Towards calibration of hyperon-nucleon interaction models using light hypernuclei

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MANY THANKS TO MY COLLABORATORS

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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, difficult to link with the underlying free-space *YN* interaction, limited predictive power
- Using **'realistic'** *YN* interaction models ...

Constraining YN interactions

- **YN scattering** – 'pure' but very difficult to realize, sparse database with large uncertainties
- Heavy-ion collisions – **production and decays** of light hypernuclei, correlation **femtoscopy**
- **Final-state interactions** in hyperon photoproduction
- **Lattice QCD**
- **Hypernuclei** – precise spectroscopy

Introduction & motivation

Theoretical analysis of hypernuclei using realistic YN interactions

- Combines modern developments of *YN* interactions based on χEFT and ab initio few- and many-body approaches
- Computationally demanding
- Can reveal deficiencies of existing YN interaction models
- $\not\pi$EFT is successful in light hypernuclei

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
- Sensitivity analysis - hypernuclear spectra **might not be sensitive** to certain parameters (LECs) of the *YN* interaction models
- **Simultaneous** fitting of other observables

Ab initio calculations of light hypernuclei

Ab initio calculations of light hypernuclei

- Ab initio methods aim to solve solve the (hyper)nuclear many-body problem starting from ‘realistic’ (free-space) interactions exactly or with controlled approximations
- Ab initio no-core shell model
  [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)]
  - Quasi-exact method to solve the few- and many-body Schrödinger equation:

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

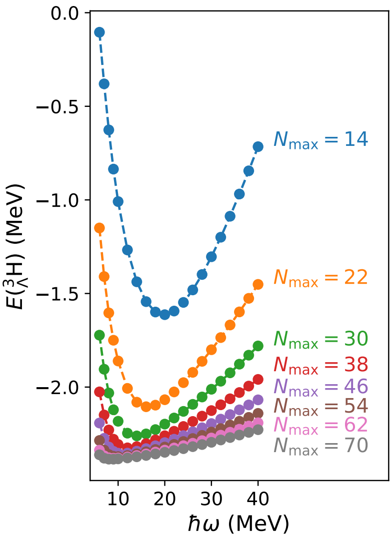
  - Wave function is expanded and Hamiltonian is diagonalized in a *finite* A-particle harmonic oscillator (HO) basis

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

  - Systematically improvable: converges to exact results for $N_{max} \to \infty$
- Input NN+NNN and YN interactions derived from χEFT
  - The NNLO$_{\text{sim}}$ 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 $(N_{\mathrm{max}}, \hbar\omega)$ recast into infrared (IR) and ultraviolet (UV) scales $(L_{\mathrm{IR}}, \Lambda_{\mathrm{UV}})$
  - In a regime with negligible UV corrections, IR corrections are universal

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

Ab initio calculations of light hypernuclei: method uncertainties

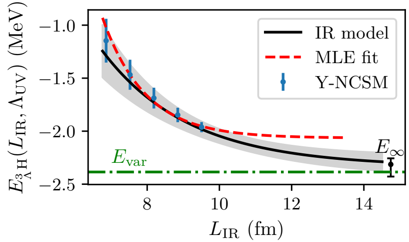
- Infrared extrapolation formulated as a Bayesian inference problem

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

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

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

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

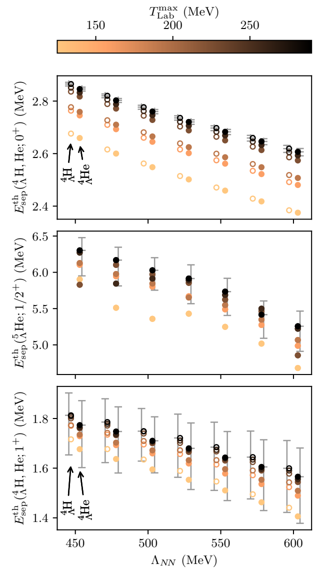


- Method uncertainty quantified by 68 % credible interval for the extrapolated energy E_∞

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

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
- 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
- We employed [DG, Htun, Forssén, PRC 106, 054001 (2022)] the family of 42 different $\mathrm{NNLO_{sim}}$ [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, $\sigma^2(\mathrm{NNLO_{sim}})$, of predictions for B_Λ

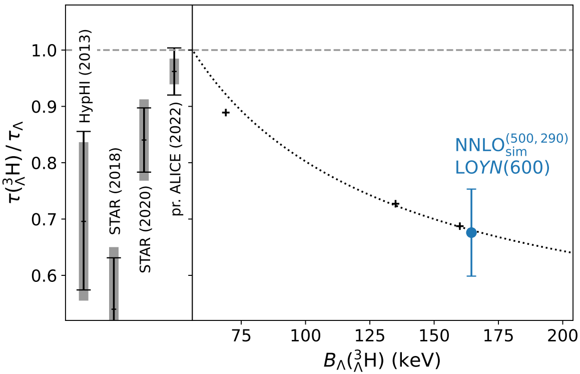
	$^3_\Lambda$H	$^4_\Lambda$H	$^4_\Lambda$He	$^5_\Lambda$He	$^4_\Lambda$H; 1^+	$^4_\Lambda$He; 1^+
σ_{model} (MeV)	0.02	0.08	0.08	0.36	0.07	0.07

Theoretical uncertainties: hypertriton lifetime

- Employed ab initio NCSM ${}^3_\Lambda$H, ^{3}He wave functions to compute the ${}^3_\Lambda$H 2-body π^- decay rate $\Gamma_{{}^3_\Lambda\mathrm{H}\to{}^3\mathrm{He}+\pi^-}$
- Accounted for significant but opposing contributions of pionic FSI and $\Sigma \to N\pi$ due to ΣNN admixtures in ${}^3_\Lambda$H

- Deduced the ${}^3_\Lambda$H lifetime $\tau({}^3_\Lambda\mathrm{H})$ by using the measured branching ratio $R_3 = \Gamma_{{}^3_\Lambda\mathrm{H}\to{}^3\mathrm{He}+\pi^-}/\Gamma_{\pi^-} = 0.35(4)$ to obtain the inclusive π^- ${}^3_\Lambda$H decay rate and employing the $\Delta T = 1/2$ rule to include all π^0 decay modes

[Pérez-Obiol, DG, Friedman, Gal, PLB 811, 135916 (2020); in preparation (2023)]



- $B_\Lambda({}^3_\Lambda\mathrm{H})$ poorly known experimentally and suffers from large theoretical uncertainties
- None of the conflicting RHI measured $\tau({}^3_\Lambda\mathrm{H})$ can be excluded but rather associated with its own value of B_Λ

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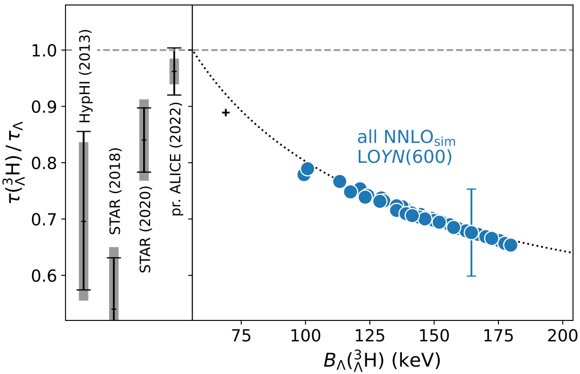

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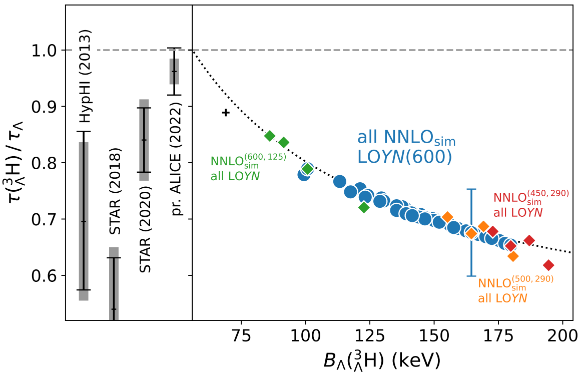

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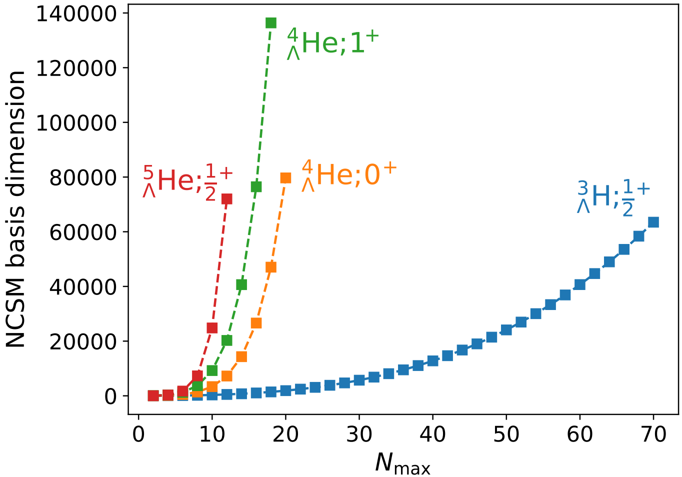
Ab initio calculations of hypernuclei: the curse of dimensionality

- 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 given their computational cost

Emulating ab initio NCSM calculations: eigenvector continuation

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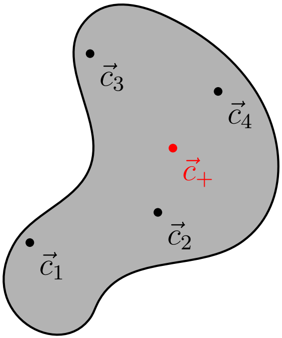
- Eigenvector continuation is based on the fact that when a Hamiltonian depends smoothly on some real-valued control parameter(s), any eigenvector is a smooth function of that parameter(s) and its trajectory is confined to a very low-dimensional subspace

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

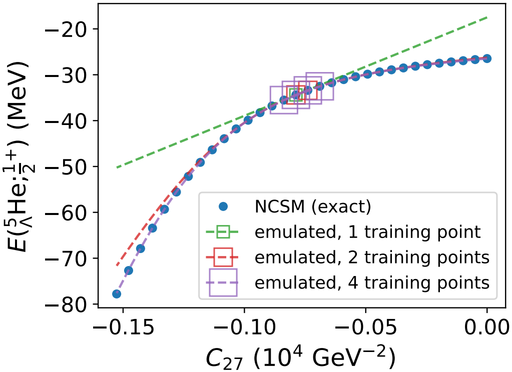
Parameter domain



- 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 $\tilde{H}(\vec{c}_+)\,|\tilde{\psi}\rangle = \tilde{E}_+\tilde{N}\,|\tilde{\psi}\rangle$, 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 SU$_f$(3) LECs and H_0 contains the kinetic energy, *NN*+*NNN* interactions, and hypernuclear meson-exchange and Coulomb interactions

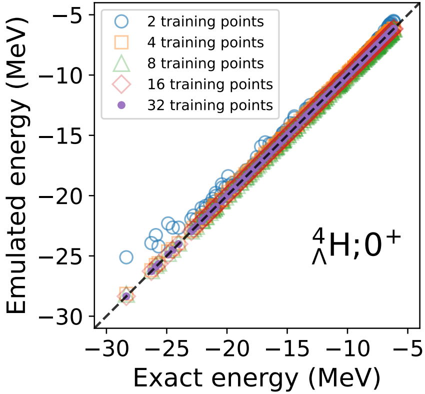


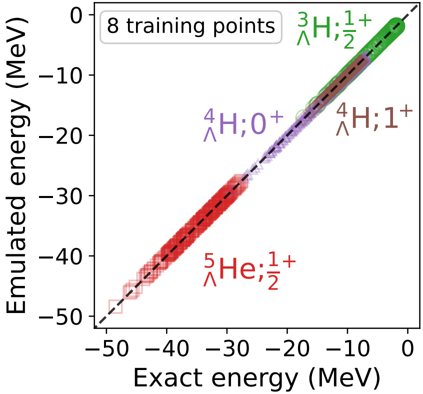
- ${}^5_\Lambda$He; $\frac{1}{2}^+$, model space truncation $N_{\max} = 12$
- Vary one LEC, C_{27}, within $\pm 100\,\%$ relative variation with respect to the nominal LO*YN*(Λ_{YN}=600 MeV) value
- Select 1, 2, 4 exact NCSM eigenvectors to construct the emulators

- Accurate and lighting-fast emulation of ab initio NCSM calculations
- Continued eigenvectors stay within the same ($N_{\max}, \hbar\omega$) model space $\rightsquigarrow$ extrapolation of observables to infinite model space is still necessary

Emulating ab initio NCSM calculations: cross validation

- Select 2, 4, 8, 16, 32 points in the 5-dimensional space of LOY*N* 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 $|\delta_{\mathrm{rel}}| < 1, 0.1, 0.002\,\%$ using 8, 16, 32 training points

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 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

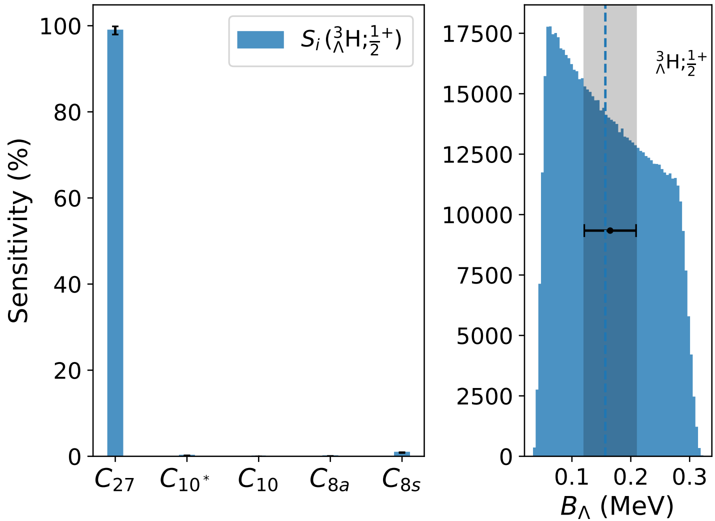
$$S_i = \frac{V_i}{\mathrm{Var}\,[Y]}, \quad S_{ij} = \frac{V_{ij}}{\mathrm{Var}\,[Y]}, \quad \cdots$$

- Total effect

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

Application: global sensitivity analysis of hypernuclear spectra

- $Y =$ Λ separation energies of ${}^{3}_{\Lambda}\mathrm{H}$, ${}^{4}_{\Lambda}\mathrm{H}_{\mathrm{gs}}$, ${}^{4}_{\Lambda}\mathrm{He}_{\mathrm{gs}}$, ${}^{4}_{\Lambda}\mathrm{H}_{\mathrm{exc}}$, ${}^{4}_{\Lambda}\mathrm{He}_{\mathrm{exc}}$, ${}^{5}_{\Lambda}\mathrm{He}_{\mathrm{gs}}$
- $\vec{\alpha} =$ the 5 LECs of the LO*YN* interaction; independent and uniformly distributed within $\pm 2\,\%$ ($\pm 20\,\%$) variation around the nominal values of LO*YN*(Λ_{YN}=600 MeV) for ${}^{3}_{\Lambda}\mathrm{H}$ ($A = 4, 5$)
- Identify the most influential LECs



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

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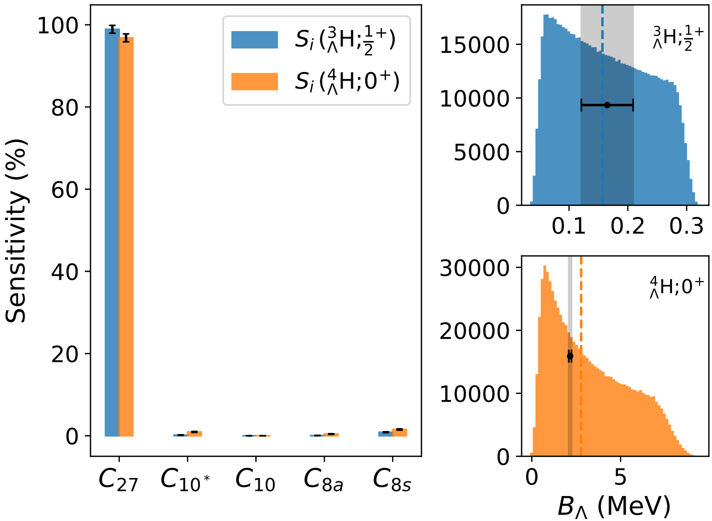

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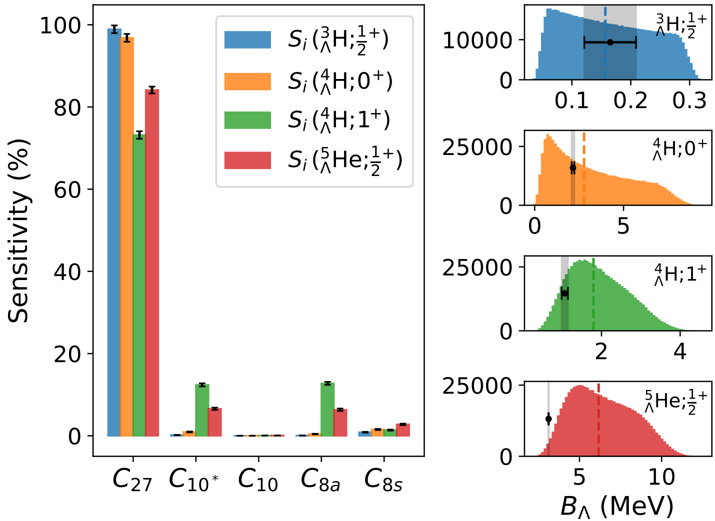

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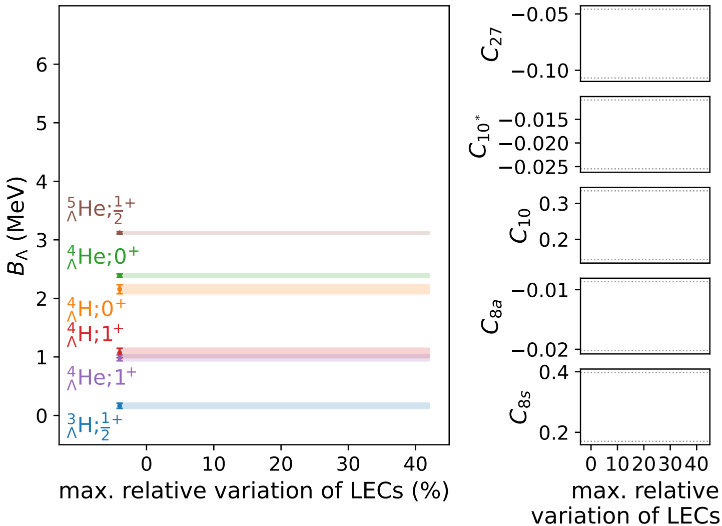
- Simultaneous fitting of *bound-state and scattering* observables is inevitable
- Can we improve the description of Λ separation energies in light hypernuclei with a small variation of LO*YN* LECs?



- Proof of principle, simple least-squares optimization
- LECs restricted up to $\pm 40\,\%$ variation around the nominal values of LO*YN*(Λ_{YN}=600 MeV)
- Theoretical precision $\sigma^2_{\text{th}} = \sigma^2_{\text{method}} + \sigma^2_{\text{model}}$

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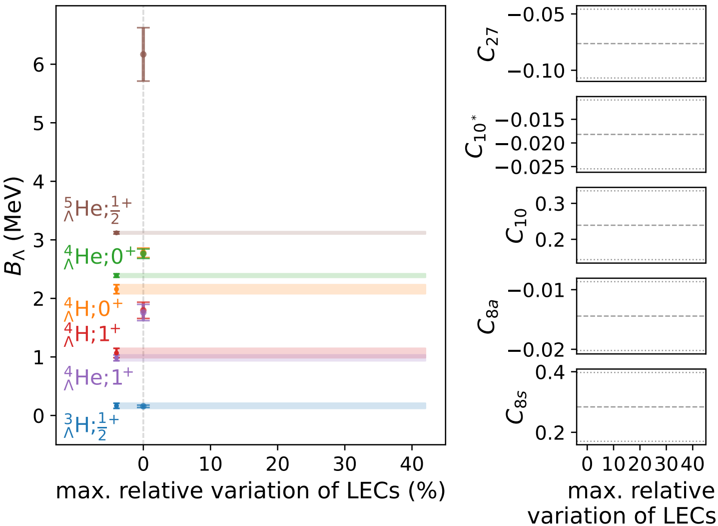

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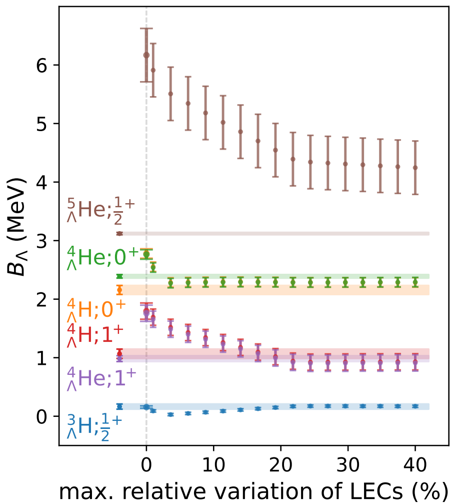

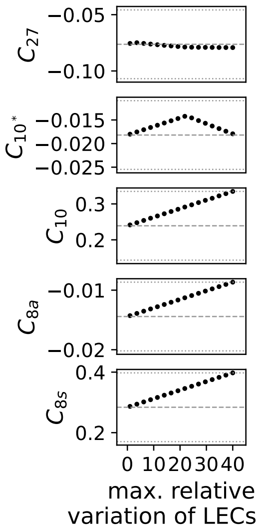

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Summary & outlook

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Ab initio calculations of light hypernuclei

- Hypernuclear observables, such as Λ **separation energies** of light hypernuclei and **hypertriton lifetime**, might 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 χEFT 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(Λ_{YN}=600 MeV) LECs

Outlook

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