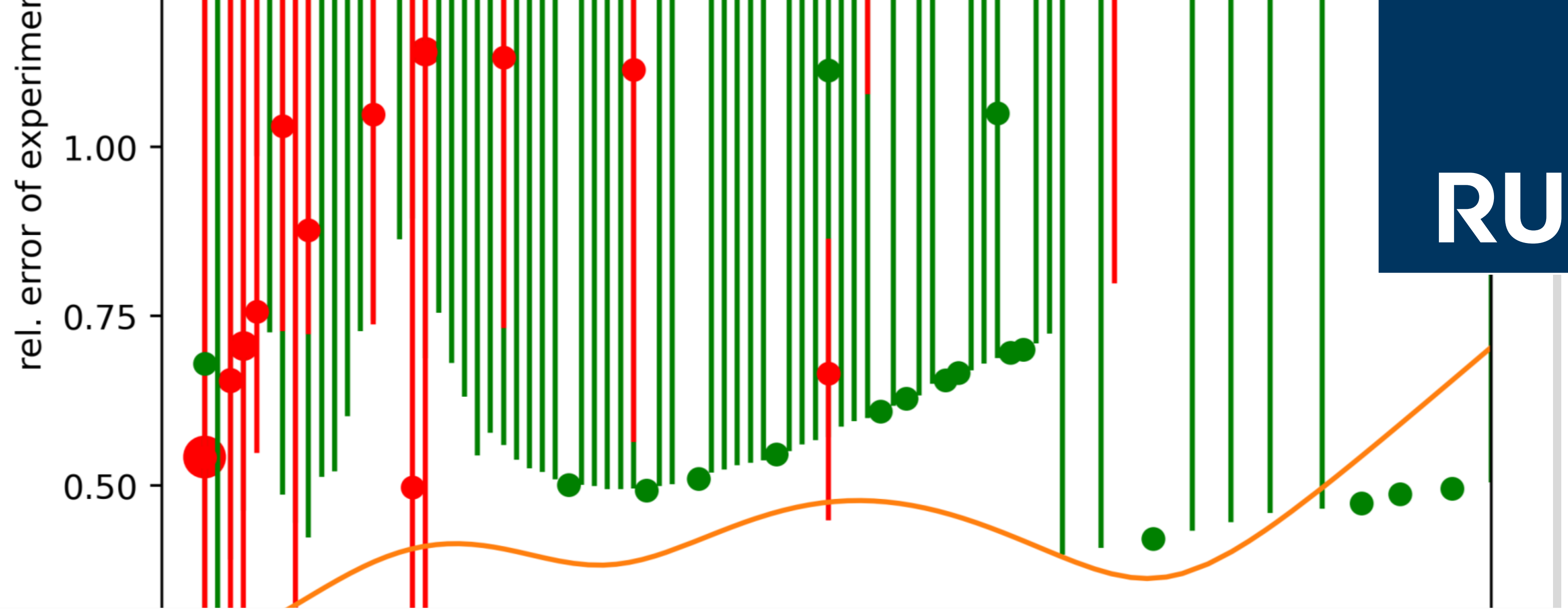

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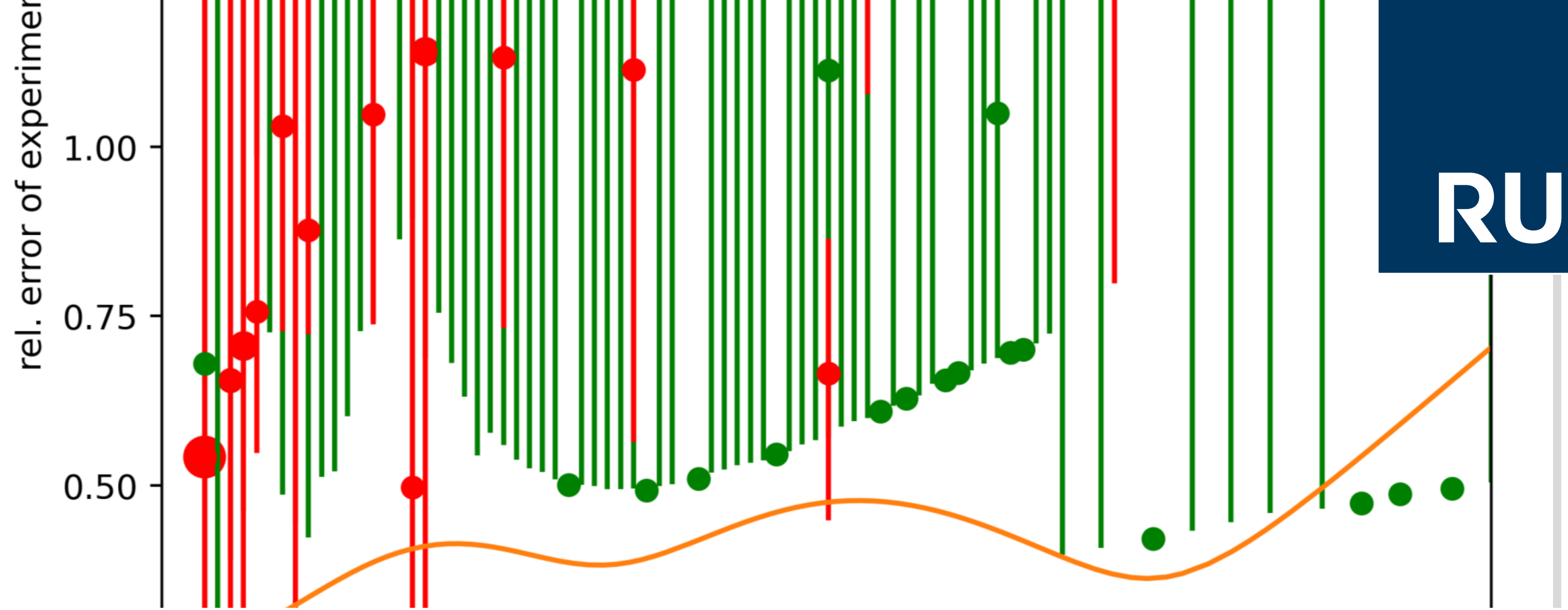
EXPLICIT ESTIMATION OF TRUNCATION UNCERTAINTIES IN CHIRAL EFT

Inverse Problems and Uncertainty Quantification in Nuclear Physics, INT, Seattle, July 11th

Sven Heihoff, Evgeny Epelbaum

contact: sven.heihoff@rub.de



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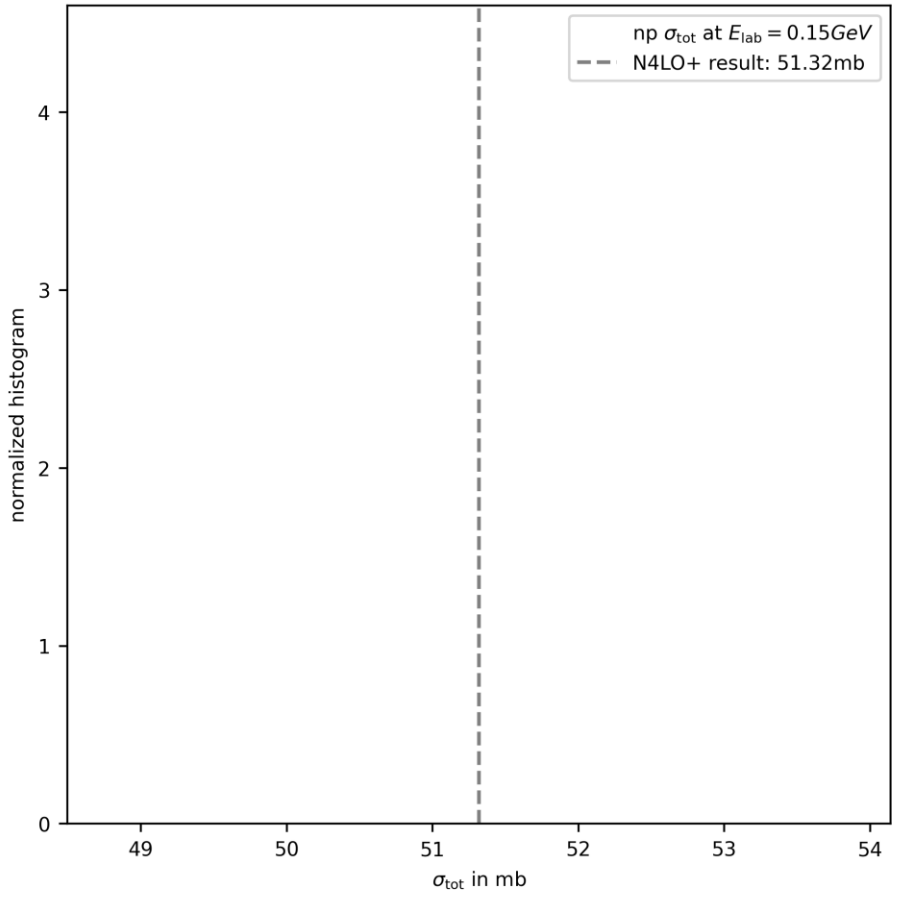
Outline

- **Aim**: Calculate some Nucleon-Nucleon scattering observable $\boldsymbol{X}$

1.) What is the theory and how to go from theory to $\boldsymbol{X}$?



Outline

- **Aim**: Calculate some Nucleon-Nucleon scattering observable $\boldsymbol{X}$

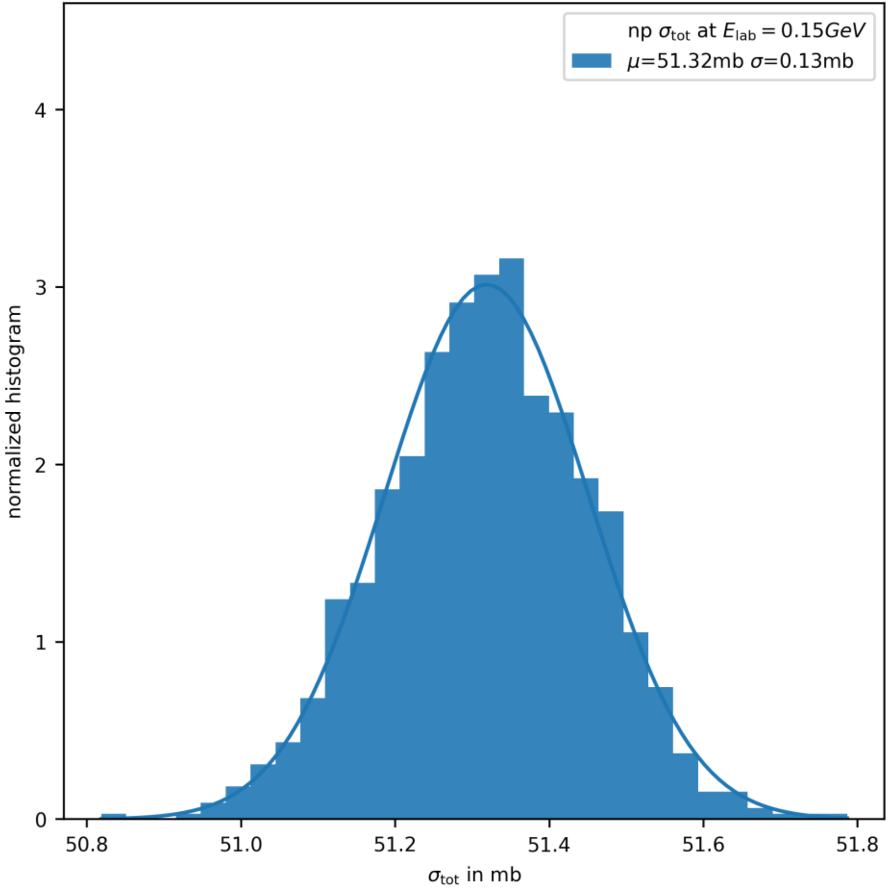
1.) What is the theory and how to go from theory to $\boldsymbol{X}$?

2.) We want: Not only central value,

but the distribution:

$$p\left(X^{(k)} \mid \text{theory}\right)$$

3.) Results – What can be learned from $p\left(X^{(k)} \mid \text{theory}\right)$?



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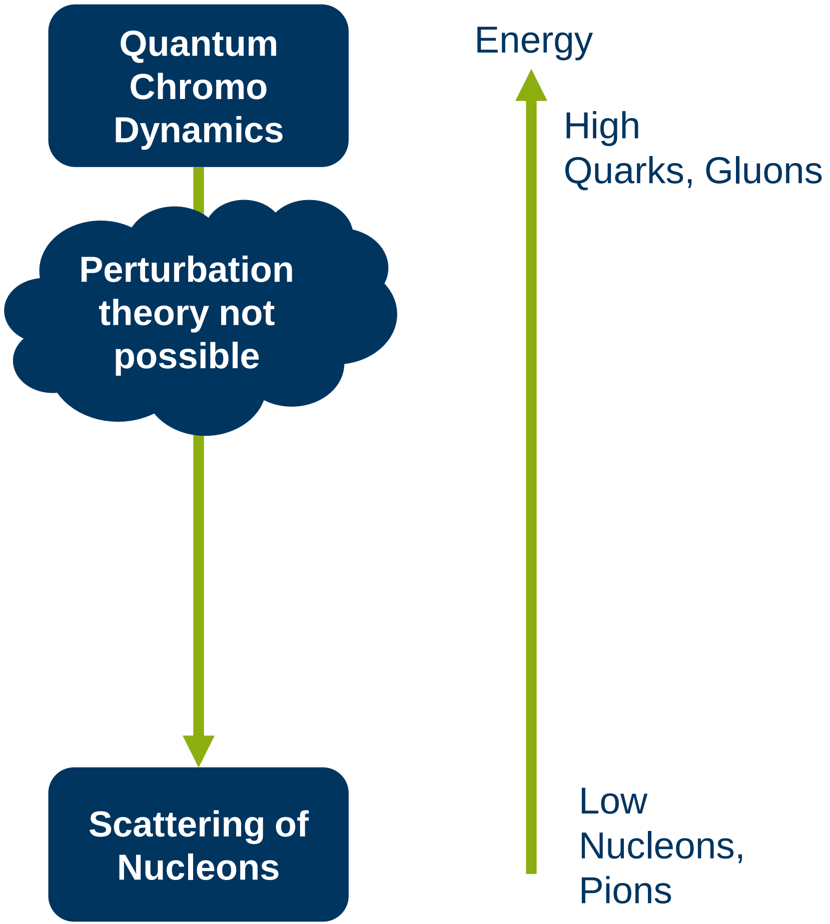
What is chiral EFT?

- QCD is best description of strong force so far
- Can not be solved at level of nucleons



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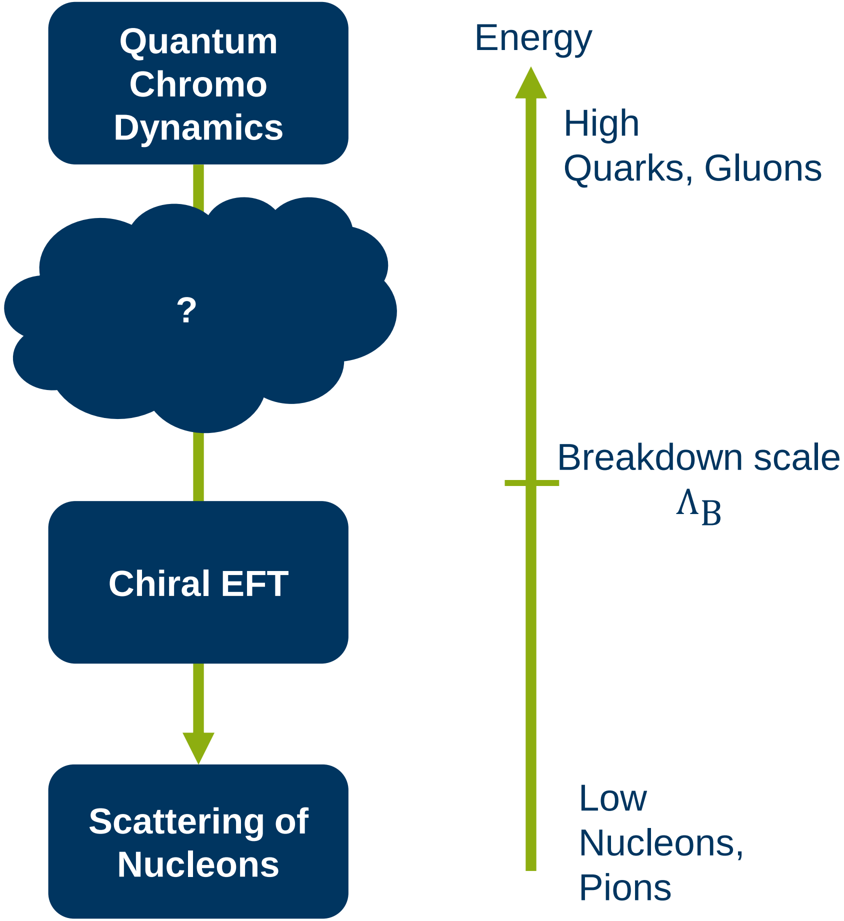
- Chiral EFT is low-energy effective theory of QCD
- Degrees of freedom: **Nucleons and pions**
- Start with most general Lagrangian ← a **lot** of terms!



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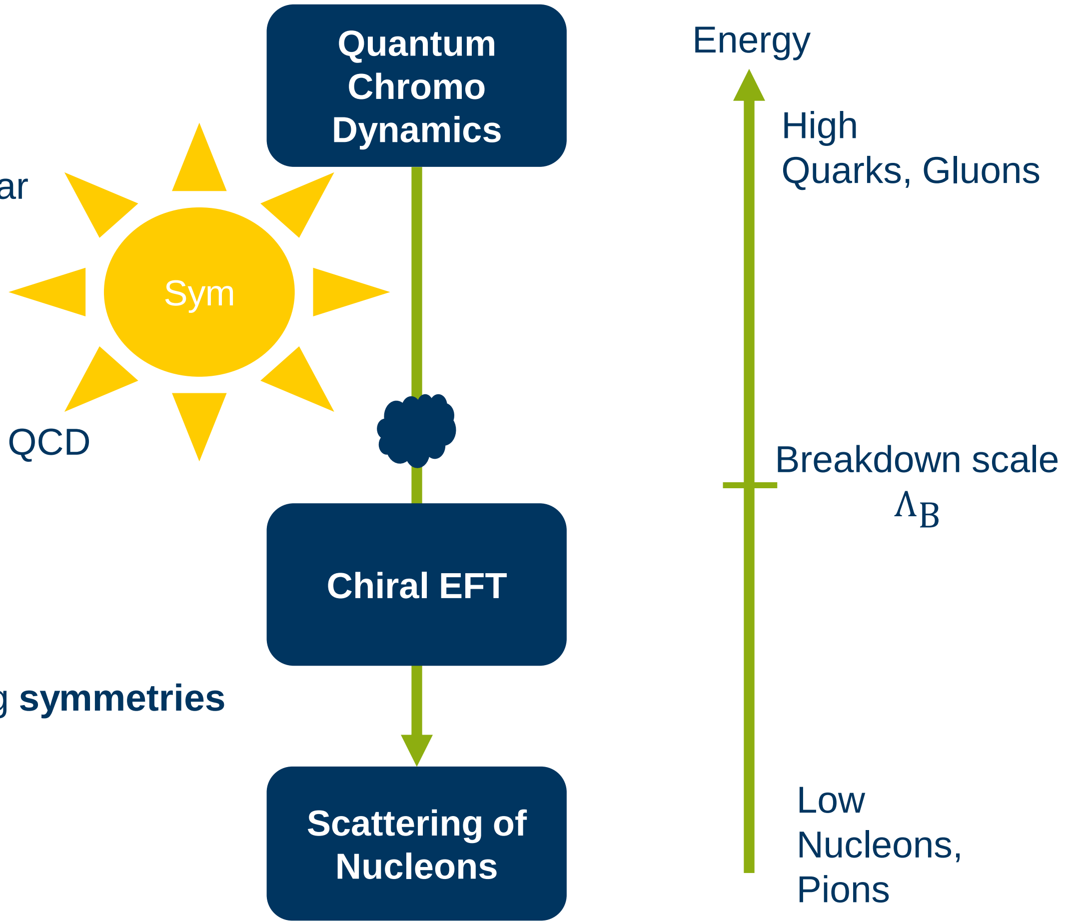

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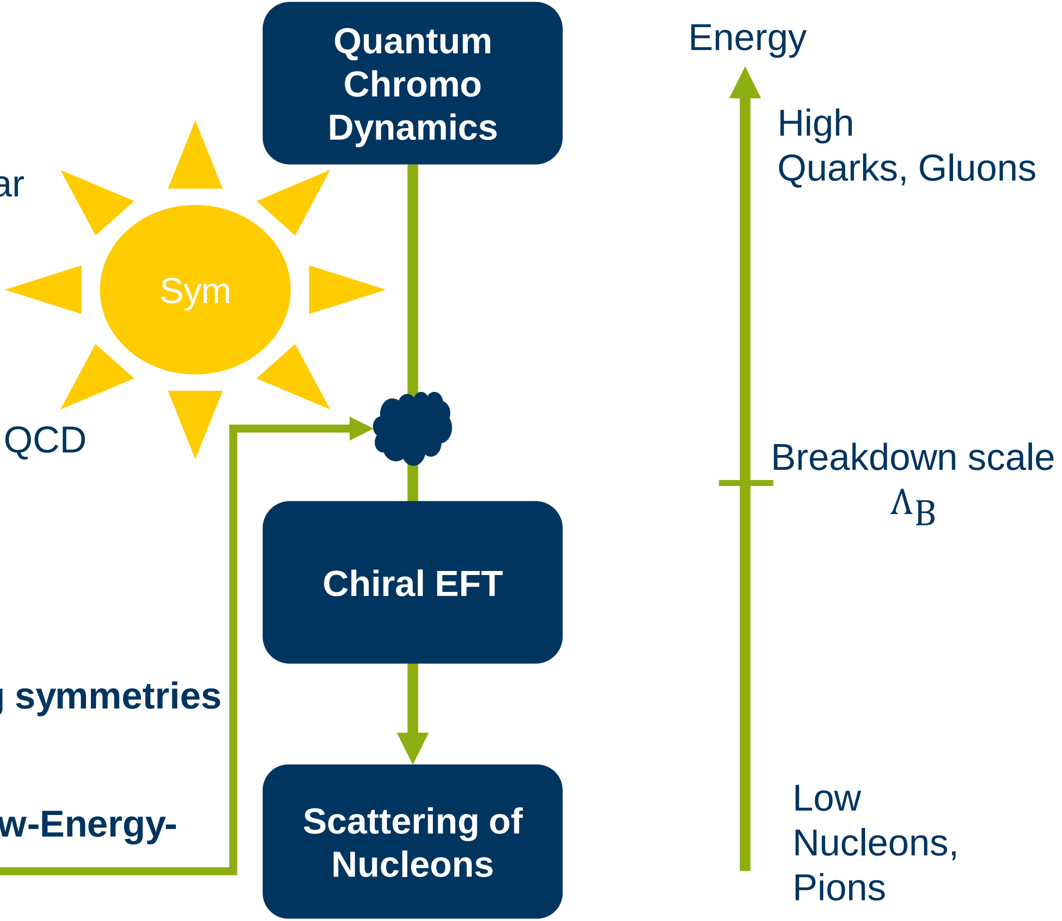
- Start with most general Lagrangian, fulfilling **symmetries**
- Chiral EFT comes with a-priori unknown **Low-Energy-Constants (LECs)**



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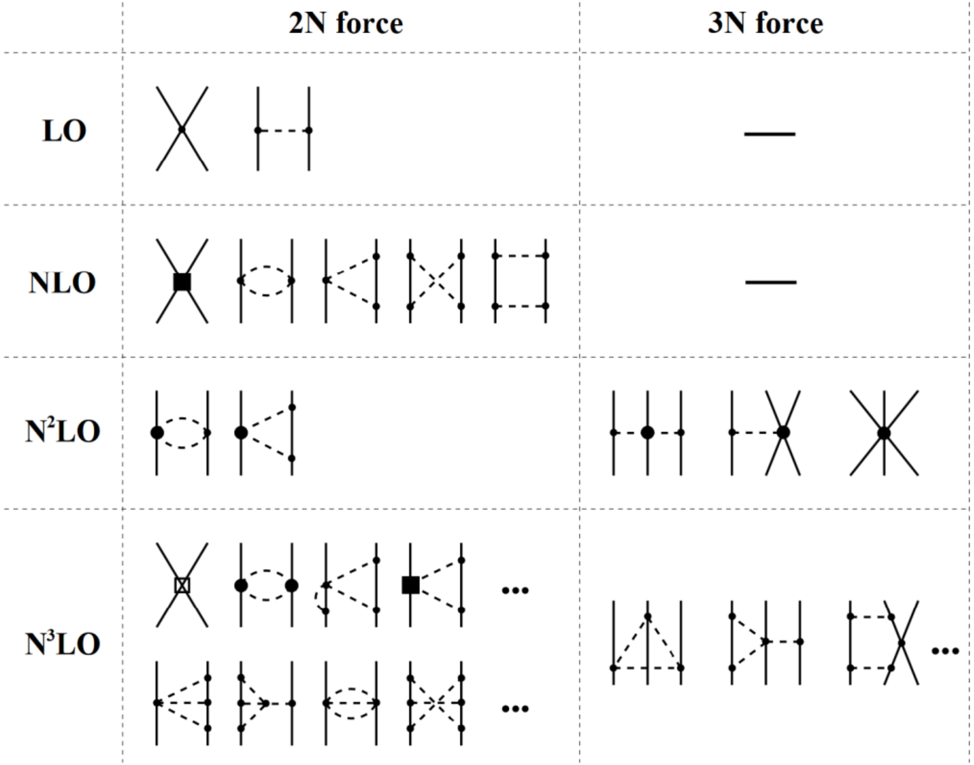
Power counting

- In principle infinitely many terms in Lagrangian
- Expansion parameter: $Q \in \left(\frac{p}{\Lambda_B}, \frac{M_\pi}{\Lambda_B}\right) \sim \frac{1}{3}$
- Each diagram is assigned to a power of Q



E. Epelbaum, Nuclear Forces from Chiral Effective Field Theory: A Primer (2010)

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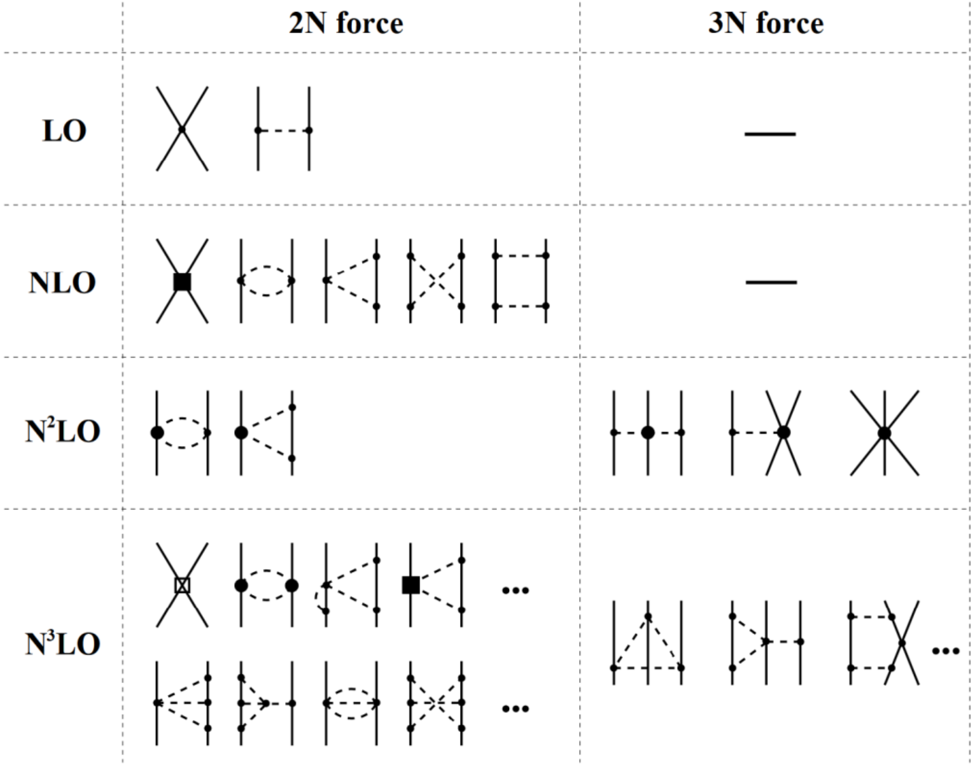
- Each diagram is assigned to a power of Q
  → Hierarchy of diagrams by their importance
  → Finite order → finite set of diagrams
  → Allows for systematic improvement of theory



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- Lagrangian looks like:

$L = A_{\text{LO}} + A_{\text{NLO}} + A_{N^2LO} + \cdots$ **with** $A_{\text{LO}} \propto Q^0$ $A_{\text{NLO}} \propto Q^2, A_{N^2LO} \propto Q^3$ **thus** $A_{\text{LO}} > A_{\text{NLO}} > A_{N^2LO}$

The final step: How to get observables?

- Finite set of diagrams can be summed into a QM potential $V = V(p, p')$
- Lippmann-Schwinger-equation:

$$T = V + VGT \Rightarrow (1 - VG)T = V$$

- With G as free propagator and T as transition matrix (directly connected to observables)
- Solved in momentum space and partial-wave decomposed

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- With G as free propagator and T as transition matrix (directly connected to observables)
- Solved in momentum space and partial-wave decomposed
- What about LECs? Fitted to experimental data! ← **inverse problem**
- 2N potential in chiral EFT leads to high-precision description of 2N data

P. Reinert, et al., Eur. Phys. J. A 54, 86 (2018)

Nice theory, but

“a physicist who has no errorbars is also just a religious person.”

Three important sources of uncertainties

- Uncertainties of the fitting protocol of the LECs
  - Numerical approximations (especially in EM contributions)
  - Fitting algorithm
  - Physical constants
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} **In this talk**

- **Aim**: probability distribution $\boldsymbol{p}\left(\boldsymbol{X}^{(\boldsymbol{k})}\right)$ of observable X at some order k of Chiral EFT.

Bayesian estimation of truncation uncertainties

- Assumption: Expansion is the same for observable $X^{(k)}$ as for potential

$$X^{(k)} = X_{\text{ref}} \cdot \left(c_0 + \sum_{i=2}^{k} c_i \cdot Q^i + \Delta_k \right)$$

- With expansion coefficients $c_i = \frac{X^{(i)}}{X_{\text{ref}} \cdot Q^i}$ and trunc. uncertainty $X_{\text{ref}} \Delta_k = X_{\text{ref}} \sum_{i=k+1}^{\infty} c_i \cdot Q^i$

J. A. Melendez, S. Wesolowski, and R. J. Furnstahl, Phys. Rev. C 96, 024003 (2017), arXiv:1704.03308

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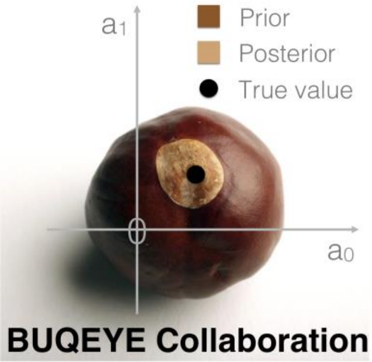
- Bayes theorem yields: $\text{p}(\{c_{j\epsilon[k+1,\infty]}\} \mid \{c_{i\epsilon[0,k]}\})$

  → Obtain a probability distribution $p(\Delta_k^h | \{c_i\})$ for $\Delta_k^h = \sum_{i=k+1}^{h} c_i \cdot Q^i$



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Issues of Bayesian approach

- Chiral EFT results at $E_{\mathrm{lab}} = 150\ \mathrm{MeV}$ and cutoff $\Lambda = 450\mathrm{MeV}$

$$\sigma_{\mathrm{tot}} = 52.15_{\mathrm{LO}} - 2.94_{\mathrm{NLO}} + 1.25_{\mathrm{N2LO}} + 0.34_{\mathrm{N3LO}} + 0.44_{\mathrm{N4LO}} + 0.07_{\mathrm{N4LO+}}$$

- Final result with Bayesian error: $\sigma_{\mathrm{tot}}^{\mathrm{N4LO+}} = 51.32 \pm 0.19\ \mathrm{mb}$

For algorithm see: E. Epelbaum et al., Eur. Phys. J. A 56, 92 (2020), arXiv:1907.03608

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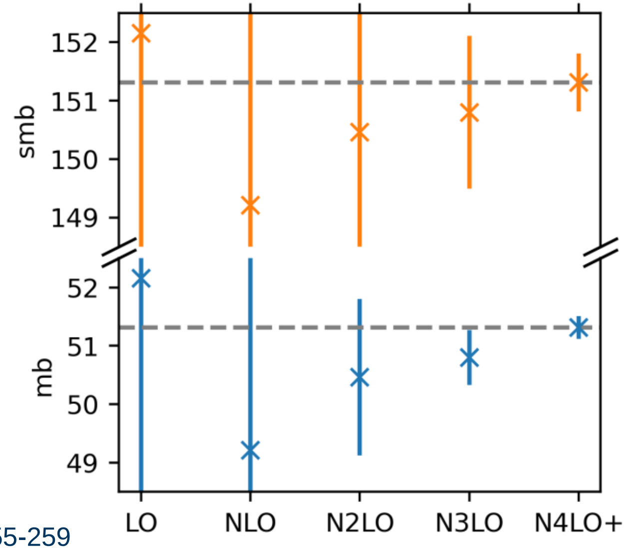
- What if, we measure in smb? $x\ \text{mb} = (x + 100)\ \text{smb}$
  - $\sigma_{\text{tot}}^{\text{N4LO+}} = 151.32 \pm 0.49\ \text{smb}$

  → Bayesian uncertainty dependent on absolute scale!



- Experiment: $51.02 \pm 0.3\ \text{mb}$ P.W. Lisowski et al.,Phys. Rev. Lett. 49 (1982), 255-259

Expansion of potential really also valid for observables?

Expansion of potential really also valid for observables?

Including next-higher order at level of nuclear potential!

Method

- How to obtain $p\left(X^{(k)}\right)$?

  1.) Include contact diagrams of next higher order $\mathrm{k}+1$ to potential

  2.) Set LECs $\vec{a}^{(k+1)}$ to natural values

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3.) Refit all lower order LECs $\vec{\mathrm{a}}^{(i\,\epsilon\,[0,\mathrm{k}])}$

4.) Repeat m times for different LECs of next higher order

→ m different values for $X^{(k)}$ ~ sample of $p\left(X^{(k)}\right)$

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- How to obtain $p\left(X^{(k)}\right)$?

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  3.) Refit all lower order LECs $\vec{\mathrm{a}}^{(i\,\in\,[0,\mathrm{k}])}$

  4.) Repeat m times for different LECs of next higher order

  → m different values for $X^{(k)}$ ~ sample of $p\left(X^{(k)}\right)$

- Mathematically: Explicitly integrating out the diagrams of order $\mathrm{k}+1$

$$p\left(X^{(k)}\right)=\int \mathrm{d}\,\vec{a}^{(k+1)}\cdot\delta\left(X^{(k+1)}\left(\vec{\mathrm{a}}^{(i\,\in\,[0,\mathrm{k}+1])}\right)-X^{(k)}\right)\cdot p\left(\vec{\mathrm{a}}^{(i\,\in\,[0,\mathrm{k}+1])}\right)$$

- Uncertainty: width of $p\left(X^{(k)}\right)$

Fitting algorithm

- Data based on Granada 2013 database
  - $0\mathrm{MeV} \leq E_{\mathrm{lab}} \leq 280\mathrm{MeV}$ (no weighting)
  - 3σ selection of data Patrick Reinert, PhD-thesis, https://doi.org/10.13154/294-9501
  - 2845 np and 2081 pp datapoints

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- Explicit constraints
  - np coherent scattering length
  - Deuteron Binding Energy

} Fixing S-waves for low scattering energies artificially!

- Fits are stable, with respect to starting values of lower-order LECs

- Levenberg-Marquardt fit algorithm form scipy‘s leastsq function

What is natural for the LECs?

- Naturalness: Every physical parameter should be in the order of 1
  - Compared to a reasonable physical scale
  - No proof, but generally accepted idea in physics
  - Here: Encoded in probability distribution for LEC values $p(a_{\mathrm{j}}^{(i)})$

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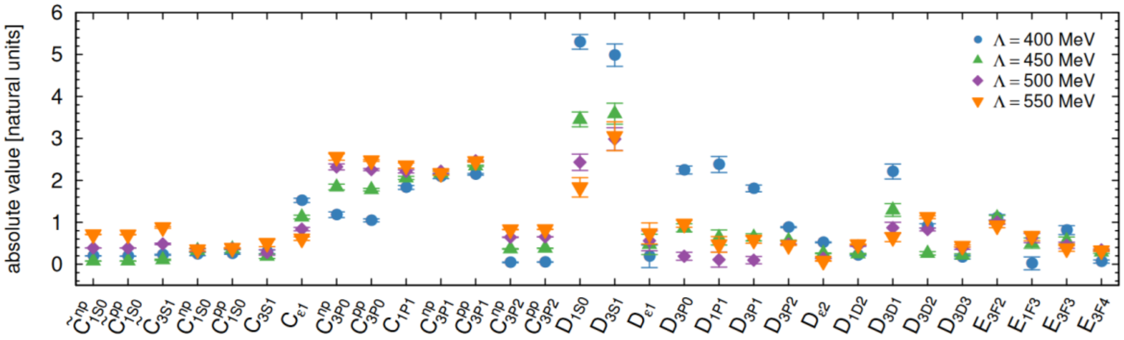
- Can we infer $p(\vec{a}^{(k+1)})$ from the LECs fitted so far?
  - Assume: $p(a_j^{(i)})$ is independet of the order i and is the same for all elements of $\vec{a}^{(i)}$
  - Assume: $p\left(a_j^{(i)}\right) \sim \mathrm{N}(0, \mathrm{w})$ follows Gaussian with mean 0 and standard deviation w
  - Bayes theorem:

$$p(w \mid \vec{\mathrm{a}}^{(i \in [0,\mathrm{k}])}) \propto p\left(\vec{\mathrm{a}}^{(i \in [0,\mathrm{k}])} \mid w\right) \cdot p(w)$$

Naturalness of known LECs

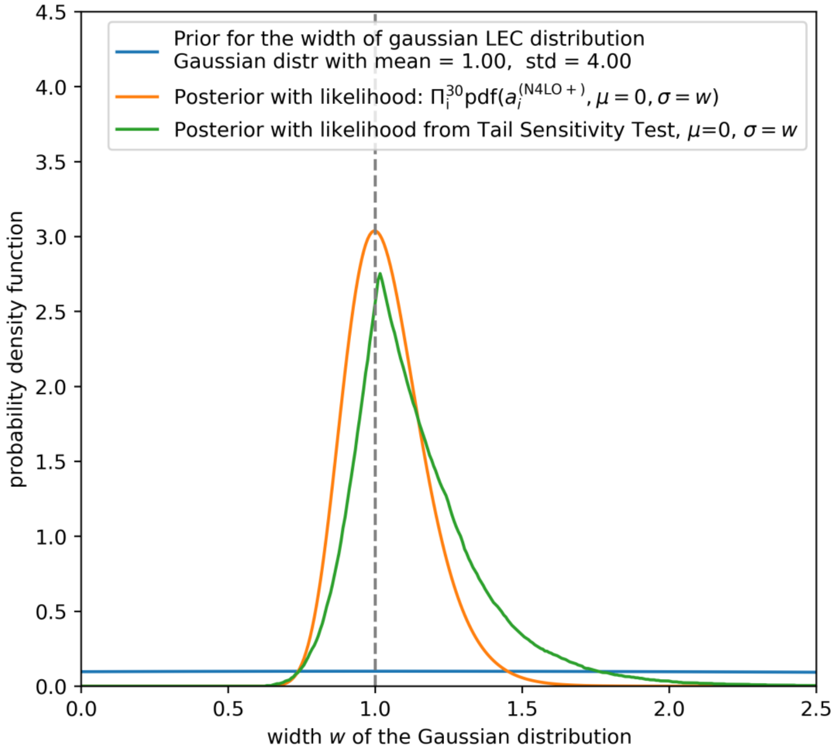
- $p(w \mid \vec{a}^{(i \in [0,k])}) \propto p\left(\vec{a}^{(i \in [0,k])} \mid w\right) \cdot p(w)$

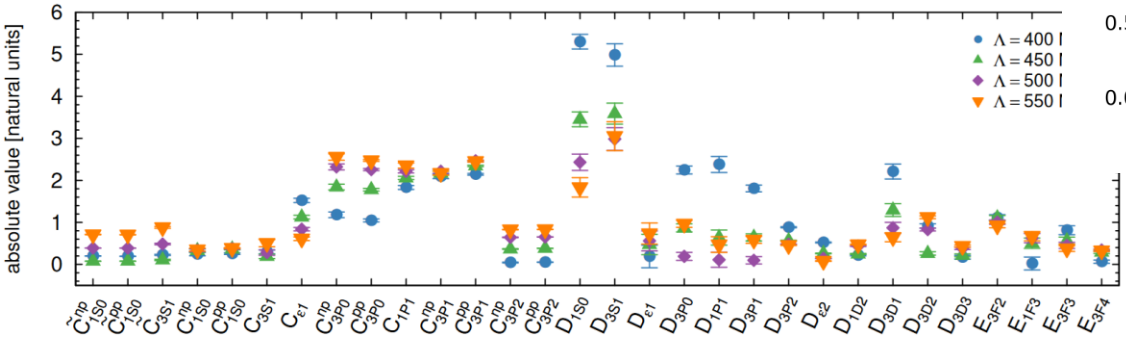


Epelbaum et al., Front. in Phys. 8, 98 (2020), arXiv:1911.11875

Naturalness of known LECs

- $p(w \mid \vec{a}^{(i\in[0,k])}) \propto p\left(\vec{a}^{(i\in[0,k])} \mid w\right) \cdot p(w)$
- What exactly is $p\left(\vec{a}^{(i\in[0,k])} \mid w\right)$?
- If assumptions are fulfilled, the LECs are indeed drawn from a Gaussian distribution with $\sigma \sim \mathbf{1}$





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What we thought we do

Calculate $X^{(k)}$ **and add randomly higher order contributions of natural size → Truncation error**

Results

PRELIMINARY!

$p\left(\sigma_{\text{tot}}^{(N4LO+)}\right)$ at 150MeV

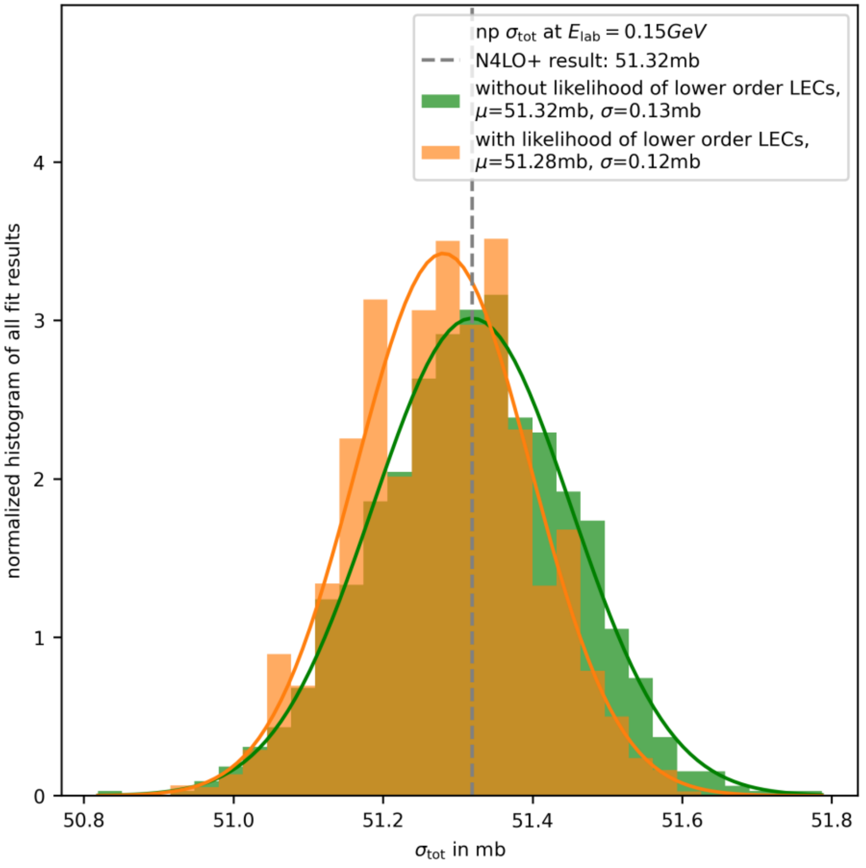
- Without likelihood of lower-order LECs

$$\int \mathrm{d}\,\vec{a}^{(k+1)} \cdot \delta\left(X^{(k+1)}\left(\vec{a}^{(i\in[0,k+1])}\right) - X^{(k)}\right) \cdot p\left(\vec{a}^{(k+1)}\right)$$

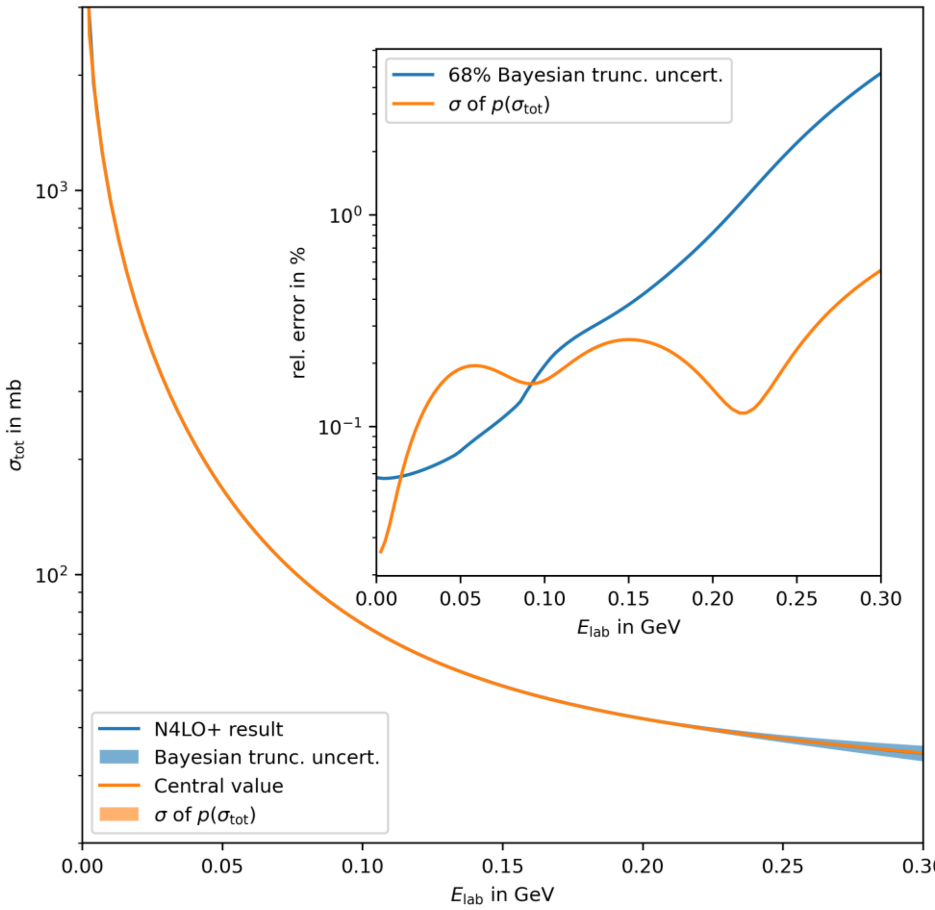
- With likelihood of lower-order LECs

$$\int \mathrm{d}\,\vec{a}^{(k+1)} \cdot \delta\left(X^{(k+1)}\left(\vec{a}^{(i\in[0,k+1])}\right) - X^{(k)}\right) \cdot p\left(\vec{a}^{(k+1)}\right) \cdot p\left(\vec{a}^{(i\in[0,k])}\right)$$

- Prior: distribution of LECs: $p\left(\vec{a}^{(k+1)}\right)$

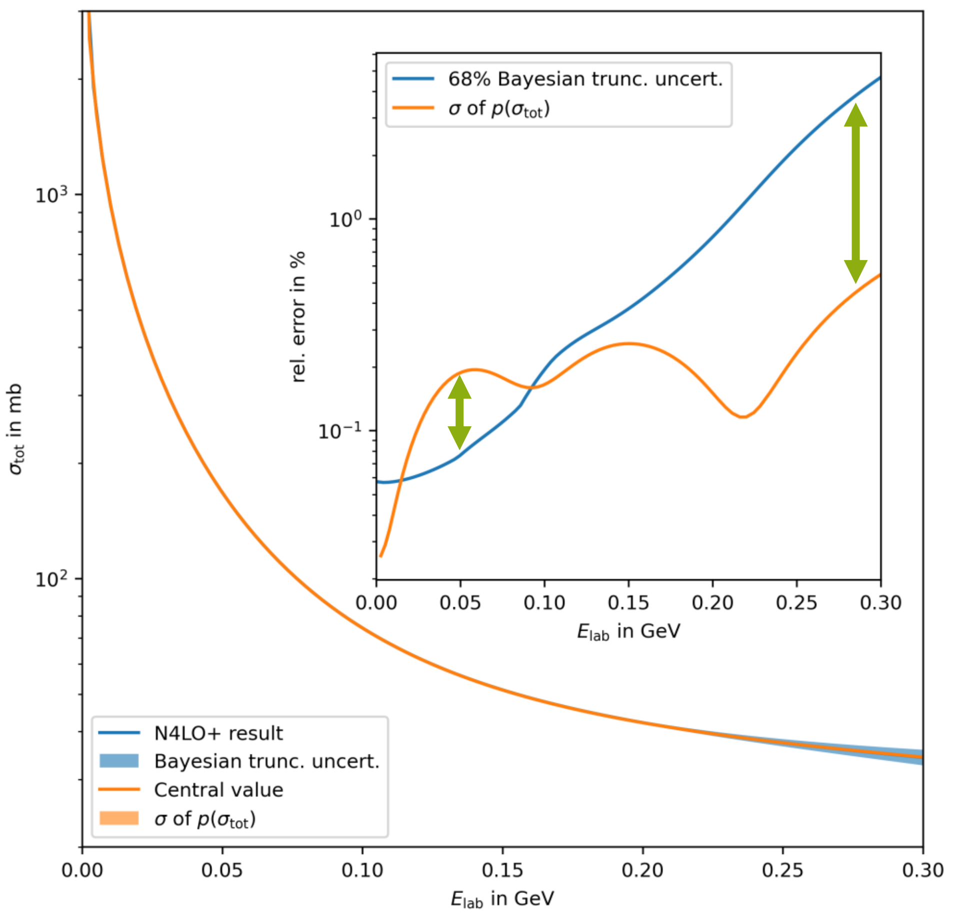


$$p\left(\sigma_{\text{tot}}^{(N4LO+)}\right)$$



$$p\left(\sigma_{\text{tot}}^{(N4LO+)}\right)$$

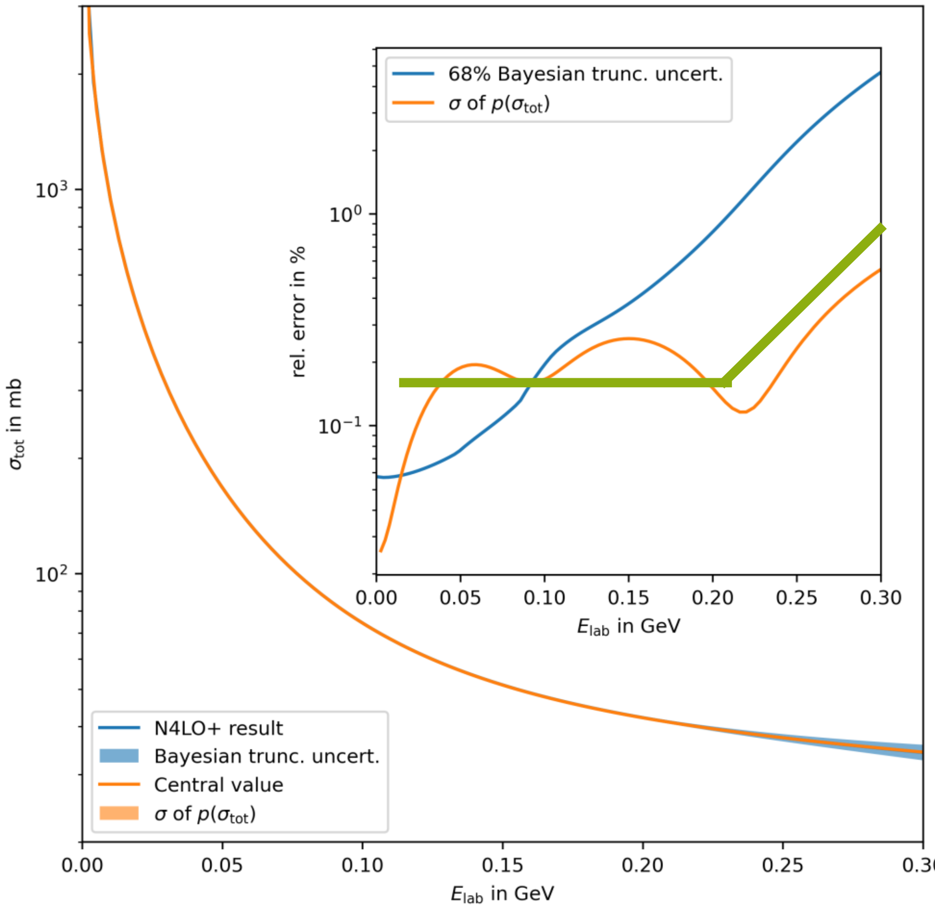
- Bayesian model underestimates for low-energy regime and overestimates for high-energy regime compared to uncertainty here



$$p\left(\sigma_{\text{tot}}^{(N4LO+)}\right)$$

- Bayesian model underestimates for low-energy regime and overestimates for high-energy regime

- Double expansion in momentum and pion mass
  → Two energy regimes



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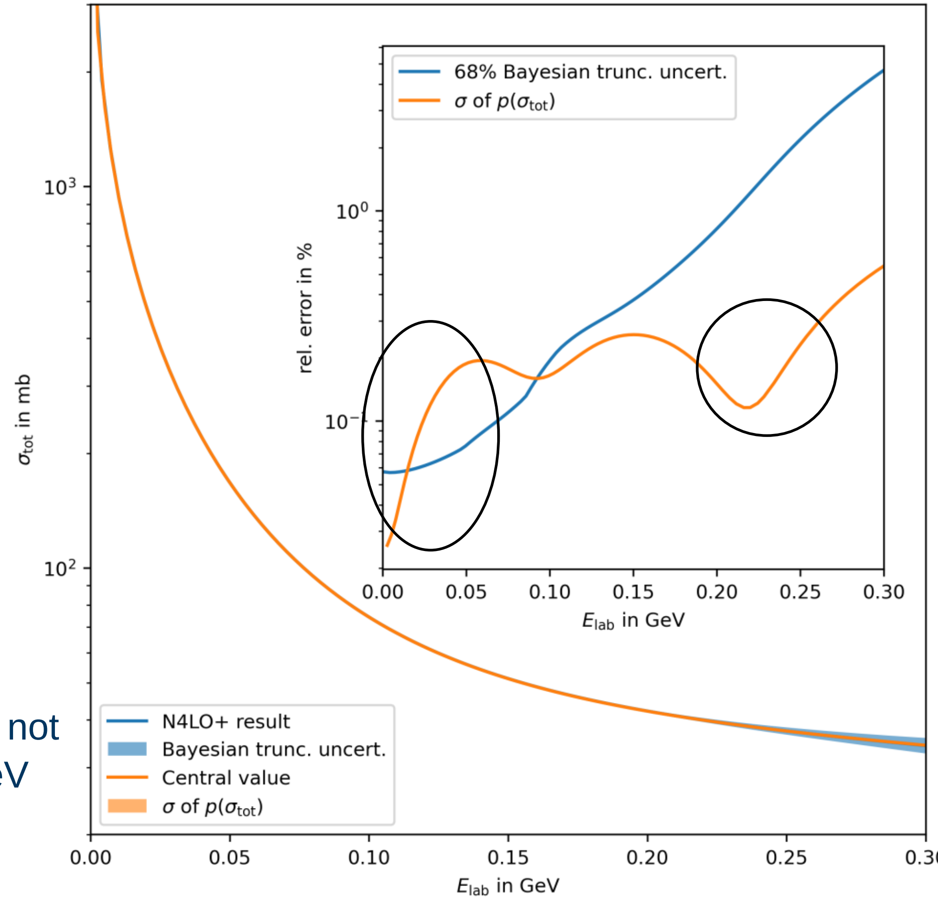
- Why the dips?
  - Number of experiments and their precision ist not equally distributed between 0MeV and 280MeV



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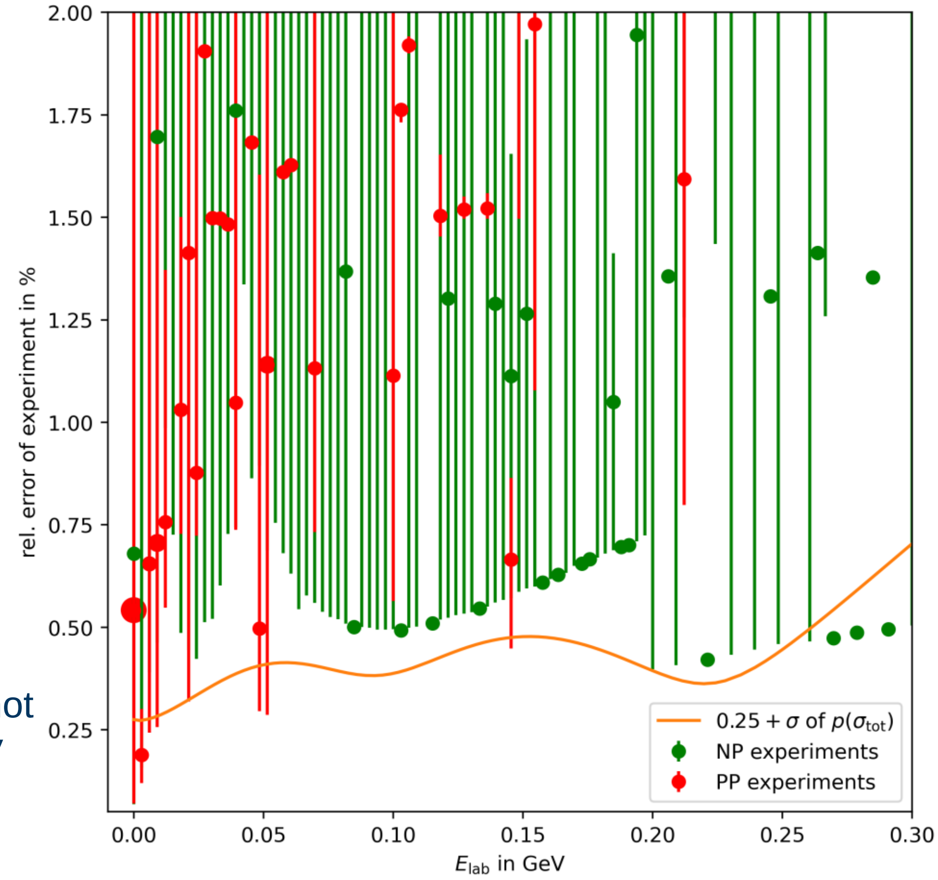


$p(X^{(k)})$ is actually not only truncation uncertainty

Theory

- Uncertainty of next-higher order contact forces

Data

- Stat. and sys. uncertainties
- Distribution of data among observables and energy ranges

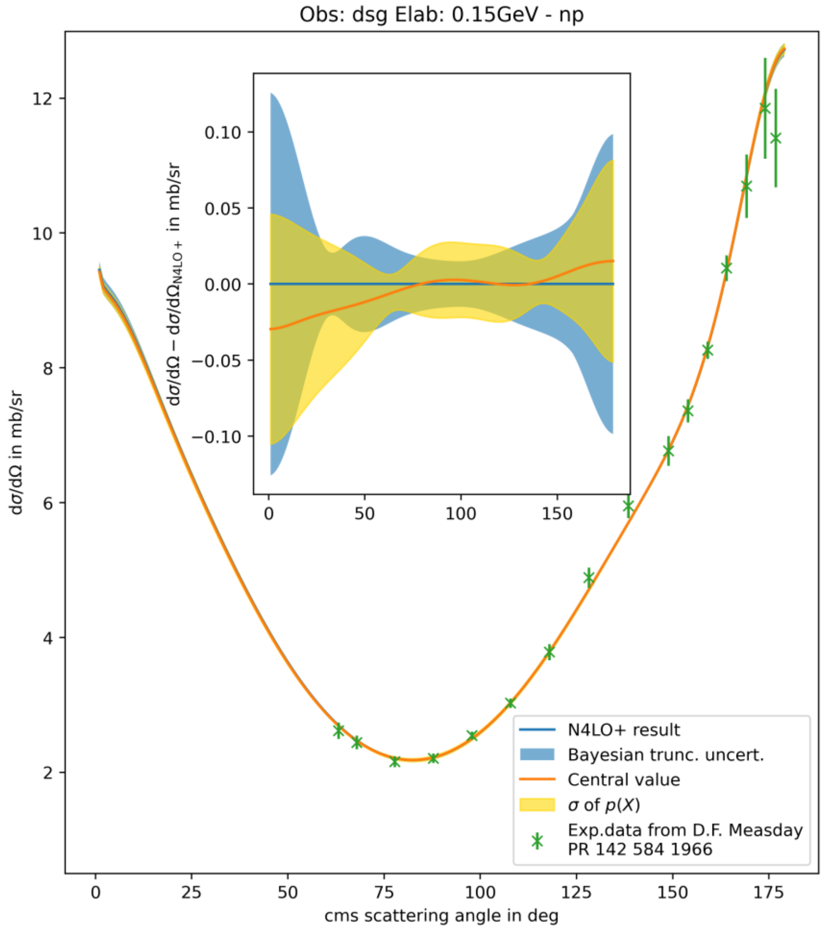
Beliefs

- Natural LECs
- No inclusion of theory‘s precision predicition in fit
- Fit protocol
- …

$$p(X^{(k)} \mid \ldots)$$

Differential cross-section

- What about angle-dependent observables?
- Bayesian model and our model agree
- No sign of another angle-dependent expansion parameter?
  - Other Mandelstam parameters do not play any role?



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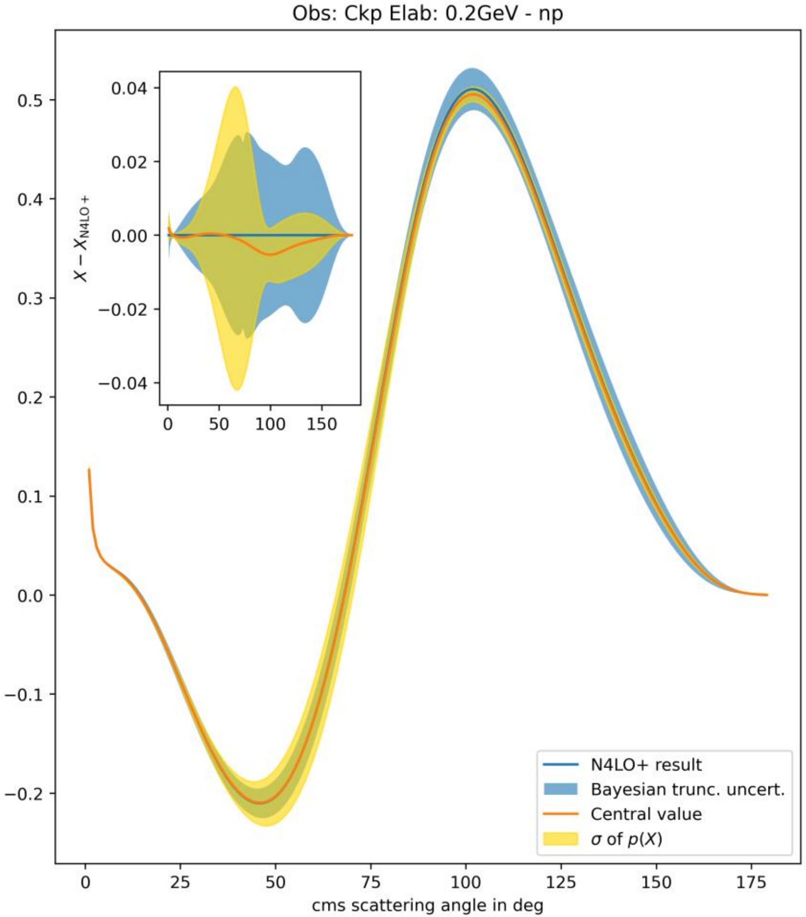
Ckp at $E_{\text{lab}} = 200\text{MeV}$

- What is our total knowledge about a certain observable?
  - → Calculate observable with well working theory
  - → Add Truncation uncertainty with experimental uncertainty

- Different angular dependence of uncertainty
  - Angular dependent expansion?
  - Impact of precisely measured experimental data?



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Conclusion

- We have obtained the **combined uncertainty** of our chiral EFT model
  - Including truncation uncertainty of contact forces, as well as uncertainty from the data
  - Using our prior beliefs

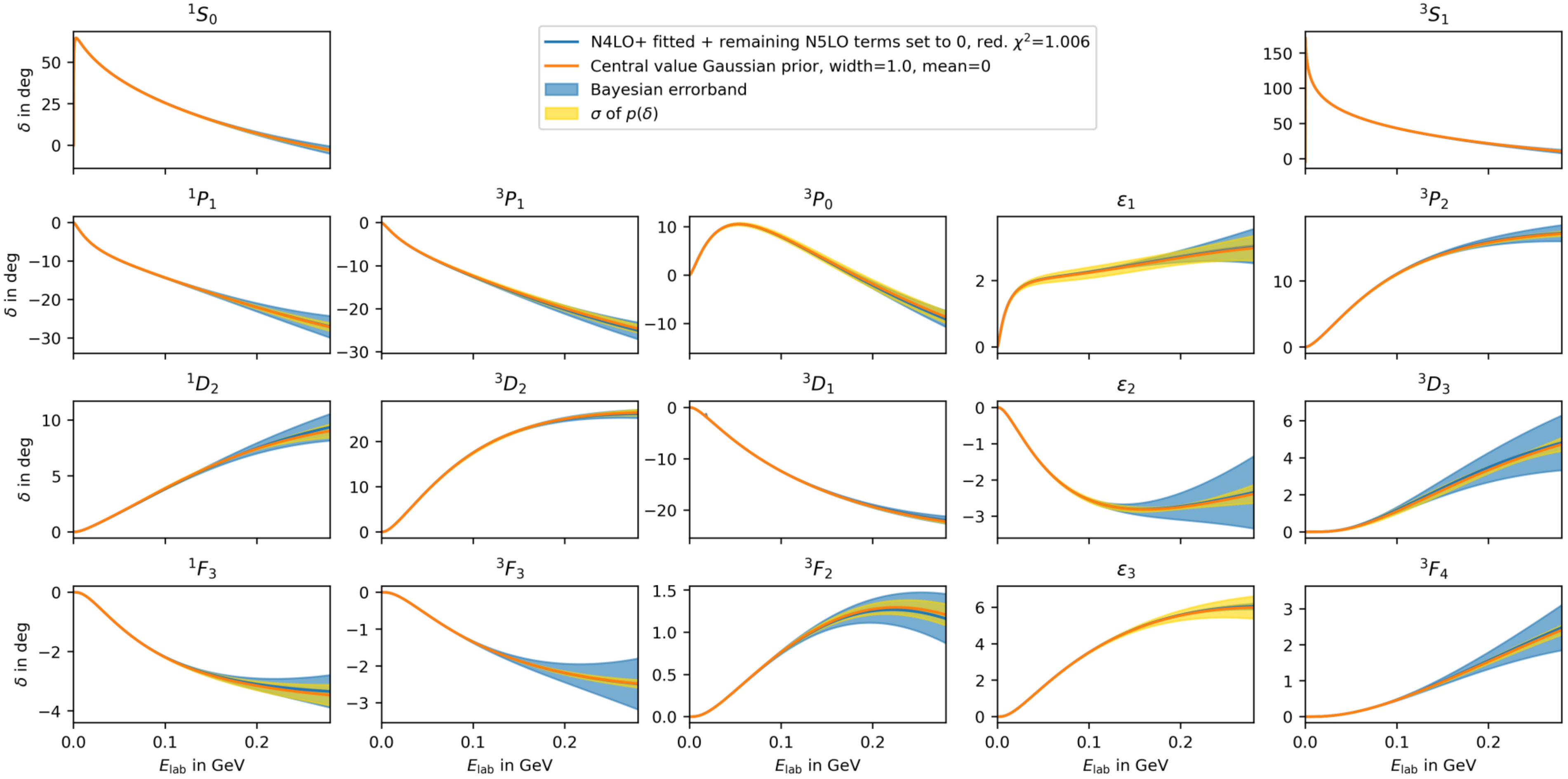
Conclusion and Outlook

- We have obtained the **combined uncertainty** of our chiral EFT model
  - Including truncation uncertainty of contact forces, as well as uncertainty from the data
  - Using our prior beliefs
- Investigate different chiral orders, different cutoffs
- So far, pion-exchange is used in calculation, but its truncation uncertainty is not yet estimated
- How to **disentangle statistical and truncation** uncertainty?
- How to propagate these uncertainties towards **few- and many-body** calculations?

Back up slides

More results, more preliminary!

Back up slides
Phaseshifts



N4LO+ fitted + remaining N5LO terms set to 0, red. χ^2=1.006
Central value Gaussian prior, width=1.0, mean=0
Bayesian errorband
σ of $p(\delta)$
$^1S_0$
$^3S_1$
$^1P_1$
$^3P_1$
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ε_1
$^3P_2$
$^1D_2$
$^3D_2$
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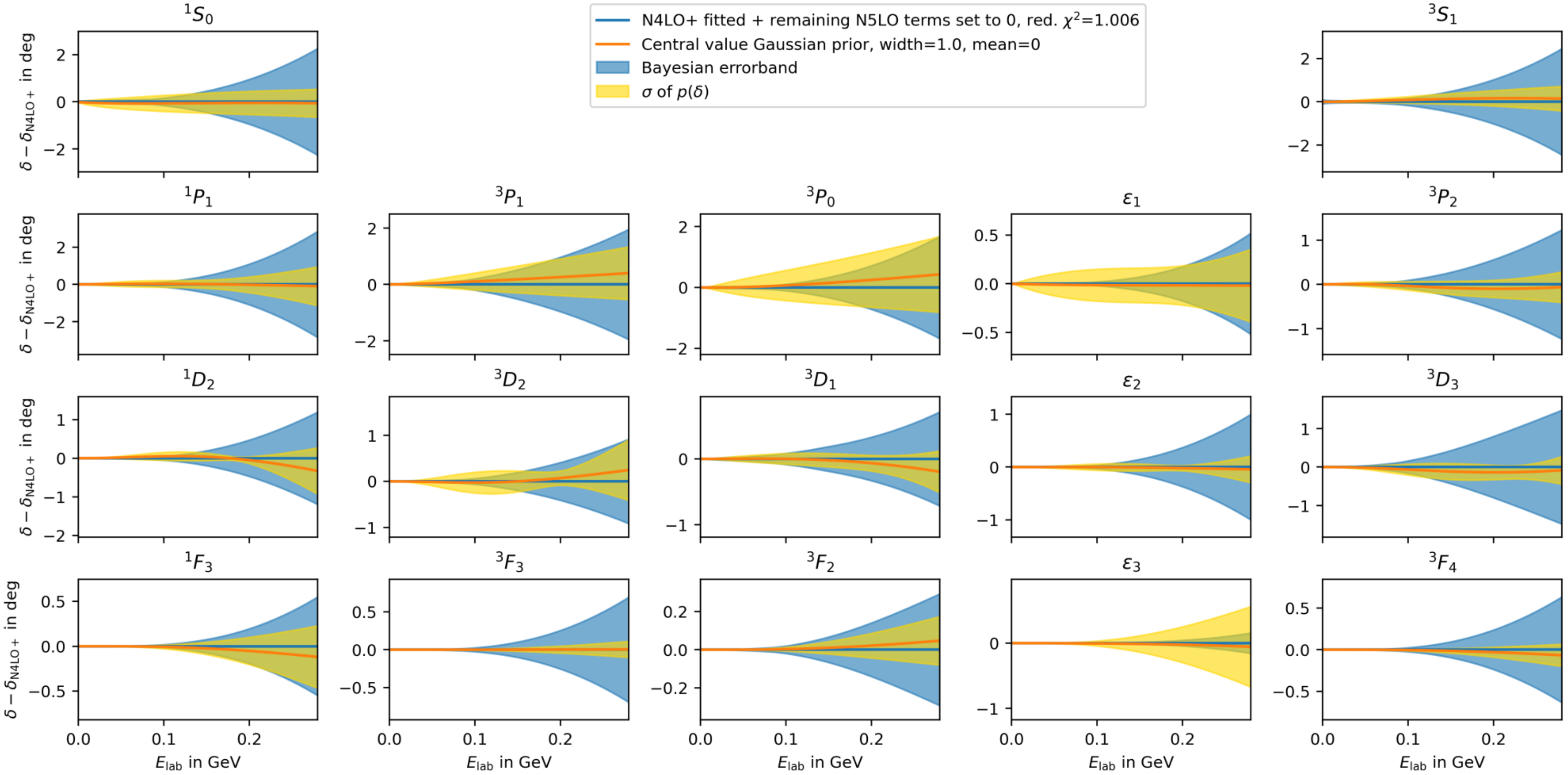
ε_2
$^3D_3$
$^1F_3$
$^3F_3$
$^3F_2$
ε_3
$^3F_4$
δ in deg
$E_{\rm lab}$ in GeV



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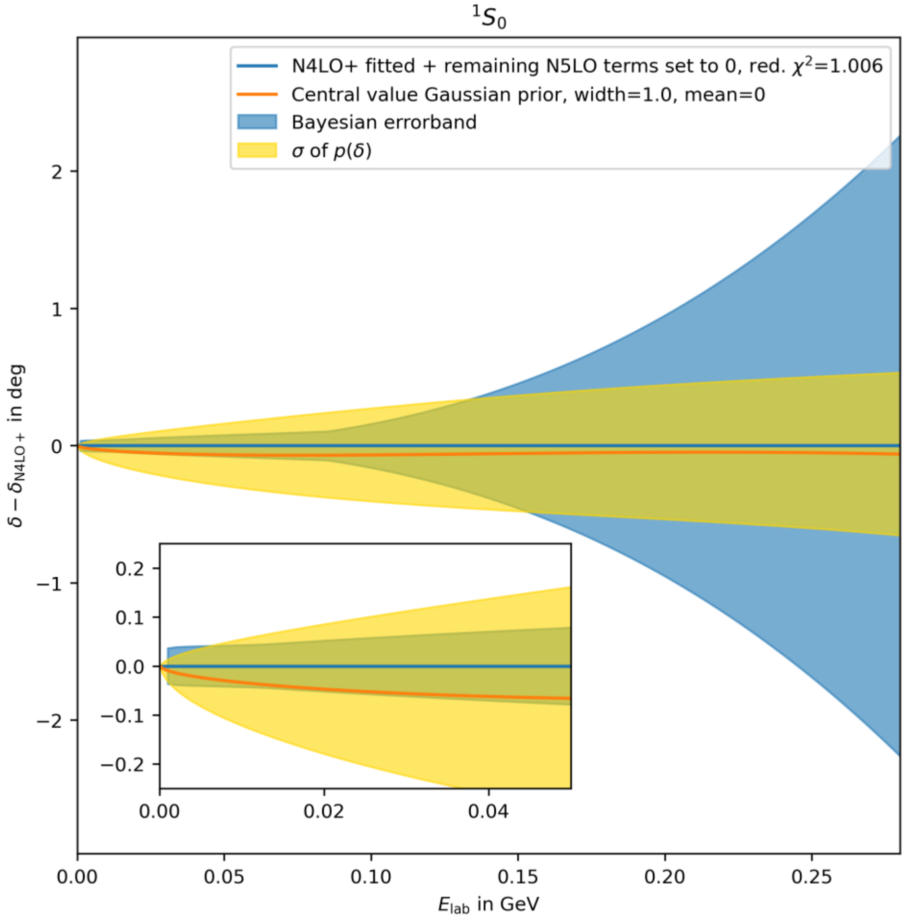
ε_2
$^3D_3$
$^1F_3$
$^3F_3$
$^3F_2$
ε_3
$^3F_4$
$\delta - \delta_{N4LO+}$ in deg
E_{lab} in GeV

1S0

- Larger uncertainty for lower energies
- Smaller uncertainty for higher energies

Compared to Bayesian estimation

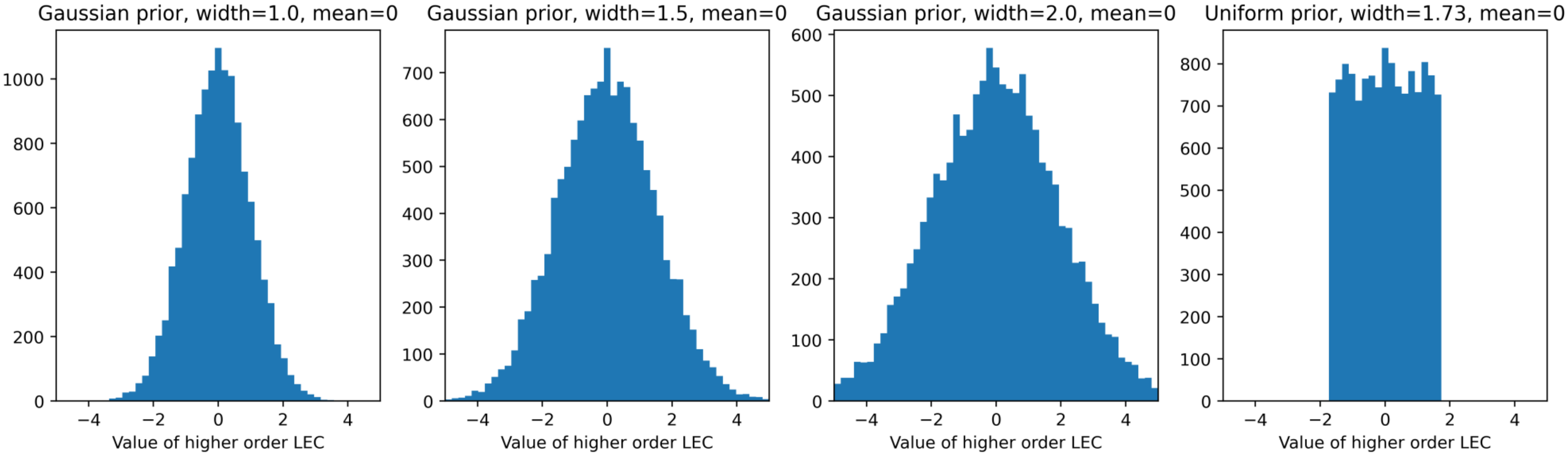


Back up slides

Using different distribution for higher-order LECs

Histograms for higher-order LECs

- Investigated 4 different distribution for higher-order LECs in total
- For each distribution 1000 fits have been conducted



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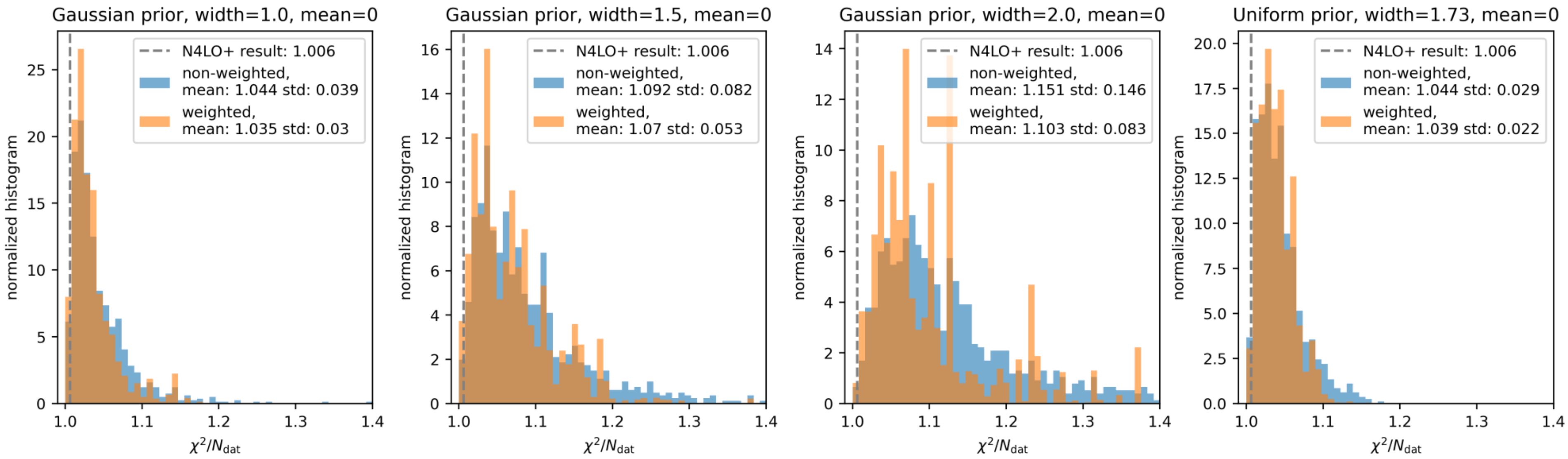
Histograms for reduced chisq

- Entem-Machleidt-Nosyk N4LO+ best $\chi^2/N_{\rm dat}$ (0-300MeV): ~ 1.2 E. Epelbaum et al., Handbook of Nuclear Physics 2022
- Fits without 2π exchange ~ 1.9 (deviates ~45σ from 1!)
- Successful PWA ($\chi^2/N_{\rm dat}$ ~ 1) and model uncertainty are two different things!



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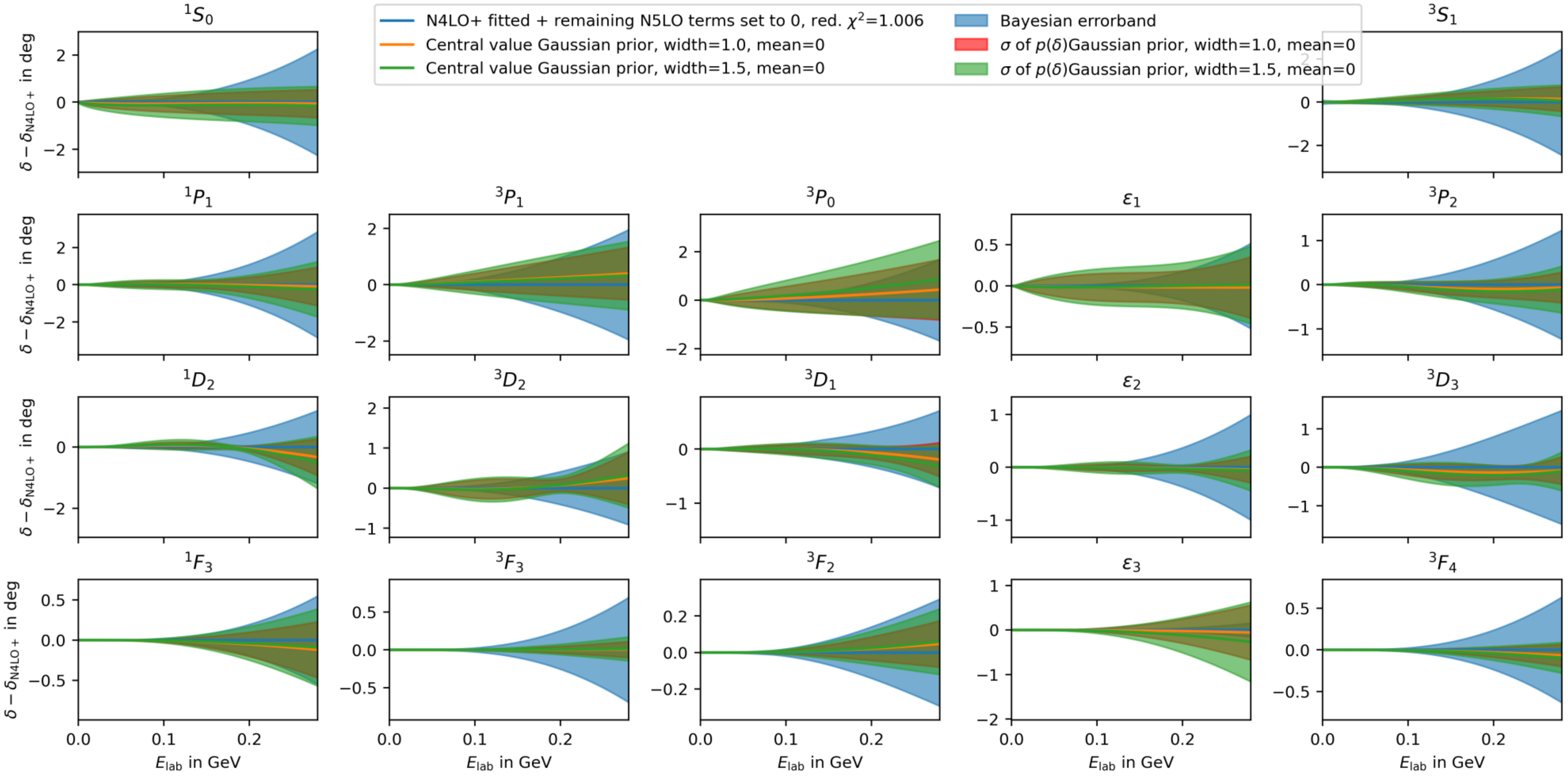
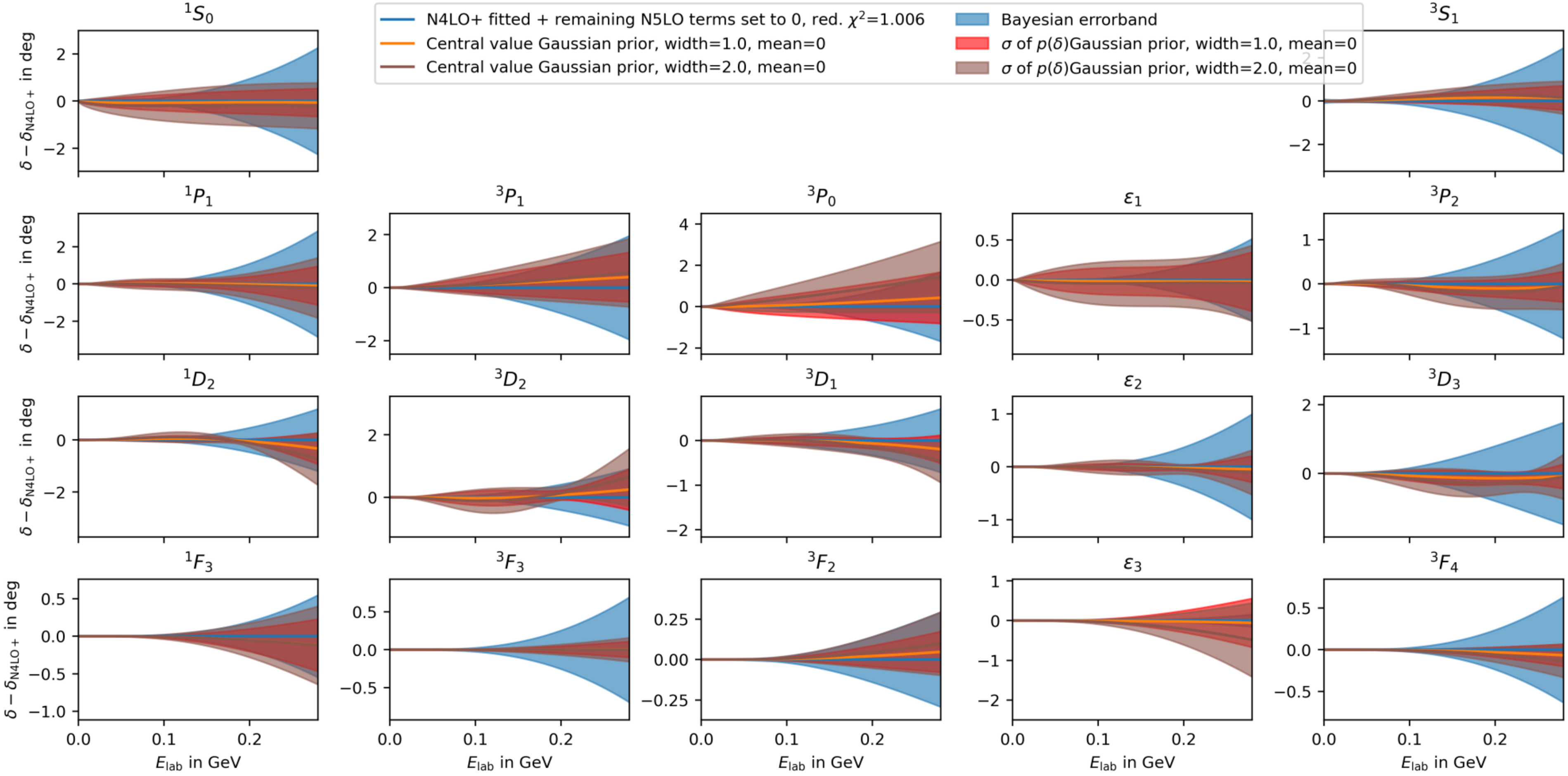

N4LO+ fitted + remaining N5LO terms set to 0, red. χ²=1.006
Central value Gaussian prior, width=1.0, mean=0
Central value Gaussian prior, width=1.5, mean=0
Bayesian errorband
σ of p(δ)Gaussian prior, width=1.0, mean=0
σ of p(δ)Gaussian prior, width=1.5, mean=0
¹S₀
³S₁
¹P₁
³P₁
³P₀
ε₁
³P₂
¹D₂
³D₂
³D₁
ε₂
³D₃
¹F₃
³F₃
³F₂
ε₃
³F₄
δ − δN4LO+ in deg
E_lab in GeV



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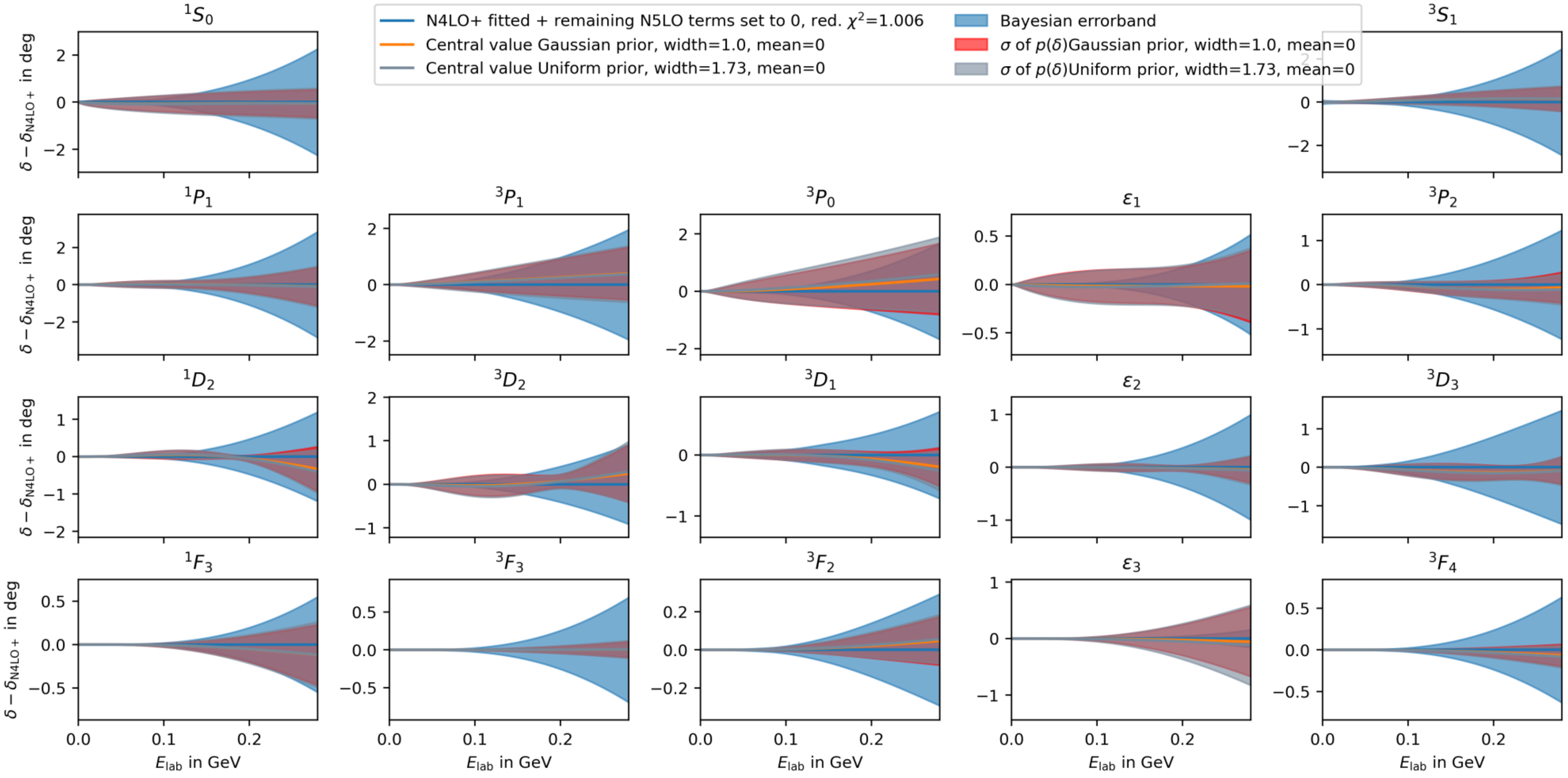

N4LO+ fitted + remaining N5LO terms set to 0, red. χ^2=1.006
Central value Gaussian prior, width=1.0, mean=0
Central value Uniform prior, width=1.73, mean=0
Bayesian errorband
σ of $p(\delta)$Gaussian prior, width=1.0, mean=0
σ of $p(\delta)$Uniform prior, width=1.73, mean=0
$^1S_0$
$^3S_1$
$^1P_1$
$^3P_1$
$^3P_0$
ε_1
$^3P_2$
$^1D_2$
$^3D_2$
$^3D_1$
ε_2
$^3D_3$
$^1F_3$
$^3F_3$
$^3F_2$
ε_3
$^3F_4$
$\delta - \delta_{\mathrm{N4LO+}}$ in deg
E_{lab} in GeV

Back up slides
Naturalness of LECs

Our general approach

- Using power counting, nuclear forces from chiral Lagrangian at some fixed chiral order are derived

- Forces are regulated, with cutoff regulator as function of external nuclear momenta and cutoff Λ
  - Regulator must leave all symmetries intact
  - Infinite number of UV-divergences, if $\Lambda \to \infty$, from iterated potential, but at finite chiral order not enough counter terms available → finite cutoff!
  - Demanding no deeply bound states

  → $\Lambda \sim \Lambda_B$ and Weinberg power counting → LECs ~ 1

- Fitting the bare(!) coefficients of the short-range operators (LECs), leaving the cutoff finite

  → Implicit renormalization of LECs (Renormalized LECs are actually unknown for pionful theory)

Epelbaum et al., Front. in Phys. 8, 98 (2020), arXiv:1911.11875

What are natural values?

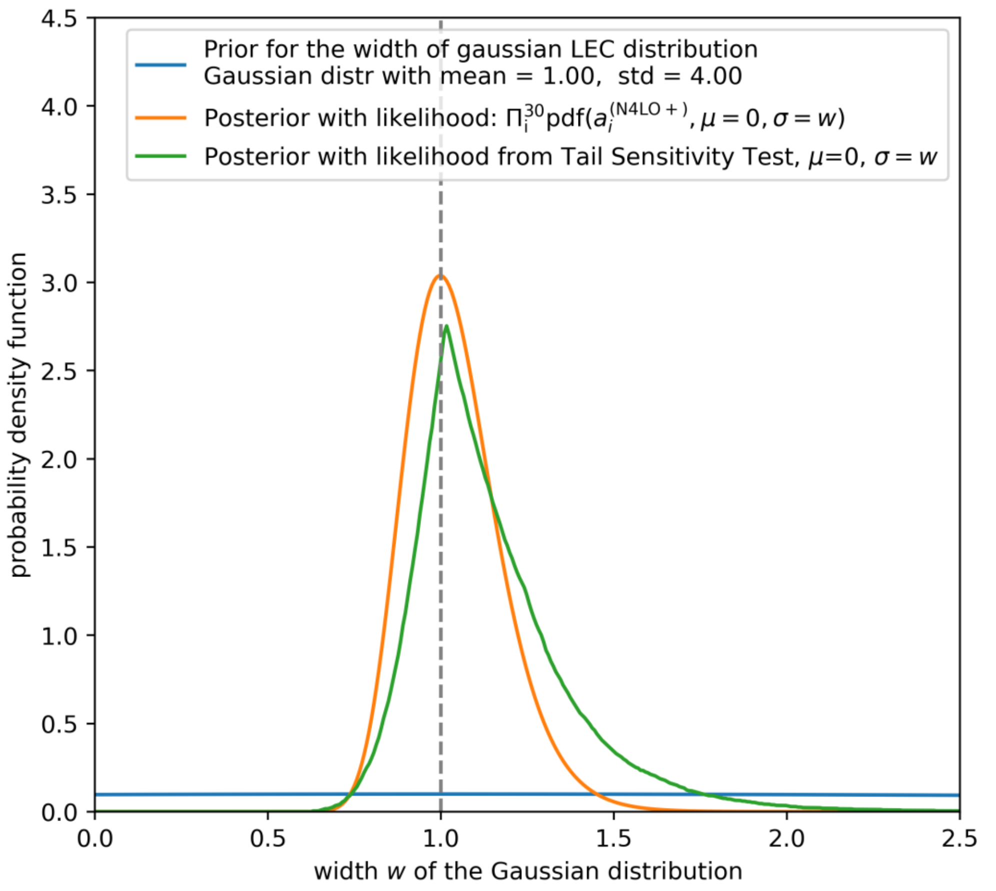
- $p(w \mid \vec{a}^{\,(i\,\epsilon\,[0,k])}) \propto p\left(\vec{a}^{\,(i\,\epsilon\,[0,k])} \mid w\right) \cdot p(w)$

- What is $p\left(\vec{a}^{\,(i\,\epsilon\,[0,k])} \mid w\right)$?

  - Product of probabilities of every element of $\vec{a}^{\,(i\,\epsilon\,[0,k])}$, that it comes from $\mathrm{N}(0, \mathrm{w})$?

  - Probability, that this set of LECs is drawn from $\mathrm{N}(0, \mathrm{w})$? Tail-sensitive test S. Aldor-Noiman et al., Am. Stat. 67, 249 (2013)

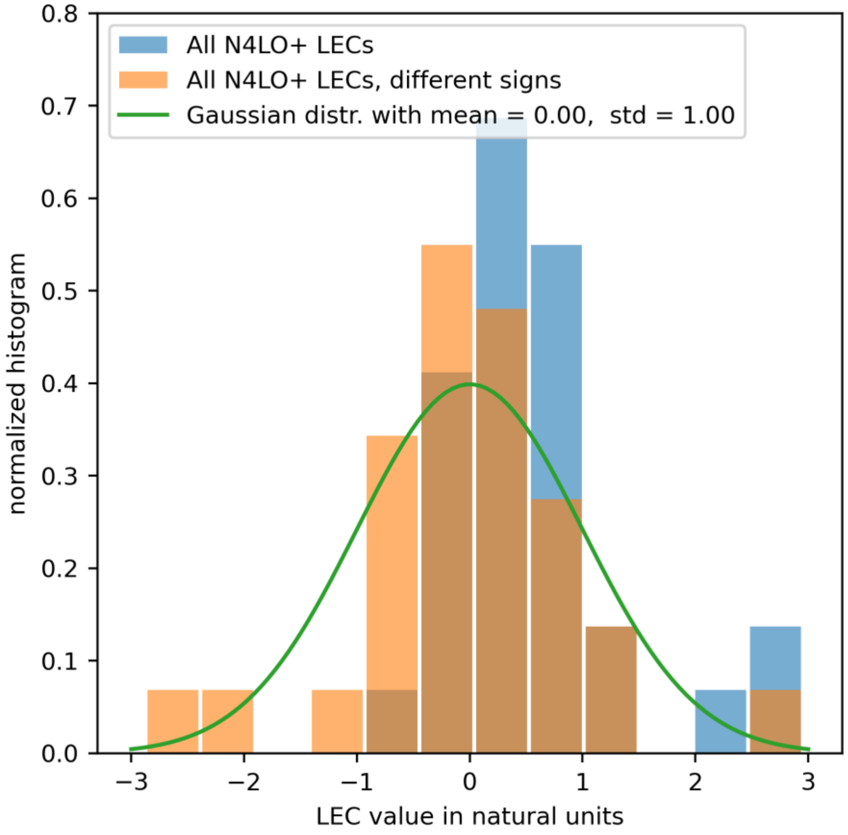
→ If assumptions are fulfilled, the LECs are indeed drawn from a distribution with $w \sim 1$



Histogram of LECs

- "Sign problem" of LECs in Chiral EFT
  - Sign of contact forces is just convention
  - → Signs of LECs can be changed without any effects for theory or observables

- What are "natural units" of LECs?
  - LECs of order Q^{2n} are given in units of $10^4 \mathrm{GeV}^{-2-2n}$



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