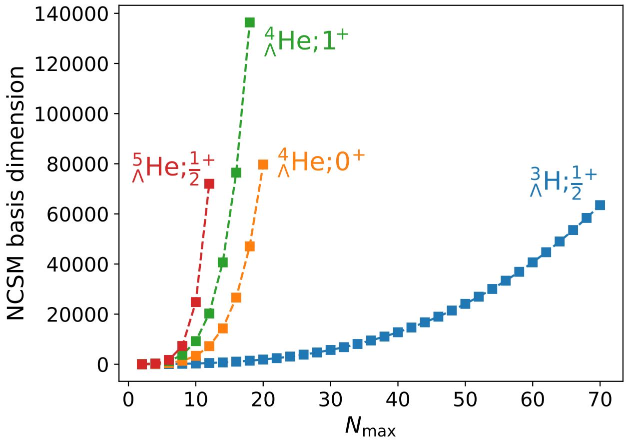


- Cf. a smaller *NN*+*NNN*-model dependence was found for NLO and NNLO *YN* interactions [Le et al., EPJA 60, 3 (2024)]

Emulating ab initio NCSM calculations

Emulating ab initio NCSM calculations

- **Ab initio methods provide a reliable link between the properties of hypernuclei and the underlying hyperon–nucleon interactions**
- Is it possible to directly incorporate them in optimization of hyperon–nucleon forces which require a large number of model evaluations?

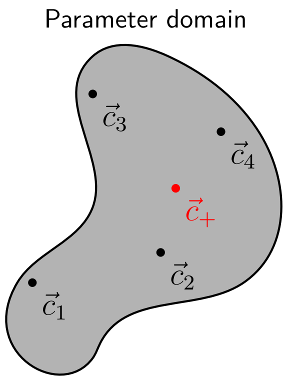


- This is not feasible for their computational cost
  (Cf. reoptimization of 2 LECs to the *p*-shell hypernuclei Λ separation energies [Knoll, Roth, PLB 846, 138258 (2023)])

Emulating ab initio NCSM calculations

- **Eigenvector continuation** is based on the fact that when a Hamiltonian depends smoothly on some real-valued control parameter(s), any eigenvector is a smooth function of that parameter(s) and its trajectory is confined to a very low-dimensional subspace

  [Frame et al., PRL 121, 032501 (2018); König et al., PLB 810, 135814 (2020)]



- Write the Hamiltonian in a **linearized** form

$$H(\vec{c}) = H_0 + \sum c_i H_i$$

- Select 'training' points $\{\vec{c}_i\}$ and solve the exact problem $H(\vec{c}_i)\,|\psi_i\rangle = E_i\,|\psi_i\rangle$
- **Project the Hamiltonian onto the subspace of training eigenvectors** $\{|\psi_i\rangle\}$ and diagonalize the generalized eigenvalue problem

$$\tilde{H}(\vec{c}_+)\,|\tilde{\psi}\rangle = \tilde{E}_+\tilde{N}\,|\tilde{\psi}\rangle\,,$$

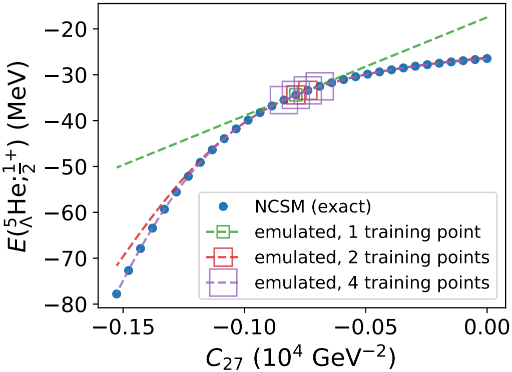
  where $\tilde{H}_{ij} = \langle\psi_i|H(\vec{c}_+)|\psi_j\rangle$, $\tilde{N}_{ij} = \langle\psi_i|\psi_j\rangle$ and $\tilde{E}_+$ approximates E_+

Emulating ab initio NCSM calculations: eigenvector continuation

- Hypernuclear Hamiltonian with LO YN interactions can be linearized,

$$H = H_0 + C_{27}V_{27} + C_{10^*}V_{10^*} + C_{10}V_{10} + C_{8a}V_{8a} + C_{8s}V_{8s},$$

where C_is are the 5 independent $\mathrm{SU}_f(3)$ LECs and H_0 contains the kinetic energy, NN+NNN interactions, and hypernuclear meson-exchange and Coulomb interactions

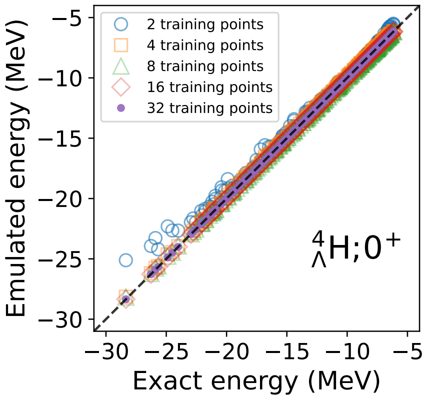


- ${}^5_\Lambda\mathrm{He}$; $\frac{1}{2}^+$, model space truncation $N_{\mathrm{max}} = 12$
- Vary one LEC, C_{27}, within $\pm100\,\%$ relative variation with respect to the nominal LOYN(Λ_{YN}=600 MeV) value
- Select 1, 2, 4 exact NCSM eigenvectors to construct the emulators

- Accurate and lighting-fast emulation of ab initio NCSM calculations

Emulating ab initio NCSM calculations: cross validation

- Select 2, 4, 8, 16, 32 points in the 5-dimensional space of LO *YN* LECs using the Latin hypercube space-filling design in a $\pm 20\,\%$ domain around the nominal values to train the emulators
- Select randomly 256 exact NCSM calculations within the same domain of LECs



- We can achieve relative accuracy of $|\delta_{\rm rel}| < 1, 0.1, 0.002\,\%$ using 8, 16, 32 training points

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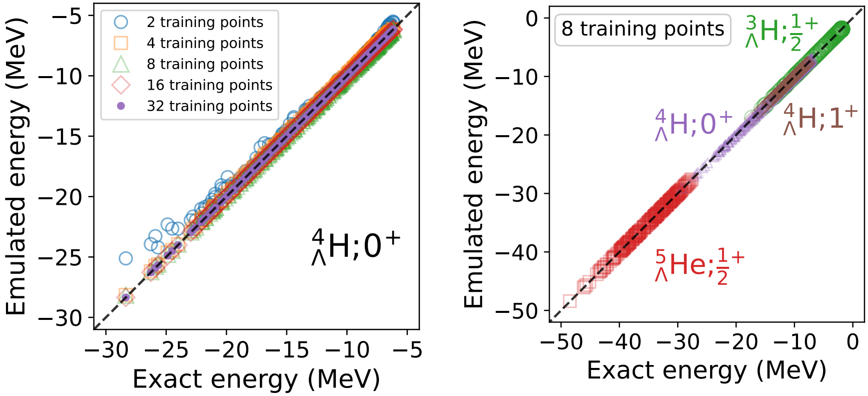

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Global sensitivity analysis of hypernuclear spectra

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Global sensitivity analysis

- Allows to identify the most influential LECs of χEFT YN interactions which determine the hypernuclear energy spectra

- For an output $Y = f(\vec{\alpha})$ of a model f, we decompose the total variance as

$$\mathrm{Var}\,[Y] = \sum_{i=1}^{d} V_i + \sum_{i<j=1}^{d} V_{ij} + \cdots\,,$$

where

$$V_i = \mathrm{Var}\,[E_{\vec{\alpha}\sim(\alpha_i)}[Y|\alpha_i]],$$
$$V_{ij} = \mathrm{Var}\,[E_{\vec{\alpha}\sim(\alpha_i,\alpha_j)}[Y|\alpha_i,\alpha_j]] - V_i - V_j,$$

are variances of conditional expectation of Y

- The variance integrals are computed by using quasi-MC sampling, including 95 % confidence intervals
- The first-, second-, and higher-order (Sobol') sensitivity indices

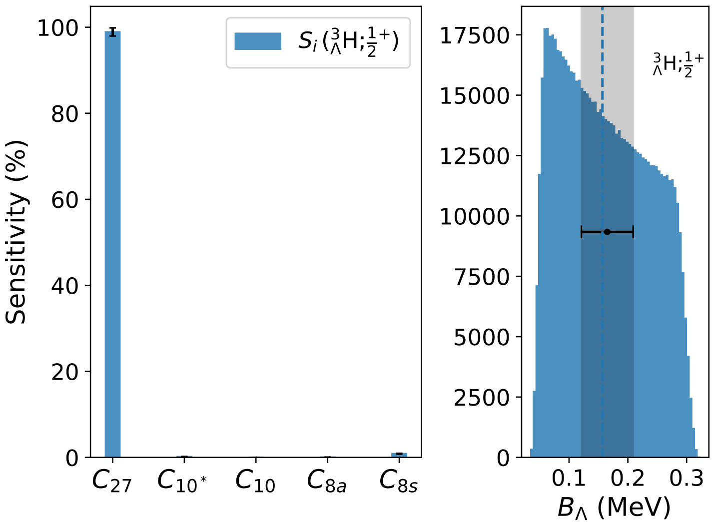
$$S_i = \frac{V_i}{\mathrm{Var}\,[Y]}, \quad S_{ij} = \frac{V_{ij}}{\mathrm{Var}\,[Y]}, \quad \ldots$$

- Total effect

$$S_{Ti} = S_i + S_{ij} + \cdots$$

Global sensitivity analysis of hypernuclear spectra

- **To identify the most influential LECs of YN interactions:**
  $Y =$ Λ separation energies of ${}^{3}_{\Lambda}\mathrm{H}_{\frac{1}{2}^+}$, ${}^{4}_{\Lambda}\mathrm{H}_{0^+}$, ${}^{4}_{\Lambda}\mathrm{He}_{0^+}$, ${}^{4}_{\Lambda}\mathrm{H}_{1^+}$, ${}^{4}_{\Lambda}\mathrm{He}_{1^+}$, ${}^{5}_{\Lambda}\mathrm{He}_{\frac{1}{2}^+}$,
  $\vec{\alpha} =$ the 5 LECs of the LO *YN* interaction; independent and uniformly distributed within $\pm 2\,\%$ (${}^{3}_{\Lambda}\mathrm{H}$) and $\pm 20\,\%$ ($A{=}4,5$) variation around the nominal values



- C_{27} is responsible for most of the variation in energy

$$C^{\Lambda\Lambda}_{^1S_0} = \frac{1}{10}(9C_{27} + C_{8s})$$
$$C^{\Lambda\Lambda}_{^3S_1} = \frac{1}{2}(C_{10^*} + C_{8a})$$
$$C^{\Sigma\Sigma}_{^3S_1} = C_{10}$$

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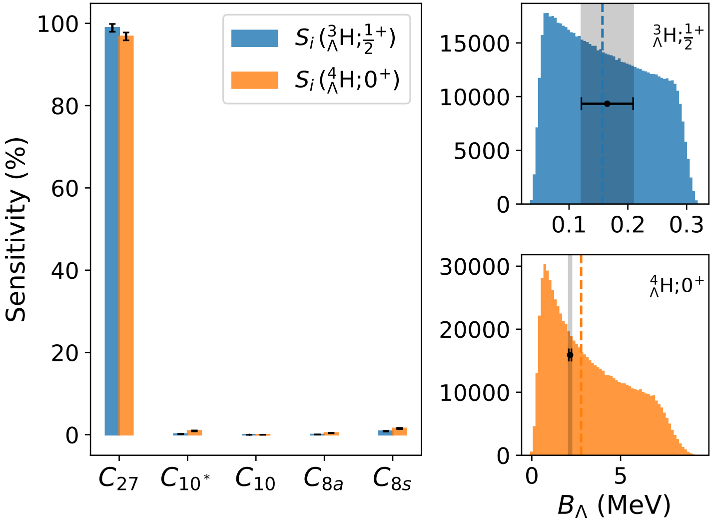

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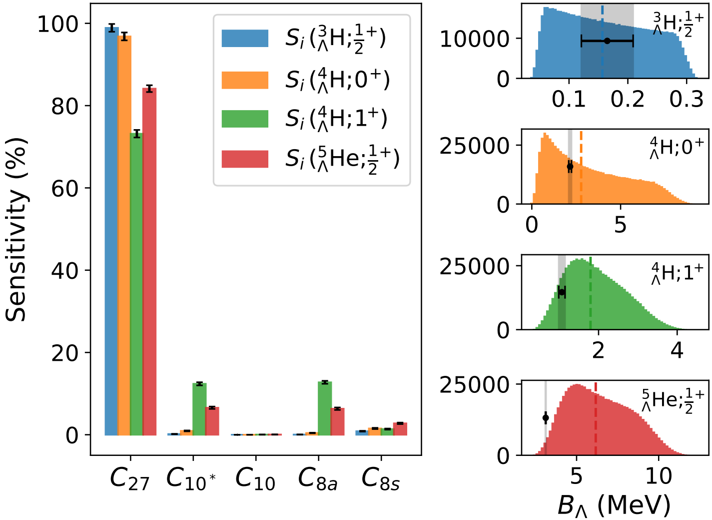

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Calibration of hyperon–nucleon interaction models

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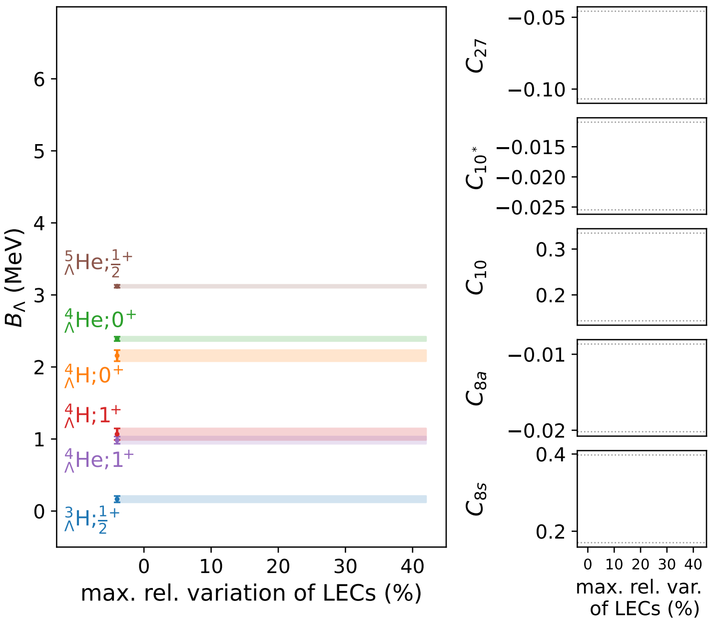
- Simultaneous fitting of *bound-state and scattering* observables is inevitable
- Can we improve the description of Λ separation energies in light hypernuclei with a small variation of LO YN LECs?



- Simple proof-of-principle least-squares optimization
- LECs restricted up to ±40 % variation around the nominal values of LOYN(Λ_{YN}=600 MeV)
- Theoretical precision $\sigma^2_{\text{th}} = \sigma^2_{\text{method}} + \sigma^2_{\text{model}}$

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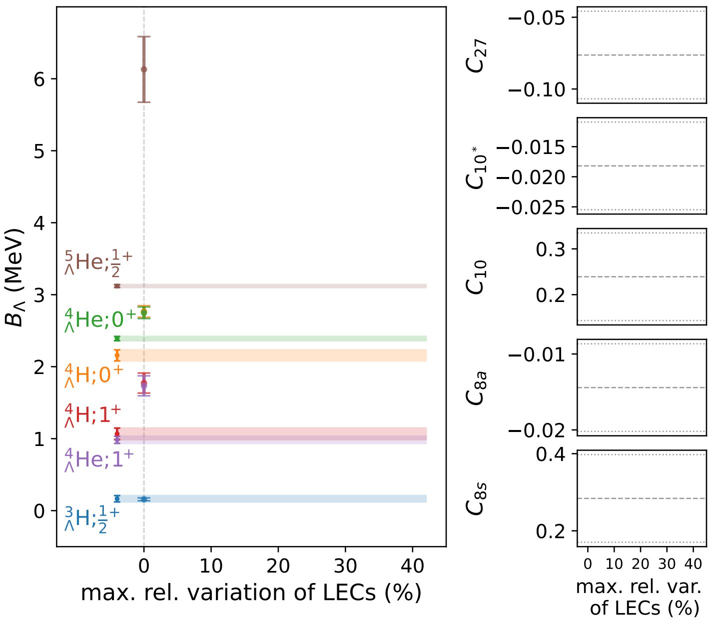

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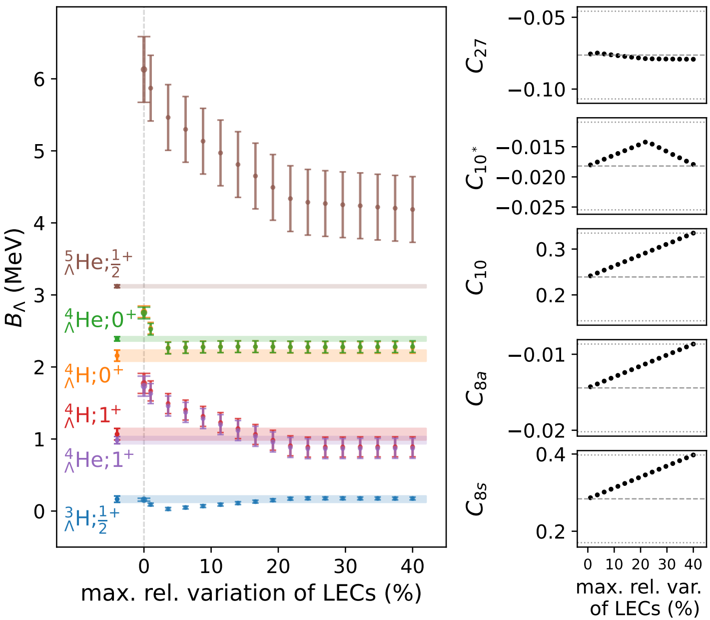

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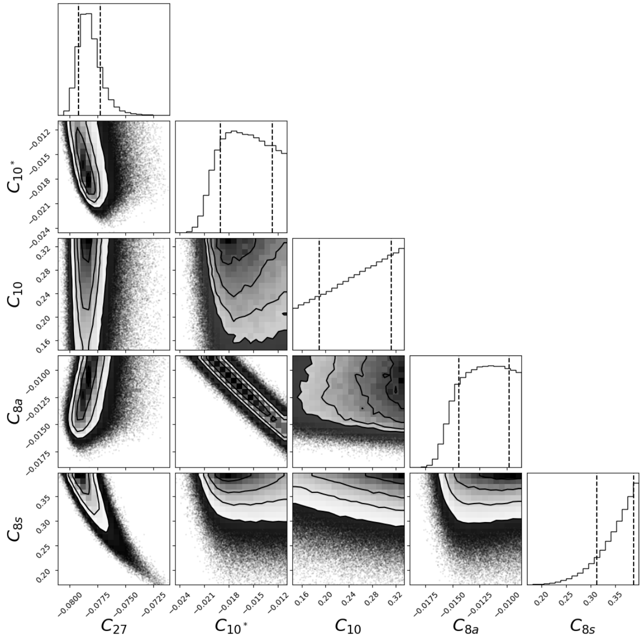
Calibration of hyperon–nucleon interaction models

- Efficiency of EC emulators $\rightarrow$ advanced Bayesian statistical methods (MCMC sampling)
- Parameter inference & predictions with quantified uncertainties!
- Proof-of-principle inference using 'flat' priors for LECs with

$$-2\log L = \sum_{i\in {}^A_\Lambda Z} \frac{(E_i^{\text{th}} - E_i^{\text{exp}})^2}{\sigma_{i,\text{th}}^2 + \sigma_{i,\text{exp}}^2}$$



Summary & outlook

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Ab initio calculations of light hypernuclei

- Energy spectra of light hypernuclei provide important constrains on *YN* interactions and can be computed reliably
- **Eigenvector continuation** provides **fast and accurate** emulation of ab initio calculations to incorporate them into the calibration of *YN* interactions
- **Global sensitivity analysis** identifies **the most influential LECs** of χEFT *YN* interactions which **determine the energy spectra** of light hypernuclei
- A **significantly better description** of energy levels of light hypernuclei can be achieved with a relatively **small variation** of *YN* interaction LECs

Outlook

- **Simultaneous optimization** of *YN* interactions using bound-state and scattering observables with accompanying **uncertainty quantification**

Thank you!