

Towards calibration of hyperon-nucleon interaction models using light hypernuclei

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Introduction & motivation

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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 \rightsquigarrow sparse database with large uncertainties
- ▶ **Final-state interactions** in hyperon photoproduction
- ▶ Heavy-ion collisions – **production and decays** of light hypernuclei, correlation **femtoscropy**
- ▶ **Lattice QCD**
- ▶ **Hypernuclei** – precise spectroscopy of hypernuclear energy levels

Introduction & motivation

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
- ▶ Can reveal deficiencies of existing YN interaction models

Calibration of YN interaction models using hypernuclei requires

- ▶ Advanced ab initio **computational methods**
- ▶ Quantified **method uncertainties**, σ_{method} – associated with the solution of the many-body problem
- ▶ Quantified **model uncertainties**, σ_{model} – associated with the choice of the nuclear interaction
- ▶ Overcoming the **computational demands** – large number of evaluations needed

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**

Ab initio no-core shell model

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

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

[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

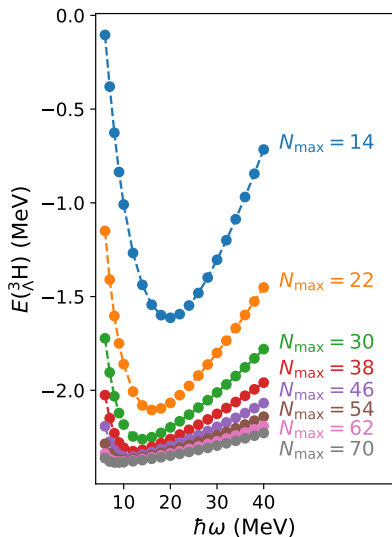
$$\Psi(\mathbf{r}_1, \dots, \mathbf{r}_A) = \sum_{N \leq N_{max}} \Phi_{N,\omega}^{HO}(\mathbf{r}_1, \dots, \mathbf{r}_A)$$

Converges to exact results for $N_{max} \rightarrow \infty$

- ▶ Input NN+NNN and YN interactions derived from χ EFT
 - ▶ The NNLO_{sim} family at NNLO [Carlsson et al., PRX 6, 011019 (2016)]
 - ▶ Jülich YN at LO [Polinder et al., NPA 779, 244 (2006)]

Ab initio calculations of light hypernuclei: 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 ($N_{\text{max}}, \hbar\omega$) recast into infrared (IR) and ultraviolet (UV) scales ($L_{\text{IR}}, \Lambda_{\text{UV}}$)
 - ▶ In a regime with negligible UV corrections, IR corrections are universal

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

Ab initio calculations of light hypernuclei: method uncertainties

- Infrared extrapolation formulated as a Bayesian inference problem

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

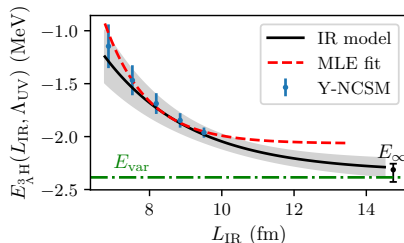
with data $\mathcal{D} = \{E(L_{\text{IR},i})\}$ calculated in different model spaces and $\vec{\epsilon}_{\text{NLO}} \sim N(0, \Sigma(\bar{\epsilon}, \rho))$ providing a stochastic model for the NLO energy correction

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

	B_{Λ}^{Exp} (MeV)	B_{Λ}^{th} (MeV)	
		median	68 % $\text{CI}_{\text{method}}$
${}^3_{\Lambda}\text{H}$	0.165(44)	0.166	$[-0.001, +0.001]$
${}^4_{\Lambda}\text{H}$	2.157(77)	2.78	$[-0.01, +0.01]$
${}^4_{\Lambda}\text{He}$	2.39(3)	2.76	$[-0.01, +0.01]$
${}^5_{\Lambda}\text{He}$	3.12(2)	6.03	$[-0.28, +0.18]$
${}^4_{\Lambda}\text{H}; 1^+$	1.067(80)	1.75	$[-0.12, +0.10]$
${}^4_{\Lambda}\text{He}; 1^+$	0.984(50)	1.71	$[-0.13, +0.10]$

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

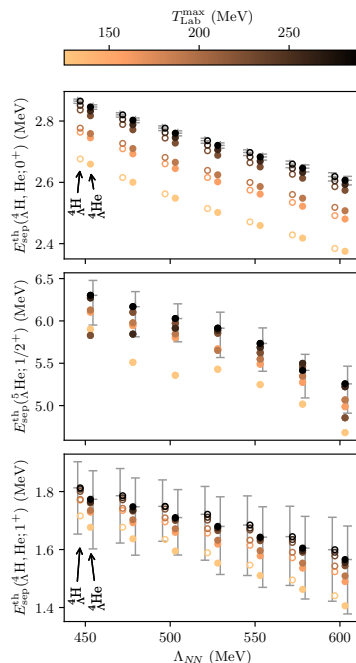
- Validation for ${}^3_{\Lambda}\text{H}$



Ab initio calculations of light hypernuclei: model uncertainties

- ▶ Energy levels of light hypernuclei are sensitive to details of the YN and $NN+NNN$ interactions
- ▶ One can naively expect that calculated Λ separation energies should be insensitive to the choice of nuclear interaction
- ▶ We employed [DG, Htun, Forssén, PRC 106, 054001 (2022)] the family of 42 different $NNLO_{sim}$ [Carlsson et al., PRX 6, 011019 (2016)] nuclear $NN+NNN$ interactions to expose the magnitude of systematic model uncertainties in B_Λ
- ▶ Model uncertainty connected to the choice of nuclear Hamiltonian quantified by variance, $\sigma^2(NNLO_{sim})$, of predictions for B_Λ

	${}^3_\Lambda\text{H}$	${}^4_\Lambda\text{H}$	${}^4_\Lambda\text{He}$	${}^5_\Lambda\text{He}$	${}^4_\Lambda\text{H}; 1^+$	${}^4_\Lambda\text{He}; 1^+$
σ_{model} (MeV)	0.02	0.08	0.08	0.36	0.07	0.07



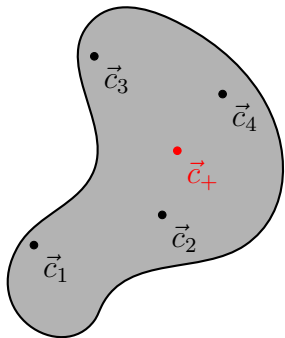
**Emulating ab initio NCSM
calculations: eigenvector
continuation**

Emulating ab initio NCSM calculations: eigenvector continuation

- ▶ 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)]

Parameter domain



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

Emulating ab initio NCSM calculations: eigenvector continuation

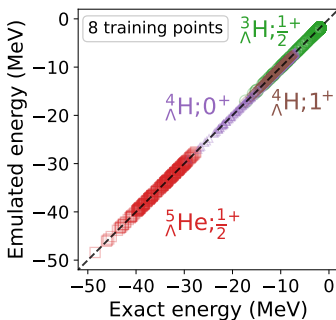
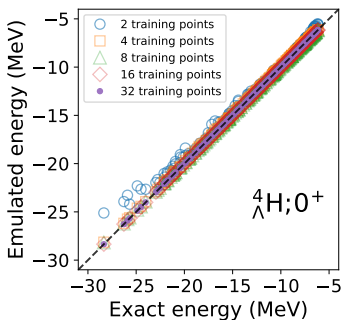
- ▶ Hypernuclear Hamiltonian with LOYN interactions can be linearized,

$$H(\vec{C}) = H_0 + C_{27}V_{27} + C_{10^*}V_{10^*} + C_{10}V_{10} + C_{8a}V_{8a} + C_{8s}V_{8s},$$

where C_j s are the 5 independent $SU_f(3)$ LECs

- ▶ Cross validation

- ▶ Select 2, 4, 8, 16, 32 points in the 5-dimensional space of LOYN LECs using the Latin hypercube space-filling design in a $\pm 40\%$ domain around the nominal values to train the emulators
- ▶ Select randomly 256 exact NCSM calculations within the same domain



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

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

**Application: global sensitivity
analysis of hypernuclear spectra**

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Global sensitivity analysis

- ▶ Addresses the question of how variance of the output of a model can be apportioned to variances of the model inputs [Saltelli et al., CPC 181, 259 (2010)]
- ▶ Allows to **identify the most influential LECs** of χ EFT 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

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

where

$$V_i = \text{Var}[E_{\vec{\alpha} \sim (\alpha_i)}[Y|\alpha_i]],$$

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

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**

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

- ▶ Total effect

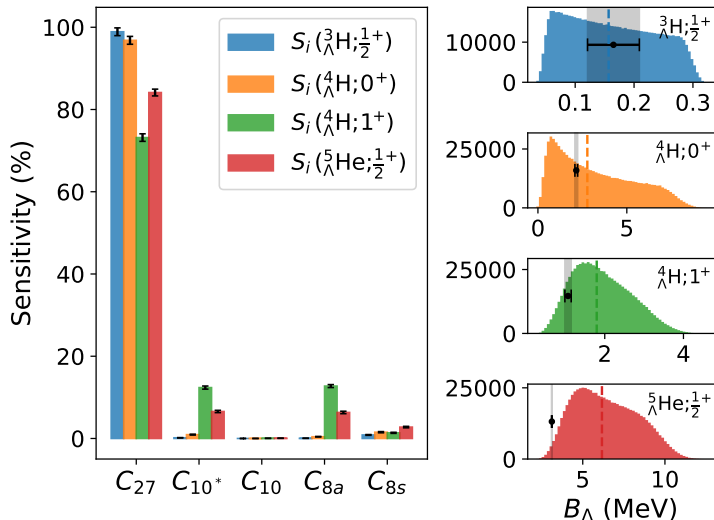
$$S_{Ti} = S_i + S_{ij} + \dots$$

Application: global sensitivity analysis of hypernuclear spectra

- Identify the most influential LECs:

$Y = \Lambda$ separation energies of ${}^3_{\Lambda}H_{\frac{1}{2}^+}$, ${}^4_{\Lambda}H_{0^+}$, ${}^4_{\Lambda}He_{0^+}$, ${}^4_{\Lambda}H_{1^+}$, ${}^4_{\Lambda}He_{1^+}$, ${}^5_{\Lambda}He_{\frac{1}{2}^+}$,

$\vec{\alpha} =$ the 5 LECs of the LOYN interaction; independent and uniformly distributed within $\pm 2\%$ ($\pm 20\%$) variation around the nominal values of LOYN ($\Lambda_{YN}=600$ MeV) for ${}^3_{\Lambda}H$ ($A = 4, 5$)



- $S_i \approx S_{Ti} \rightsquigarrow$ energies are additive in all LECs
- C_{27} is responsible for most of the variation in energy

$$C_{1S_0}^{\Lambda} = \frac{1}{10}(9C_{27} + C_{8s})$$

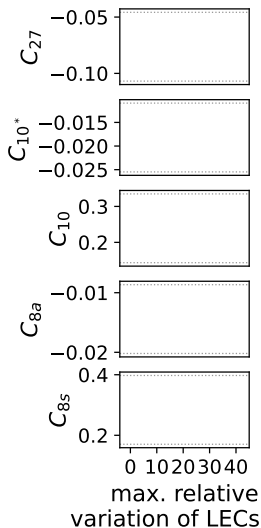
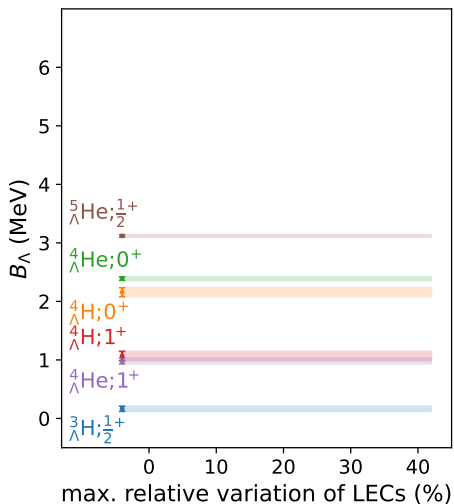
$$C_{3S_1}^{\Lambda} = \frac{1}{2}(C_{10^*} + C_{8a})$$

$$C_{3S_1}^{\Sigma\Sigma} = C_{10}$$

Application: 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 LOYN LECs?

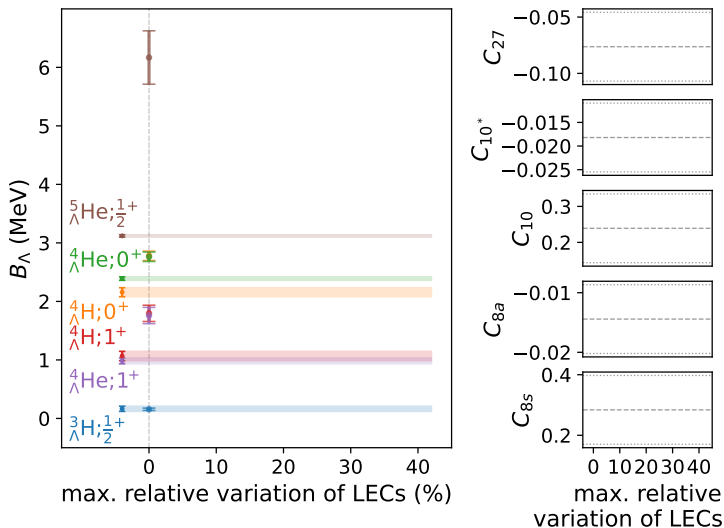


- ▶ Proof of principle, simple least-squares optimization
- ▶ LECs restricted up to $\pm 40\%$ variation around the nominal values of LOYN ($\Lambda_{YN}=600$ MeV)
- ▶ Theoretical precision

$$\sigma_{\text{th}}^2 = \sigma_{\text{method}}^2 + \sigma_{\text{model}}^2$$

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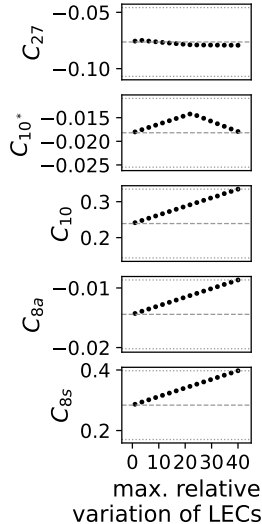
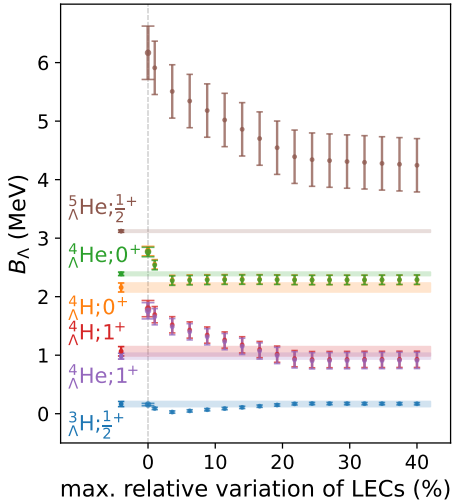


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Summary & outlook

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Ab initio calculations of light hypernuclei

- ▶ Hypernuclear observables, such as **Λ separation energies** in light hypernuclei, suffer from **sizable theoretical uncertainties** associated with the choice of nuclear interaction

Emulating ab initio NCSM

- ▶ **Eigenvector continuation** provides **fast and accurate** emulation of ab initio calculations of light hypernuclei
- ▶ Global sensitivity analysis identifies **the most influential LECs** of χ EFT YN interaction 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 the LOYN($\Lambda_{YN}=600$ MeV) LECs

Outlook

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