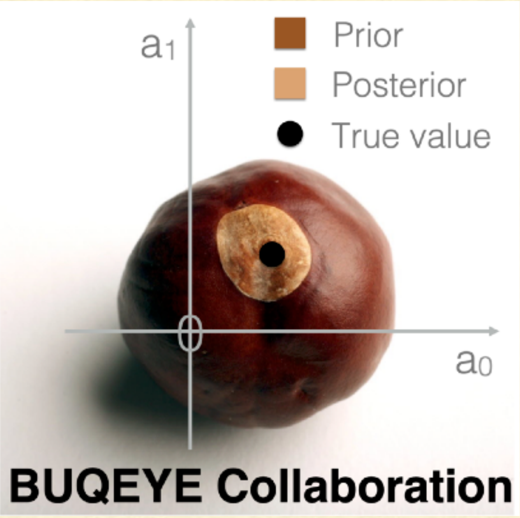
Building error models in an EFT: how and why. Plus an interesting failure mode.

Daniel Phillips



OHIO UNIVERSITY

BAND
Bayesian Analysis of Nuclear Dynamics

Research supported by the US DoE, the NSF Office of Advanced Cyberinfrastructre, and the Swedish Research Council

Outline

- Uncovering the statistical properties of EFTs
- Why?
  - (Get well-calibrated uncertainties)
  - Test EFT convergence (aka power counting)
  - Do accurate LEC inference (no over-fitting, stability with fit region)
  - (Accurate predictions)
- A failure mode: symmetry-protected observables
- Summary

Generic EFT expansion

Consider χEFT, where we have two light scales, p and m_π

- General χEFT series for observable to order k: $y = y_{\rm ref} \sum_{n=0}^{k} c_n(p_{\rm typ}/m_\pi) Q^n$:

$$Q = \frac{(p_{\rm typ}, m_\pi)}{\Lambda_b}; \quad \Lambda_b \approx 600 \text{ MeV}$$

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Higher-order uncertainties

- Exist
- Have a characteristic size $\sim Q^{k+1}$
- Are correlated across the input space
- Have a characteristic correlation length of order the light scale
- Can be modeled statistically

From predictions to coefficients

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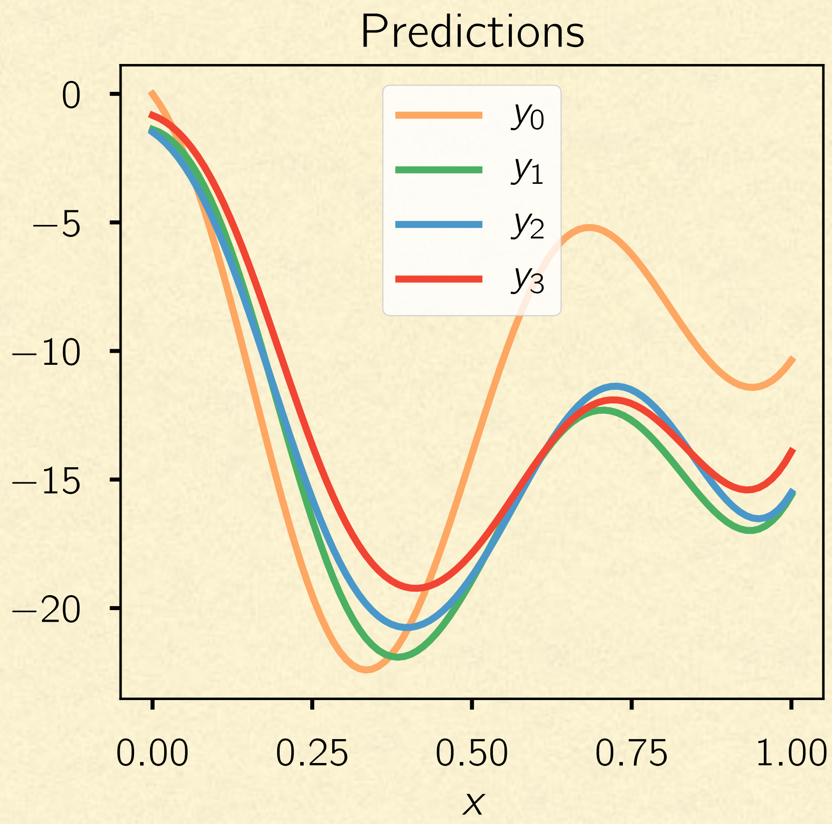

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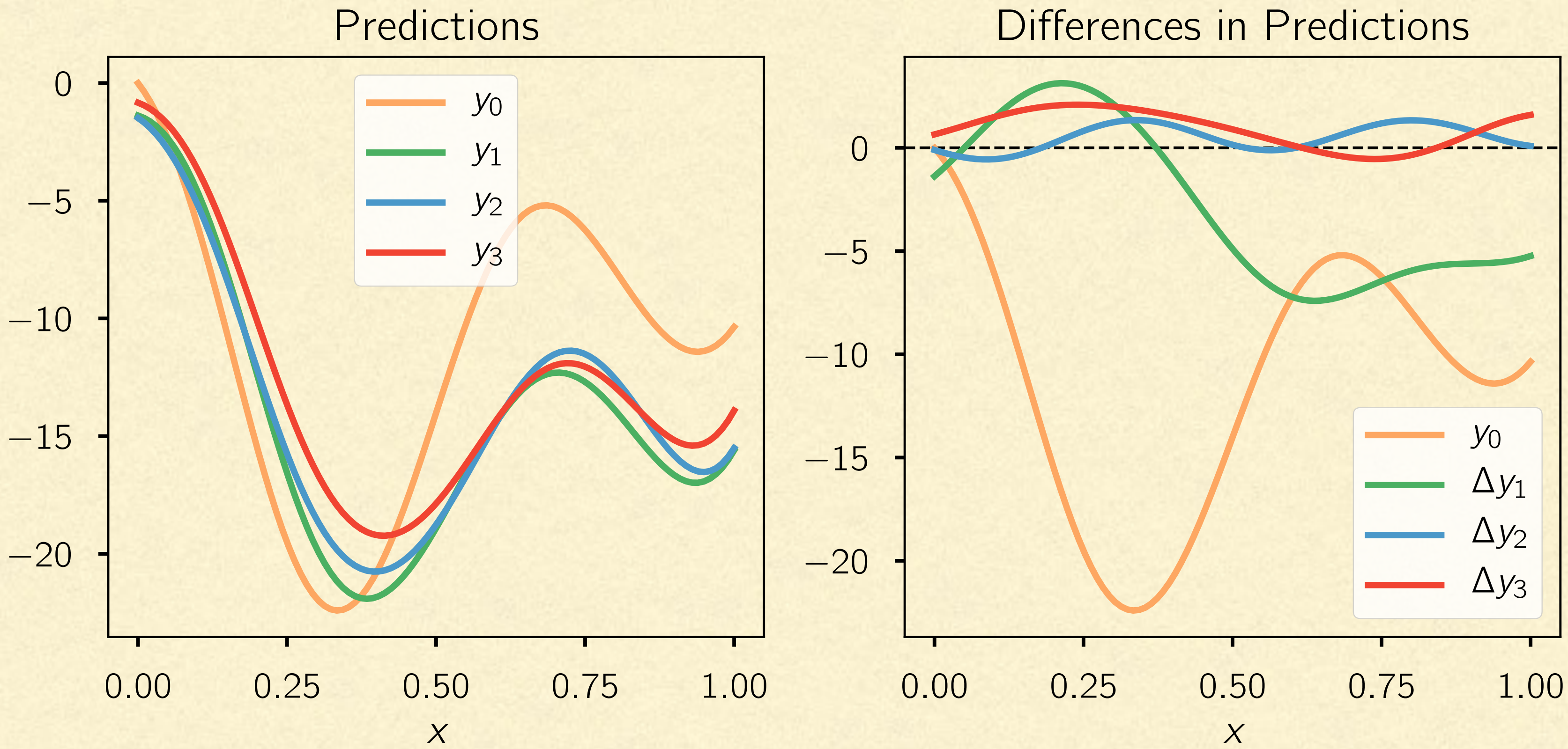

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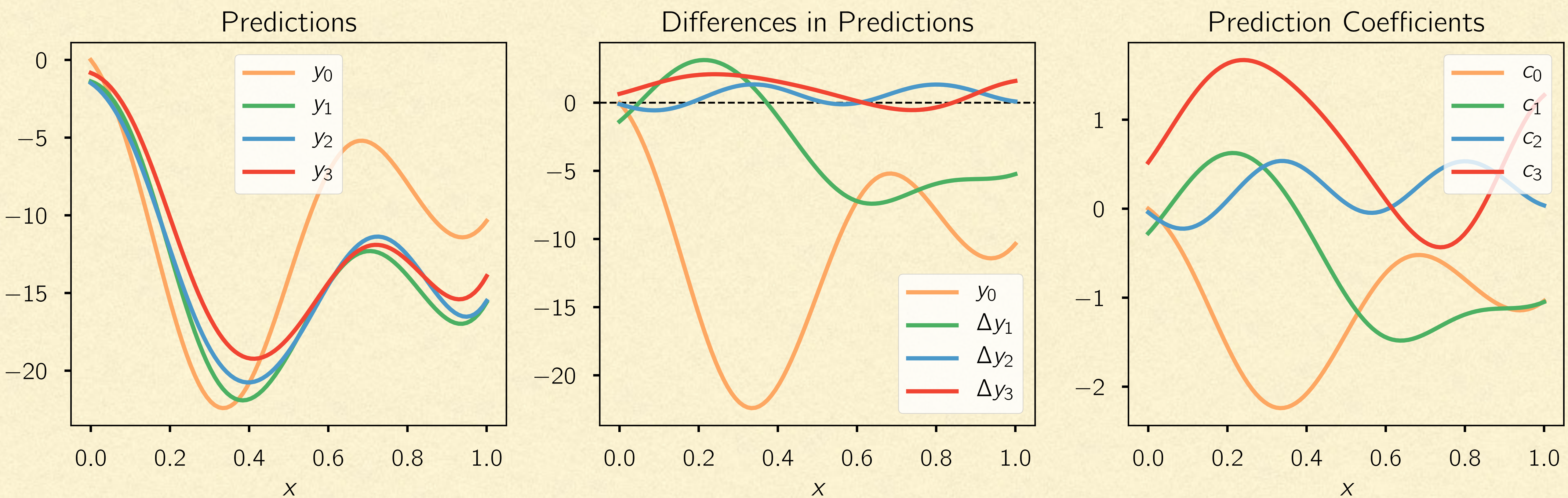

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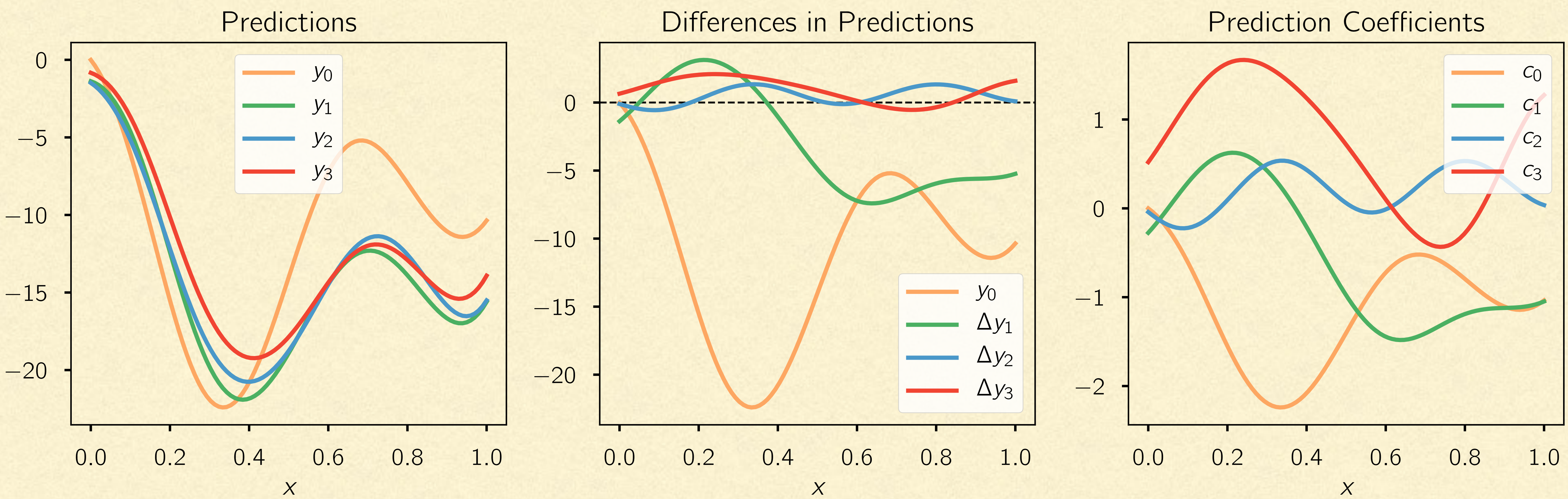

This is what a healthy observable expansion looks like: bounded coefficients, that do not grow or shrink with order.

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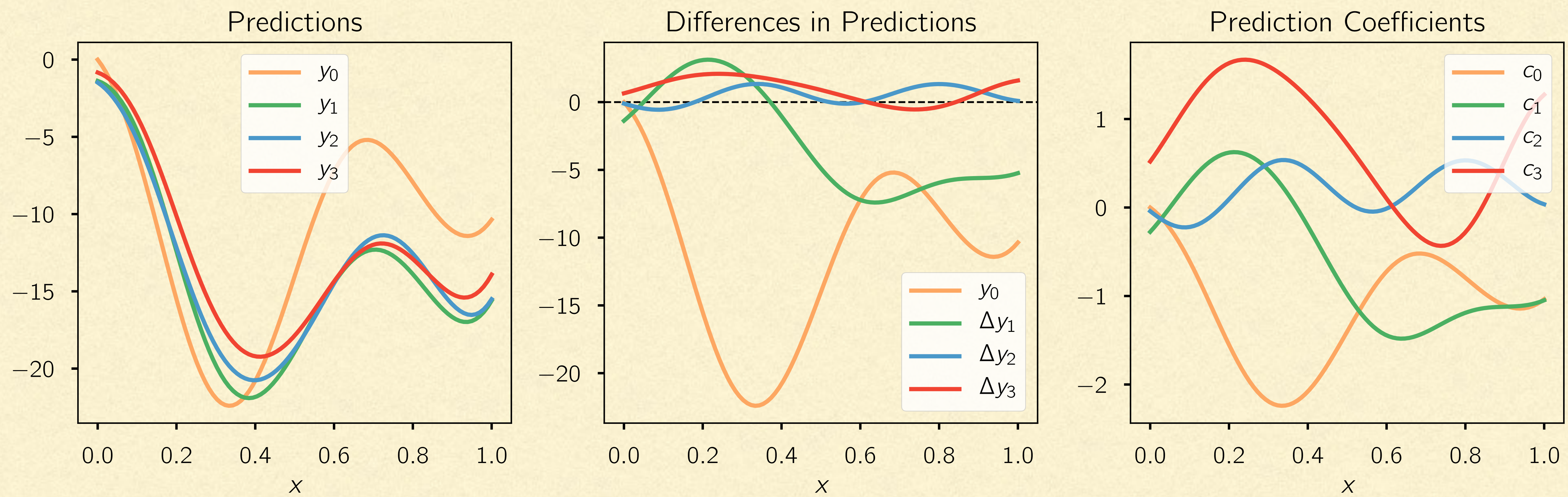

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Data for analysis: EFT predictions at different orders across “input space”

Statistica properties of coefficient curves

Melendez, Wesolowski, Furnstahl, DP, Pratola, PRC (2019)

$$y = y_{\rm ref} \sum_{n=0}^{k} c_n(p/m_\pi) Q^n$$

Function c_n is not a constant.
But the c_n's at different values of p aren't independent random variables either

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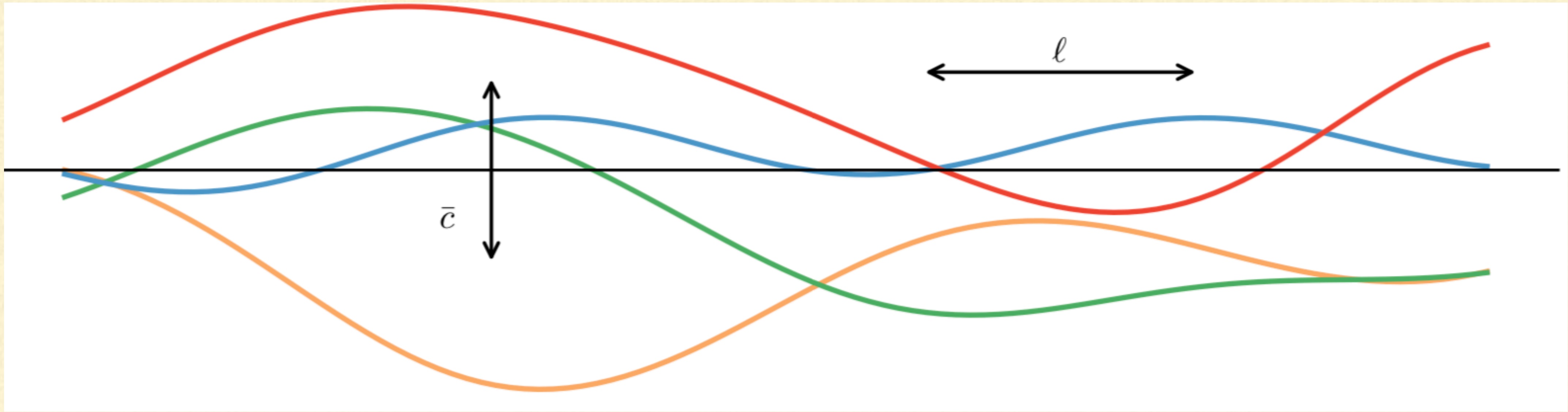

- Gaussian distribution at each point
- With correlation structure parameterized by a single $\bar{c}^2$ and ℓ at all orders

A bit more on Gaussian Processes

- Non-parametric, probabilistic model for a function
- Specify how f(y) is correlated with $f(x_1)$, $f(x_2)$, …..; don't specify underlying functional form.
- But value of f(y) is not deterministic: it's given by a (Gaussian) probability distribution.
- Correlation decreases as points get further away from each other.
- Specify correlation matrix of f at x and y, e.g.:

$$k(f(x), f(y)) = \bar{c}^2 \exp\left(-\frac{(x-y)^2}{2\ell^2}\right)$$

- $\mathrm{pr}(\bar{c}^2 \,|\, I) \sim \chi^{-2}(\nu_0, \tau_0^2); \mathrm{pr}(\ell \,|\, I)$ uniform

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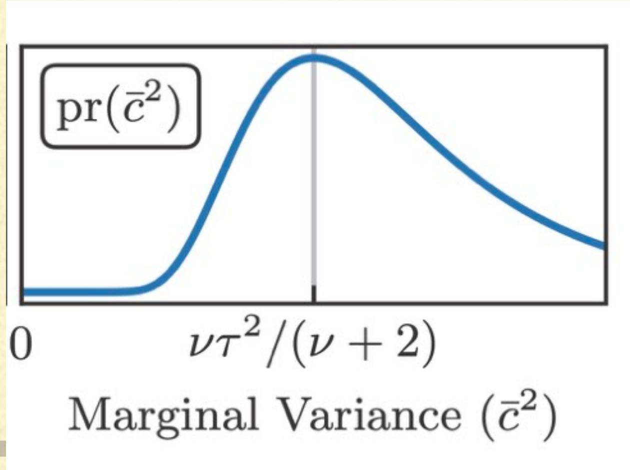
Statistical model choices

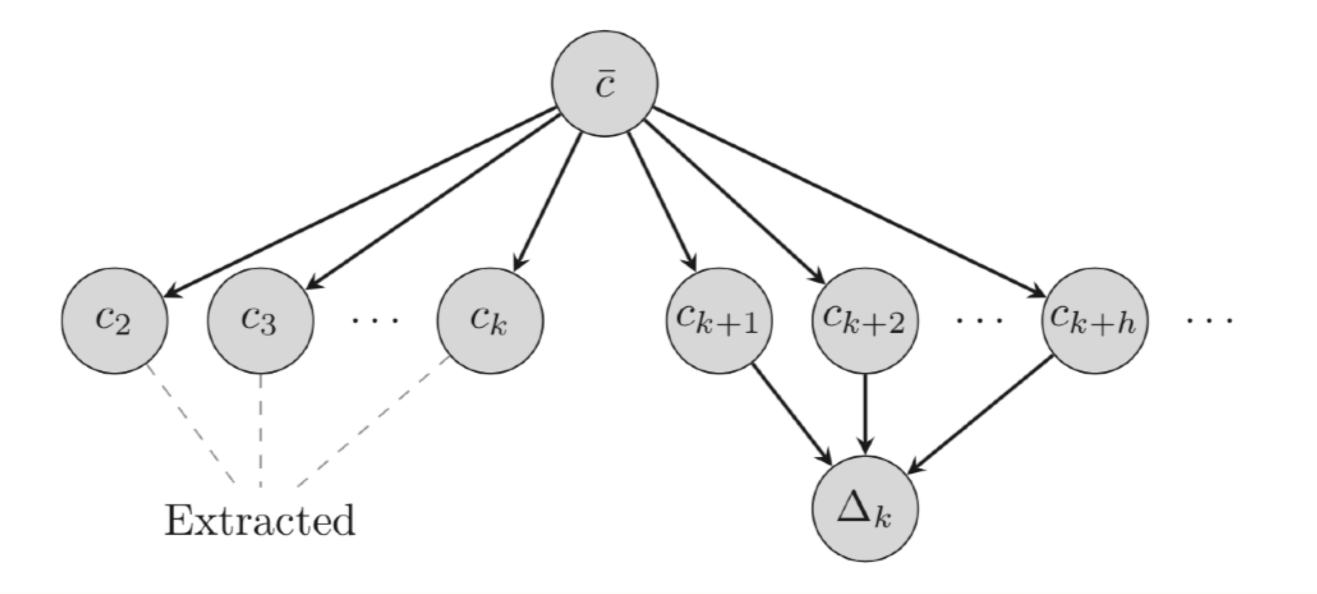
- $\mathrm{pr}(\bar{c}^2 \,|\, I) \sim \chi^{-2}(\nu_0, \tau_0^2)$; $\mathrm{pr}(\ell \,|\, I)$ uniform

$$\nu = \nu_0 + n_c;$$

$$\nu\tau^2 = \nu_0\tau_0^2 + \vec{c}_k^{\,2}$$



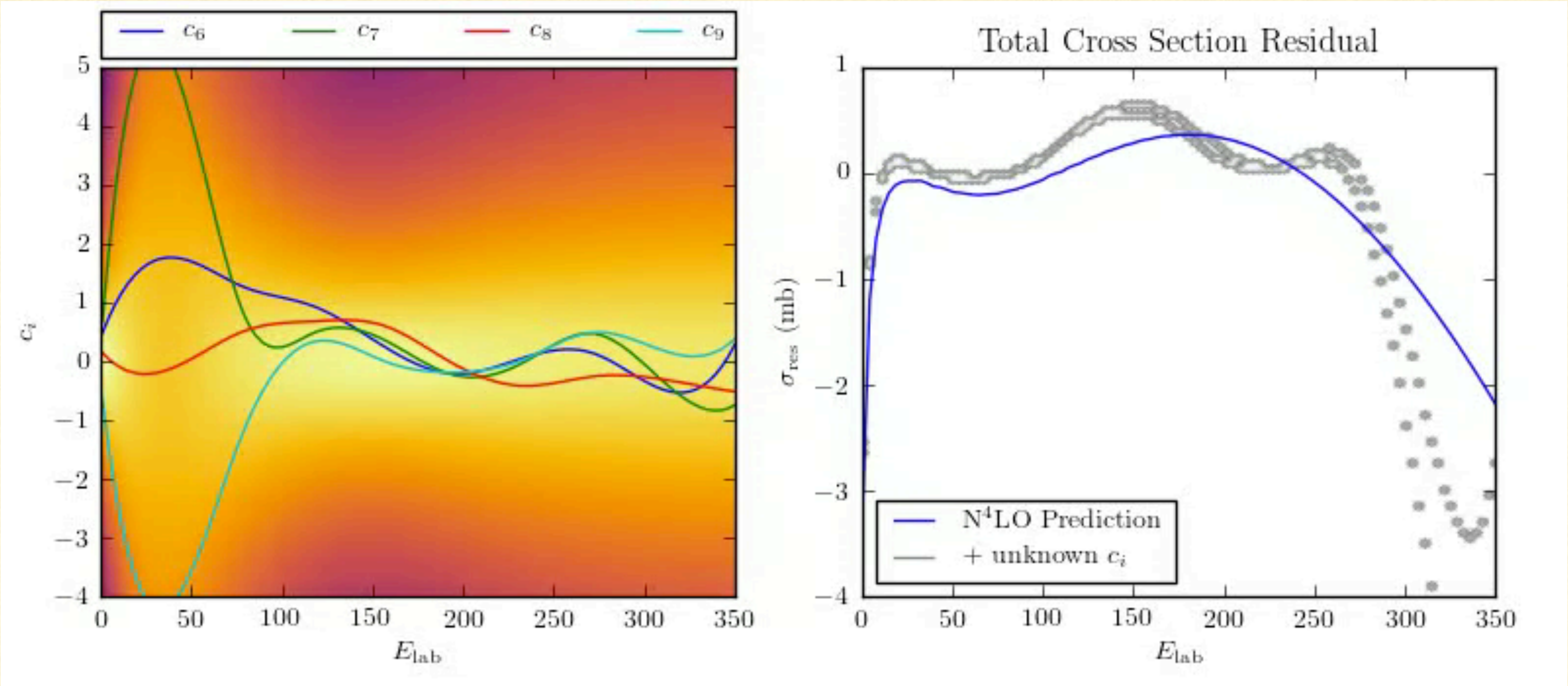
Inferring the next coefficient(s)



- Learn size of higher-order c_n's based on ones you have
- Avoid unintended spurious precision from assumption that model is arbitrarily precise to arbitrarily high energy/short distances

Gaussian process "model" for χEFT coefficients, trained on c_2 -c_5, can be used to predict distribution of N^{5}LO corrections

Inferring the next coefficient(s)



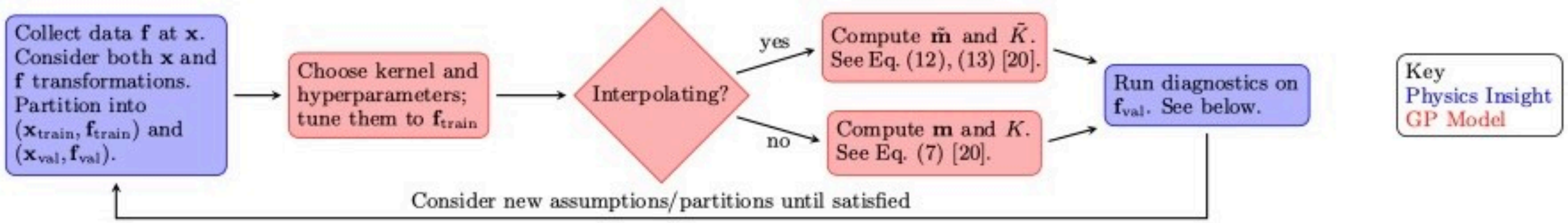
Gaussian process "model" for χEFT coefficients, trained on c_2 -c_5, can be used to predict distribution of N^{5}LO corrections

$$\Delta\sigma(E) = \sigma_{\mathrm{ref}}[c_6(E)Q^6 + c_7(E)Q^7 + c_8(E)Q^8 + c_9(E)Q^9 + c_{10}(E)Q^{10}]$$

Model checking

https://github.com/buqeye/gsum

Melendez et al. (2019), Millican et al. (2024),
Bastos & O'Hagan (2009)

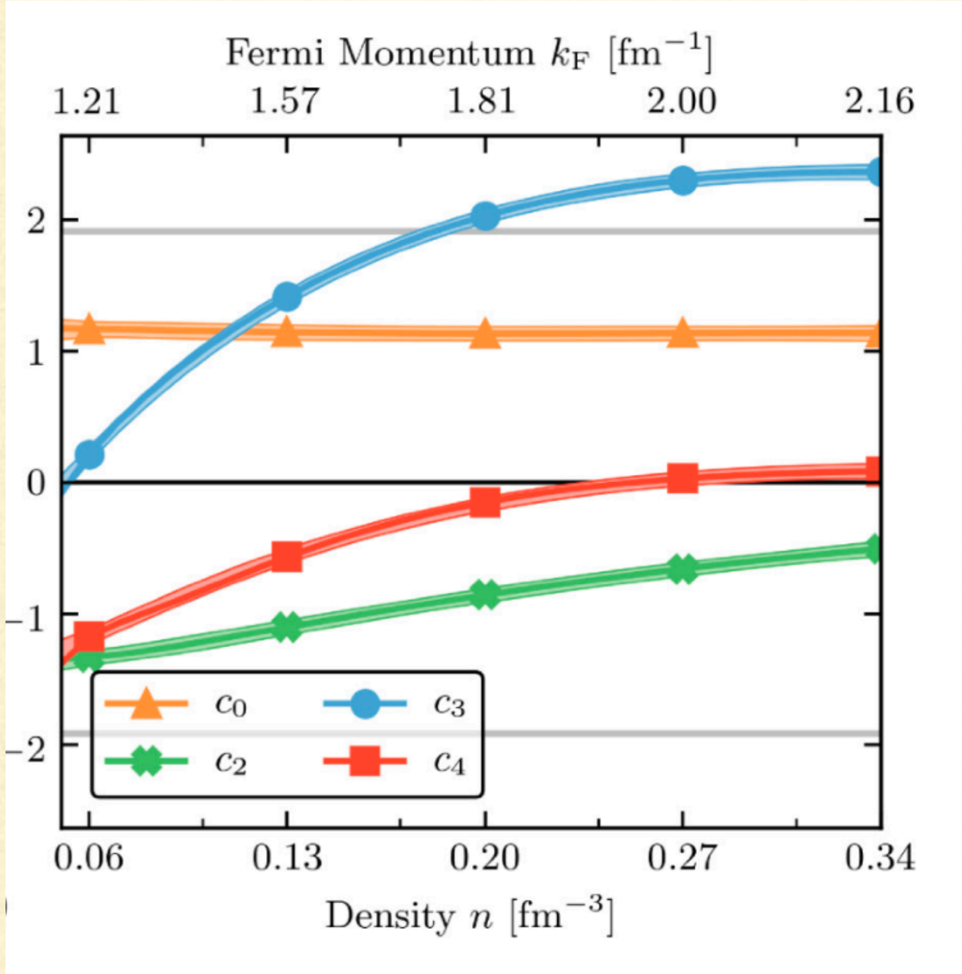


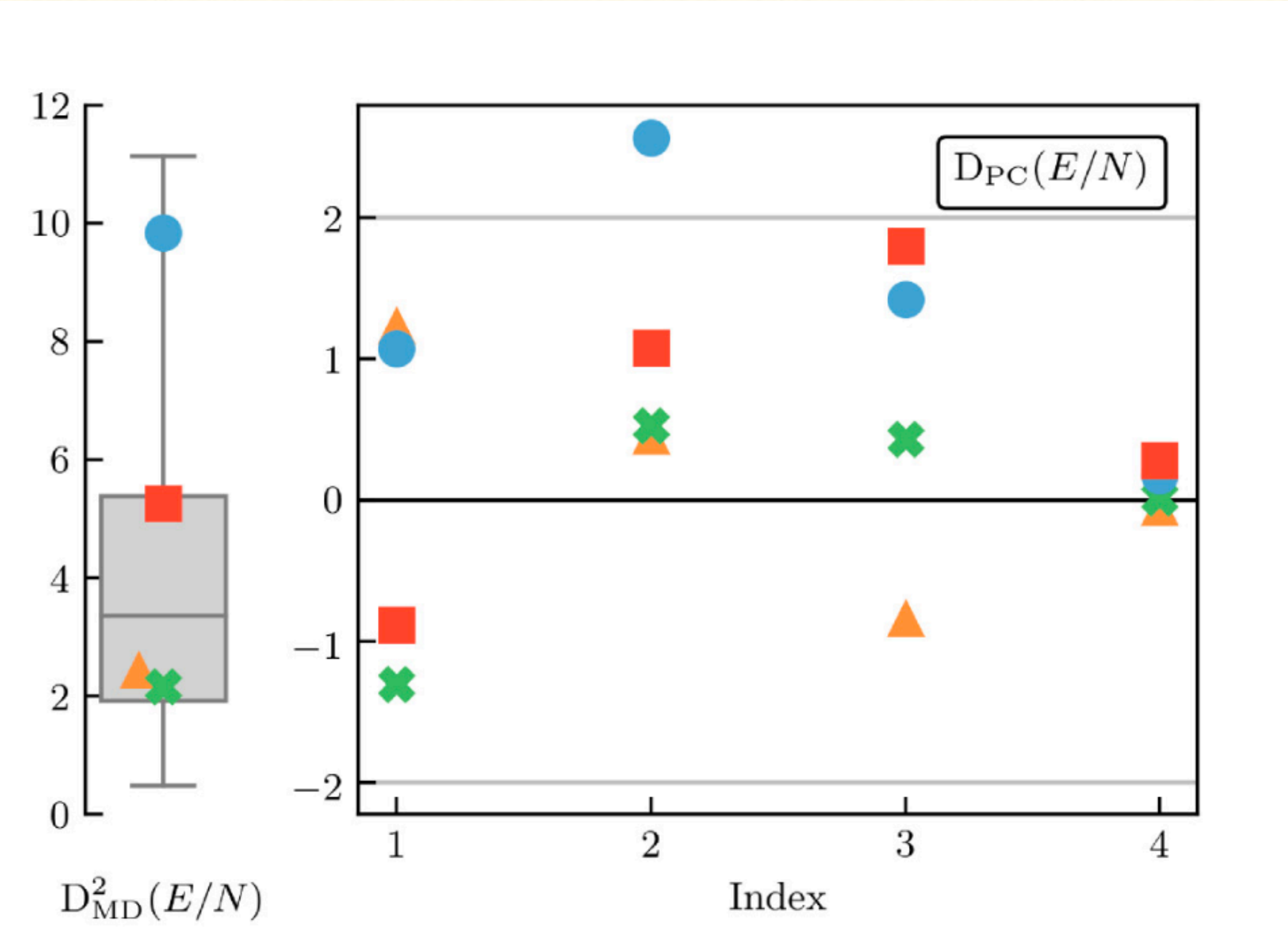
Diagnostic	Formula	Motivation	Success	Failure
Visualize the function	—	Does $\mathbf{f}_{\text{val}}$ look like a draw from a GP? What kind of GP?	$\mathbf{f}_{\text{val}}$ "looks similar" to draws from a GP	$\mathbf{f}_{\text{val}}$ "stands out" compared to GP draws
Mahalanobis Distance $\mathrm{D}^2_{\mathrm{MD}}$	$(\mathbf{f}_{\text{val}} - \mathbf{m})^\intercal K^{-1}(\mathbf{f}_{\text{val}} - \mathbf{m})$	Can we *quantify* how much the $\mathbf{f}_{\text{val}}$ looks like a GP?	$\mathrm{D}^2_{\mathrm{MD}}$ follows its theoretical distribution (χ^2_M)	$\mathrm{D}^2_{\mathrm{MD}}$ lies too far away from the expected value of M
Pivoted Cholesky $\mathbf{D}_{\mathrm{PC}}$	$G^{-1}(\mathbf{f}_{\text{val}} - \mathbf{m})$	Can we understand why $\mathrm{D}^2_{\mathrm{MD}}$ is failing?	At each index, points follow standard Gaussian	Many cases (see below)
Credible Interval $\mathrm{D}_{\mathrm{CI}}(P)$ for $P \in [0,1]$	$\frac{1}{M}\sum_{i=1}^{M} \mathbf{1}[\mathbf{f}_{\text{val},i} \in \mathrm{CI}_i(P)]$	Do $100P\%$ credible intervals capture data roughly $100P\%$ of the time?	Plot $\mathrm{D}_{\mathrm{CI}}(P)$ for $P \in [0,1]$; the curve should be within errors of $\mathrm{D}_{\mathrm{CI}}(P) = P$,	$\mathrm{D}_{\mathrm{CI}}(P)$ is far from $100P\%$, particularly for large $100P\%$ (e.g., 68% and 95%).

Variance	Length Scale	Observed Pattern in $\mathbf{D}_{\mathrm{PC}}$
$\sigma_{\text{est}} = \sigma_{\text{true}}$	$\ell_{\text{est}} = \ell_{\text{true}}$	Points are distributed as a standard Gaussian, with no pattern across index (e.g., only $\approx 5\%$ of points outside 2σ lines).
$\sigma_{\text{est}} = \sigma_{\text{true}}$	$\ell_{\text{est}} > \ell_{\text{true}}$	Points look well distributed at small index but expand to a too-large range at high index.
$\sigma_{\text{est}} = \sigma_{\text{true}}$	$\ell_{\text{est}} < \ell_{\text{true}}$	Points look well distributed at small index but shrink to a too-small range at high index.
$\sigma_{\text{est}} > \sigma_{\text{true}}$	$\ell_{\text{est}} = \ell_{\text{true}}$	Points are distributed in a too-small range at all indices.
$\sigma_{\text{est}} < \sigma_{\text{true}}$	$\ell_{\text{est}} = \ell_{\text{true}}$	Points are distributed in a too-large range at all indices.

Example: E/N for pure neutron matter

Drischler, Melendez, Furnstahl, DP, PRL, PRC (2020)





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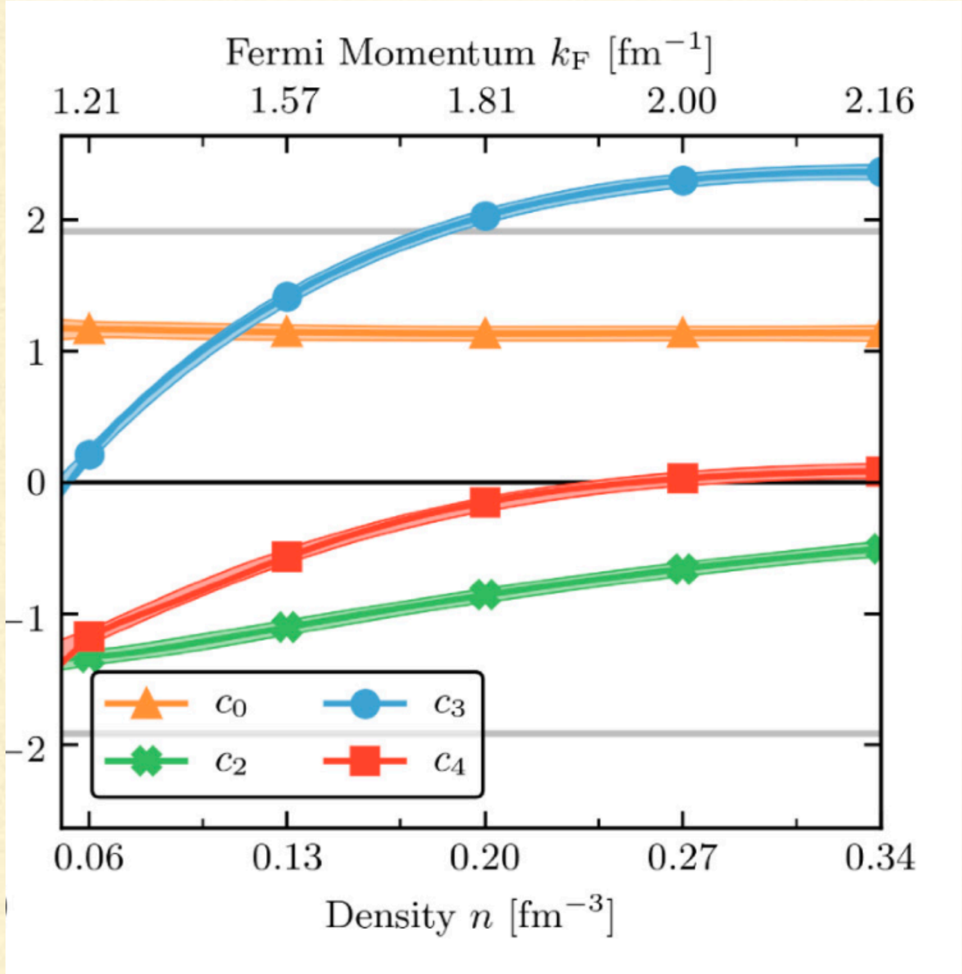
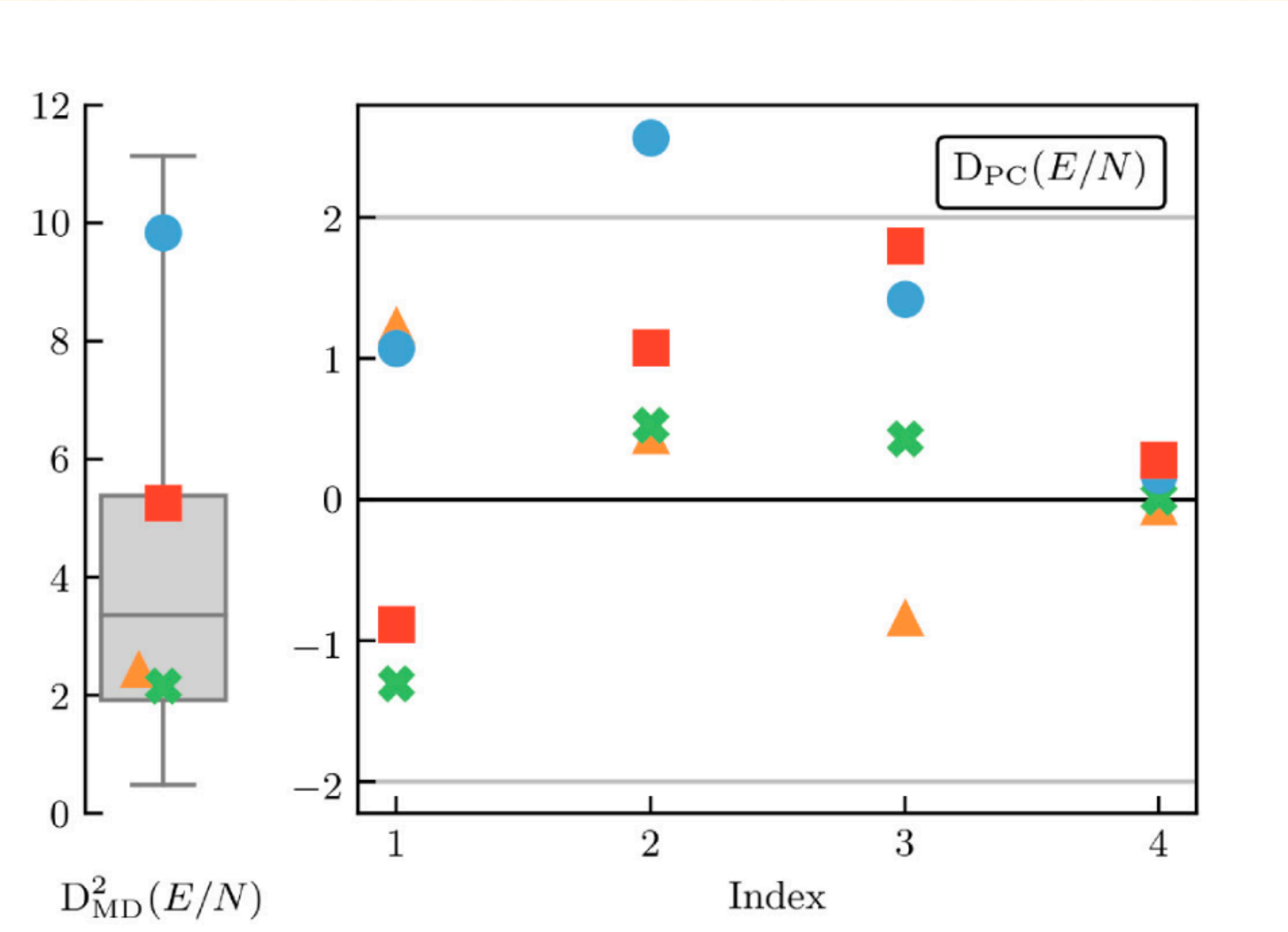
- Order-by-order uncertainties for pure neutron matter
- Obtained by applying BUQEYE™ approach to truncation errors





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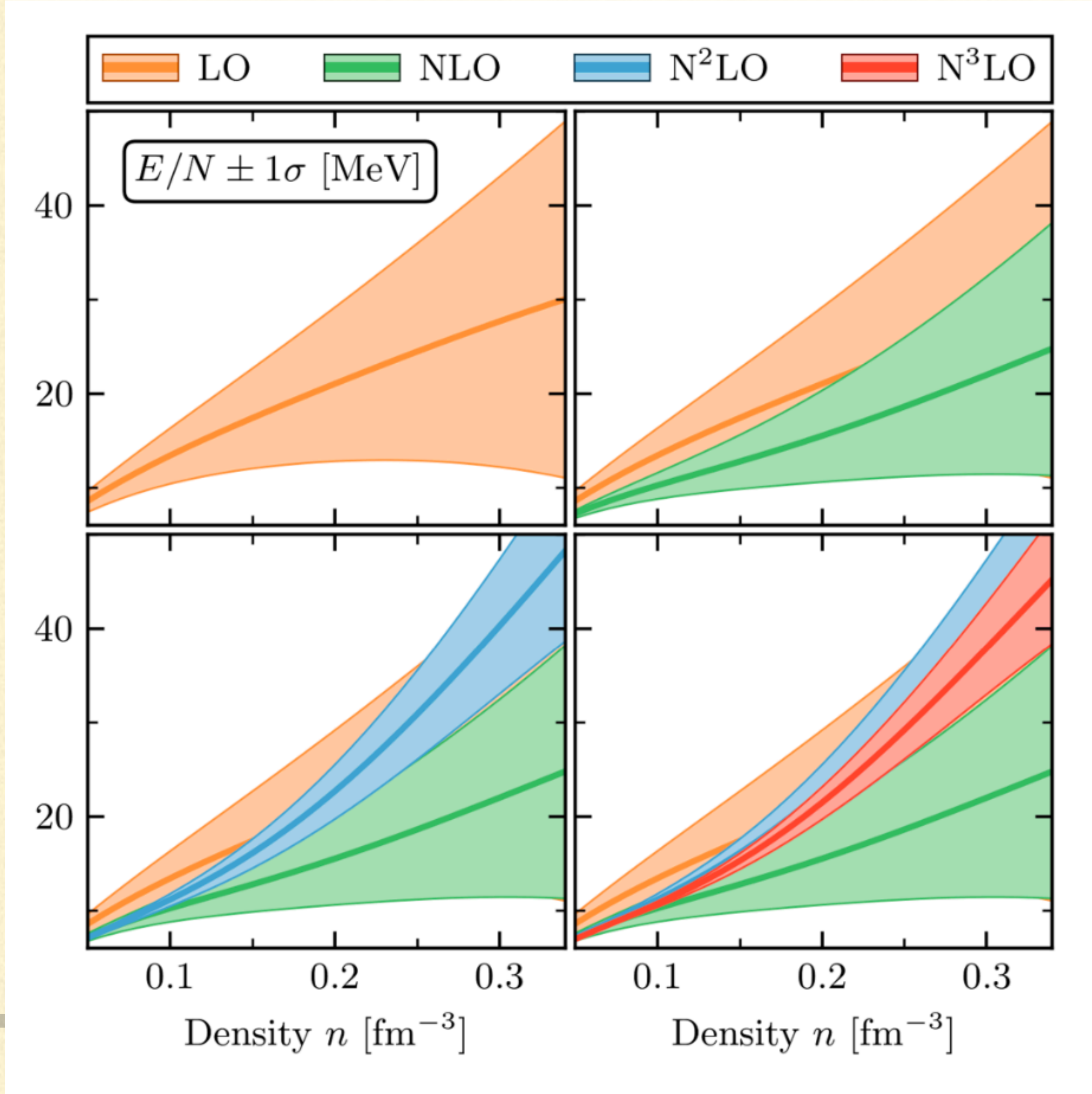
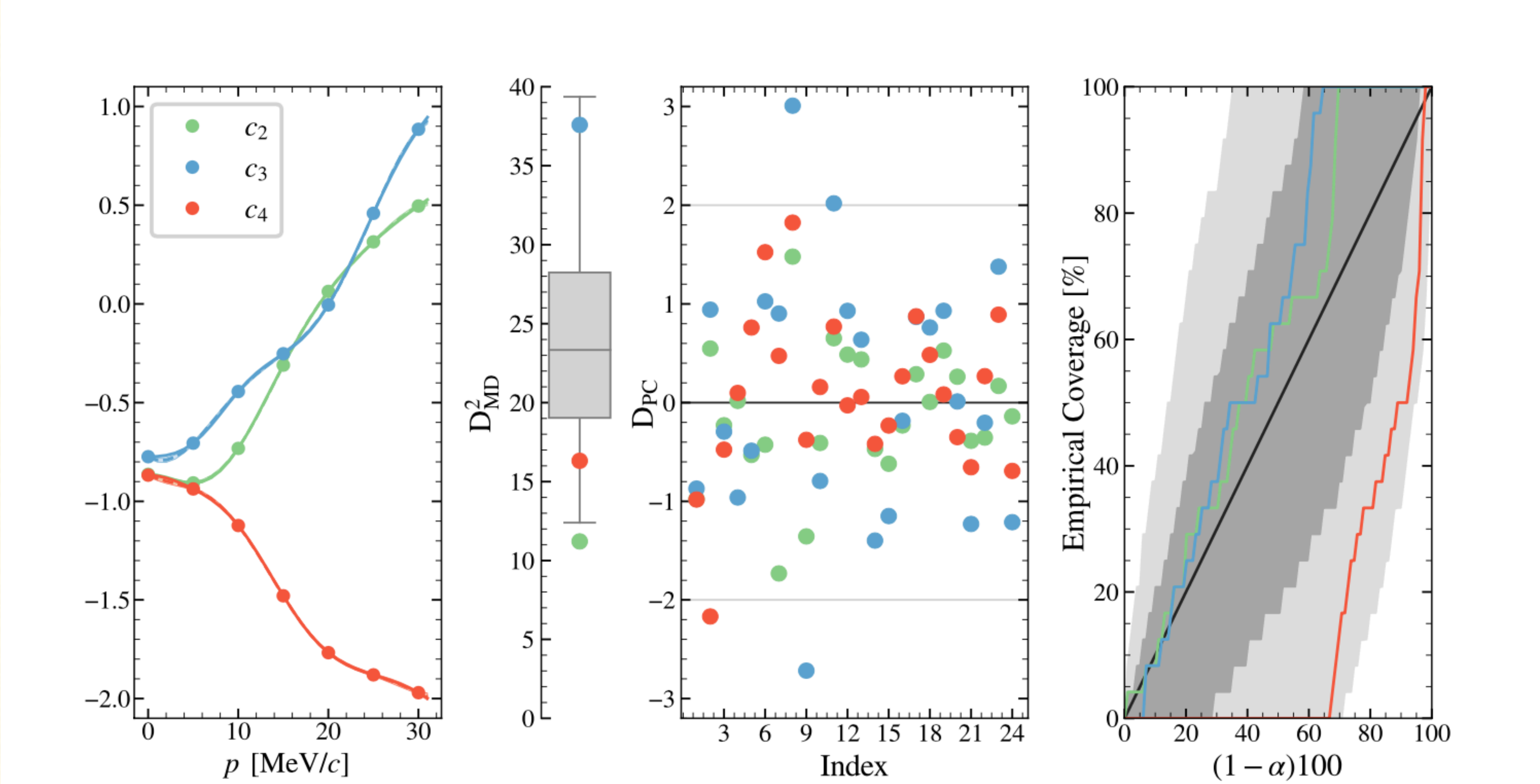


Example: np→dγ

Acharya, Bacca, PLB (2022)



(a) (b) (c) (d)

Publicly available package: https://github.com/buqeye/gsum

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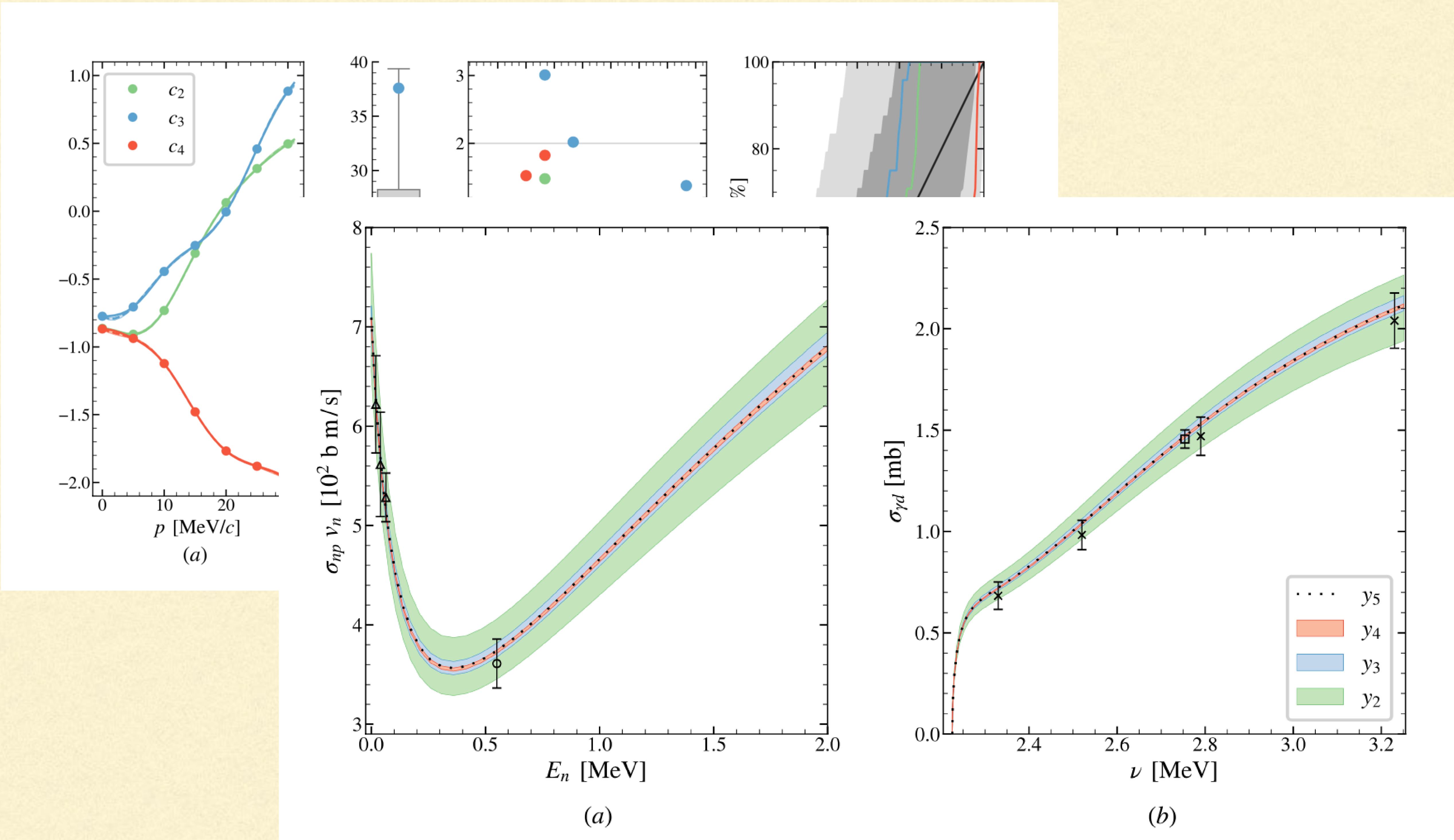

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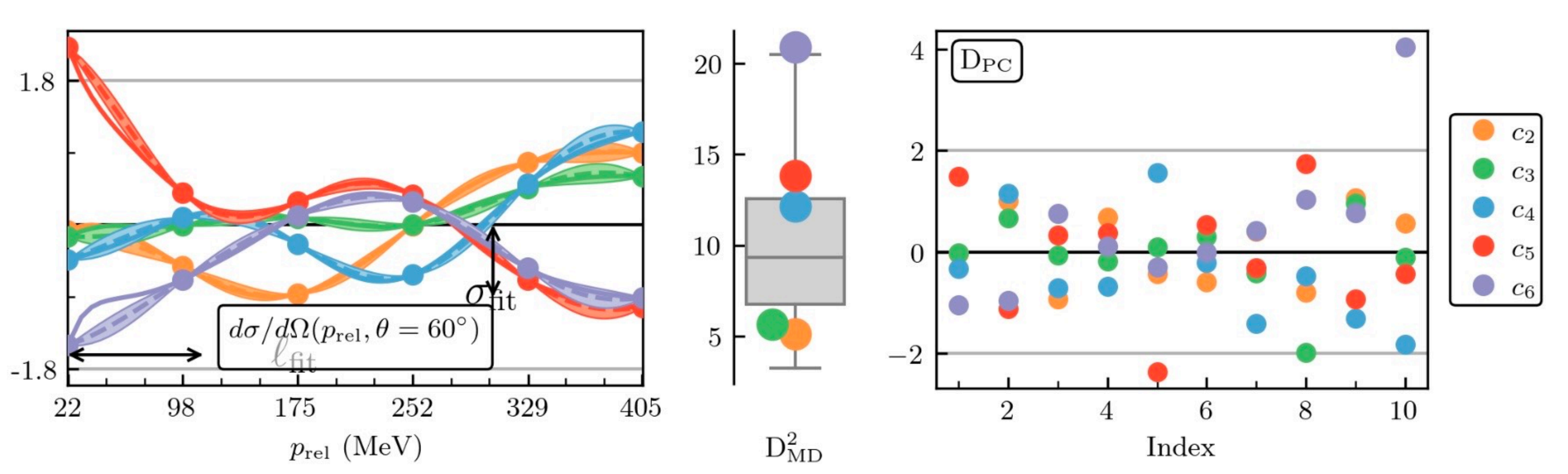
Example: NN differential cross section

Millican, Furnstahl, Melendez, DP, Pratola (2024)



What about amplitudes?

McClung, Elster, DP, submitted to PRC (2025)

Wolfenstein amplitudes

Wolfenstein & Ashkin (1952)

$$
\begin{aligned}
\overline{M}(q,\theta) = & A(q,\theta)\mathbb{1} \\
& + iC(q,\theta)(\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2)\cdot\hat{\mathbf{n}} \\
& + M(q,\theta)(\boldsymbol{\sigma}_1\cdot\hat{\mathbf{n}})(\boldsymbol{\sigma}_2\cdot\hat{\mathbf{n}}) \\
& + [G(q,\theta) - H(q,\theta)](\boldsymbol{\sigma}_1\cdot\hat{\mathbf{q}})(\boldsymbol{\sigma}_2\cdot\hat{\mathbf{q}}) \\
& + [G(q,\theta) + H(q,\theta)](\boldsymbol{\sigma}_1\cdot\hat{\boldsymbol{\mathcal{K}}})(\boldsymbol{\sigma}_2\cdot\hat{\boldsymbol{\mathcal{K}}}).
\end{aligned}
$$

$$\mathbf{K} = \frac{1}{2}(\mathbf{p} + \mathbf{p}'); \mathbf{q} = \mathbf{p}' - \mathbf{p}; \mathbf{n} = \mathbf{p}\times\mathbf{p}'$$

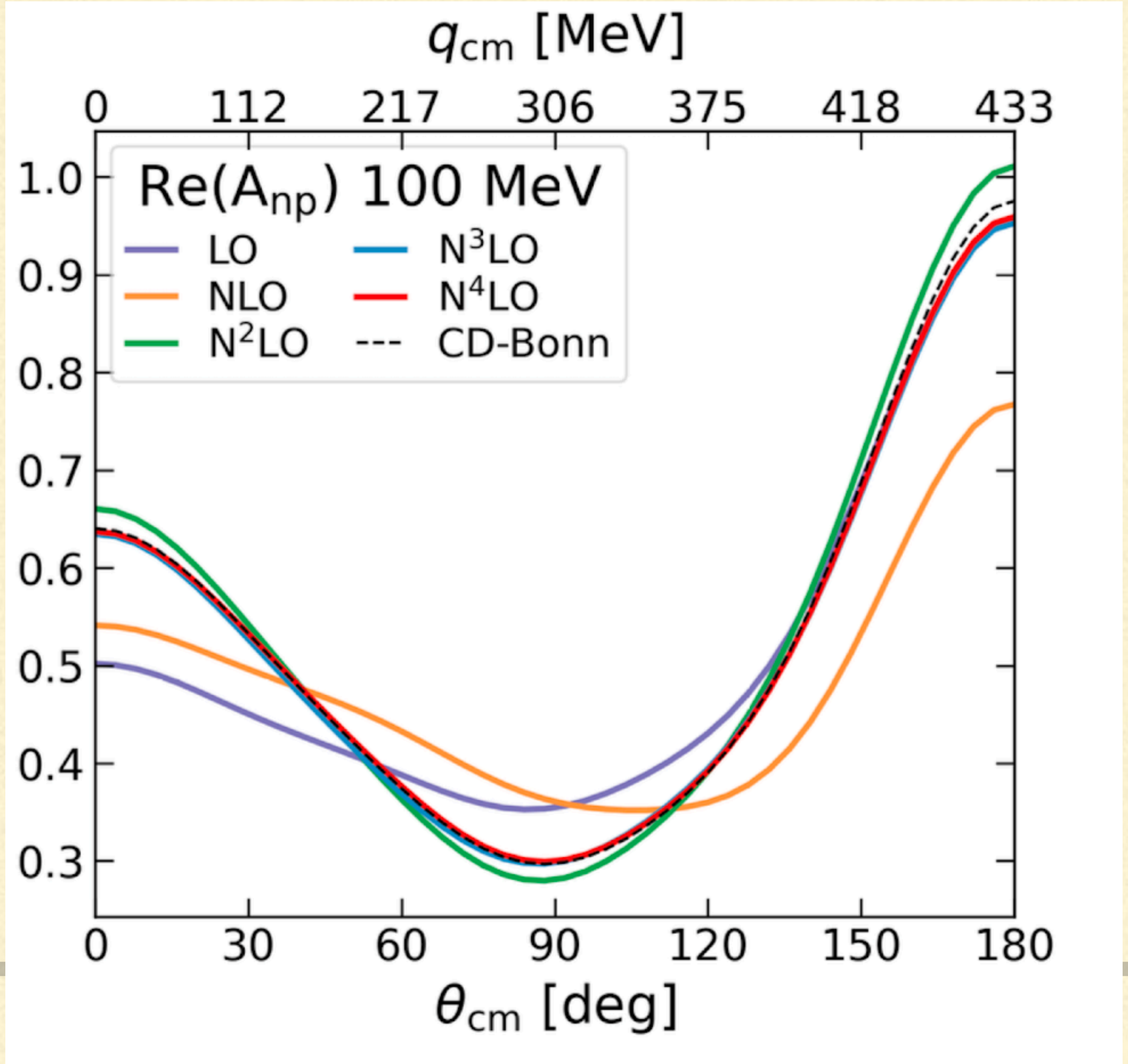
A: central part

C: spin-orbit

M, G, and H: tensor effects

Works well for amplitudes at 100 MeV

- y_{ref}=Im(A)
- $Q = \dfrac{\max(p,q) + m_\pi}{\Lambda_b + m_\pi}$



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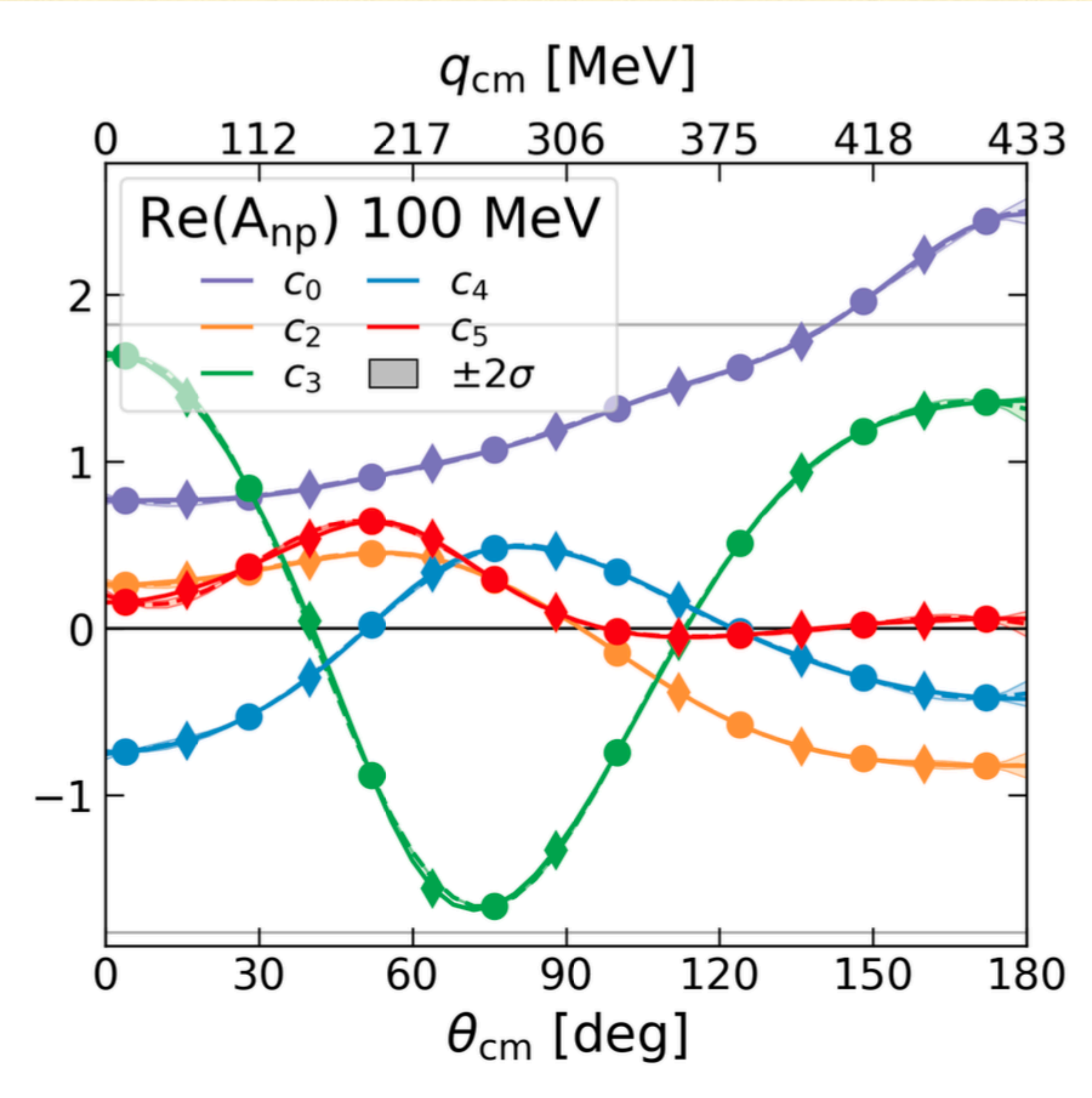

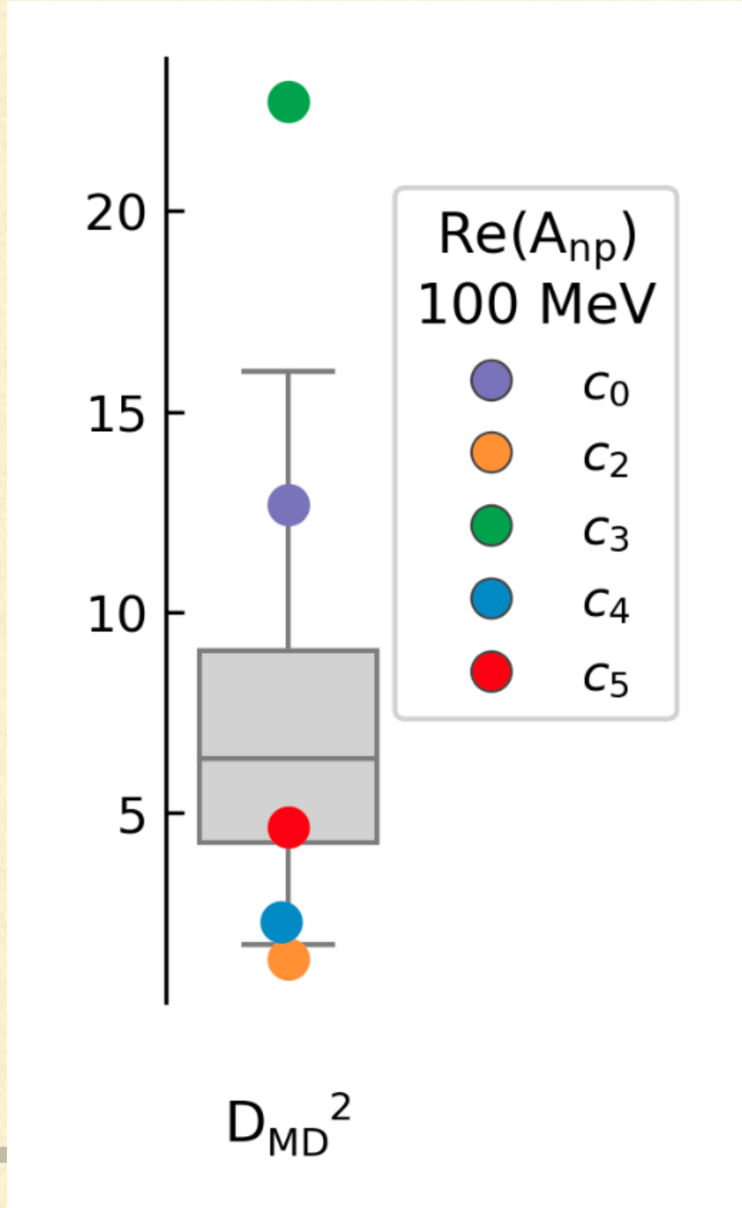

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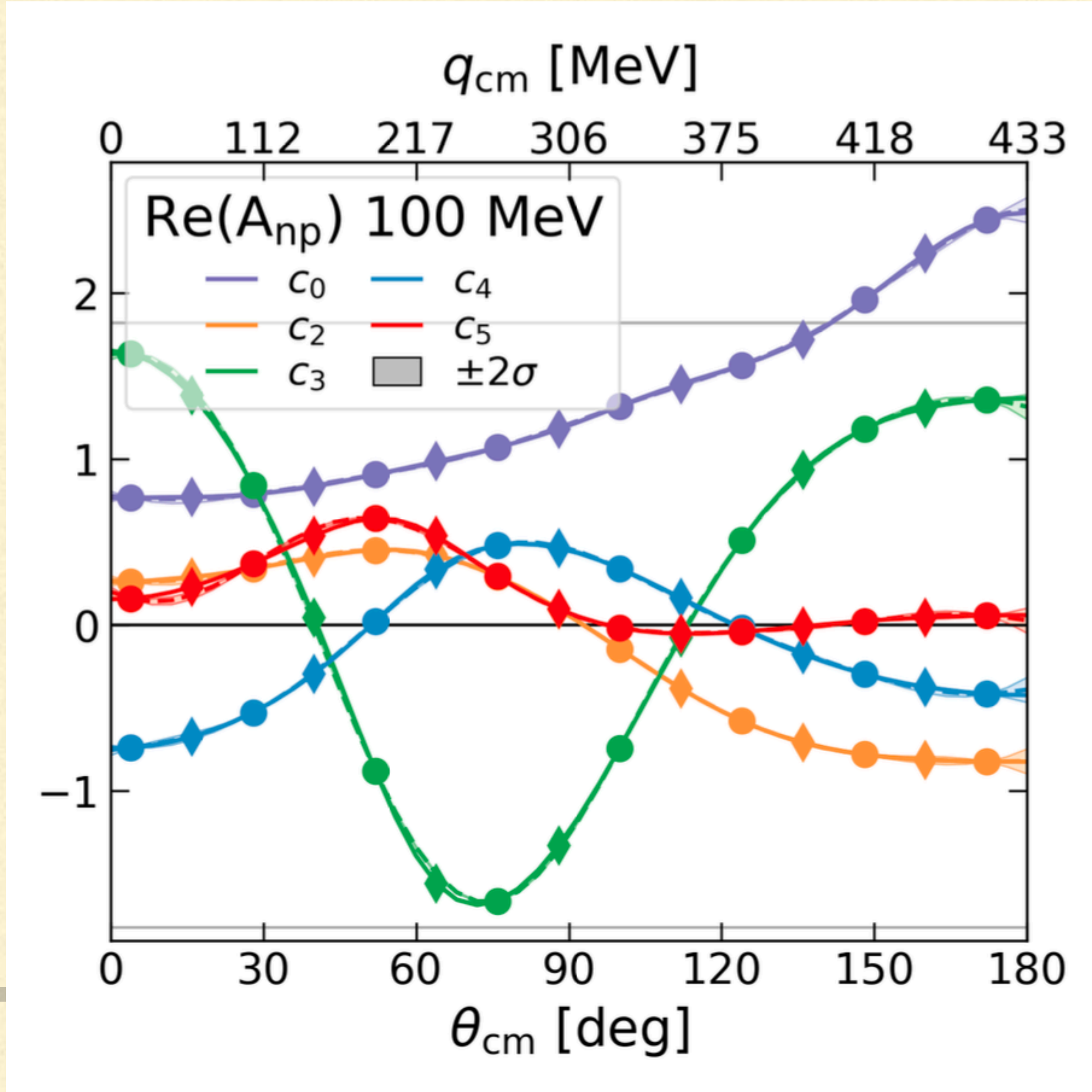
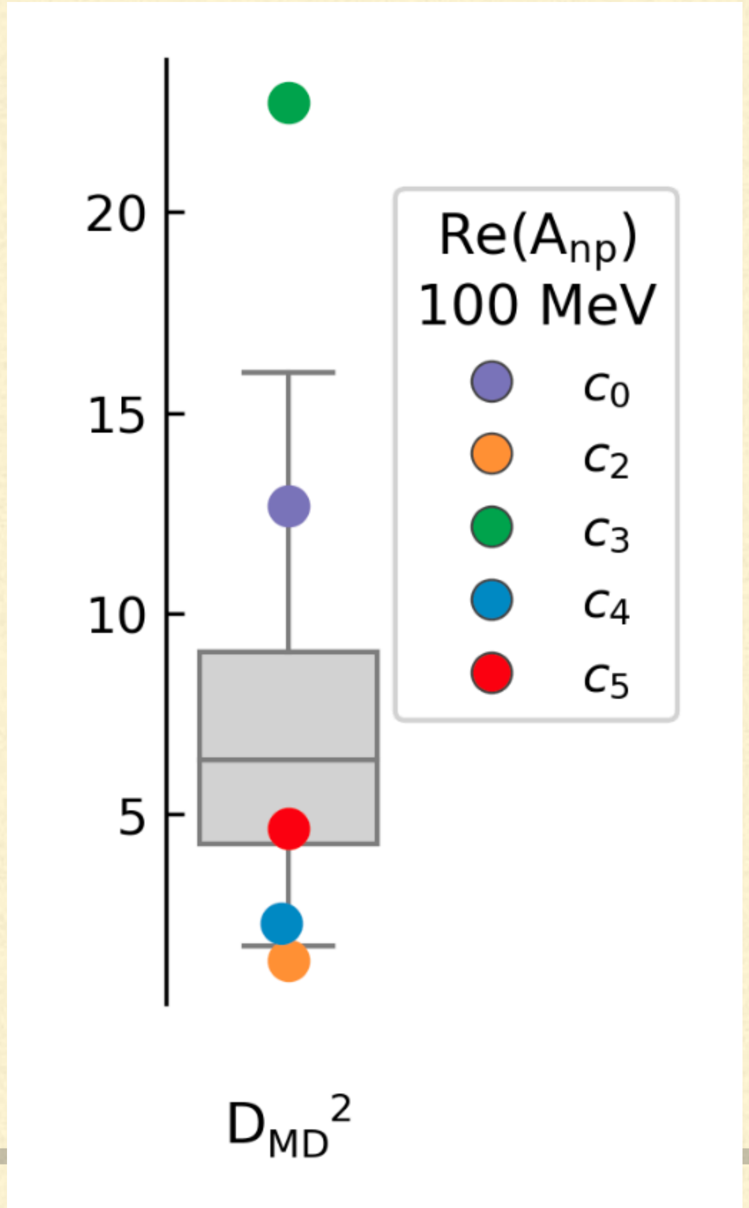
See ℓ_q is constant with energy





Why: assessing breakdown

Melendez et al., PRC (2019)

If Q too big then c_n will shrink with n
(and so will error bars)

If Q too small then c_n will grow with n
(and so will error bars)

Once we have $\mathrm{pr}(\vec{\mathbf{c}}_k \,|\, \ell, I)$ we derive

$$\mathrm{pr}(\mathbf{Q} \,|\, \vec{\mathbf{y}}_k, \ell, I) \propto \frac{\mathrm{pr}(Q \,|\, I)}{\tau^{\nu} \prod_{i,n} |\, Q^n(x_i) \,|}$$

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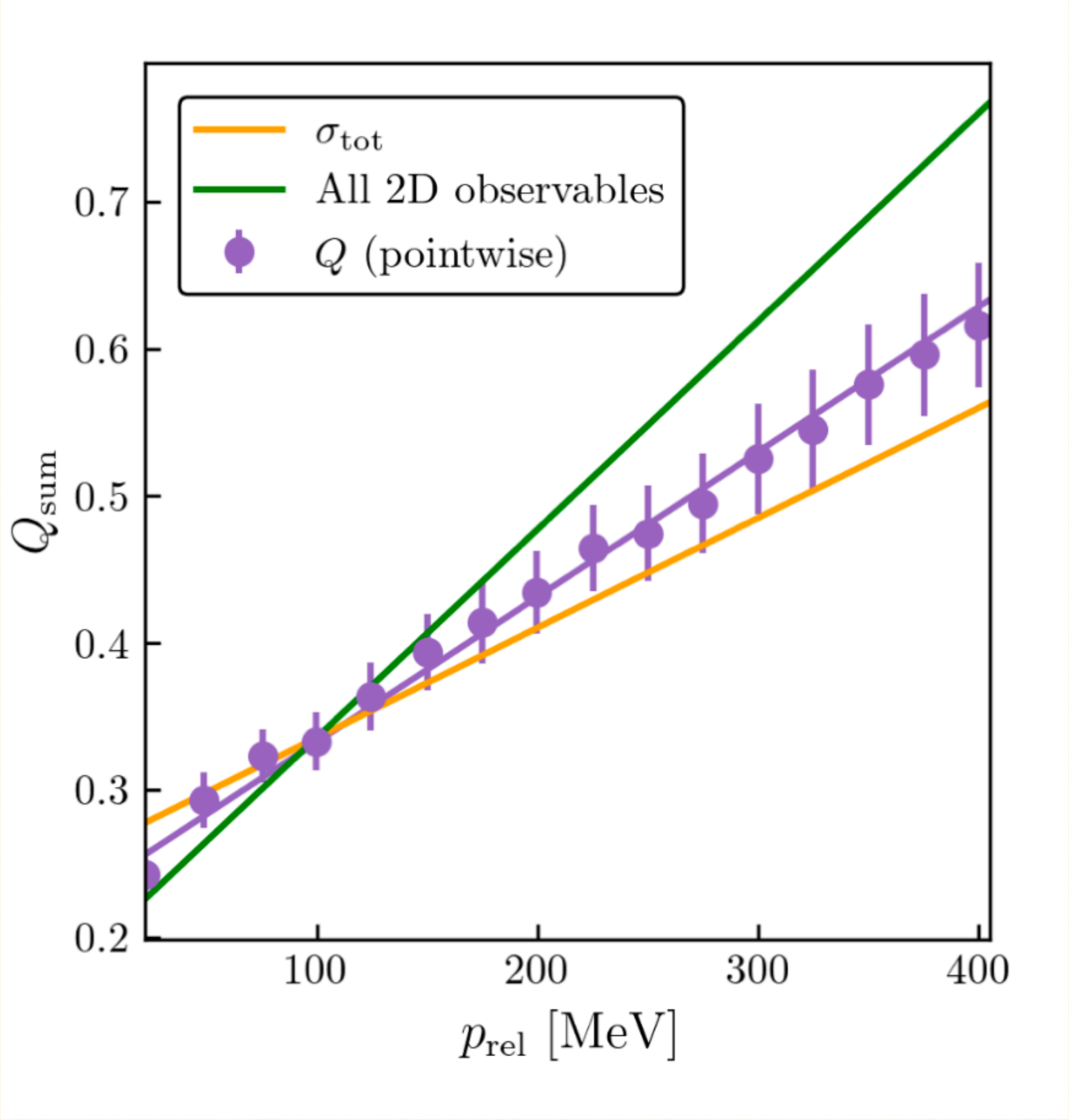


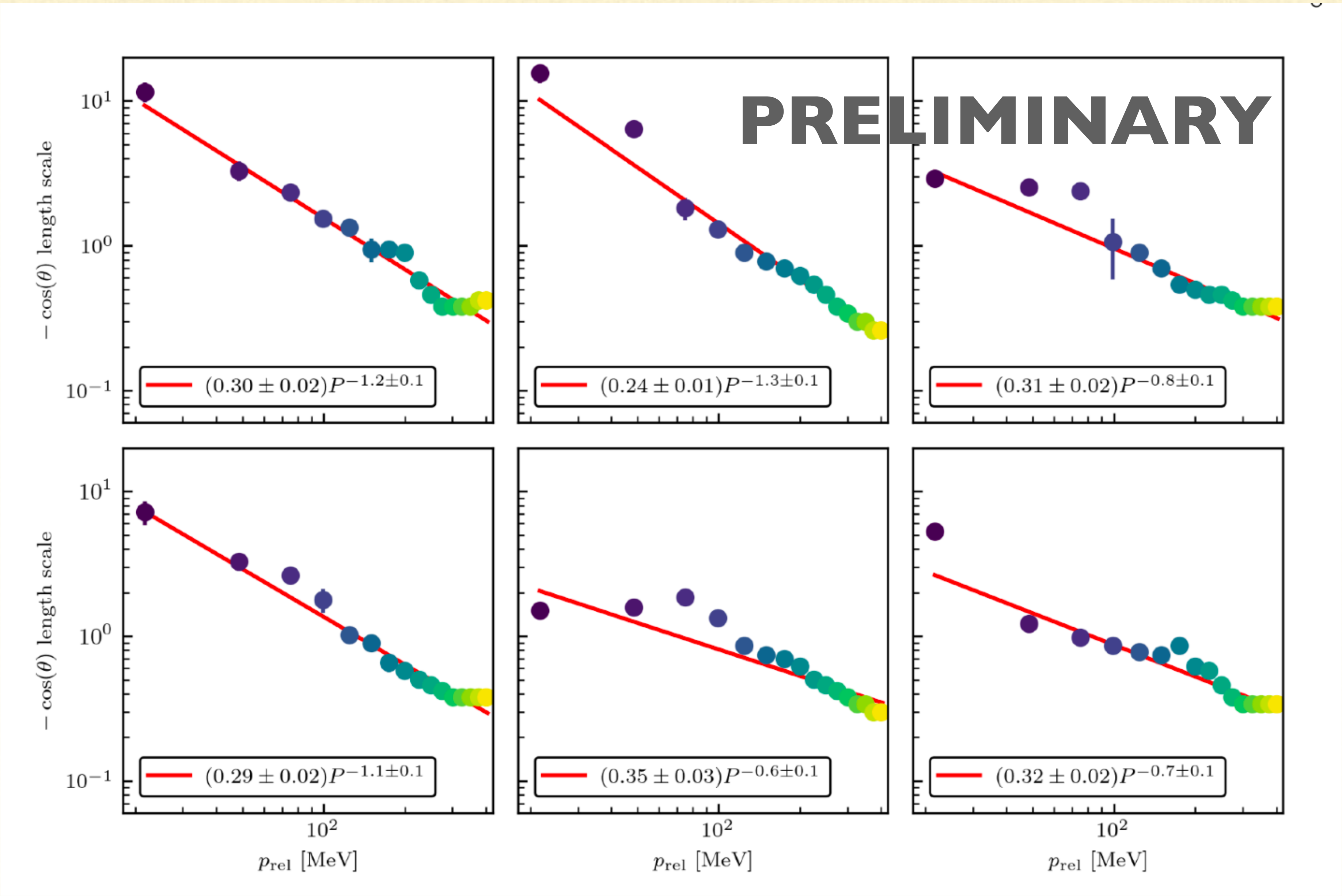
$Q_{max} = \dfrac{(\mathrm{p}, \mathrm{m}_\pi)}{\Lambda_b}$ or $Q_{sum} = \dfrac{p + m_\pi}{\Lambda_b + m_\pi}$?

Millican et al., PRC (2024)

But GP is **not** 2D stationary

Millican et al. (2025)

SMS 500 MeV



$$P = \frac{p_{\mathrm{rel}}}{405\ \mathrm{MeV}}$$

- $\ell_\theta \sim 1/p$
- "Warp" input space to account for 1/p effect

Results for Λ_b

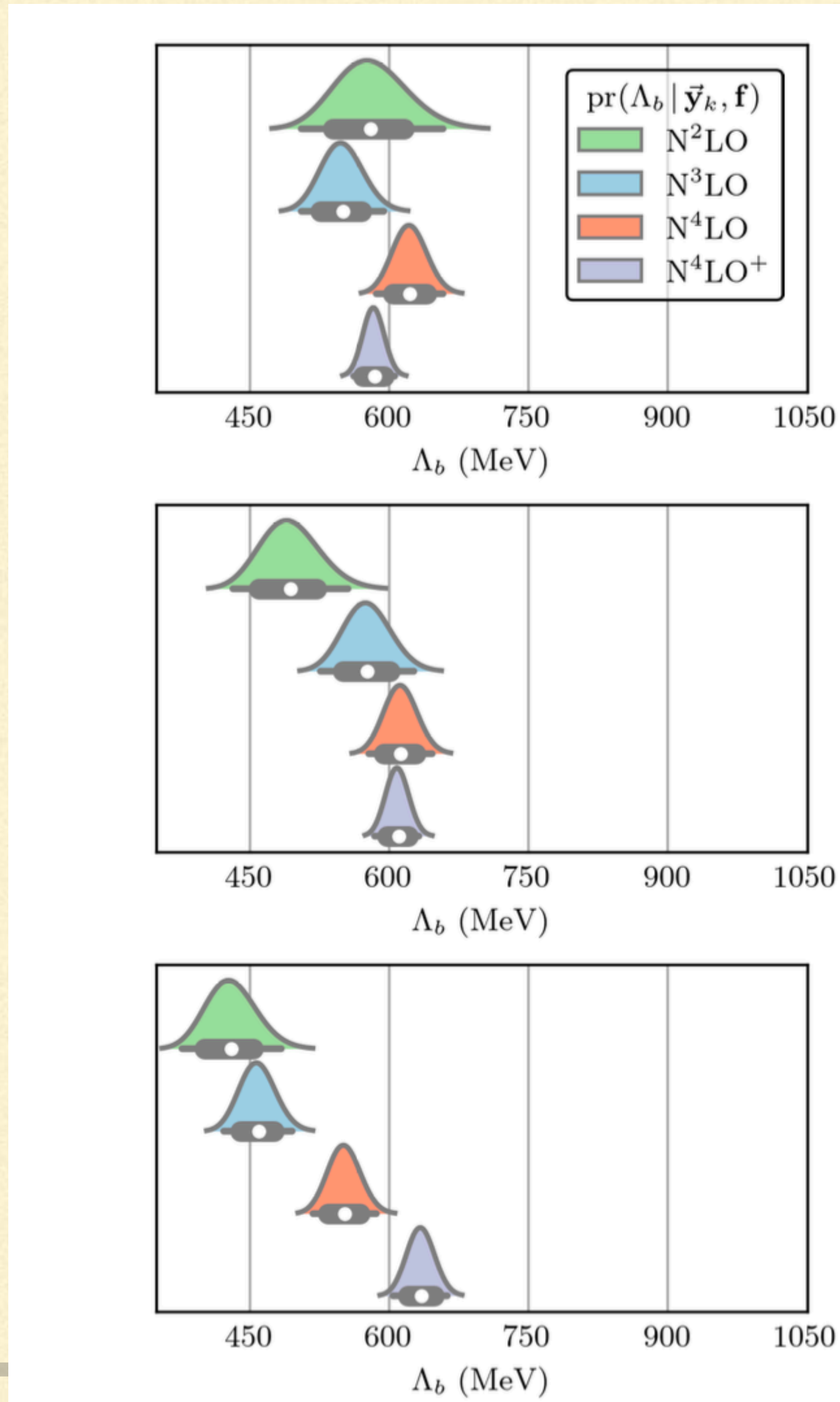
PRELIMINARY

Millican et al., in preparation (2025)

SMS 450 MeV

SMS 500 MeV

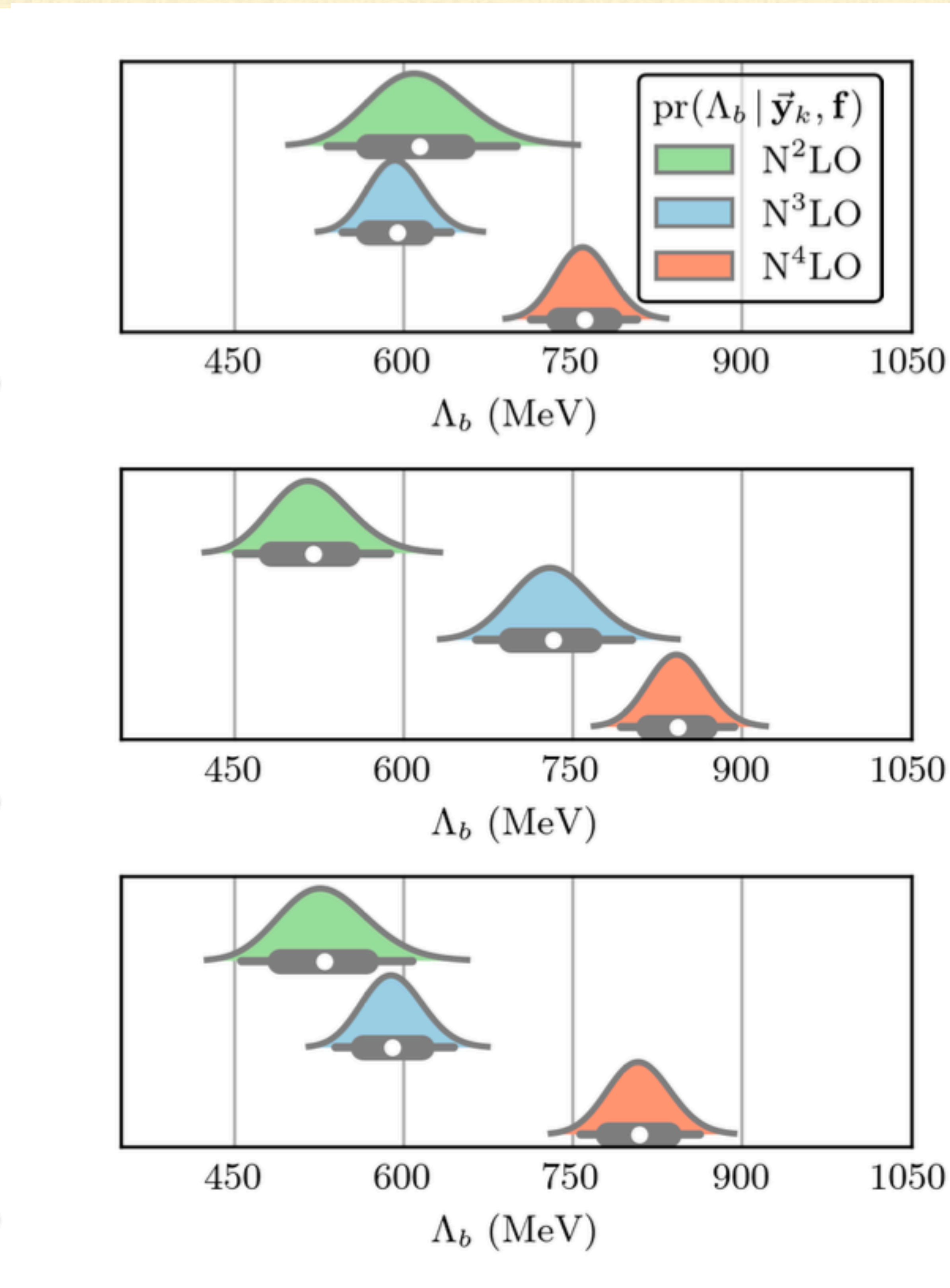
SMS 550 MeV



SCS 1.0 fm

SCS 0.9 fm

EMN 500 MeV



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δy_{exp}: let's take normally distributed, uncorrelated errors

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- $\delta y_{\text{th}} = y_{\text{ref}}(p)[c_{k+1} Q^{k+1} + c_{k+2} Q^{k+2} + \ldots]$
- Predictions for model discrepancy size AND growth with p

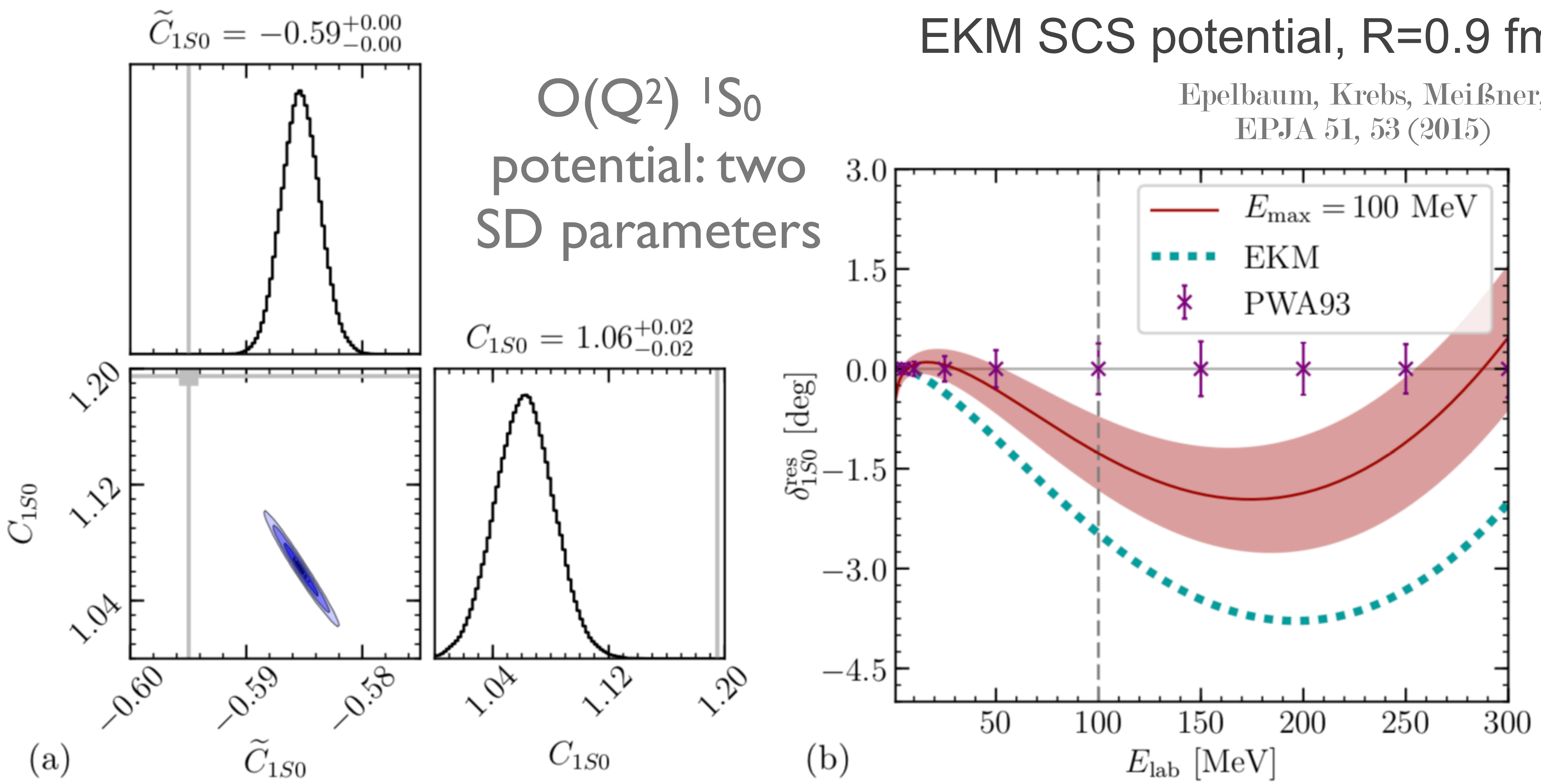
Parameter estimates: $^1S_0$

Wesolowski, Furnstahl, Melendez, DP (2019)

O(Q²) $^1S_0$ potential: two SD parameters

EKM SCS potential, R=0.9 fm

Epelbaum, Krebs, Meißner, EPJA 51, 53 (2015)



Including truncation errors changes central values and (esp.) errors

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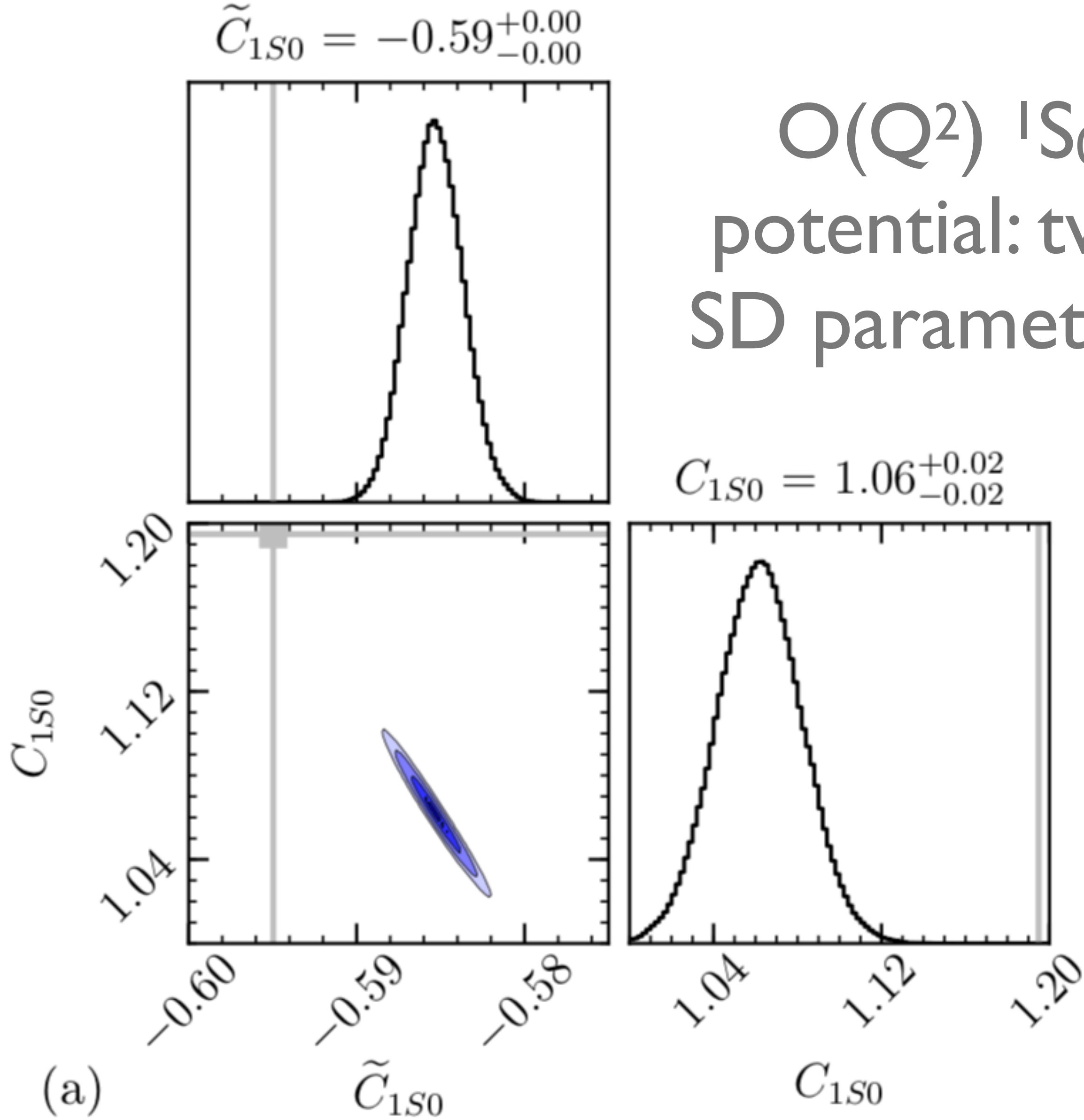
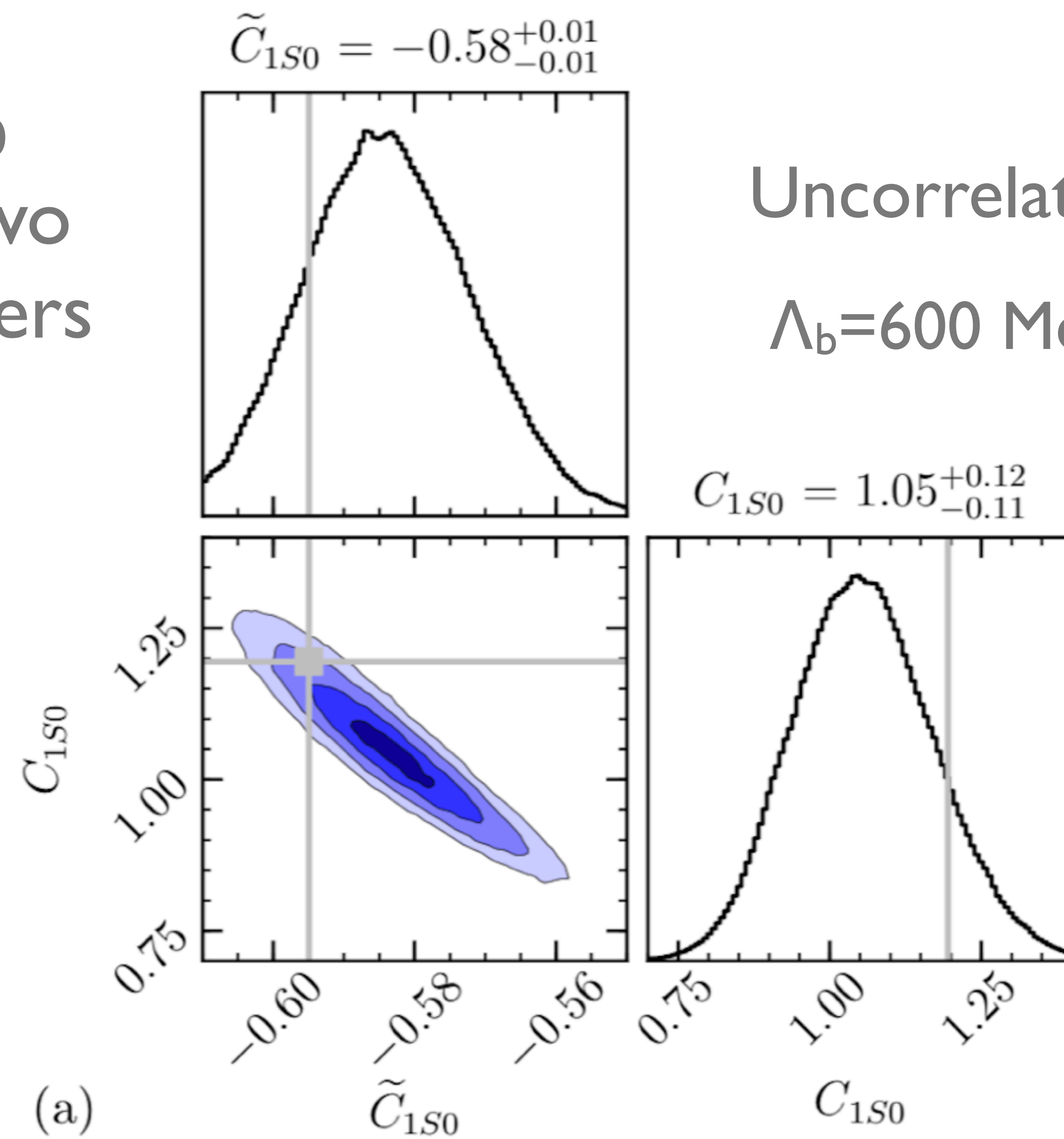


O(Q²) $^1S_0$ potential: two SD parameters



Uncorrelated

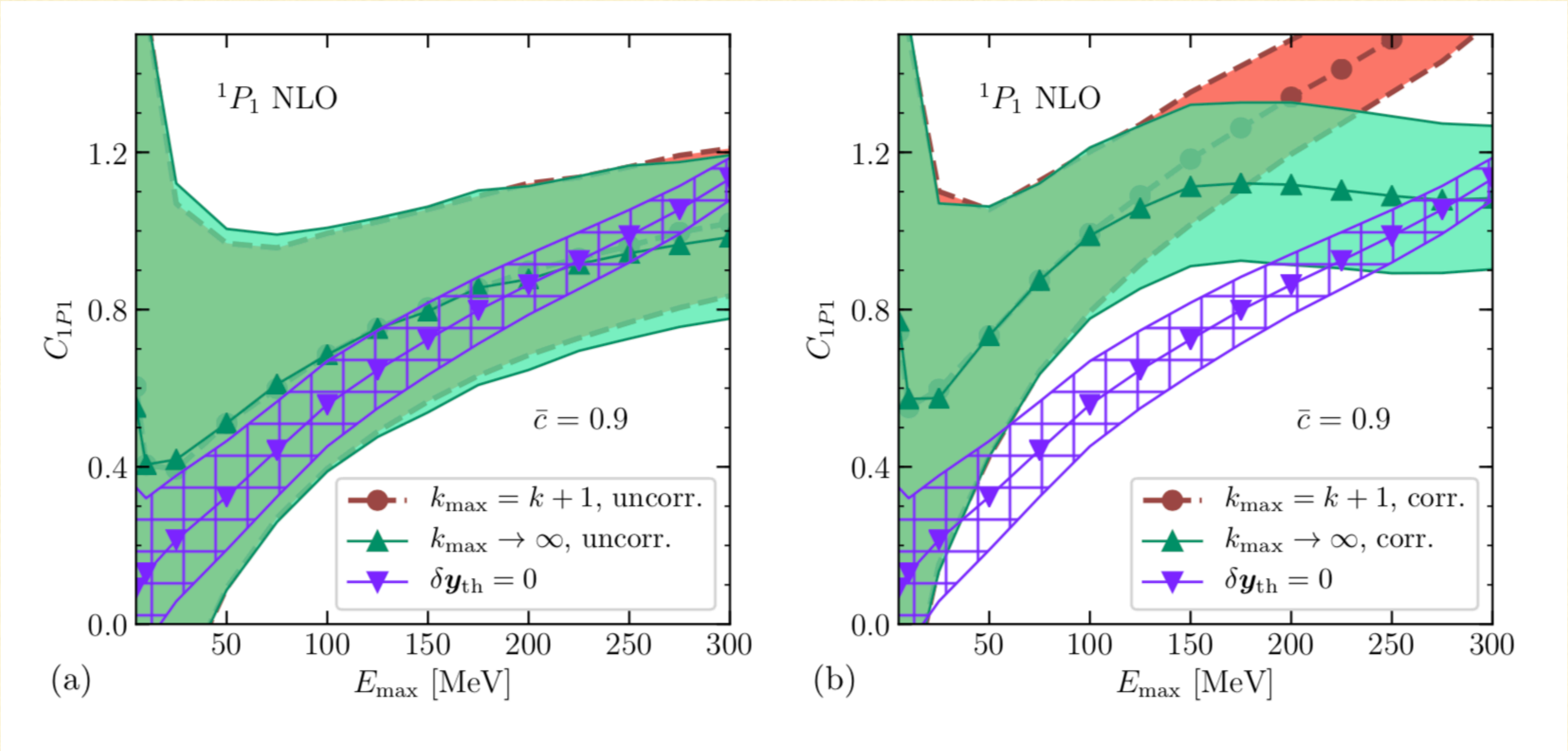
Λ_b=600 MeV

Including truncation errors changes central values and (esp.) errors

$$(\boldsymbol{\Sigma}_{\rm th,uncorr})_{ij} = (\mathbf{y}_{\rm ref})^2 \bar{c}^2 \delta_{ij} \sum_{n=k+1}^{k_{\max}} Q_i^{2n}$$

E_{max} plots in the $^1P_1$

Wesolowski, Furnstahl, Melendez, DP, J. Phys. G. (2019)

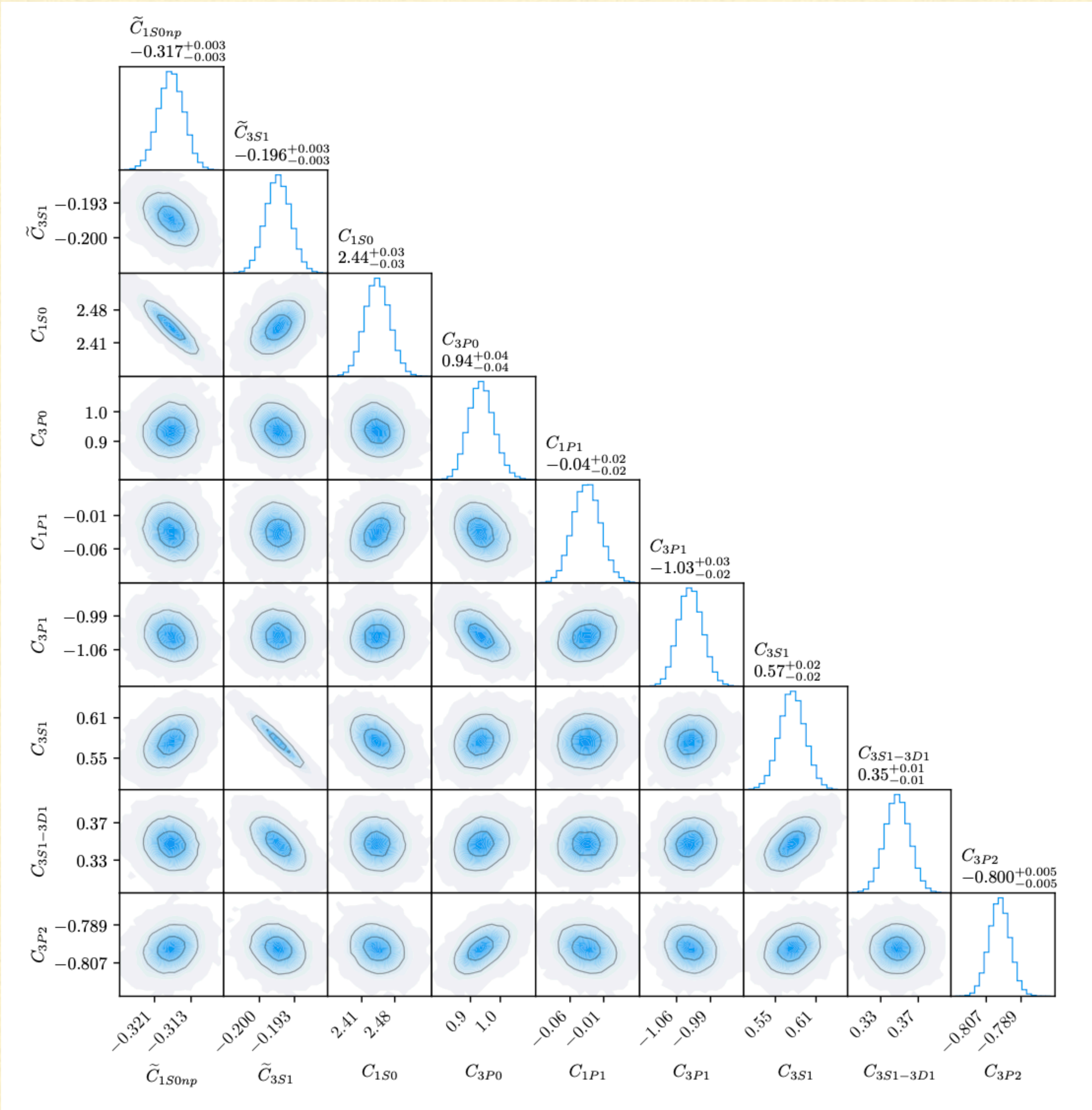


$$(\boldsymbol{\Sigma}_{\text{th,uncorr}})_{ij} = (\mathbf{y}_{\text{ref}})^2 \bar{c}^2 \delta_{ij} \sum_{n=k+1}^{k_{\max}} Q_i^{2n} \qquad (\boldsymbol{\Sigma}_{\text{th,corr}})_{ij} = (\mathbf{y}_{\text{ref}})_i (\mathbf{y}_{\text{ref}})_j \bar{c}^2 \sum_{n=k+1}^{k_{\max}} Q_i^n Q_j^n$$

- Can resum truncation error to all orders (under assumptions about its correlation across orders): tests validity of FOTA

Calibrating NN LECs with a GP error model

Svennson, Ekstróm, Forssén, PRC (2024)



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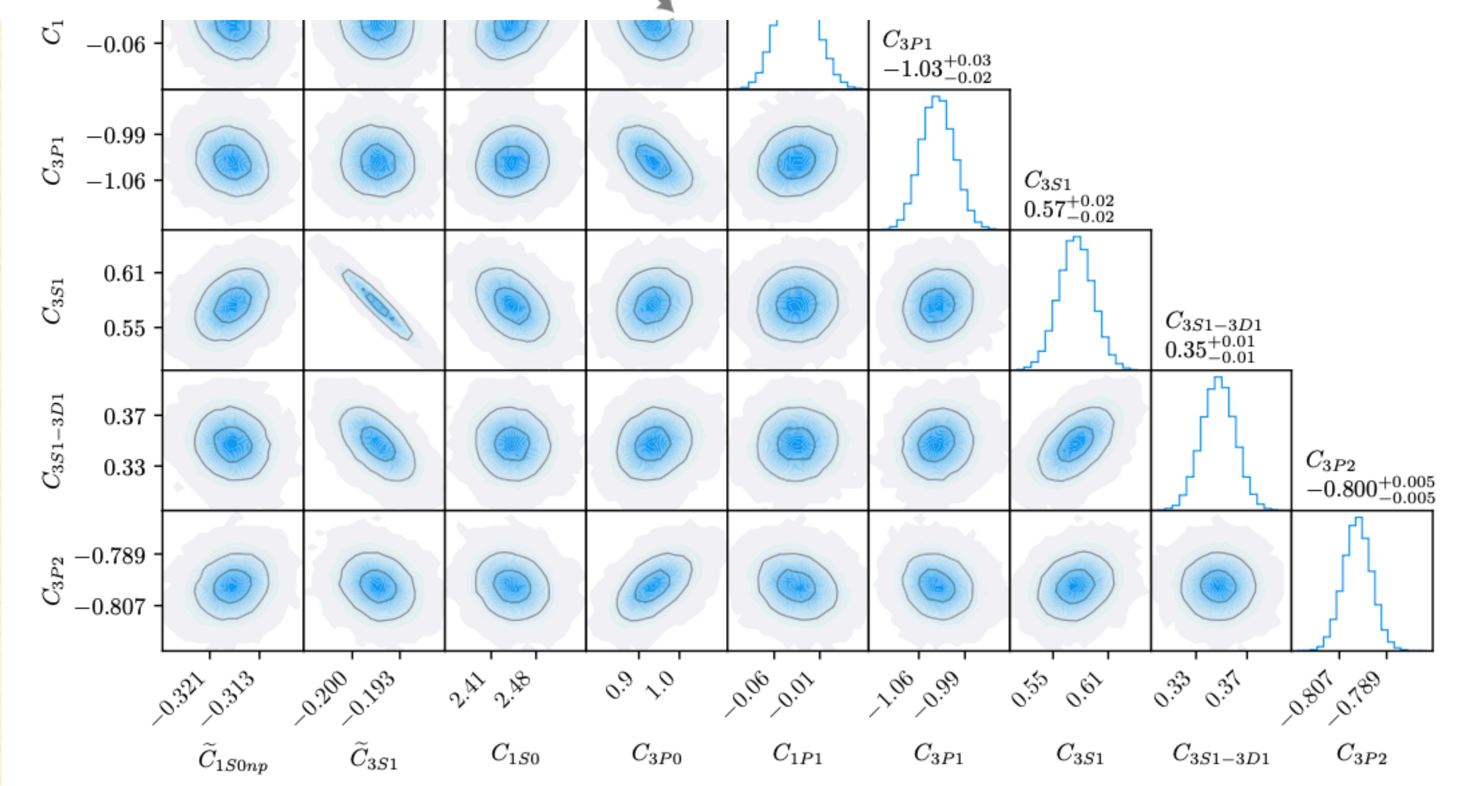
Notation	Definition	Acronym	$N_{d,y}$	$N_{T_{\text{lab}},y}$	n_{eff}	$\widehat{\ell_{T_{\text{lab}}}}$ (MeV)	$\widehat{\bar{c}^2}$
σ_{tot}	total cross section	SGT	119	113	30.8	49	0.56^2
σ_T	$\sigma_{\text{tot}}(\uparrow\downarrow) - \sigma_{\text{tot}}(\uparrow\uparrow)$	SGTT	3	3	—	—	—
σ_L	$\sigma_{\text{tot}}(\leftrightarrows) - \sigma_{\text{tot}}(\rightrightarrows)$	SGTL	4	4	3.8	47	1.95^2

Notation	Tensor	Illustration	Acronym	$N_{d,y}$	$N_{T_{\text{lab}},y}$	n_{eff}	$\widehat{\ell_{T_{\text{lab}}}}$ (MeV)	$\widehat{\ell_\theta}$ (deg)	$\widehat{\bar{c}^2}$
$\sigma(\theta)$	I_{0000}		DSG	1207	68	352.9	73	39	0.61^2
$A(\theta)$	D_{s0k0}		A	5	1	5.0	68	37	0.65^2



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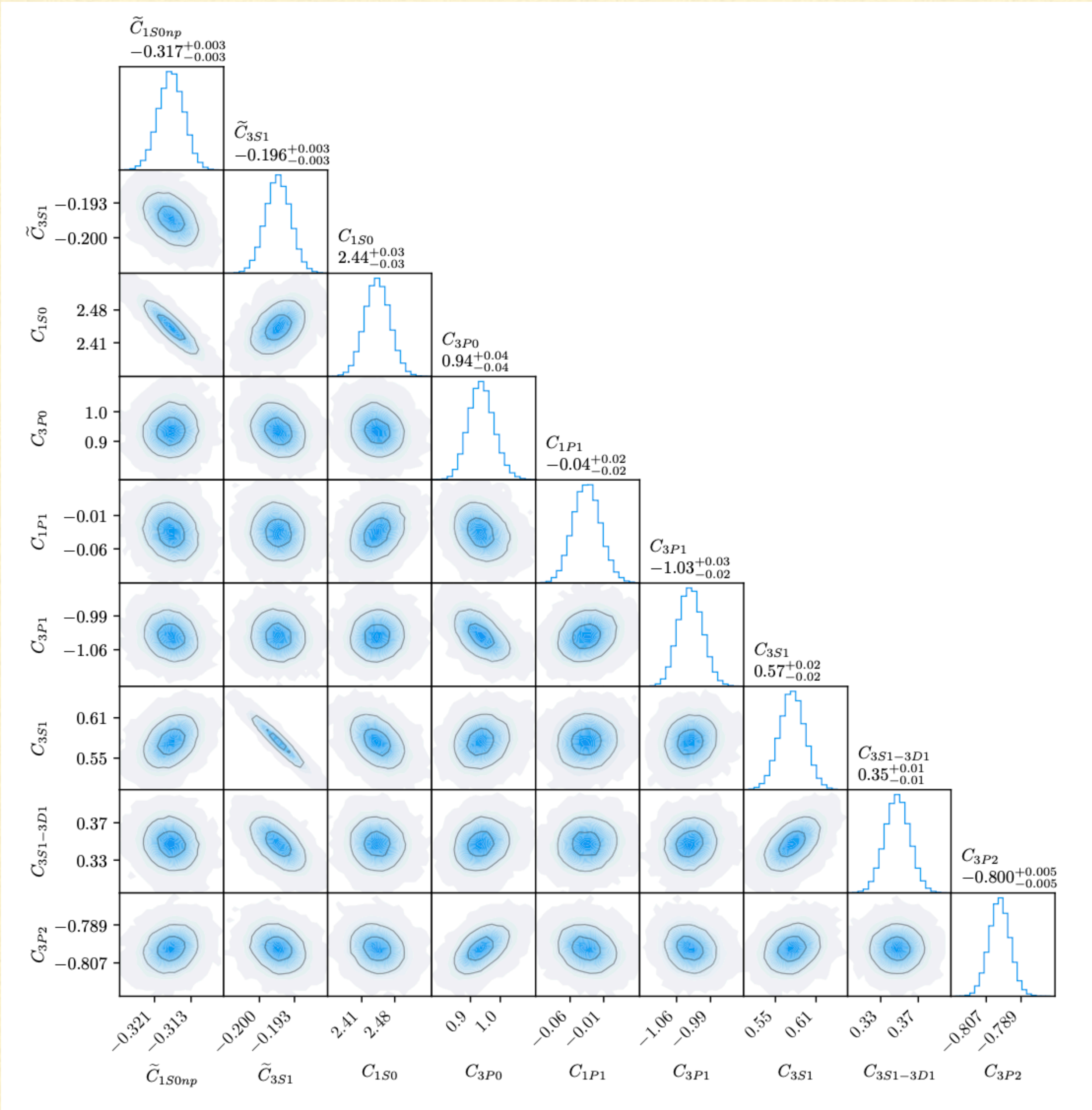

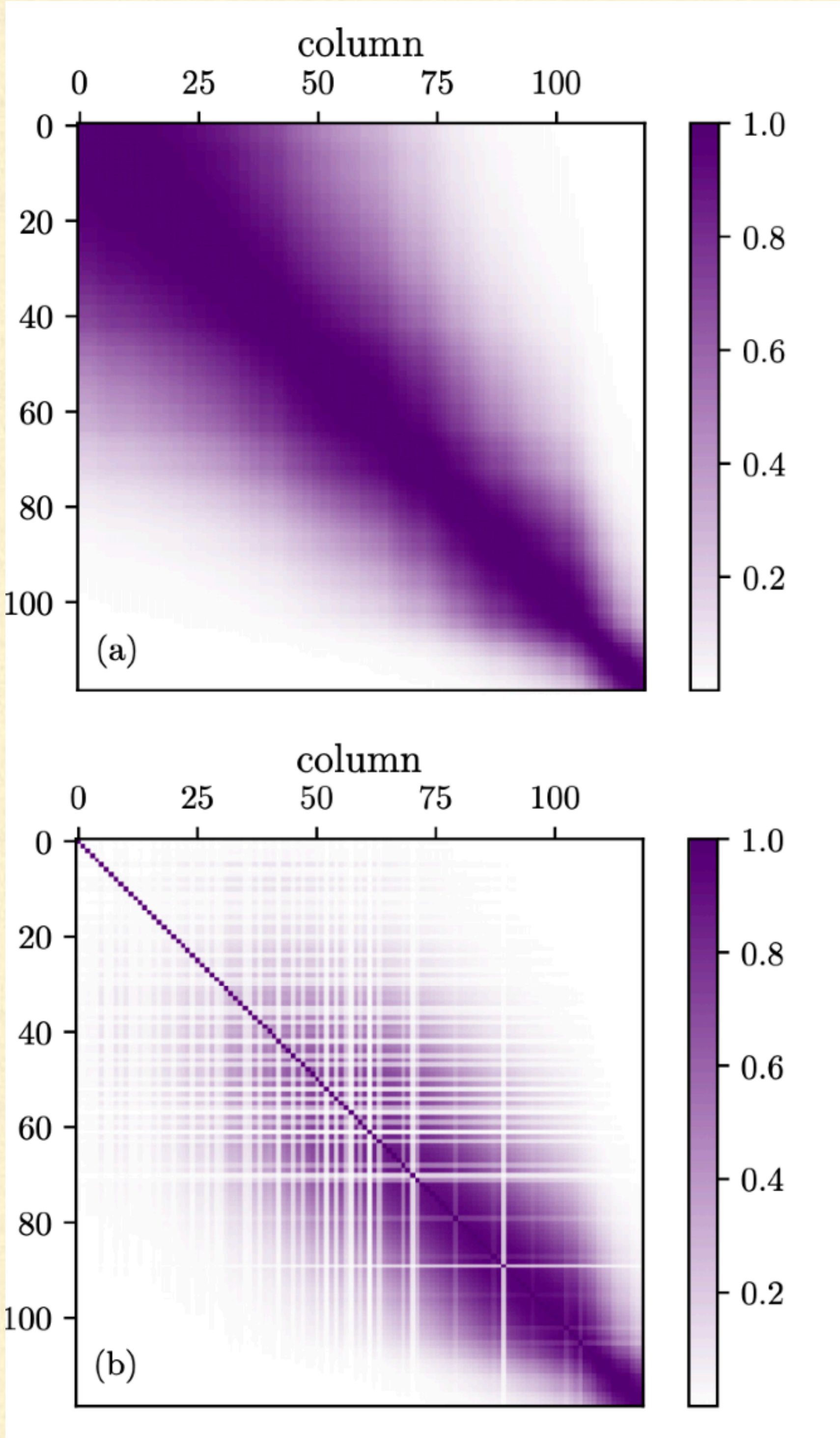

σ_{tot} correlations by data index

All at once: LECs & truncation errors together

Wesolowski, Svennson, Ekström, Forssén, Furnstahl, Melendez, DP, Phys. Rev. C (2022)

$$y_{\rm exp} = y_{\rm th} + \delta y_{\rm exp} + \delta y_{\rm th}$$

- This time Q is not obvious: we will actually make it a parameter and sample it. We will also sample $\bar{c}^2$, the mean-square value of the higher-order coefficients. $\bar{c}^2$and Q are also constrained by information from the lower-order calculations.
- NN force refit at $O(Q^0)$, $O(Q^2)$ and $O(Q^3)$; in last case with πN LECs from Roy-Steiner analysis
- Propagate uncertainties from NN LECs to final result for c_D and c_E by sampling the full 13-dimensional parameter space and marginalizing over NN parameters

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$$y_{\rm th}(p) = y_{\rm ref}(p) \sum_{i=0}^{k} c_i(\{a_j\}) Q^i$$

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Posterior and priors

Truncation errors

Naturalness

Posterior and priors

$$\mathrm{pr}(\mathbf{a}, \bar{c}^2, Q \,|\, D, I) \propto \exp\left(-\frac{1}{2}\mathbf{r}^T(\boldsymbol{\Sigma}_{\mathrm{exp}} + \boldsymbol{\Sigma}_{\mathrm{th}})^{-1}\mathbf{r}\right) \exp\left(-\frac{\mathbf{a}^2}{2\bar{a}^2}\right) \mathrm{pr}(\bar{c}^2 \,|\, Q, \bar{a}, I)\mathrm{pr}(Q \,|\, \mathbf{a}, I)$$

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Truncation errors

Naturalness

- We take uncorrelated error model for $\boldsymbol{\Sigma}_{\mathrm{th}}$: $(\boldsymbol{\Sigma}_{\mathrm{th,uncorr}})_{ij} = (\mathbf{y}_{\mathrm{ref}})^2 \bar{c}^2 \delta_{ij} \sum_{n=k+1}^{\infty} Q^{2n}$.
- Experimental errors are negligible in comparison
- Can include NN in "fit" by expanding meaning of **a** to include NN parameters. Incorporate NN information by using posterior from that analysis as a prior on that $\mathbf{a}_{\mathrm{NN}}$, the NN piece of **a**, here
- $\mathrm{pr}(\bar{c}^2 \,|\, Q, \vec{a}, I)$ is taken to be an inverse-χ^2 distribution. Information on the order-to-order shifts NLO-LO and NNLO-NLO included there
- $\mathrm{pr}(Q \,|\, \mathbf{a}, I)$ then also affected by that information. Starts as weakly informative Beta distribution before any updating from NLO-LO and NNLO-NLO shifts

Results for 3NF parameters, Q, $\bar{c}^2$

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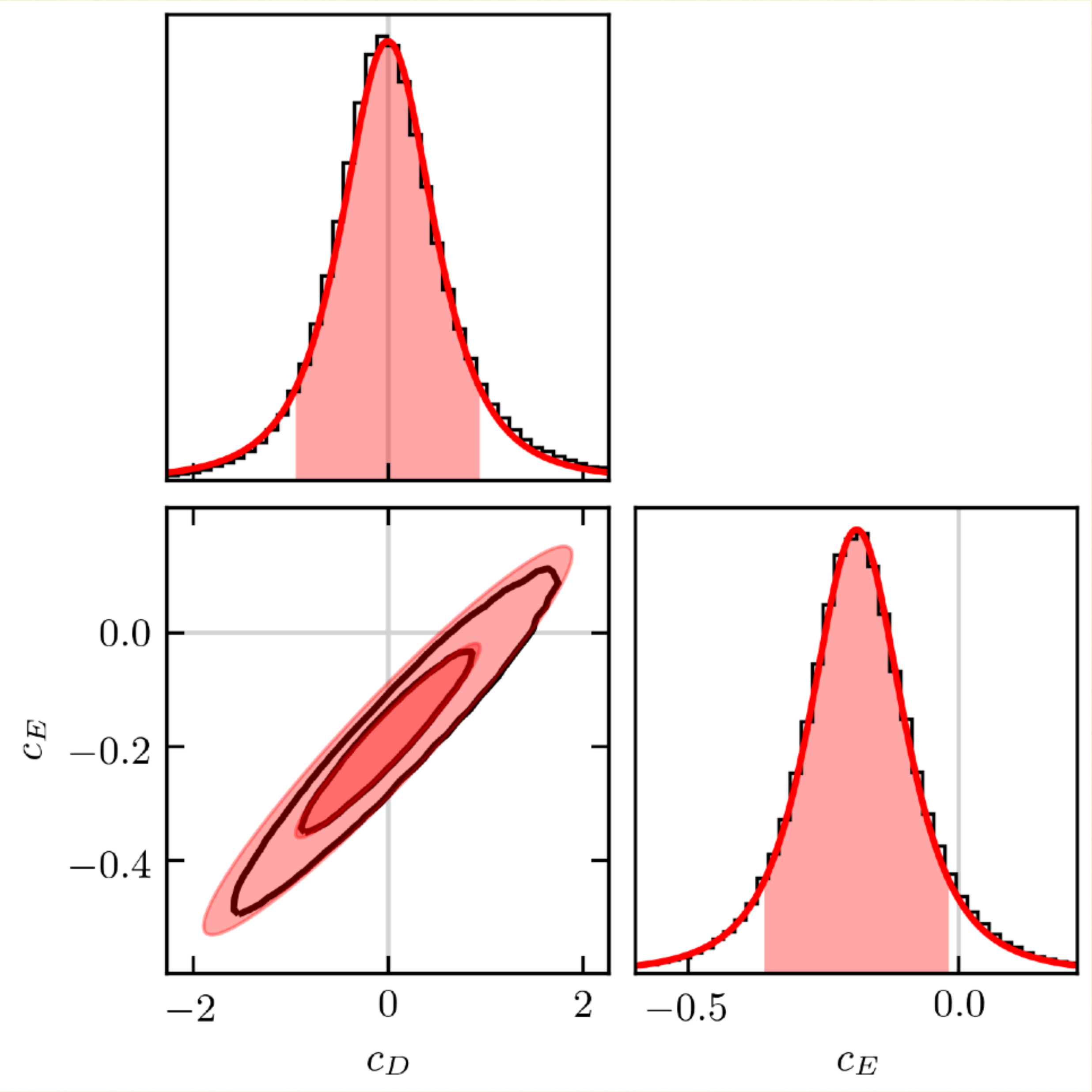

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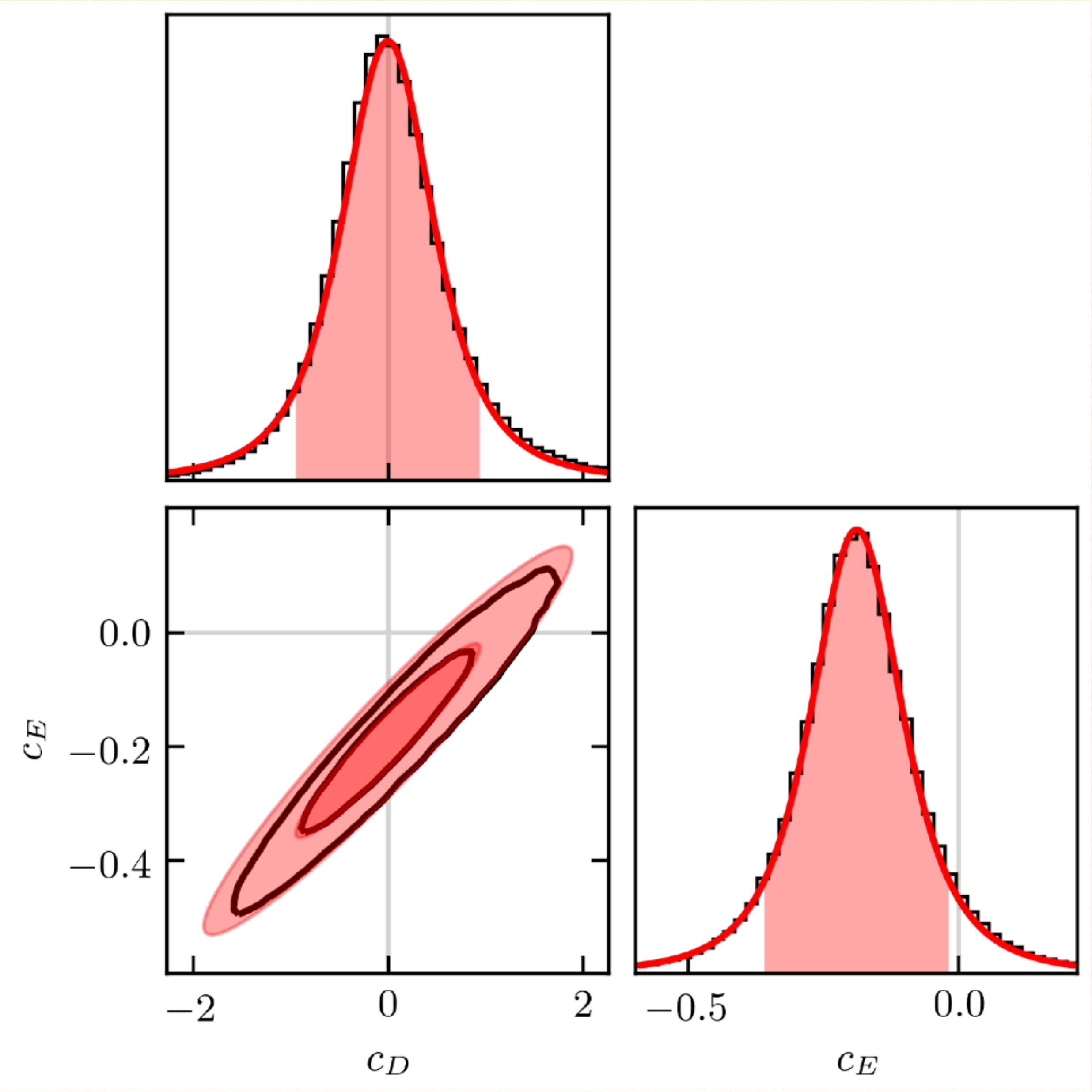

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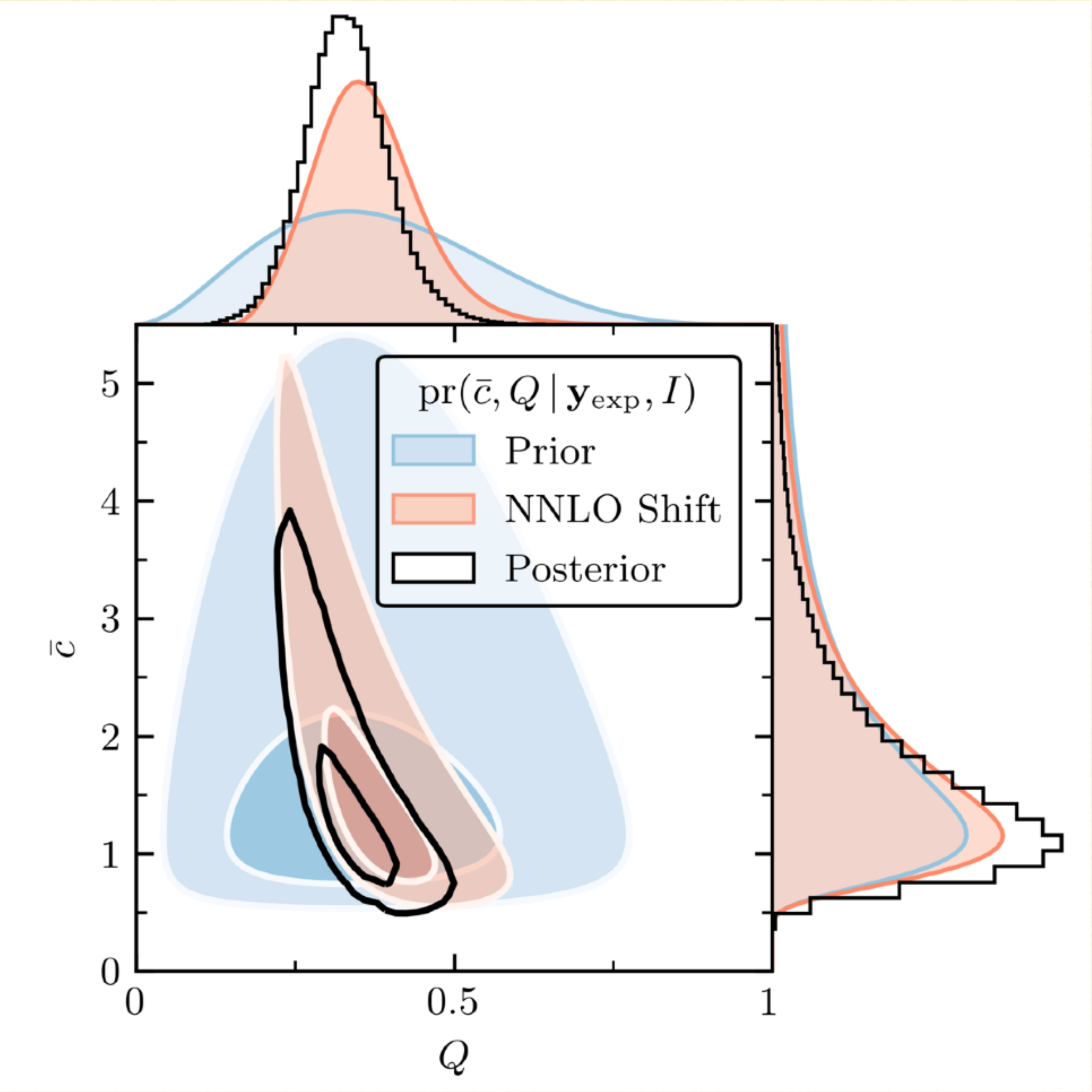
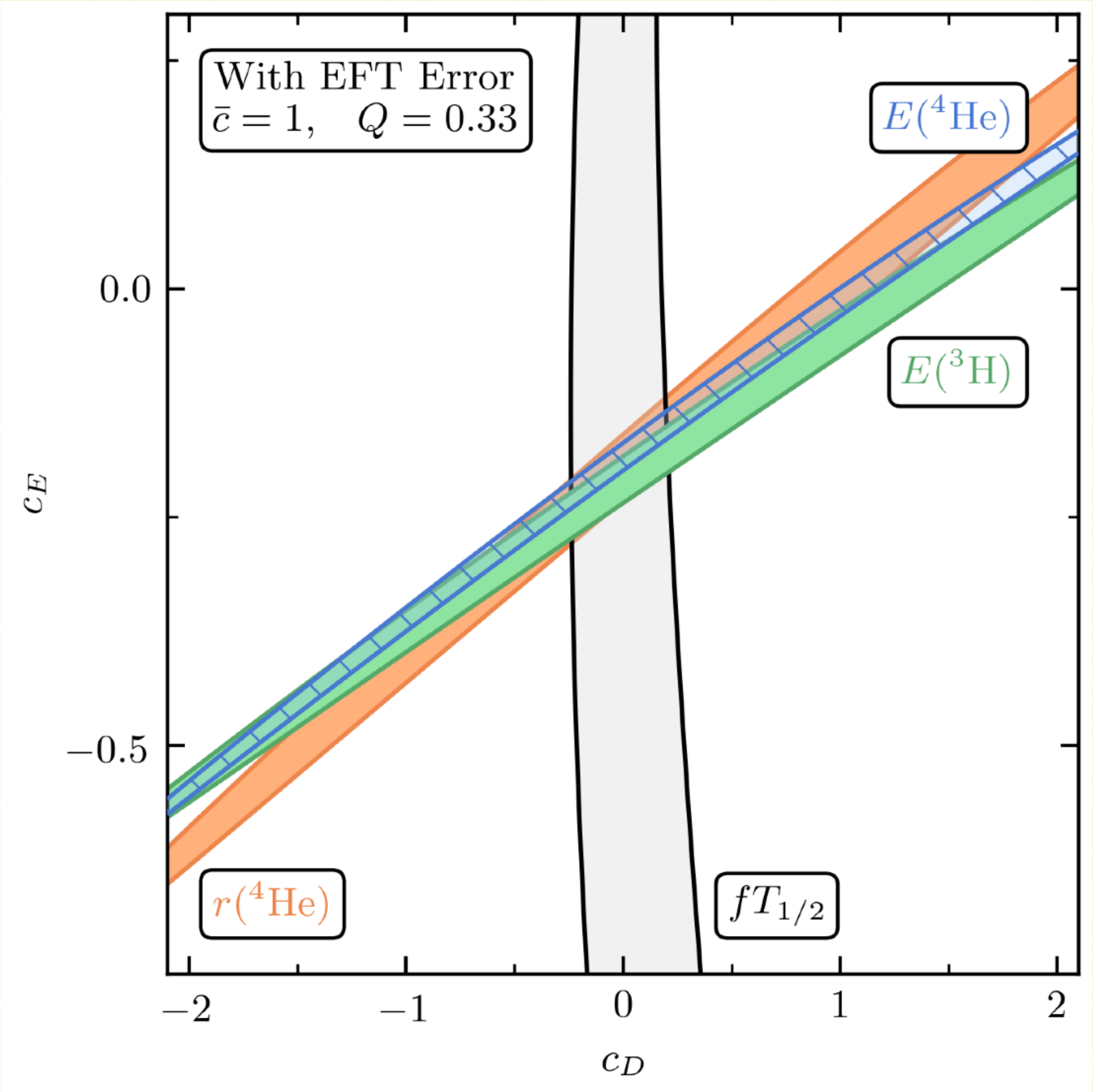


Q inferred from data, convergence pattern

Different constraints and truncation errors



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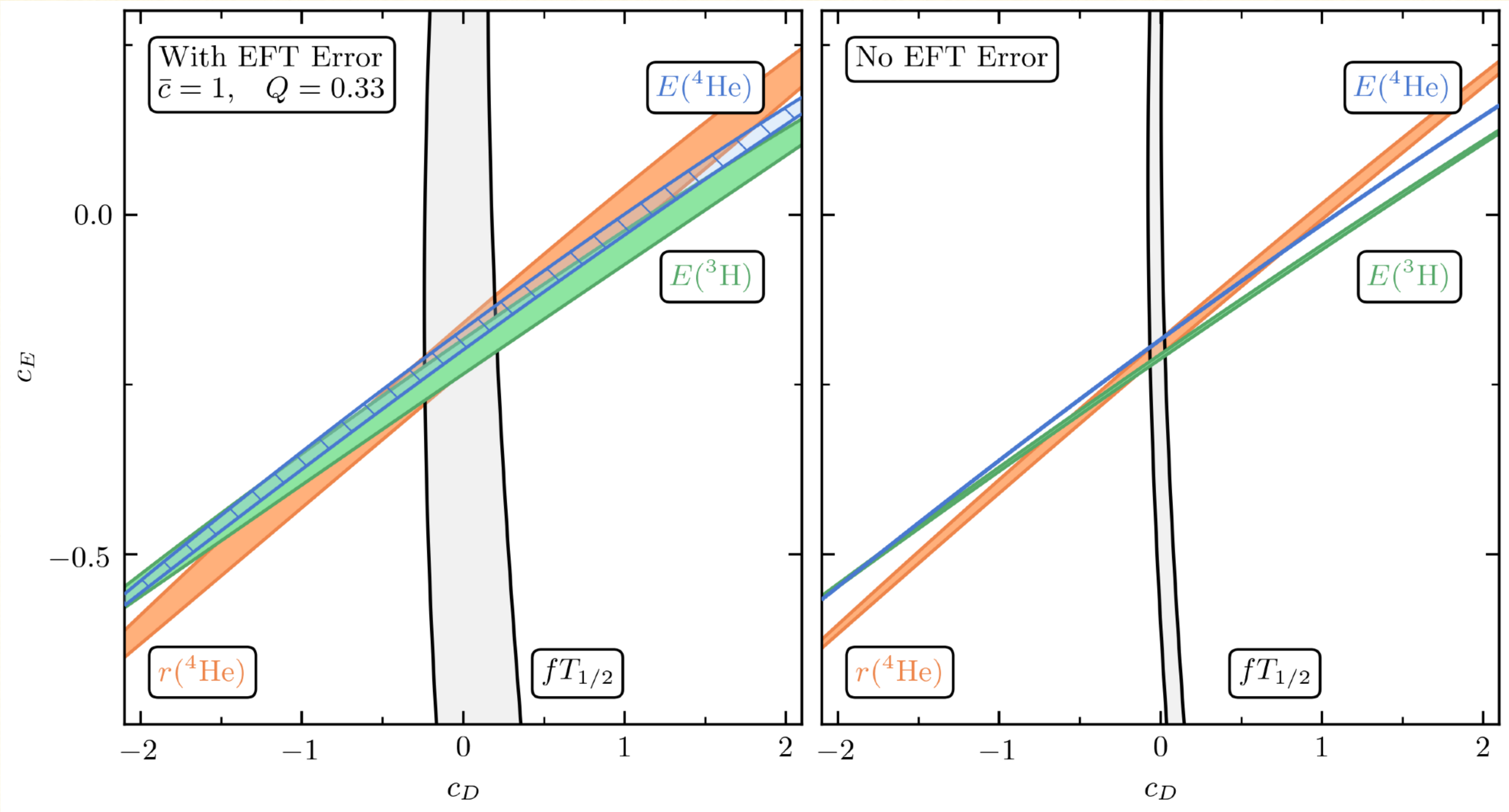
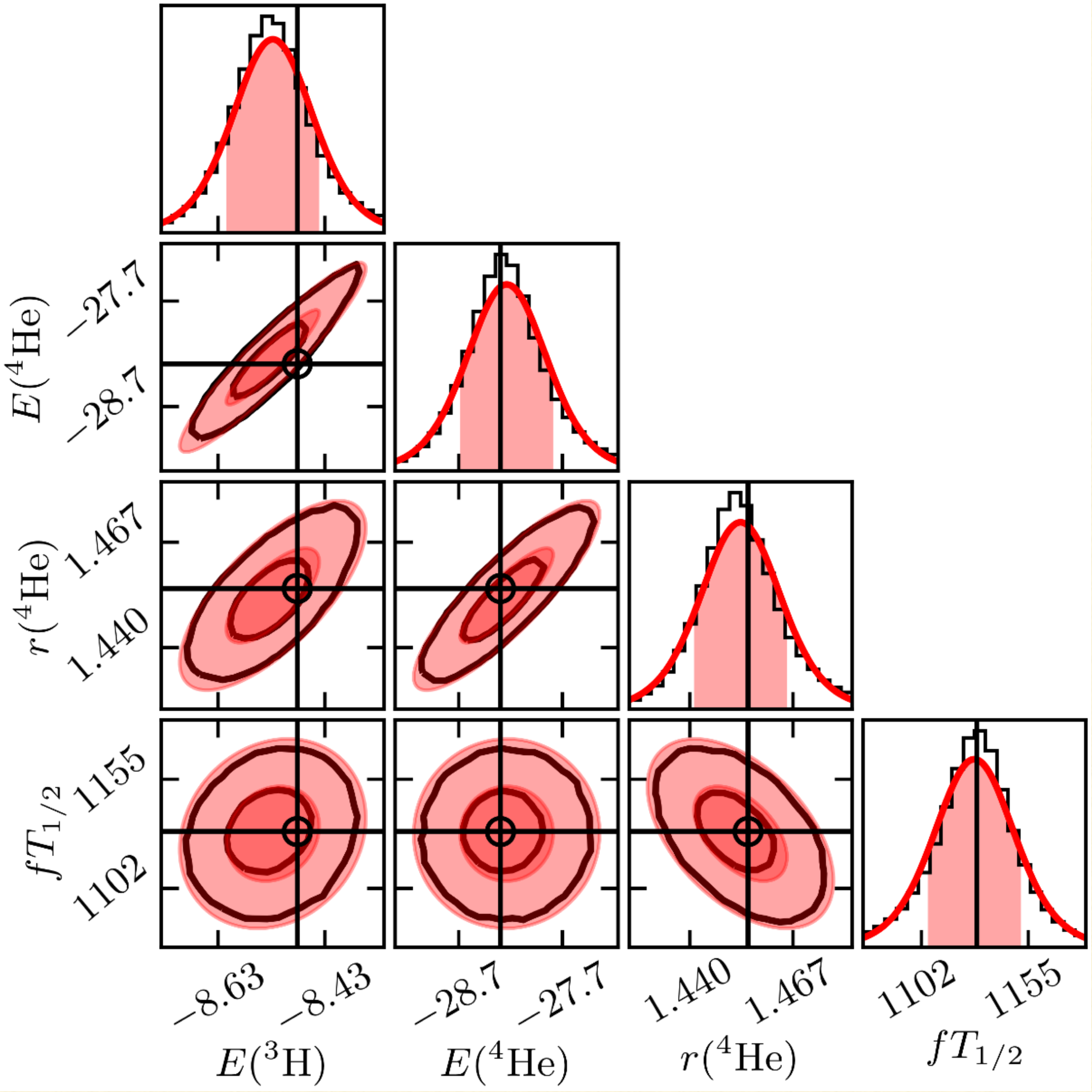


Posterior predictive distribution



χEFT can describe all these data once truncation errors are accounted for

Part 3: an interesting way to fail

Li Muli, Djärv, Forssén, DP, arXiv:2503.16372

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King et al., Phys. Rev. C 102, 025501 (2020)

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- SU(4) also explains suppression of nd→tγ at threshold in EFT($\not\pi$)

Lin, Singh, Springer, Vanasse, PRC 108, 104401 (2022)

SU(4) decomposition for A=4 to 8

- Gamow-Teller operator is a generator of SU(4) with no spatial dependence, therefore at LO in χEFT we have

$$\langle\Psi'|j_5^{ST}|\Psi\rangle = \sum_{C_2} d'(C_2)d(C_2)\langle C_2|j_5^{ST}|C_2\rangle$$

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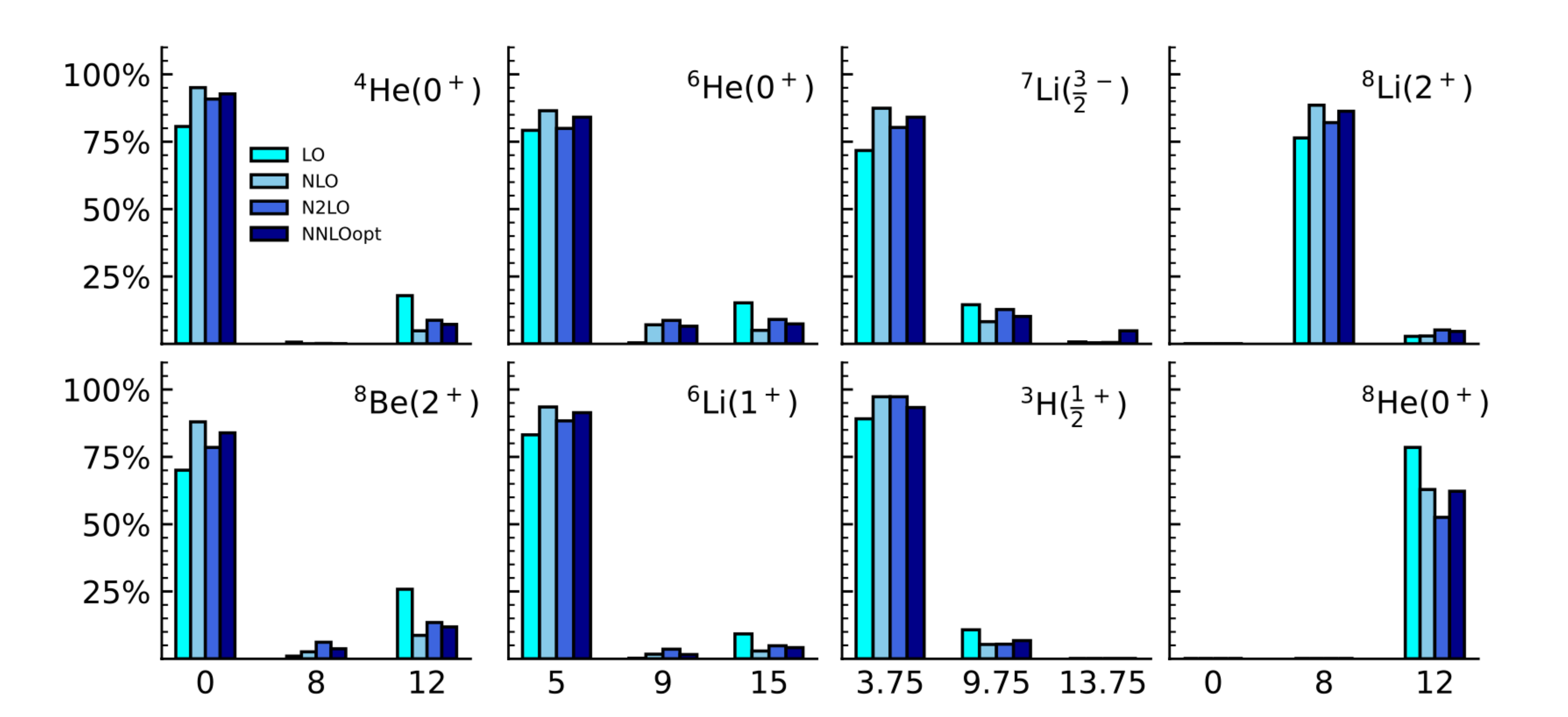


Implications

- β-decay matrix element is protected by Wigner's SU(4)-symmetry
- Cannot expect "regular" EFT convergence for symmetry protected observables
- EFT expansion for SU(4)-symmetry breaking part? Dual expansion?
- Why? Unitarity limit, QCD in limit of large-N_C, ….

Reaction	Eq. (3)	*ab initio*	[7]
$^3H(\frac{1}{2}^+)$ [1,1,1,0] → $^3He(\frac{1}{2}^+)$ [1,1,1,0]	2.449	2.313	//
$^6He(0^+)$ [2,2,1,1] → $^6Li(1^+)$ [2,2,1,1]	2.449	2.260	2.200
$^7Be(\frac{3}{2}^-)$ [2,2,2,1] → $^7Li(\frac{3}{2}^-)$ [2,2,2,1]	2.582	2.357	2.317
$^7Be(\frac{3}{2}^-)$ [2,2,2,1] → $^7Li(\frac{1}{2}^-)$ [2,2,2,1]	2.309	2.175	2.157
$^8Li(2^+)$ [3,2,2,1] → $^8Be(2^+)$ [3,2,2,1]	0.0	0.093	0.147
$^8He(0^+)$ [3,3,1,1] → $^8Li(1^+)$ [3,3,1,1]	0.0	0.335	0.386

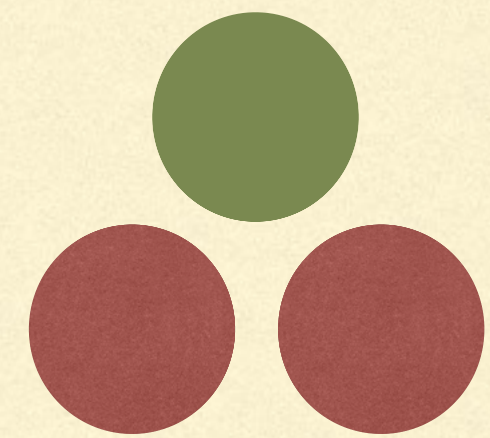
Summary

- The uncertainty induced in amplitudes—and hence in observables—by truncation of an EFT series can be modeled using Bayesian methods
- The BUQEYE collaboration has modeled the coefficients (≠ LECs) in the EFT expansion as Gaussian Processes
- The truncation-error model must be tested to ensure its statistical properties describes the orders already computed
- Benefits: well-calibrated uncertainties, breakdown scale information, full uncertainty quantification for LECs, predictions with uncertainties
- β-decay in s- and p-shell nuclei needs a different statistical model of truncation errors. Wigner's SU(4) symmetry protects matrix elements from corrections and so alters the EFT convergence pattern

3N data

For the moment we stick to bound-state observables

- Binding energy of three-nucleon nuclei: ^3H
- Binding energy of ^4He
- Charge radius of ^4He
- Beta-decay half-life of ^3H, aka "GT matrix element"



Solve Schrödinger equation for ^3He and ^4He and compute radii, GT matrix element

Done at $O(Q^0)$, $O(Q^2)$, $O(Q^3)$

Emulation via Eigenvector Continuation make fast evaluation possible