Bayes of My Life:
Bayesian analysis of nucleon-nucleon scattering data in pionless EFT

Jason Bub

In collaboration with: Maria Piarulli, Dick Furnstahl, Saori Pastore, and Daniel Phillips

The Nuclear Interaction: Post-Modern Developments @ ECT*
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Washington University in St. Louis

Outline

- Motivation/Bayesian EFT Model Calibration
- BUQEYE Formalism
- Interaction Choice
- Results
- Questions

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$$\mathrm{pr}(\vec{\mathrm{a}}\,|\,\vec{\mathrm{y}}, \mathrm{I}) \propto \mathrm{pr}(\vec{\mathrm{y}}\,|\,\vec{\mathrm{a}})$$

where $\vec{a}$ is the vector of parameters, $\vec{y}$ is a vector of data, and I is additional external information.

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$$y_{\mathrm{exp}} = y_{\mathrm{th}}(\vec{a}) + \delta y_{\mathrm{exp}}, \quad \delta y_{\mathrm{exp}} \sim \mathcal{N}(0,\sigma^2)$$

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- Ex: LECs are natural, i.e., order 1 $\rightarrow \mathrm{pr}(\vec{\mathrm{a}}\,|\,\mathrm{I}) \sim \mathcal{N}\left(\vec{0}, \Sigma_{\mathrm{pr}}\right)$

Parameter Estimation vs. Parameter Fitting

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Bayesian calibration with $\mathrm{pr}(\vec{a} \mid \vec{y}, I) \propto \mathrm{pr}(\vec{y} \mid \vec{a})\, \mathrm{pr}(\vec{a} \mid I)$ is vastly different from least-squares

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• Use of prior information	• Informed only by data
• Robust handling of data outliers	• Sensitive to data outliers
• Rigorous uncertainties	• Approximate uncertainties
• Easy extension to full model uncertainties	• Convoluted extension to model uncertainties

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$$\sigma_i^2 \longrightarrow \sigma_i^2 \to \sigma_i^2 + \sigma_{\text{th},i}^2$$

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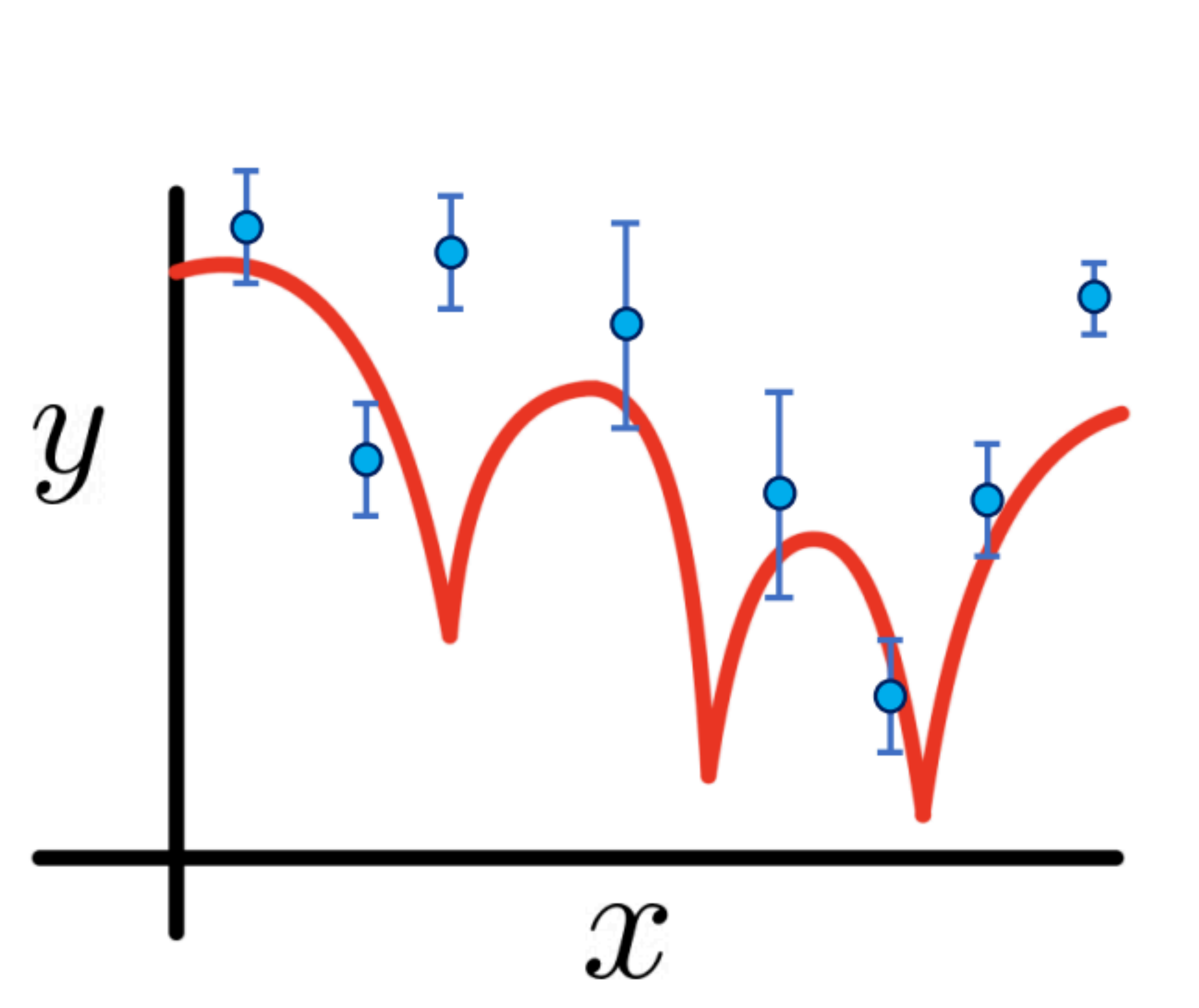

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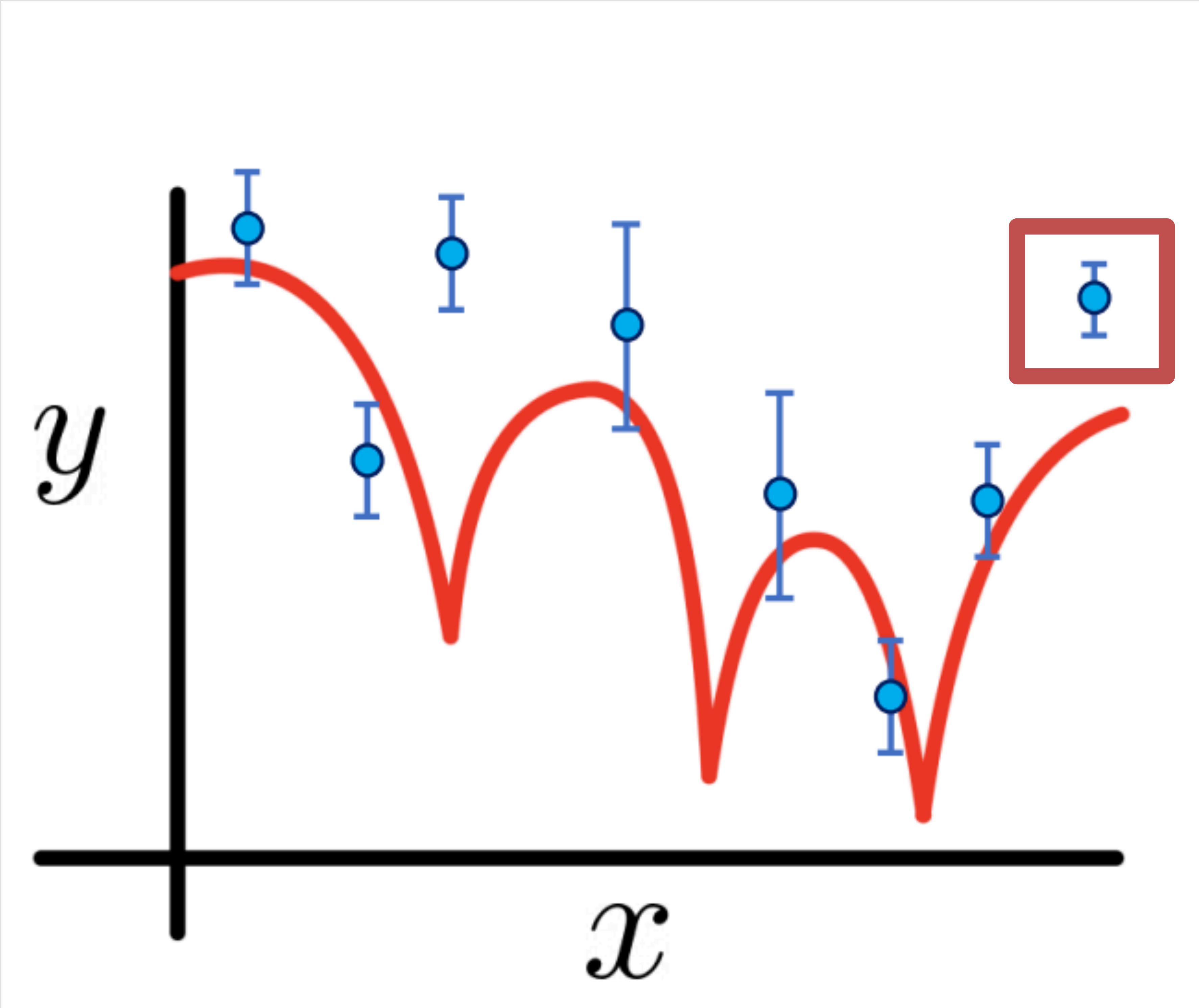

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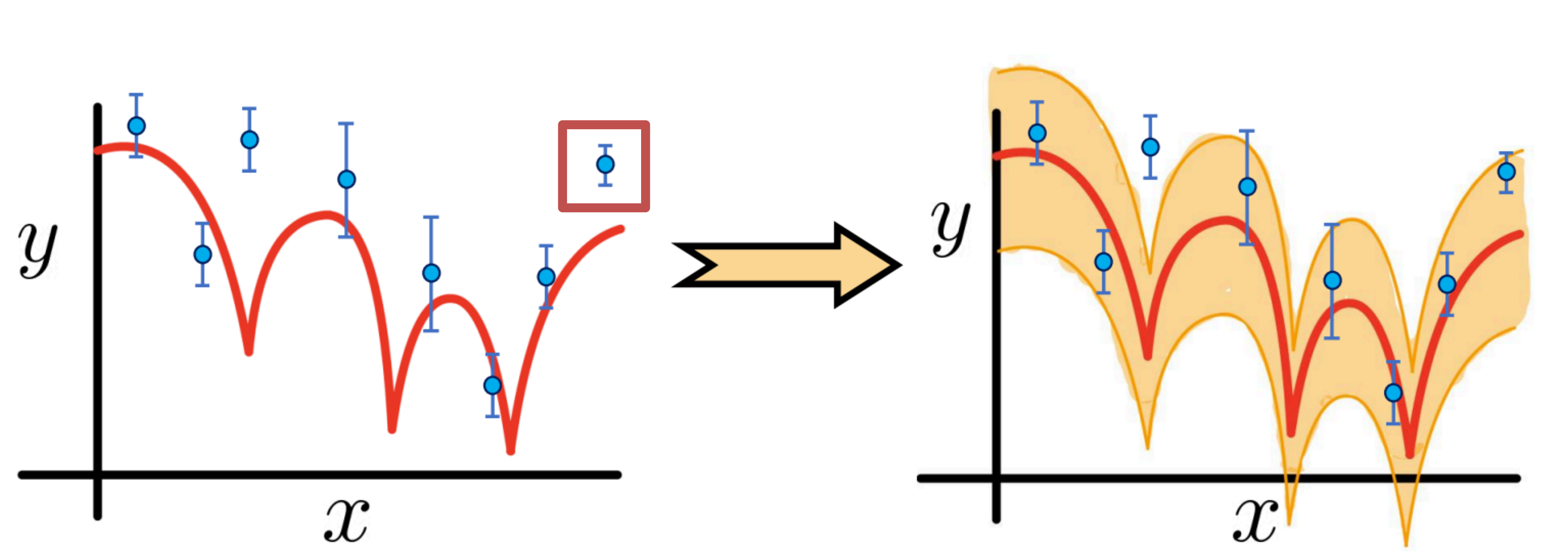

Figure courtesy of Pablo Giuliani

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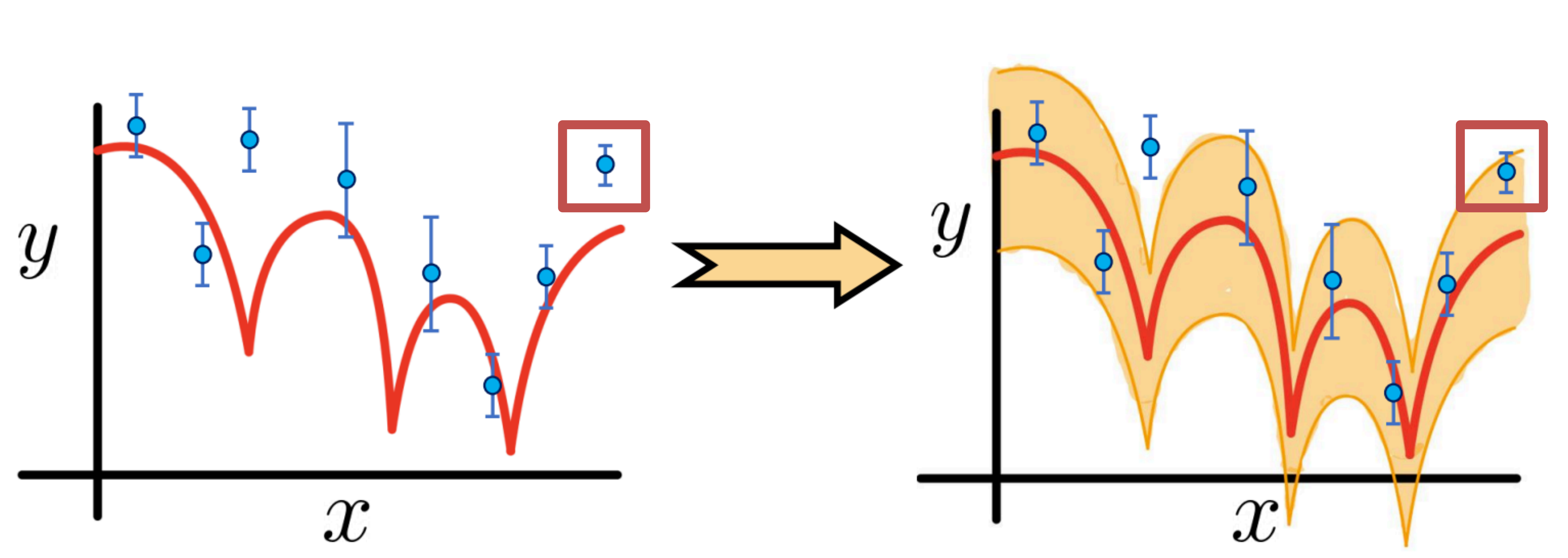

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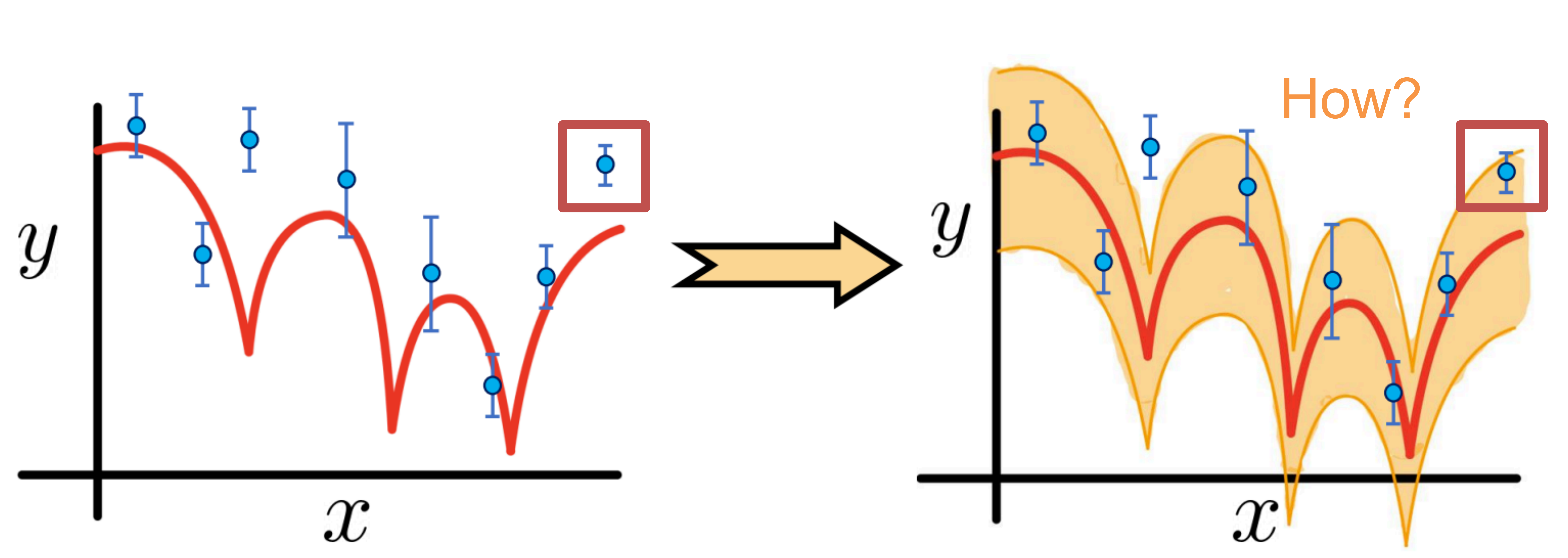

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$$y_{\mathrm{th}}(x) = y_{\mathrm{ref}}(x) \sum_{n=0}^{\infty} c_n(x) Q^n(x), \quad Q \equiv \frac{\max[p_{soft}, p]}{\Lambda_b},$$

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where $y_{\rm ref}(x)$ sets a reference scale for the observable $y_{\rm th}$ and Λ_b is the EFT breakdown scale.

This series follows the truncation scheme of the EFT:

$$y_{\rm th}(x) = y_{\rm ref}(x) \sum_{n=0}^{k} c_n Q^n + y_{\rm ref}(x) \sum_{n=k+1}^{\infty} c_n Q^n = y_{\rm th}^{(k)}(x) + \delta y_{\rm th}^{(k)}(x).$$

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Where we assume that $c_n \,|\, \bar{c} \sim \mathcal{N}\left(0, \bar{c}^2\right)$.

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From the truncation uncertainty, we can construct a covariance matrix, assuming δy_{th} is normally distributed,

$$\Sigma_{ij}^{\text{th}} = \frac{\left(y_{\text{ref},i}\,\bar{c}\,Q_i^{(k+1)}\right)\left(y_{\text{ref},j}\,\bar{c}\,Q_j^{(k+1)}\right)}{1 - Q_i Q_j} r(x_i, x_j; \vec{l}),$$

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were we introduce a kernel $r(x_i, x_j; \vec{l})$ to smooth and handle correlations.

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Correlated version of χ^2

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$$\underbrace{\mathrm{pr}(\vec{a}, \bar{c}^2, \Lambda_b \,|\, \vec{y}_{exp}, I)}_{\text{Total posterior}} \propto \underbrace{\mathrm{pr}(\vec{y}_{exp} \,|\, \vec{a}, \Sigma, I)}_{\text{Likelihood for } \vec{a}} \; \underbrace{\mathrm{pr}(\vec{a} \,|\, I)}_{\text{Prior for } \vec{a}} \; \underbrace{\mathrm{pr}(\bar{c}^2 \,|\, \Lambda_b, \vec{a}, I)}_{\text{Posterior for } \bar{c}^2} \; \underbrace{\mathrm{pr}(\Lambda_b \,|\, \vec{a}, I)}_{\text{Posterior for } \Lambda_b} \; .$$

We can find a closed form of $\mathrm{pr}(\bar{c}^2 \,|\, \Lambda_b, \vec{a}, I)$ and $\mathrm{pr}(\Lambda_b \,|\, \vec{a}, I)$.

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With all our components, we can estimate our parameters.

Outline

- Motivation/Bayesian EFT Model Calibration
- BUQEYE Formalism
- Interaction Choice
- Results
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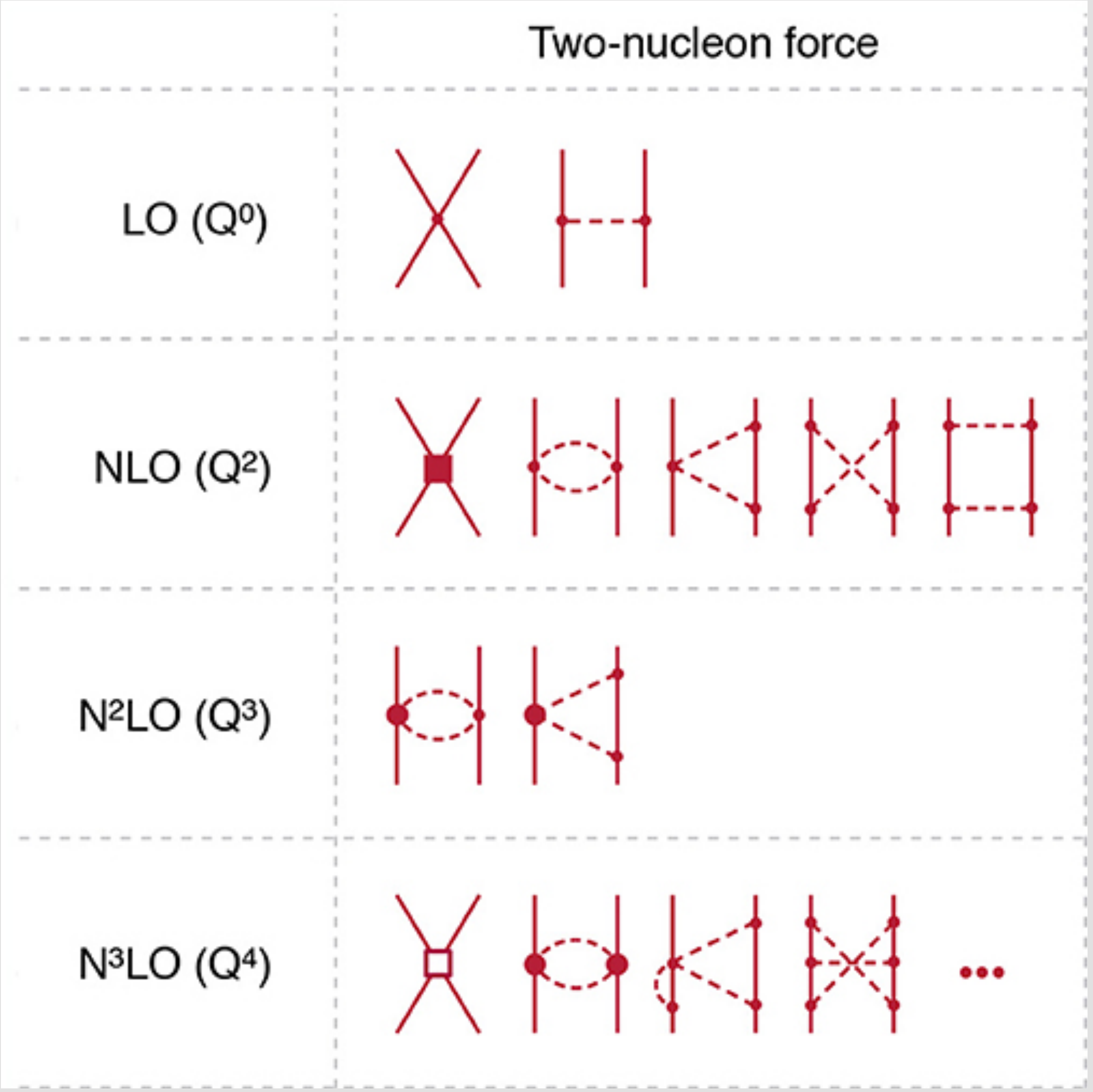

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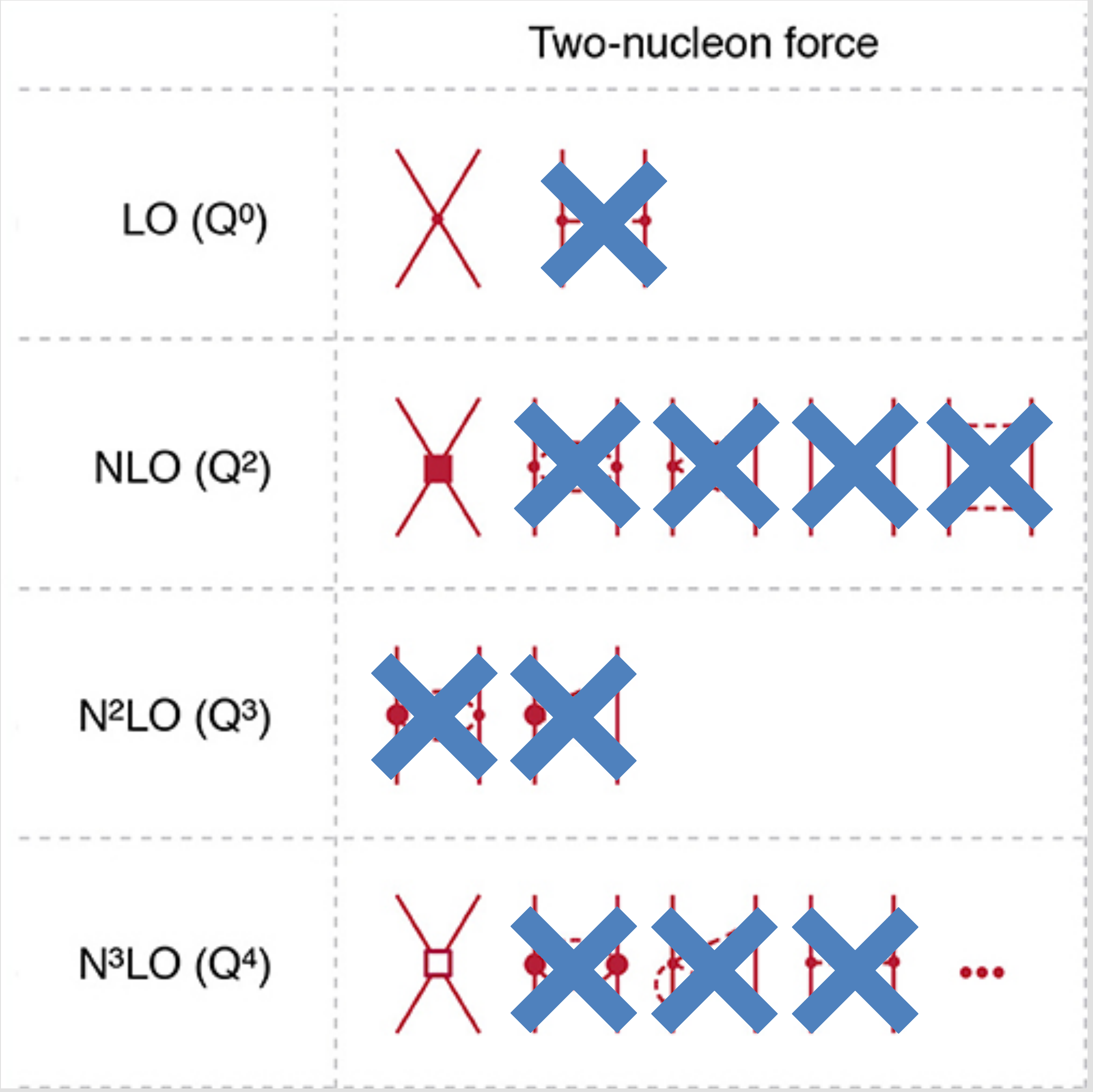

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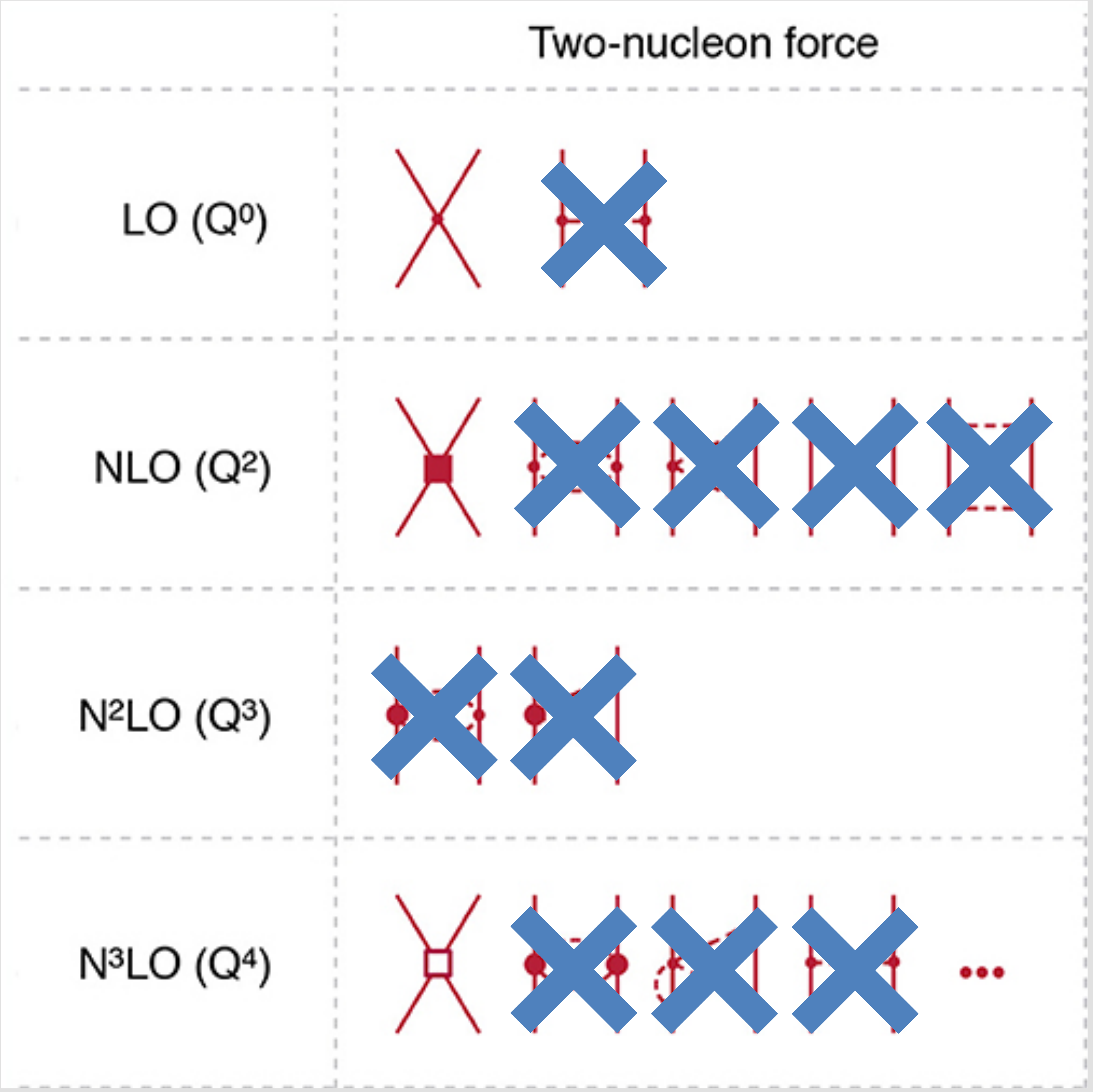

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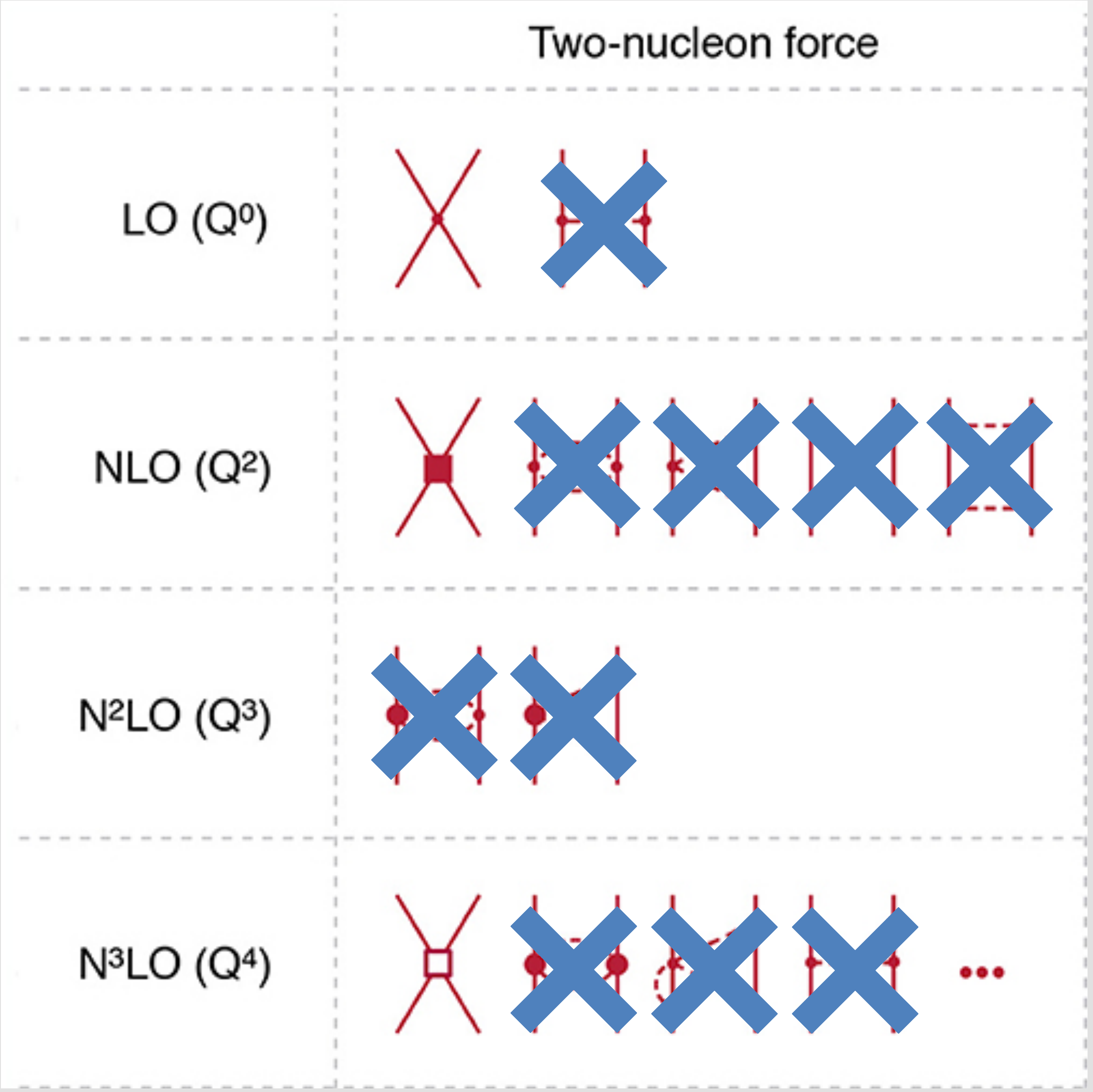

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$$+ i C_5 \vec{S} \cdot (\vec{K} \times \vec{k}) + C_6 k^2 \tau_1 \cdot \tau_2 \sigma_1 \cdot \sigma_2 + C_7 S_{12}(k) \tau_2 \cdot \tau_2$$

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We choose $R_s \in [1.5, 2.0, 2.5]$ fm which are $\sim \frac{400}{R_s}$ MeV in momentum space.

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Our choice of data is the pp and np Granada database (251 differential cross sections, 133 total cross sections, 4 polarized cross sections) up to 5 MeV + deuteron binding energy + nn scattering length.

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We then use Markov Chain Monte Carlo (MCMC) to sample the posteriors at LO $\left(Q^0\right)$, NLO $\left(Q^2\right)$, and N3LO $\left(Q^4\right)$, allowing for the order-by-order convergence analysis for LO→NLO and NLO→N3LO to estimate $\bar{c}$ and Λ_b.

Prior Choices

- $\mathrm{pr}(\vec{\mathrm{a}}\,|\,\mathrm{I}) \sim \mathcal{N}\left(\vec{\mathrm{a}}^{\mathrm{MAP}}_{\mathrm{p.s.}}, \overrightarrow{10^2}\right)$
- $\mathrm{pr}(\Lambda_\mathrm{b}\,|\,\mathrm{I}) \sim \mathcal{N}\left(500\ \text{MeV}, 1000^2\ \text{MeV}^2\right)$
- $\mathrm{pr}(\bar{\mathrm{c}}^2\,|\,\mathrm{I}) \sim \chi^{-2}(\nu_0 = 1.5, \tau_0^2 = 1.5^2)$
- $r(x_i, x_j; \vec{l}) = e^{|p_i - p_j|/2l_p} e^{|\theta_i - \theta_j|/2l_\theta} \delta_{\mathrm{type}_i,\mathrm{type}_j}, \quad l_p = 0.3\ \text{MeV}, l_\theta = 20°$
- $p_{\mathrm{soft}} = \begin{cases} p_d \sim 45\ \text{MeV}/c, & \text{for } np \text{ scattering} \\ 1/{}^1a_{\mathrm{pp}} \sim 25\ \text{MeV}, & \text{for } pp \text{ scattering}. \end{cases}$

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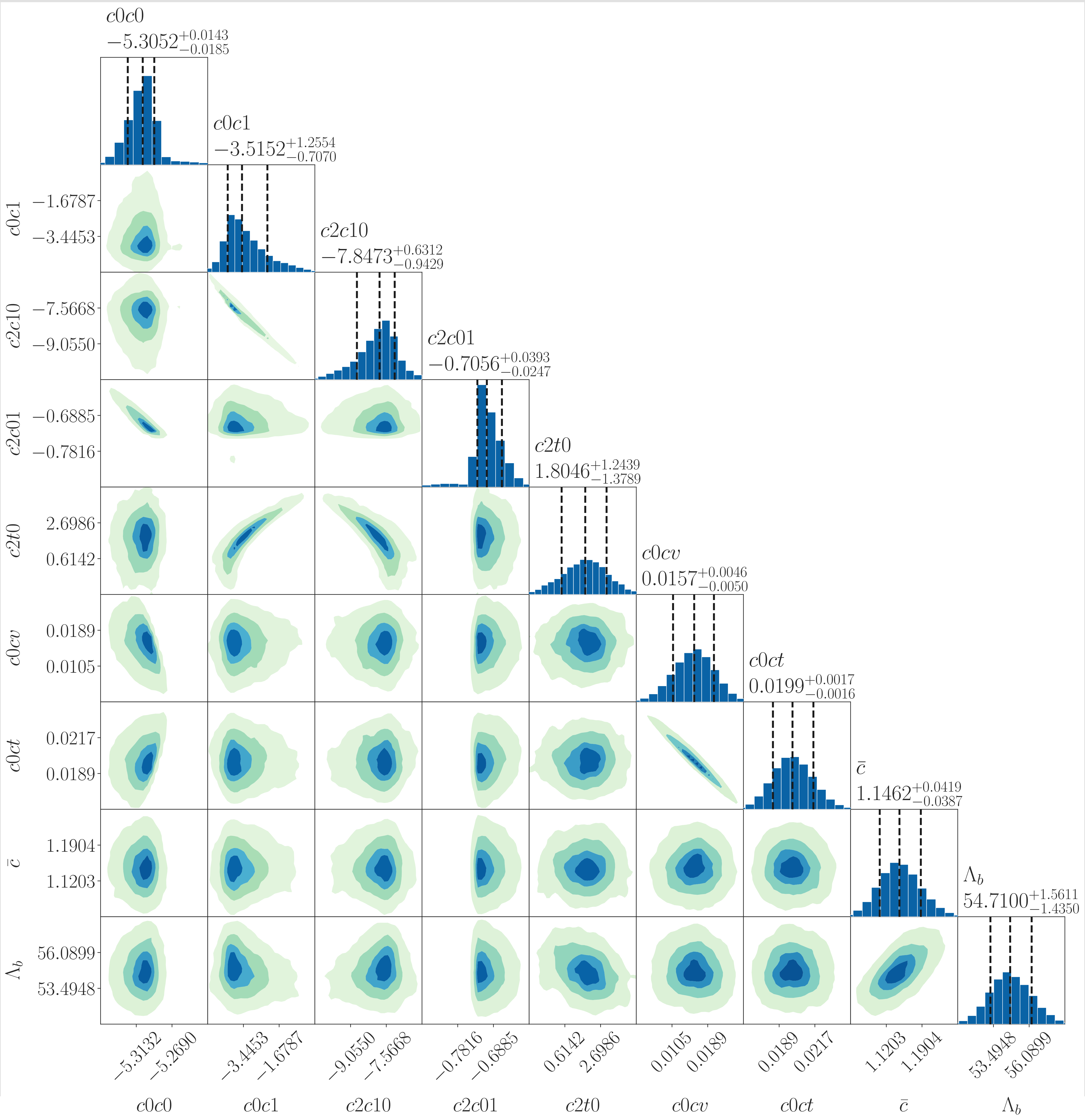
NLO Posterior

Figures:

NLO Posterior



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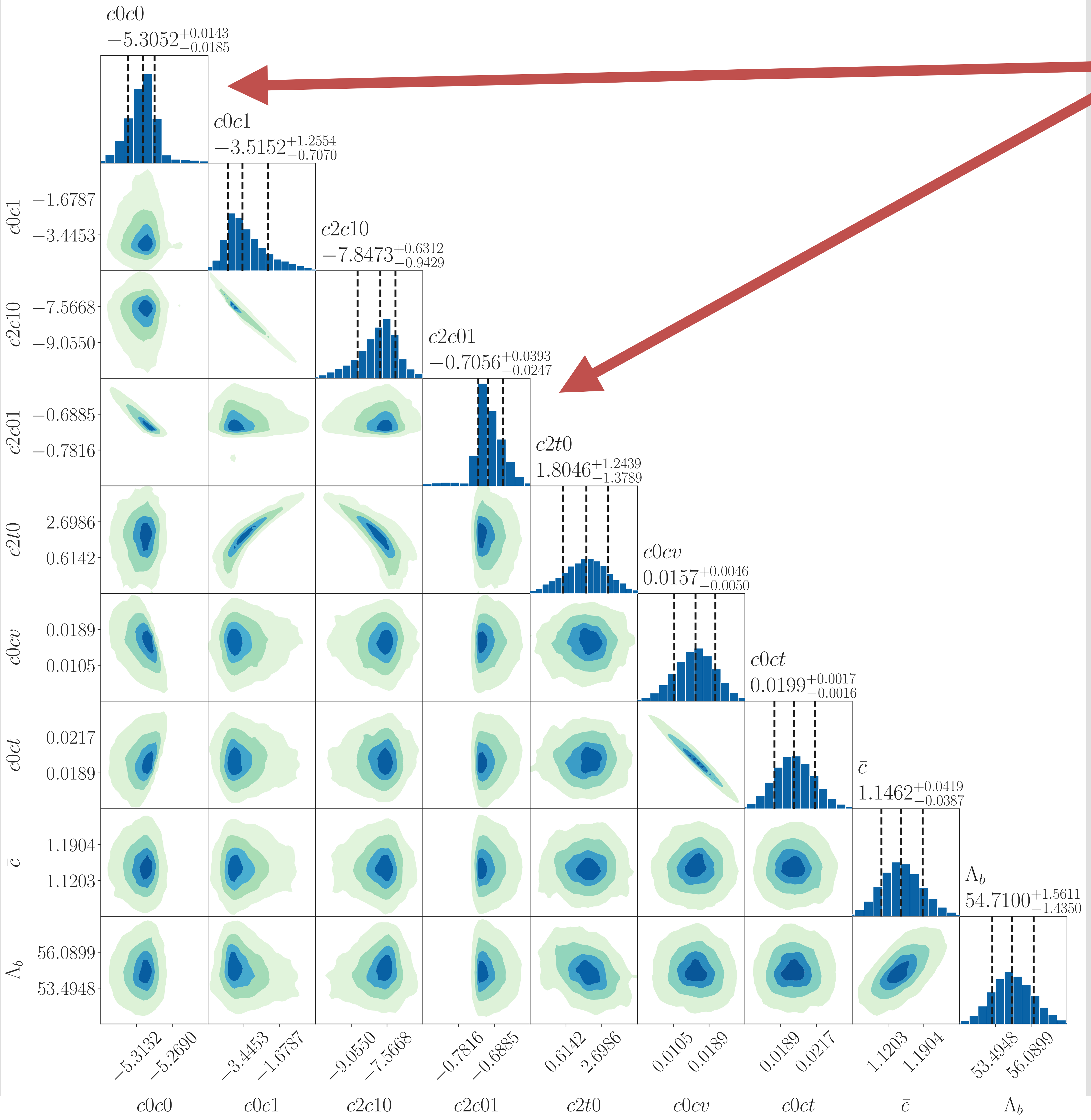

$(S, T) = (0,1)$

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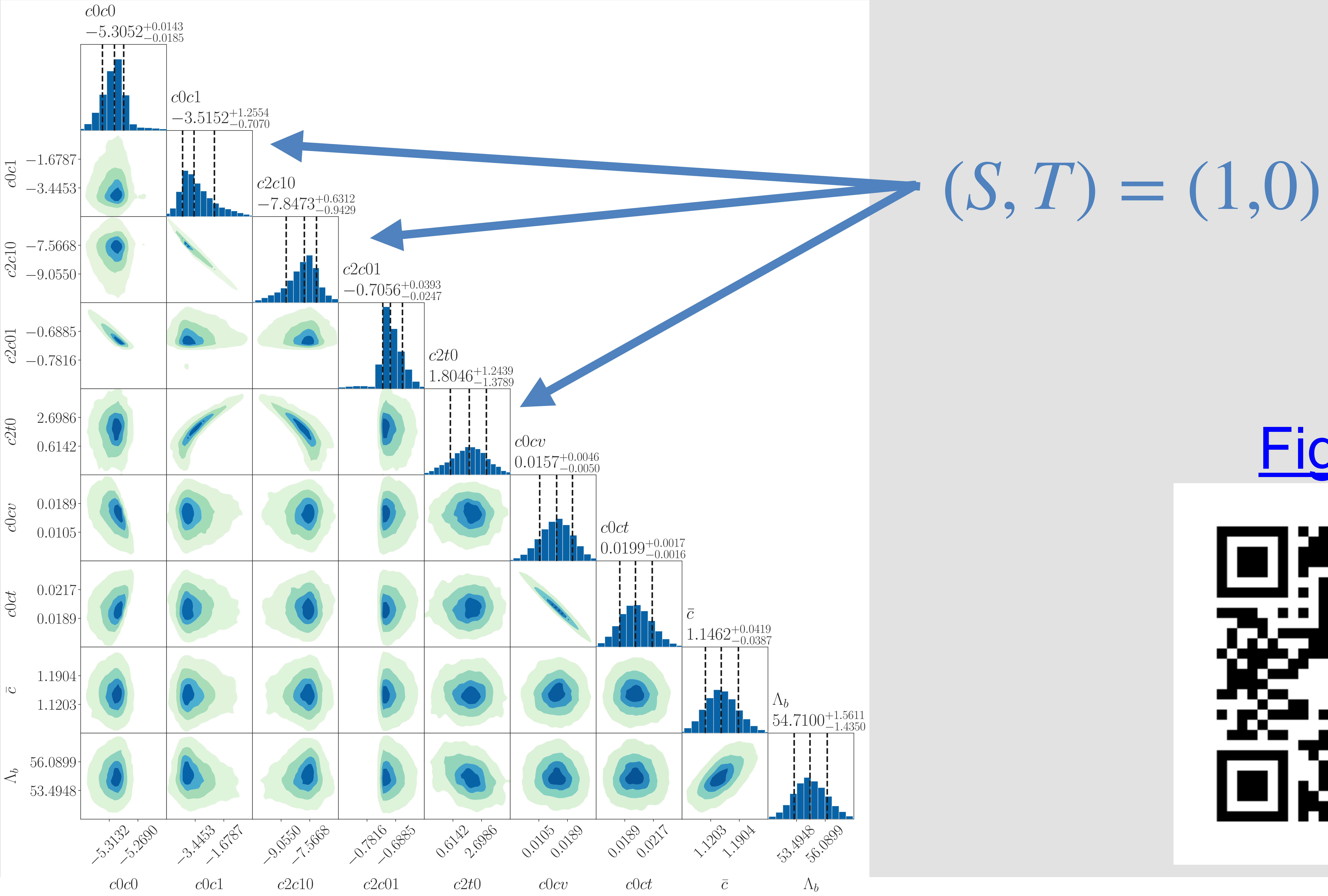

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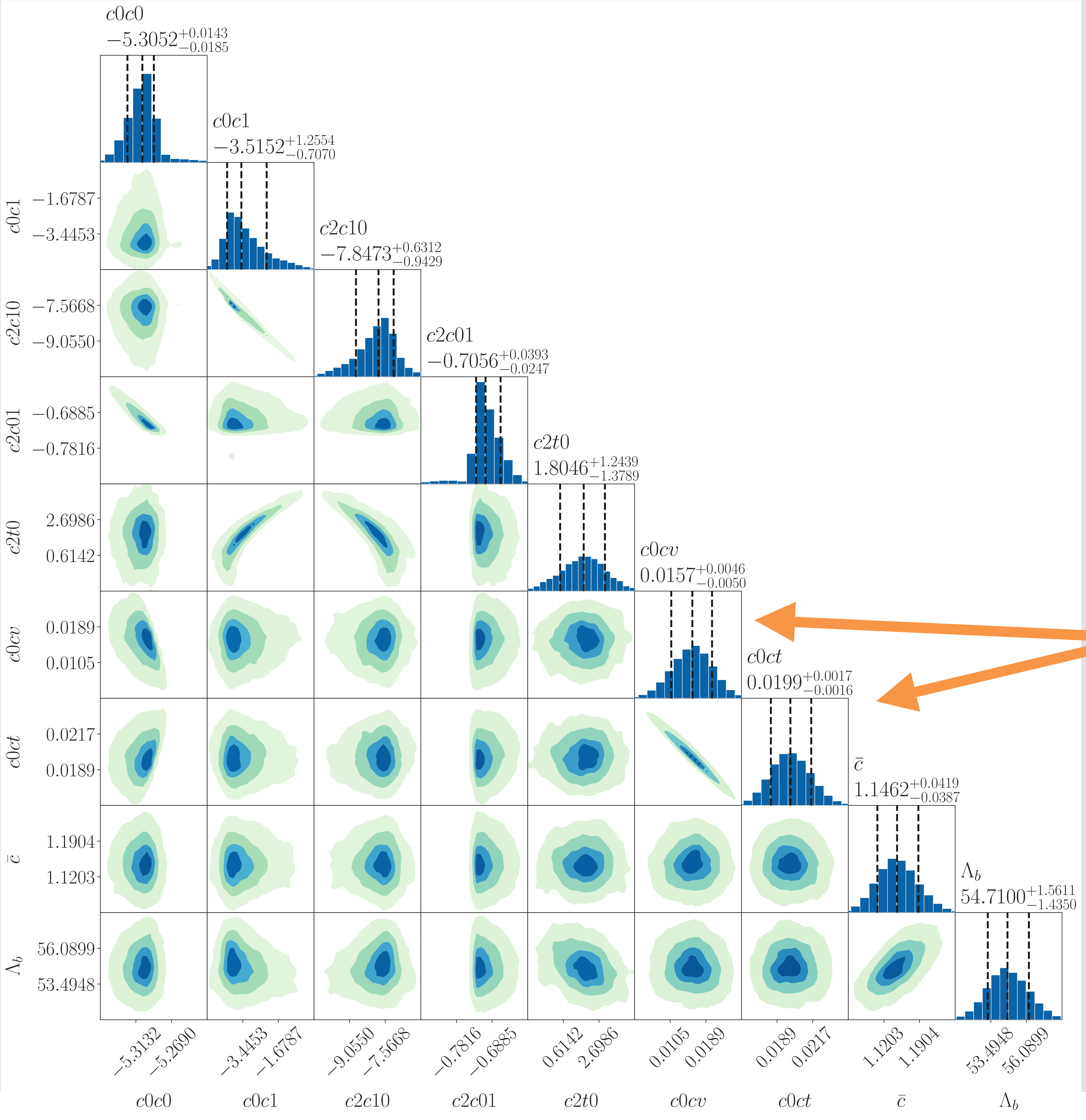
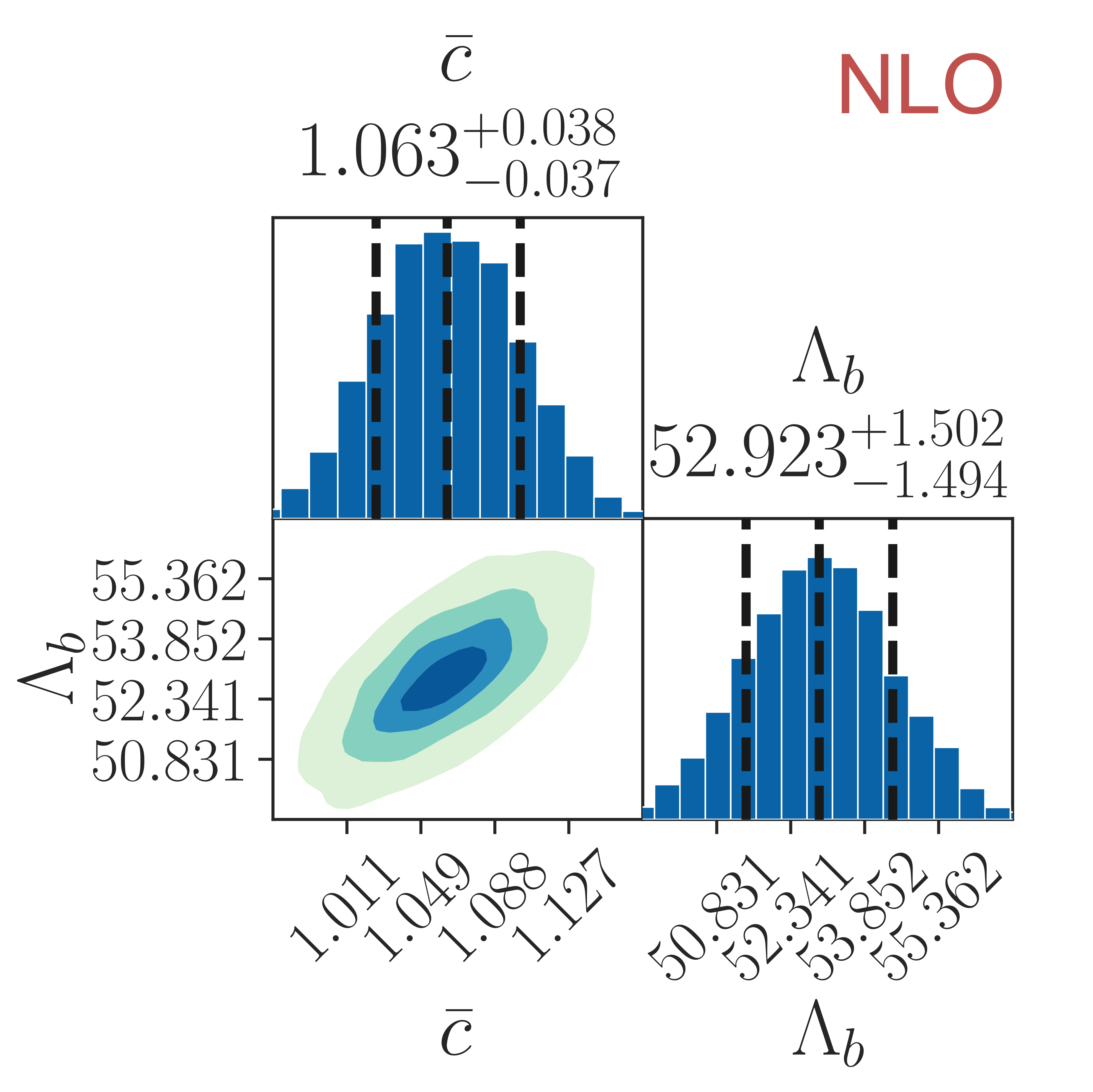
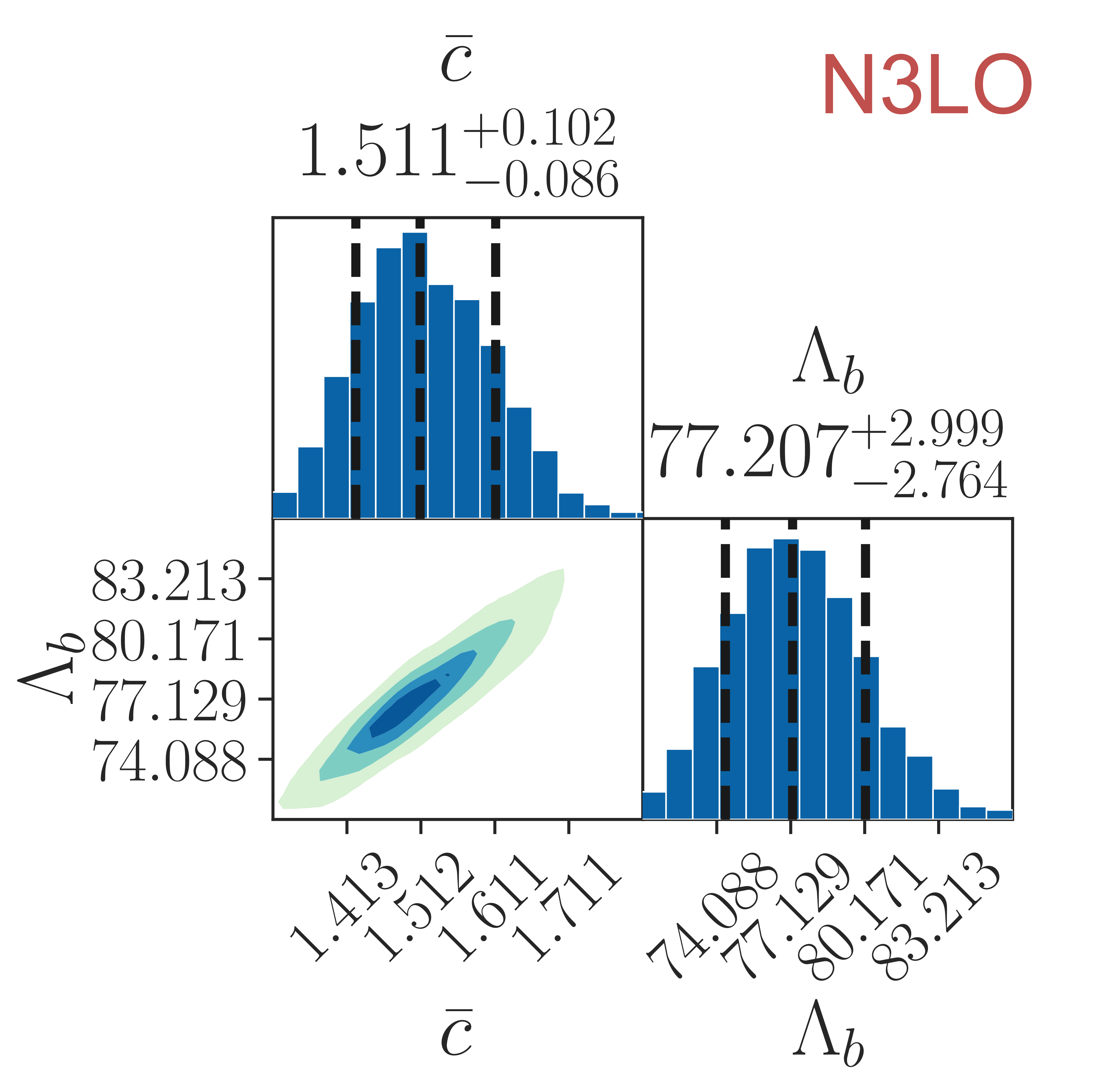


C^{CD}

[Figures:](#)

2.5 fm $\bar{c}$ and Λ_b Posteriors





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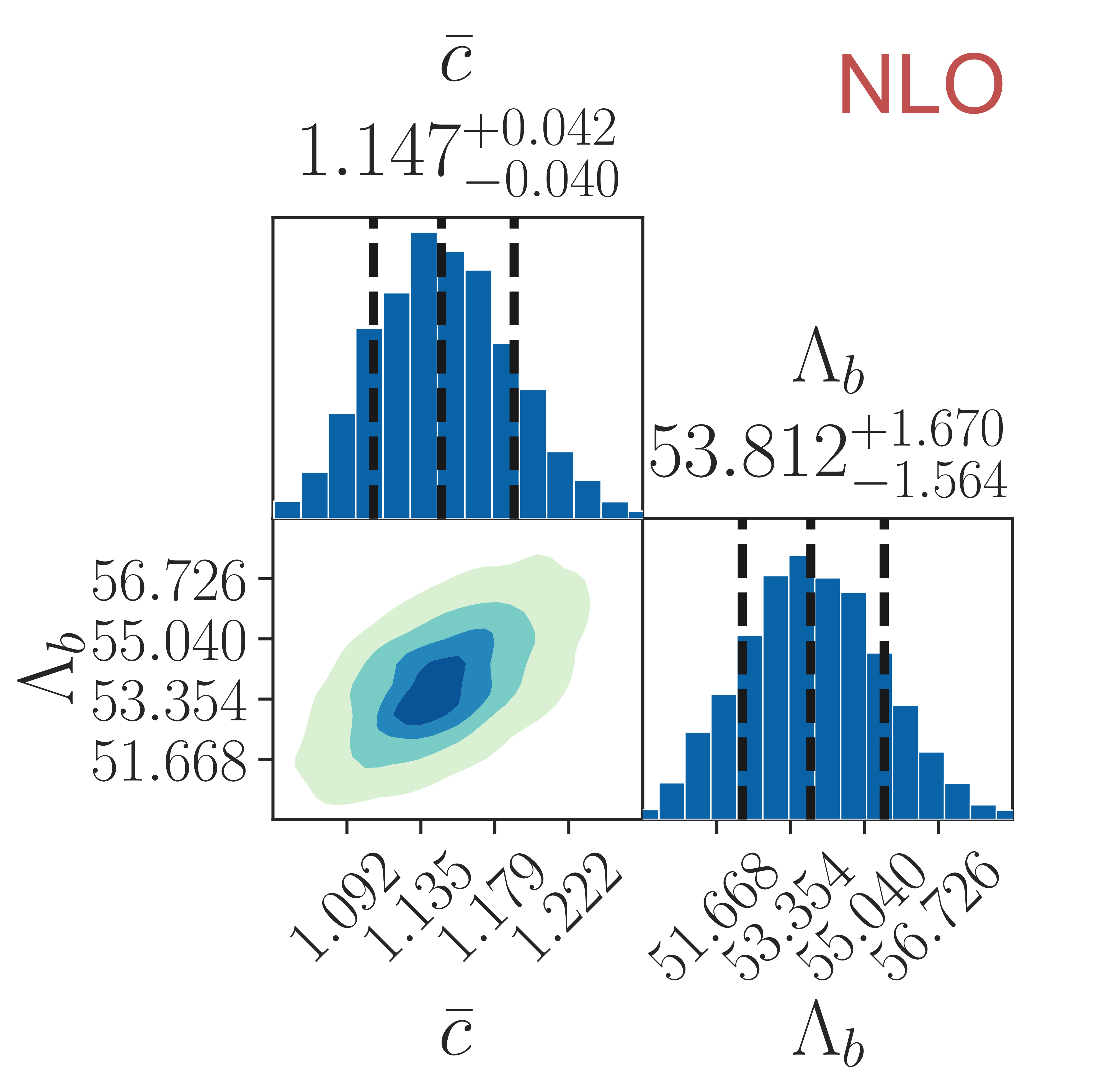
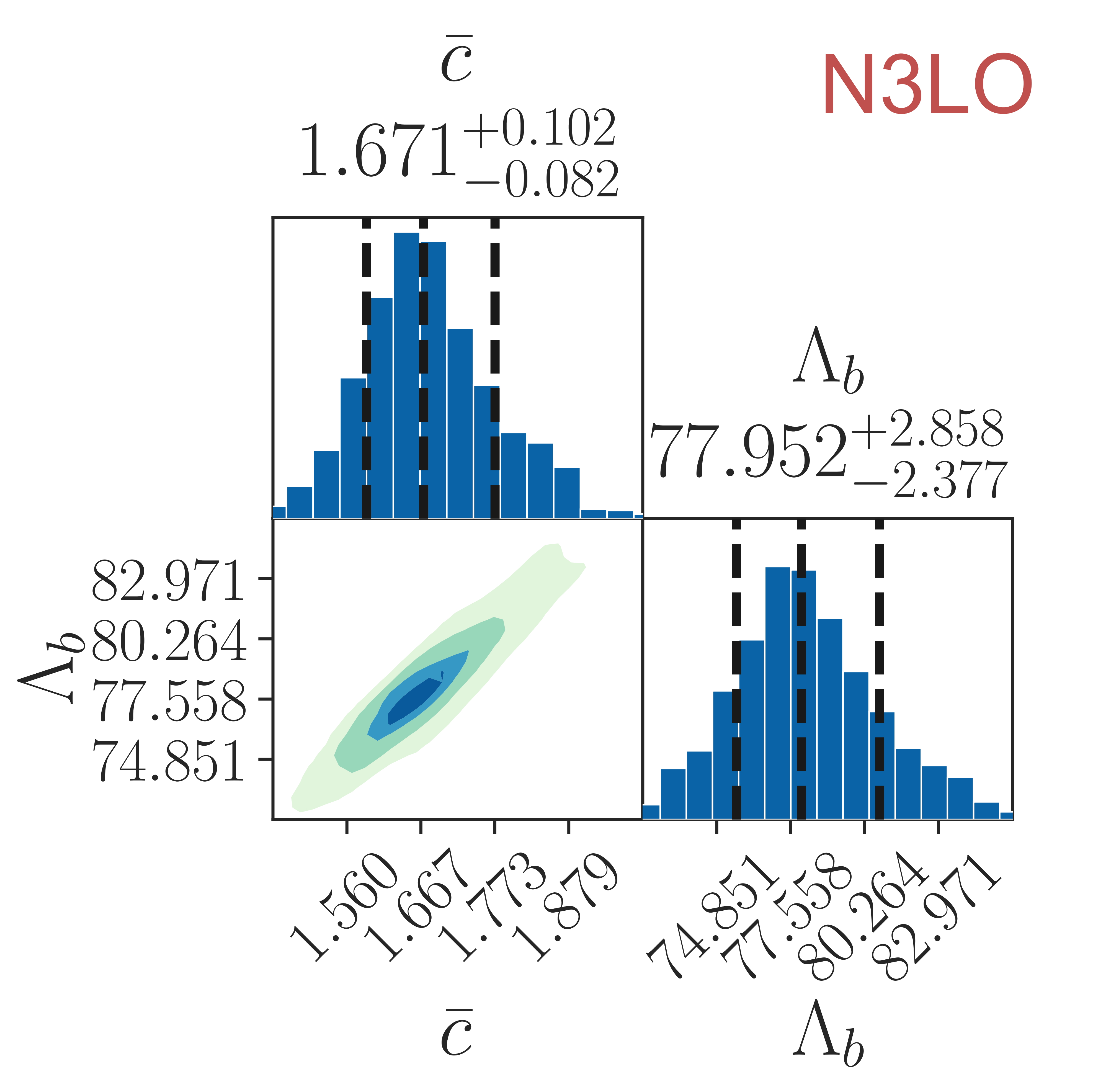
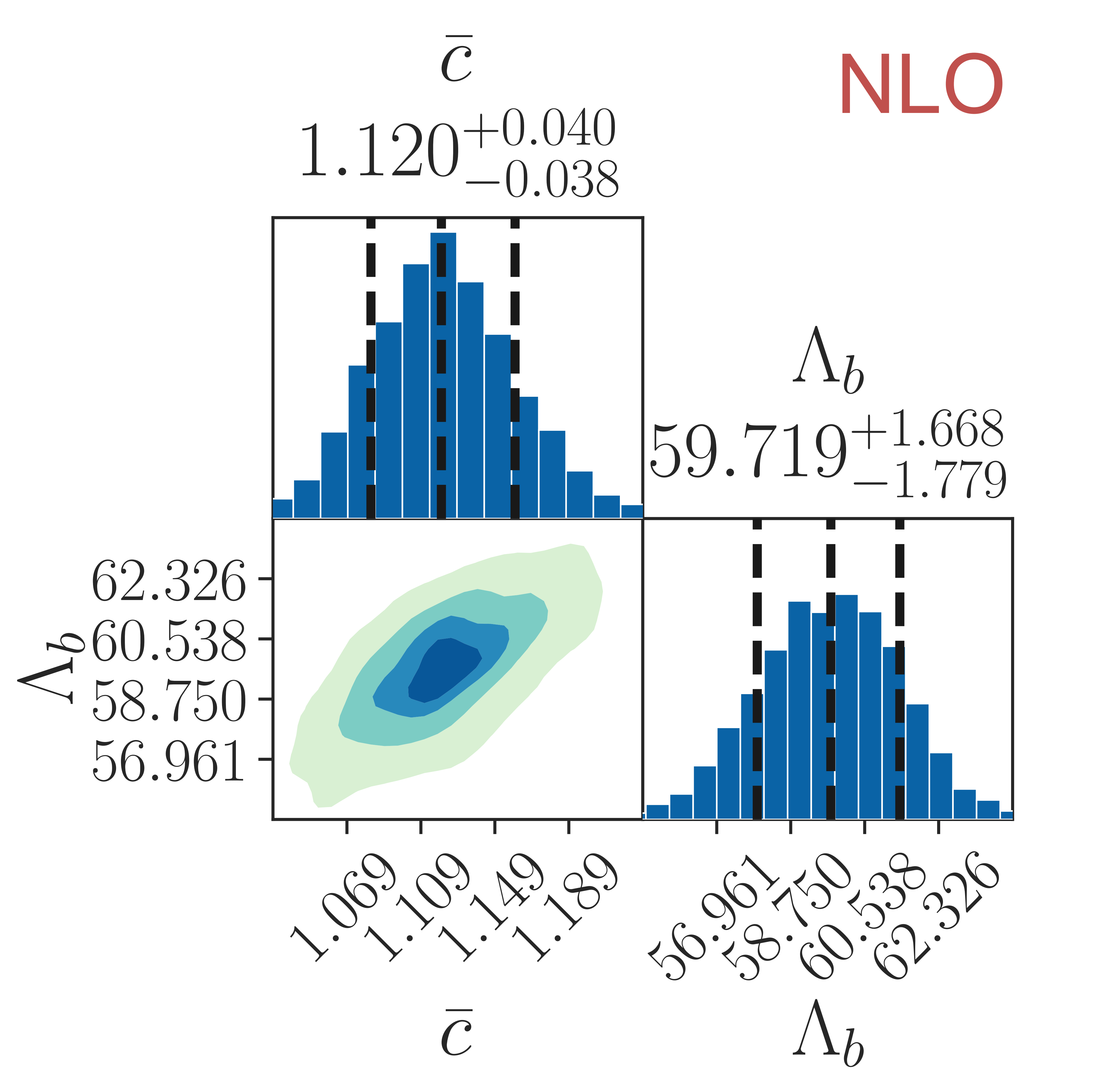
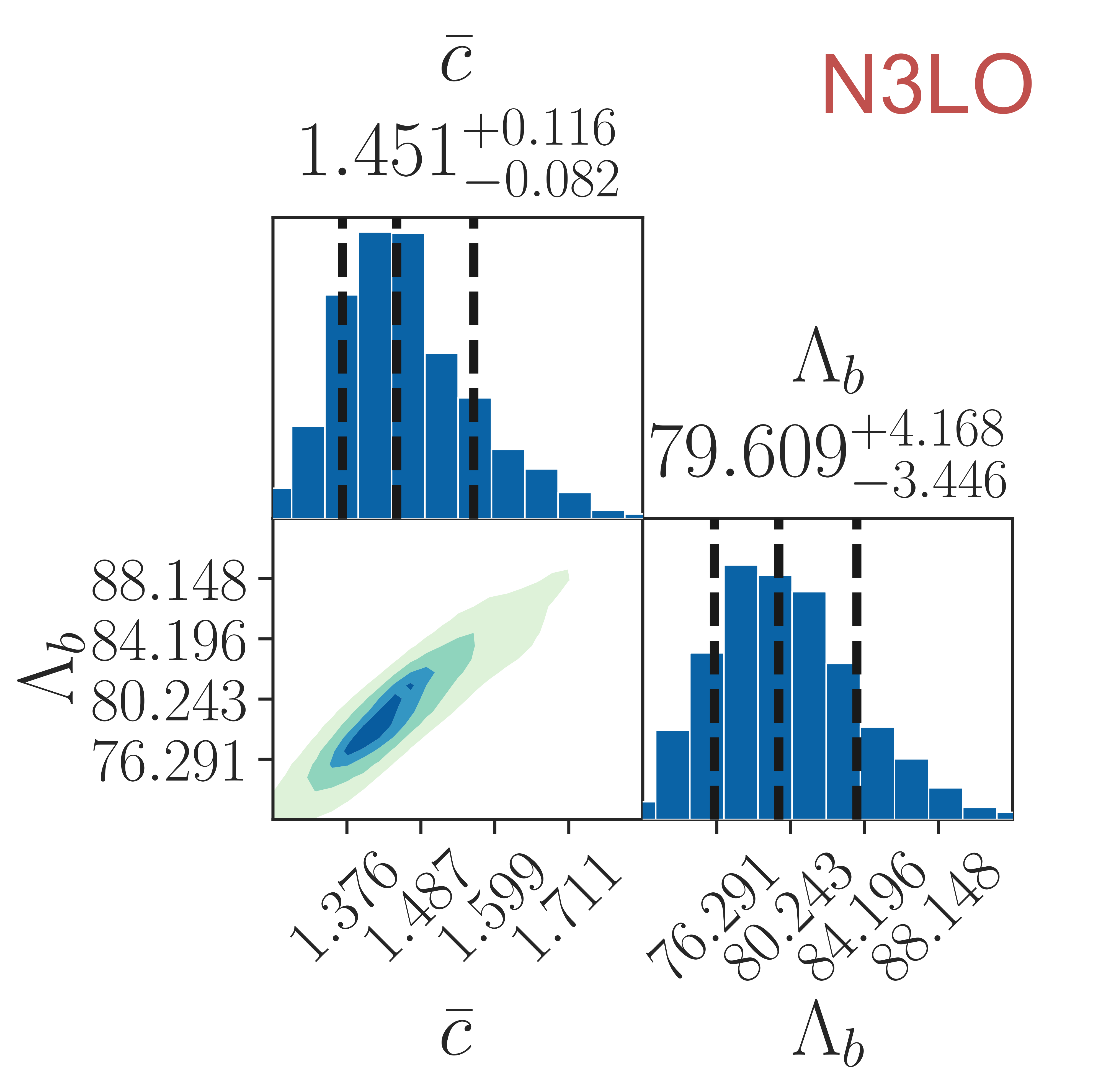


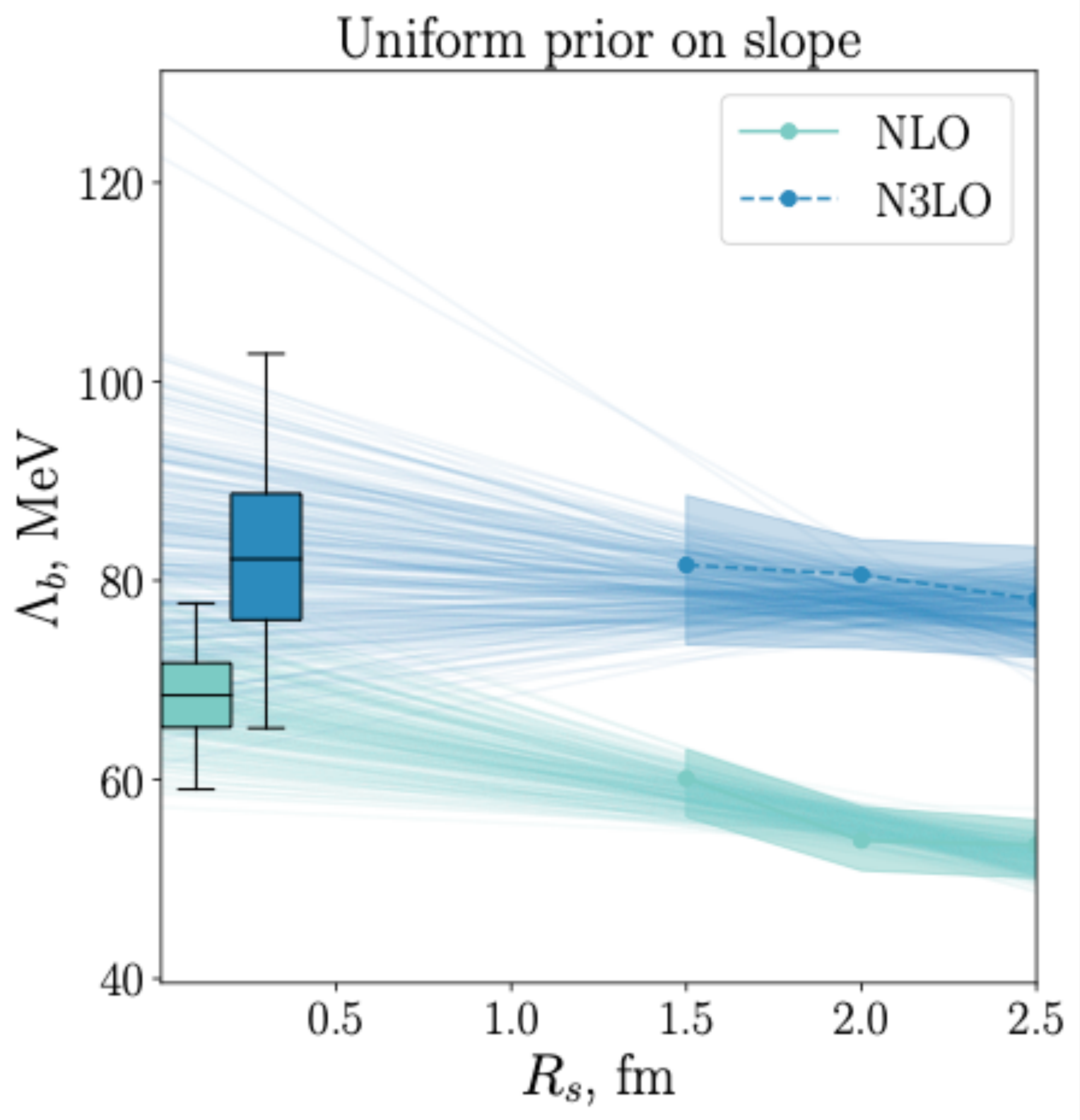


1.5 fm $\bar{c}$ and Λ_b Posteriors





Extrapolation to Remove Artifacts



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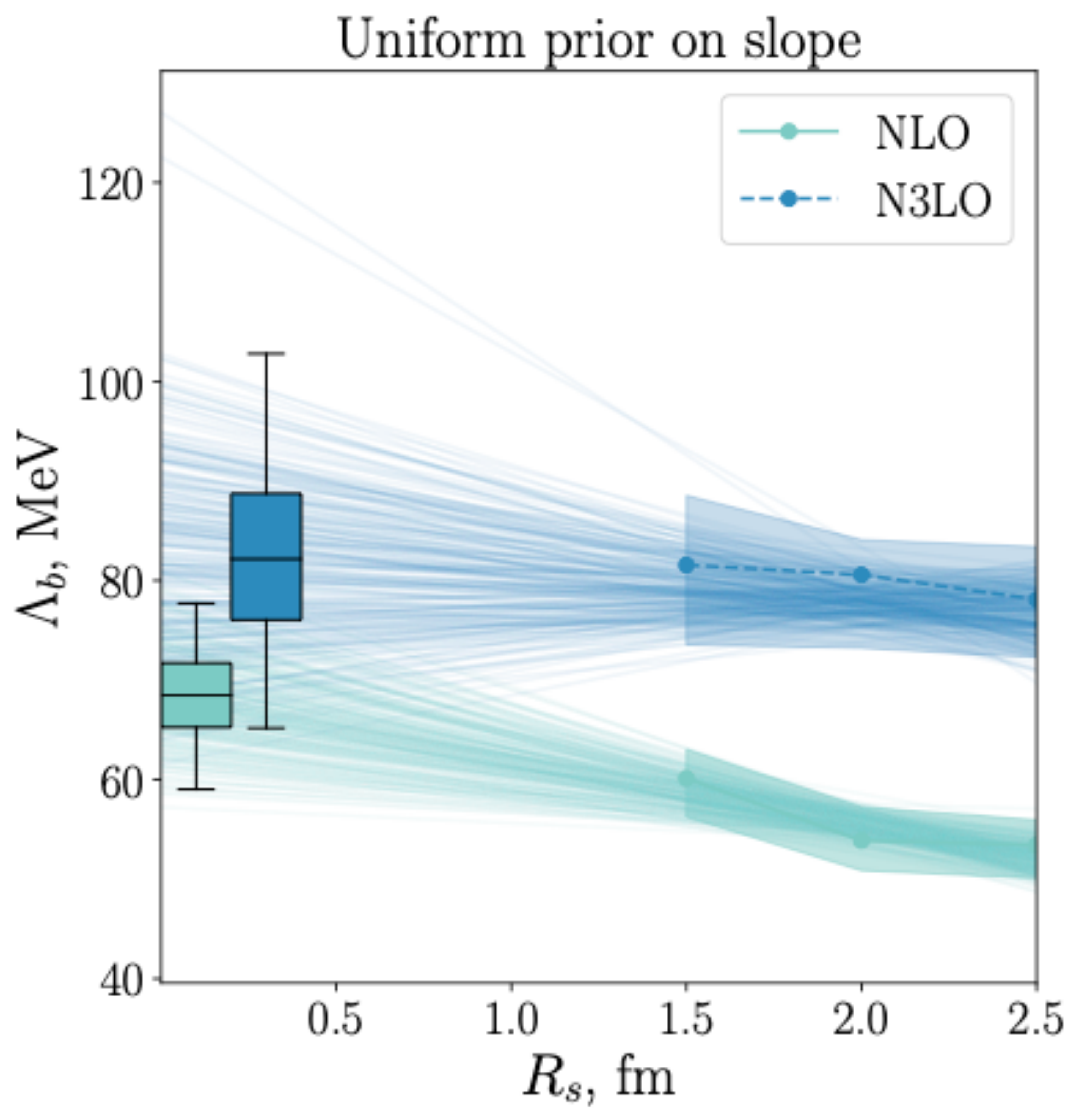

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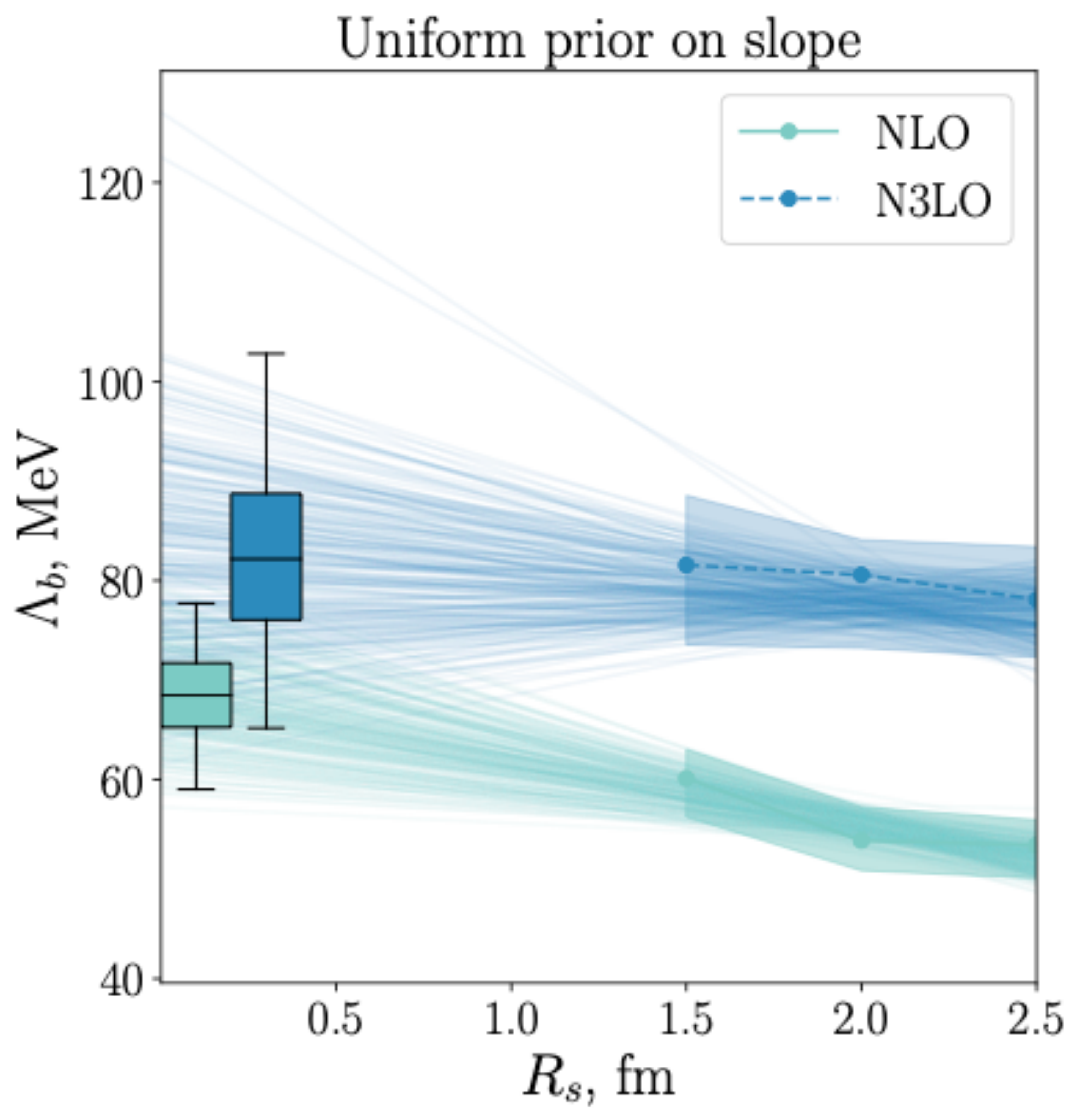

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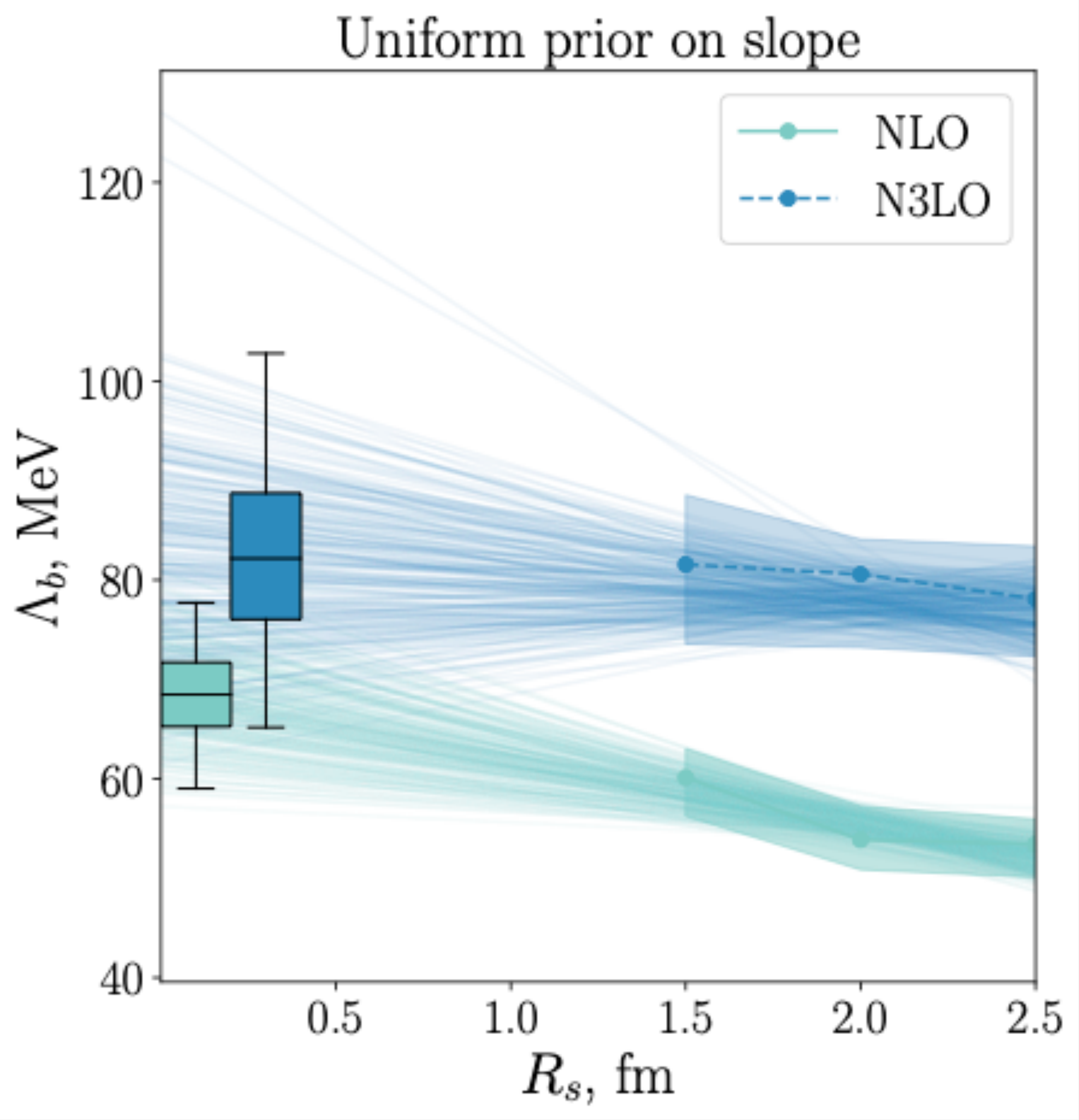

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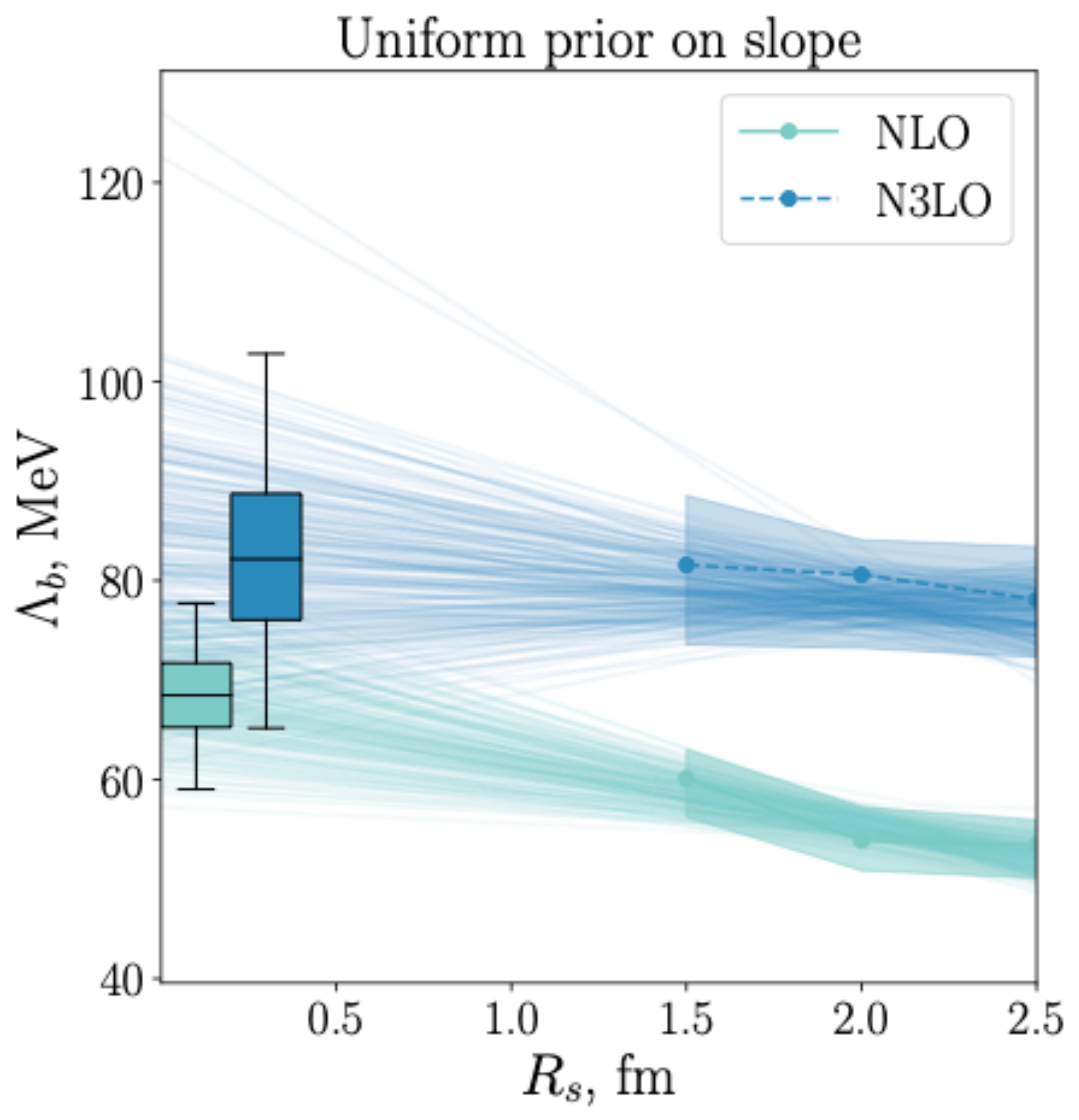

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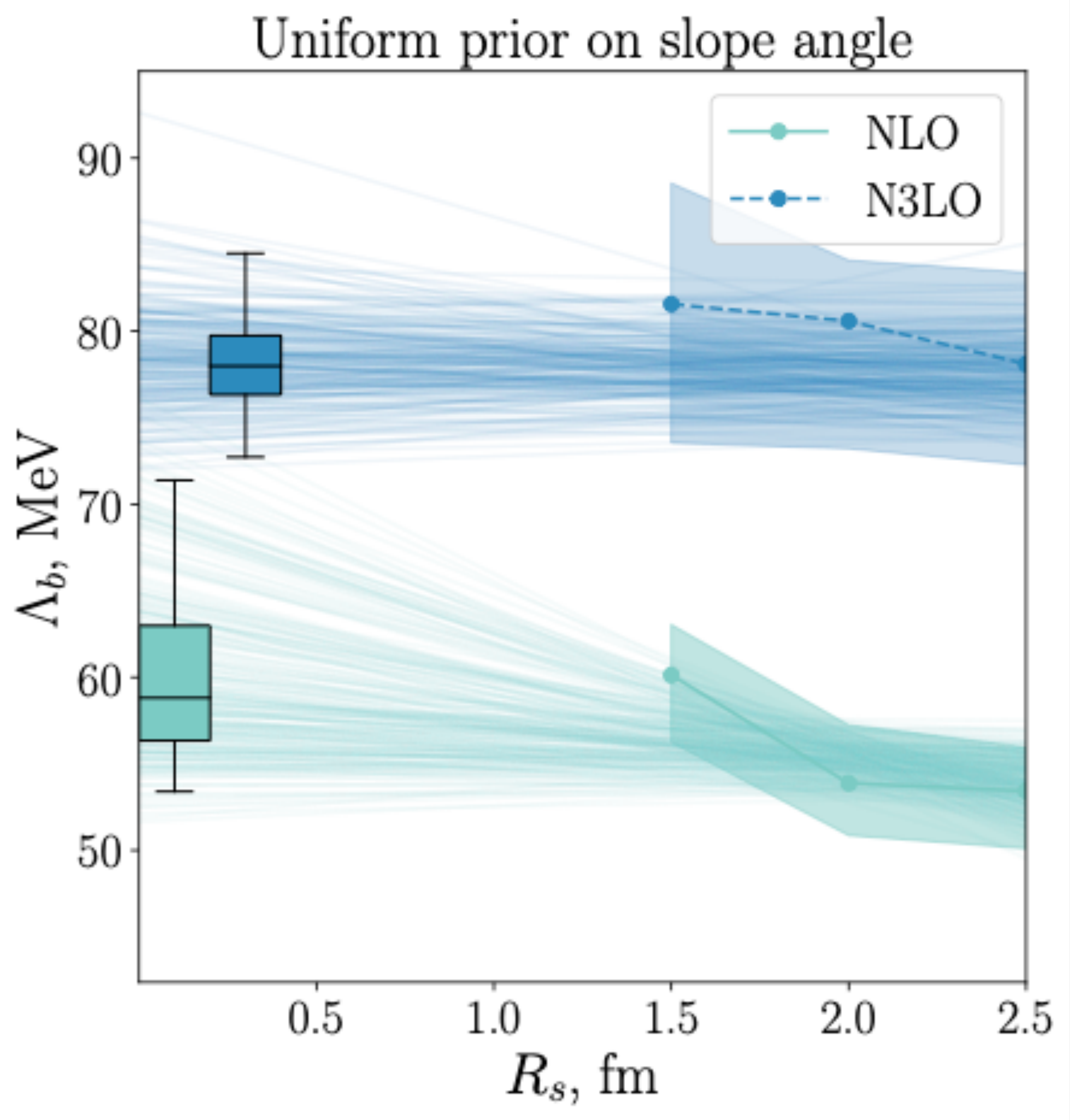

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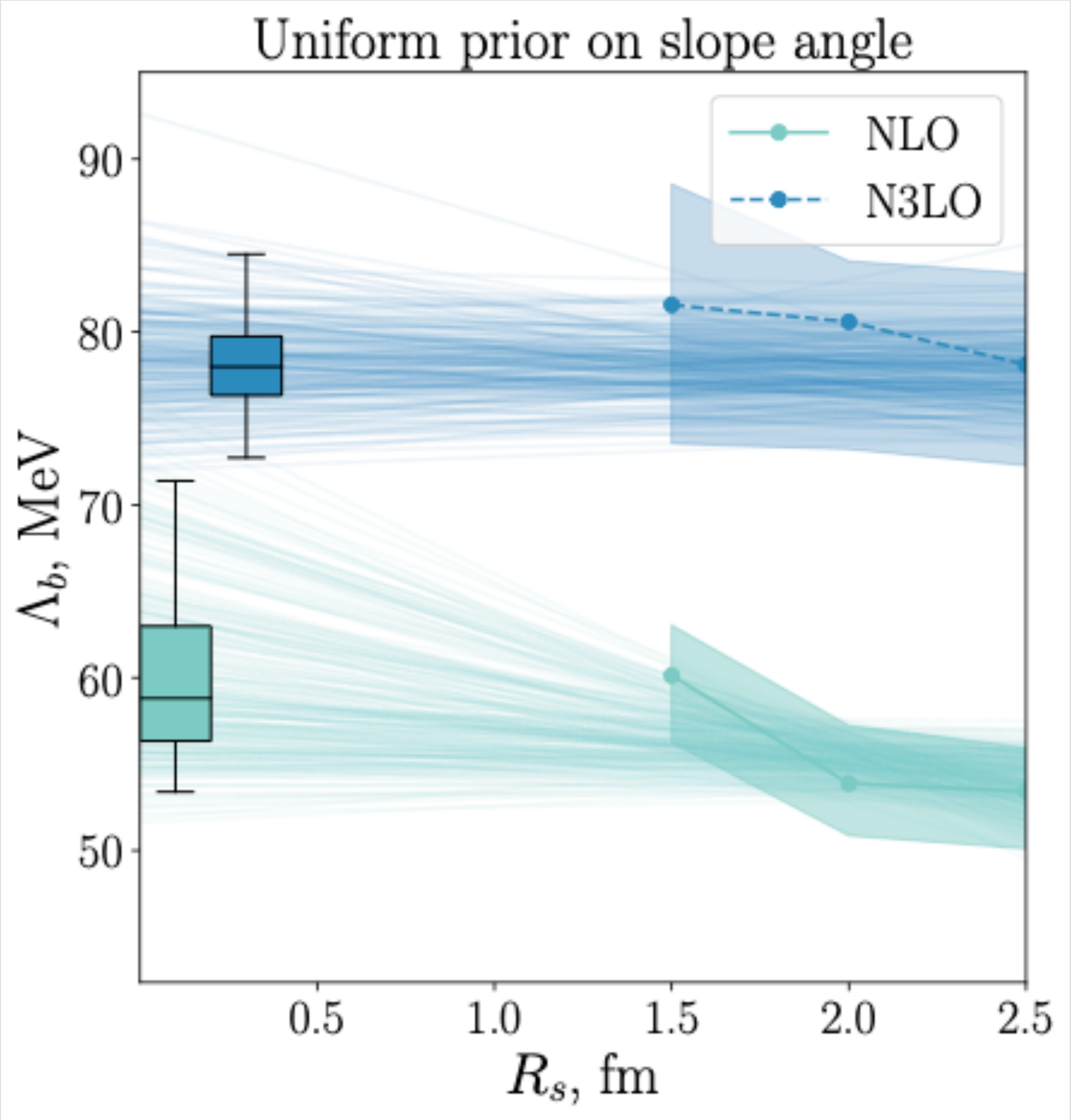

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The data is telling us that our “Weinberg-ized” pionless EFT is predominantly *s*-wave physics!

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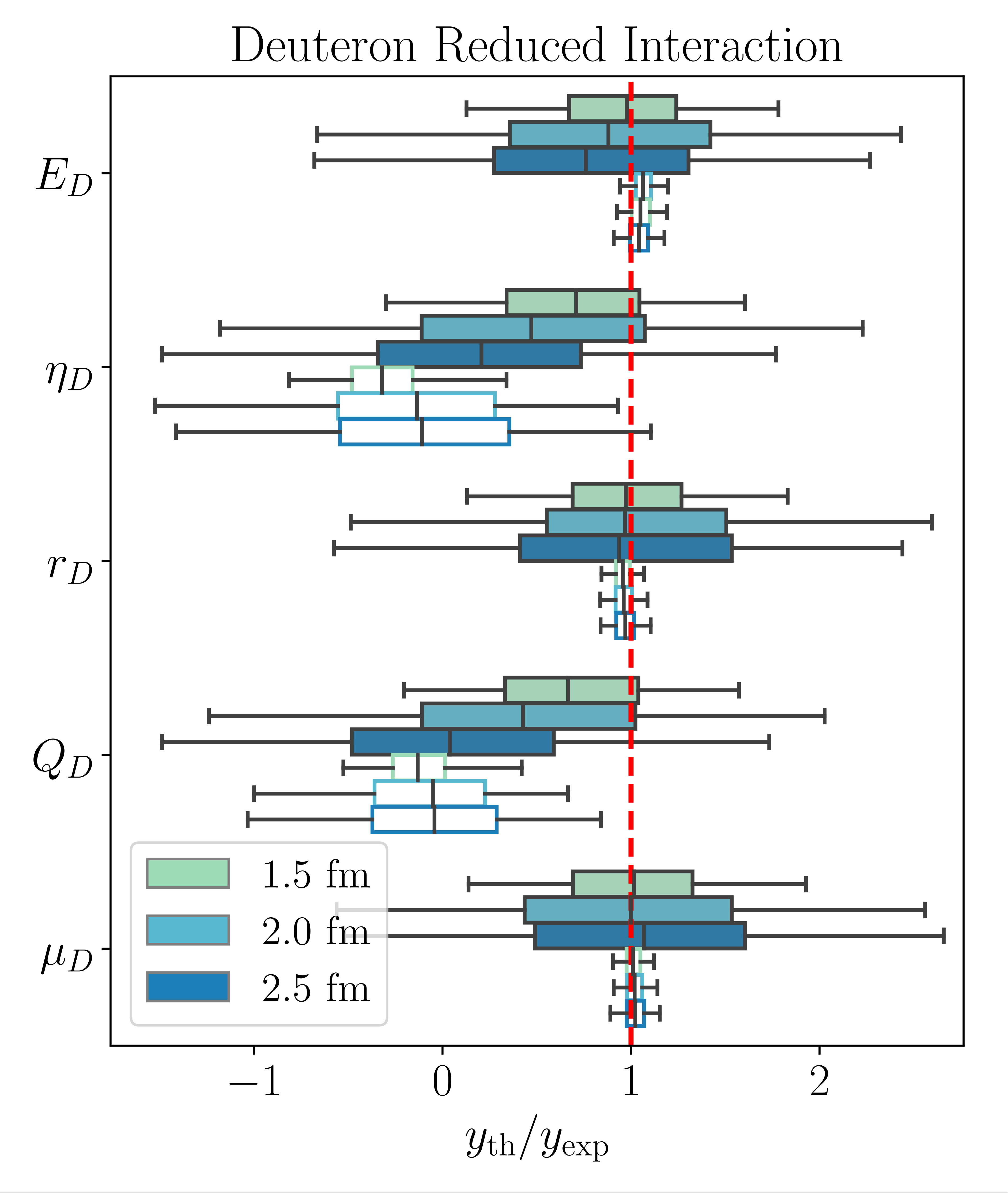
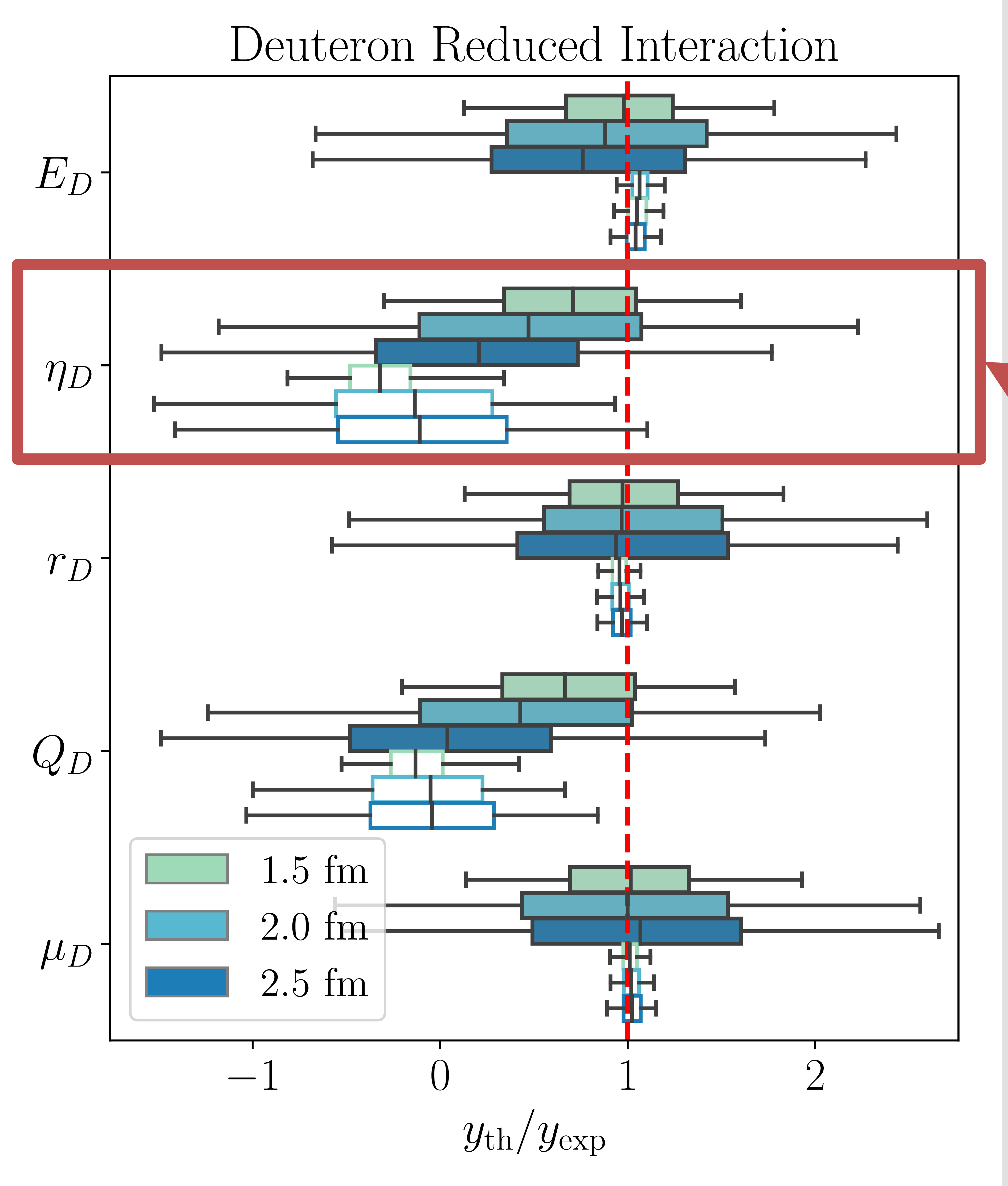
This can be done for **any** calculation of nuclear observables.

Propagation of Errors for Deuteron

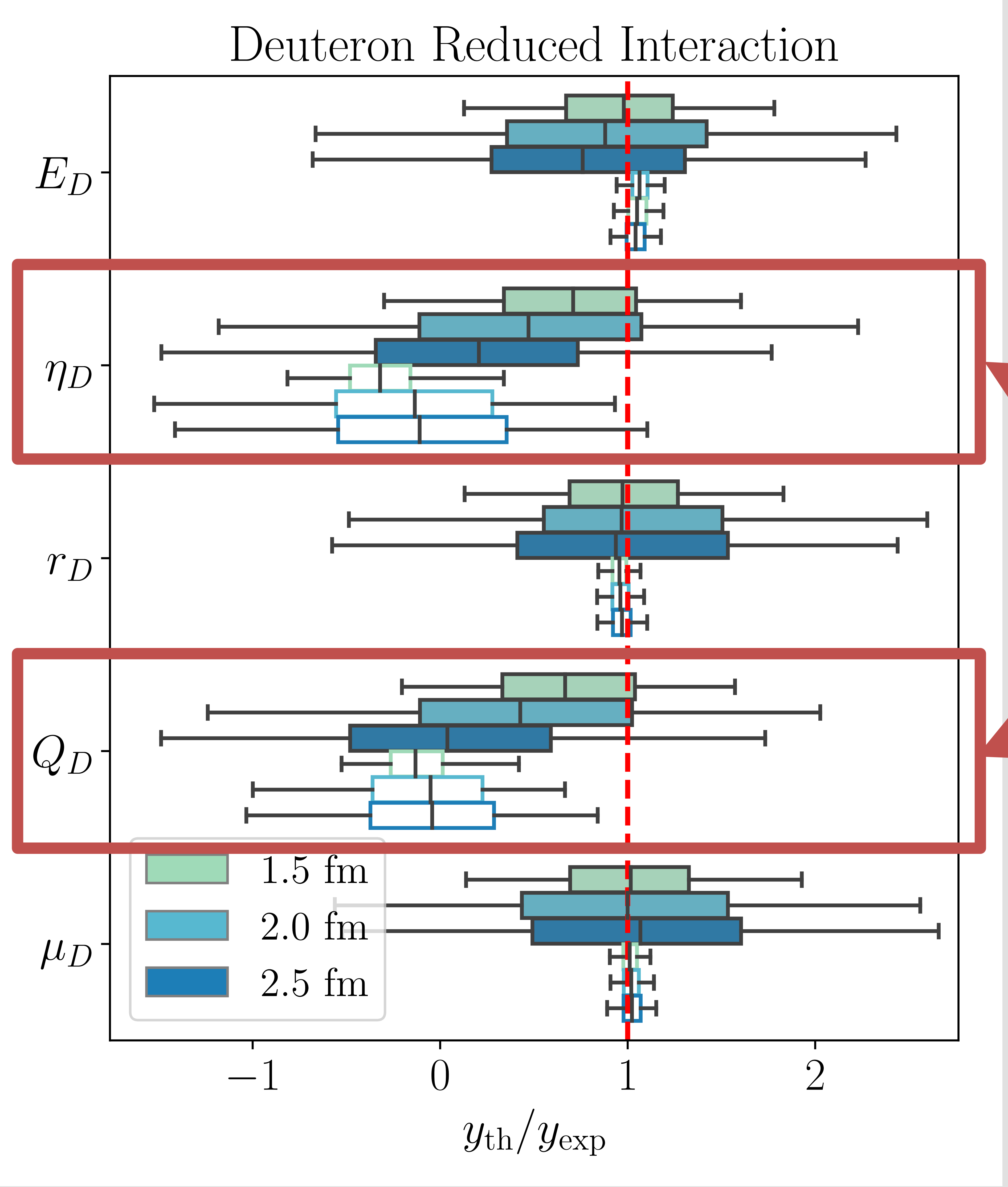


Propagation of Errors for Deuteron



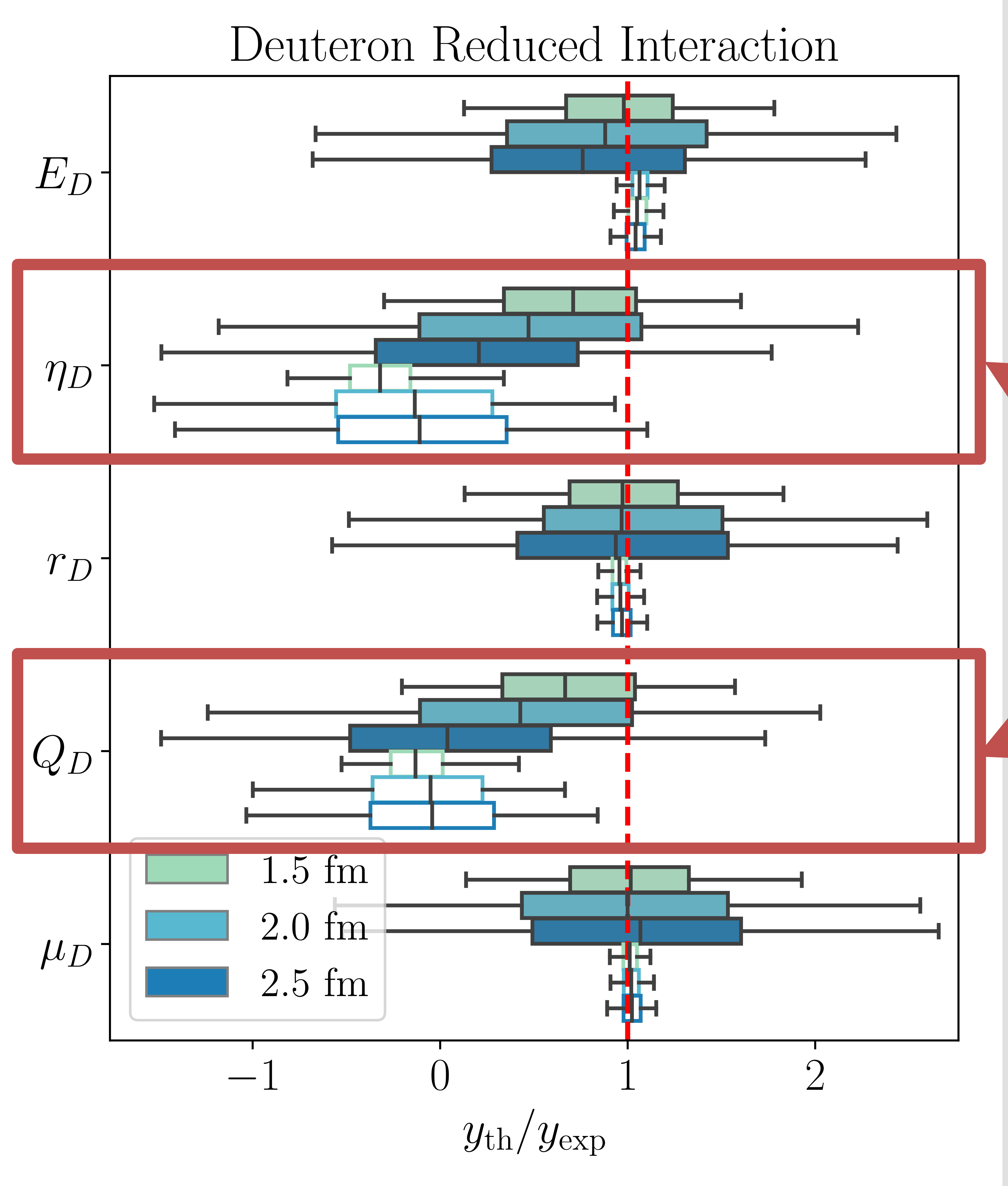
- Poorly constrained d-waves

Propagation of Errors for Deuteron



- Poorly constrained d-waves
- 2b corrections at $O(Q^5)$

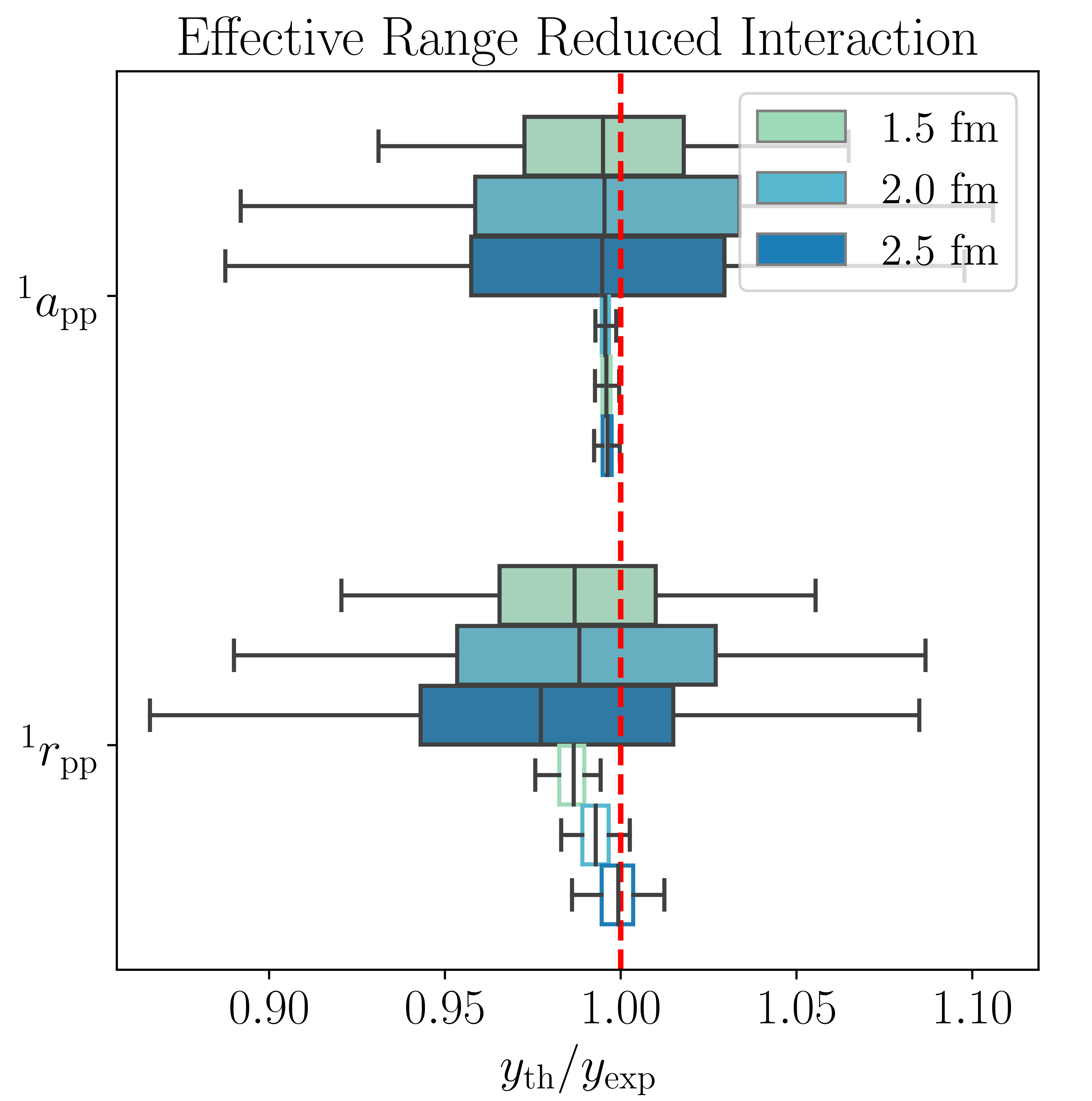
Propagation of Errors for Deuteron

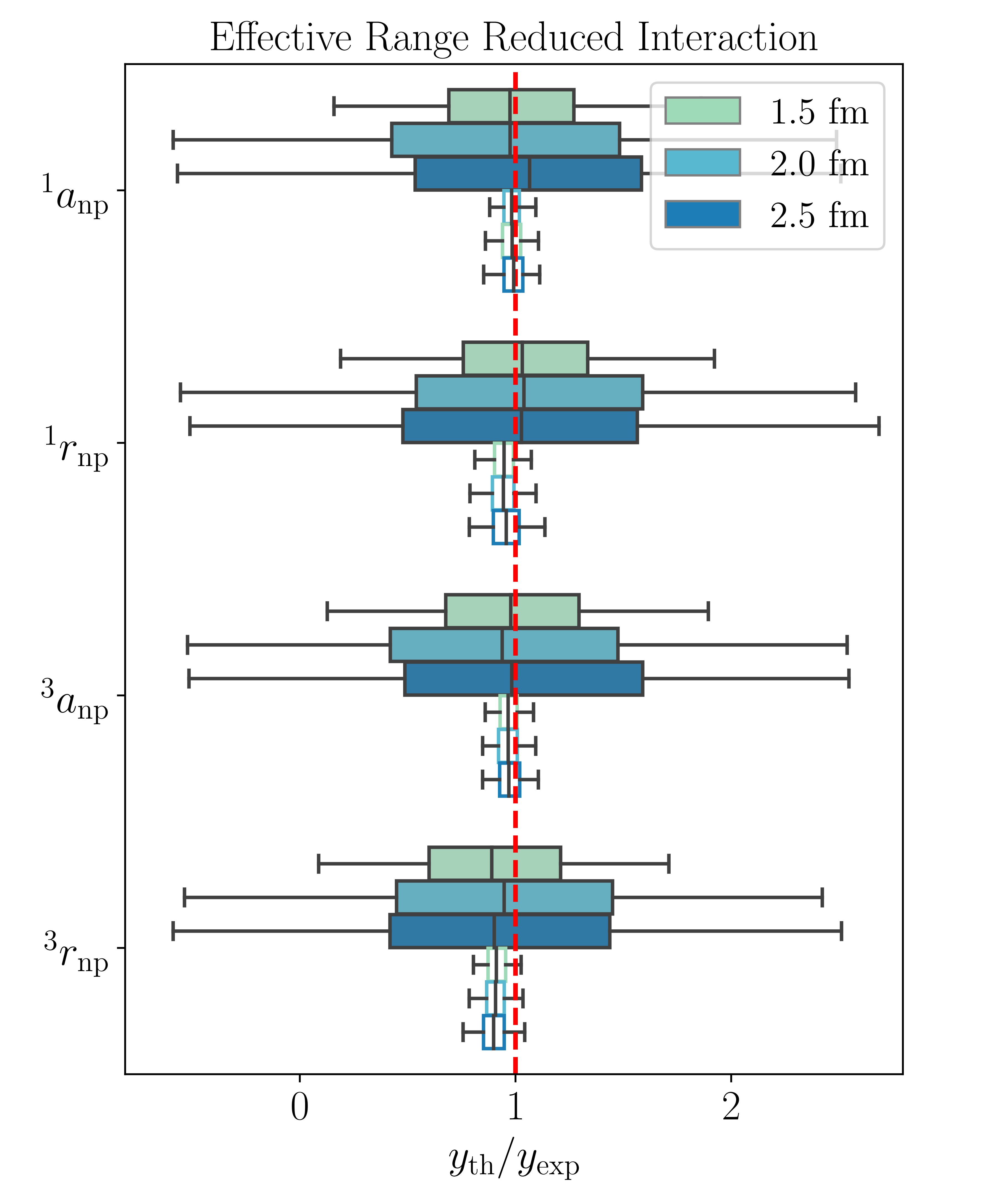


- Poorly constrained d-waves
- 2b corrections at $O(Q^5)$

→SHOULD BE CONSISTENT WITH 0

Propagation of Errors for ERPs





More Degrees of Freedom

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- For pion- and Δ-full interactions, we must look at higher energy data (~200 MeV)

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$\sim 10^5$ parallel sample steps at ~4 min. per step

$\rightarrow$280 days of wall time on an HPC

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Gaussian Process Emulation

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Gaussian Process Emulation

Reduced Basis Methods via Galerkin Projection

Outline

- Motivation/Bayesian EFT Model Calibration
- BUQEYE Formalism
- Interaction Choice
- Results
- Questions

Open Questions

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- Can Bayesian machinery help us identify consistent power counting? E.x. breakdown discrepancies across orders?
- Data can inform us about EFTs if we work consistently. How do we move towards consistent order-by-order inclusion of many-body forces and currents?

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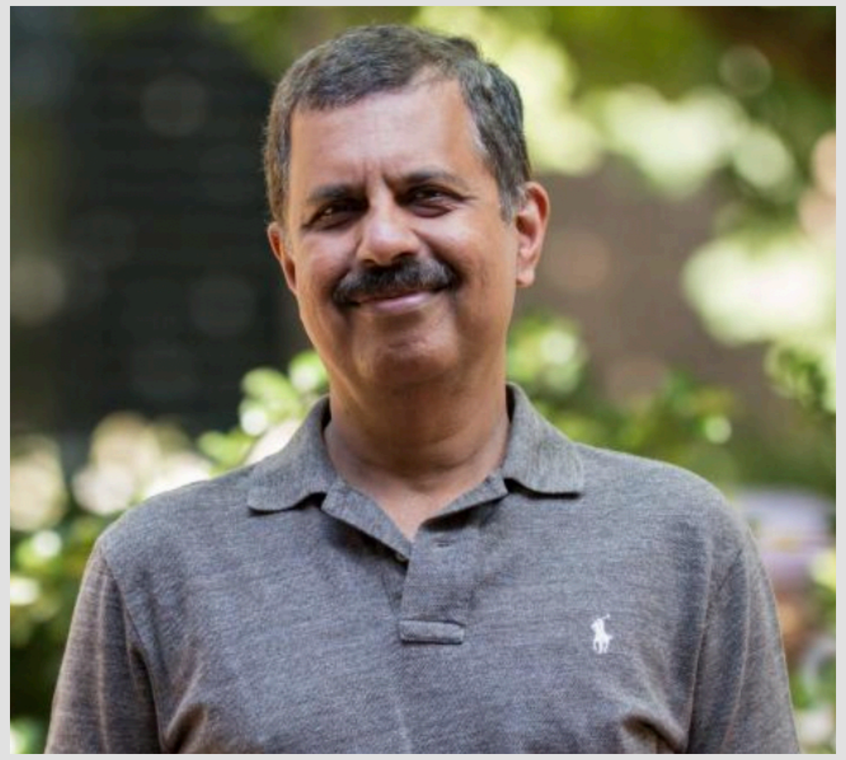

Sai Iyer
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Fellowship/Travel

BAND Bayesian Analysis of Nuclear Dynamics

Collaborations

NTNP

NUCLEI
Nuclear Computational Low-Energy Initiative
A SciDAC-5 Project