UNCERTAINTY QUANTIFICATION AND CHIRAL DYNAMICS

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for the BUQEYE collaboration
(Bayesian Uncertainty Quantification: Errors for Your EFT)

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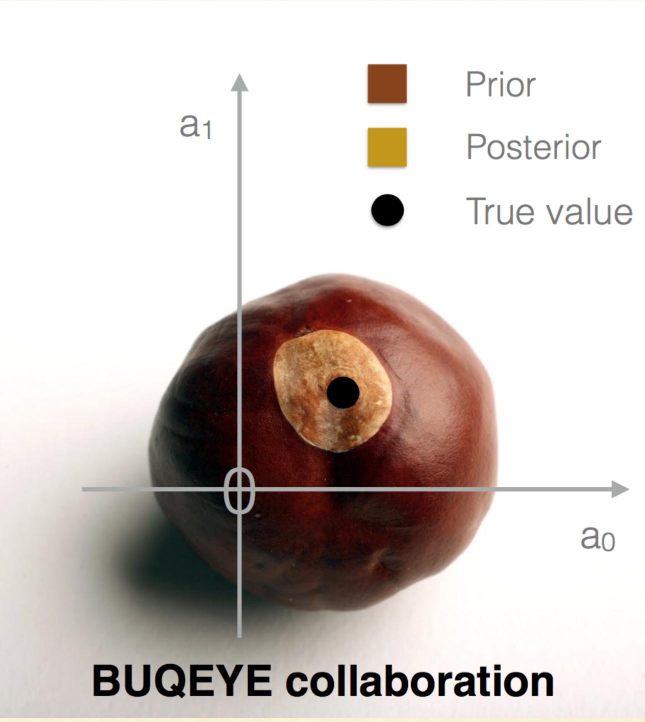

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UNCERTAINTY QUANTIFICATION

Physical Review A Editorial, 29 April 2011

The purpose of this Editorial is to discuss the importance of including uncertainty estimates in papers involving theoretical calculations of physical quantities.

It is not unusual for manuscripts on theoretical work to be submitted without uncertainty estimates for numerical results. In contrast, papers presenting the results of laboratory measurements would usually not be considered acceptable for publication in *Physical Review A* without a detailed discussion of the uncertainties involved in the measurements….

The question is to what extent can the same high standards be applied to papers reporting the results of theoretical calculations…..There are many cases where it is indeed not practical to give a meaningful error estimate for a theoretical calculation….However, there is a broad class of papers where estimates of theoretical uncertainties can and should be made.

Papers presenting the results of theoretical calculations are expected to include uncertainty estimates for the calculations whenever practicable, and especially under the following circumstances:

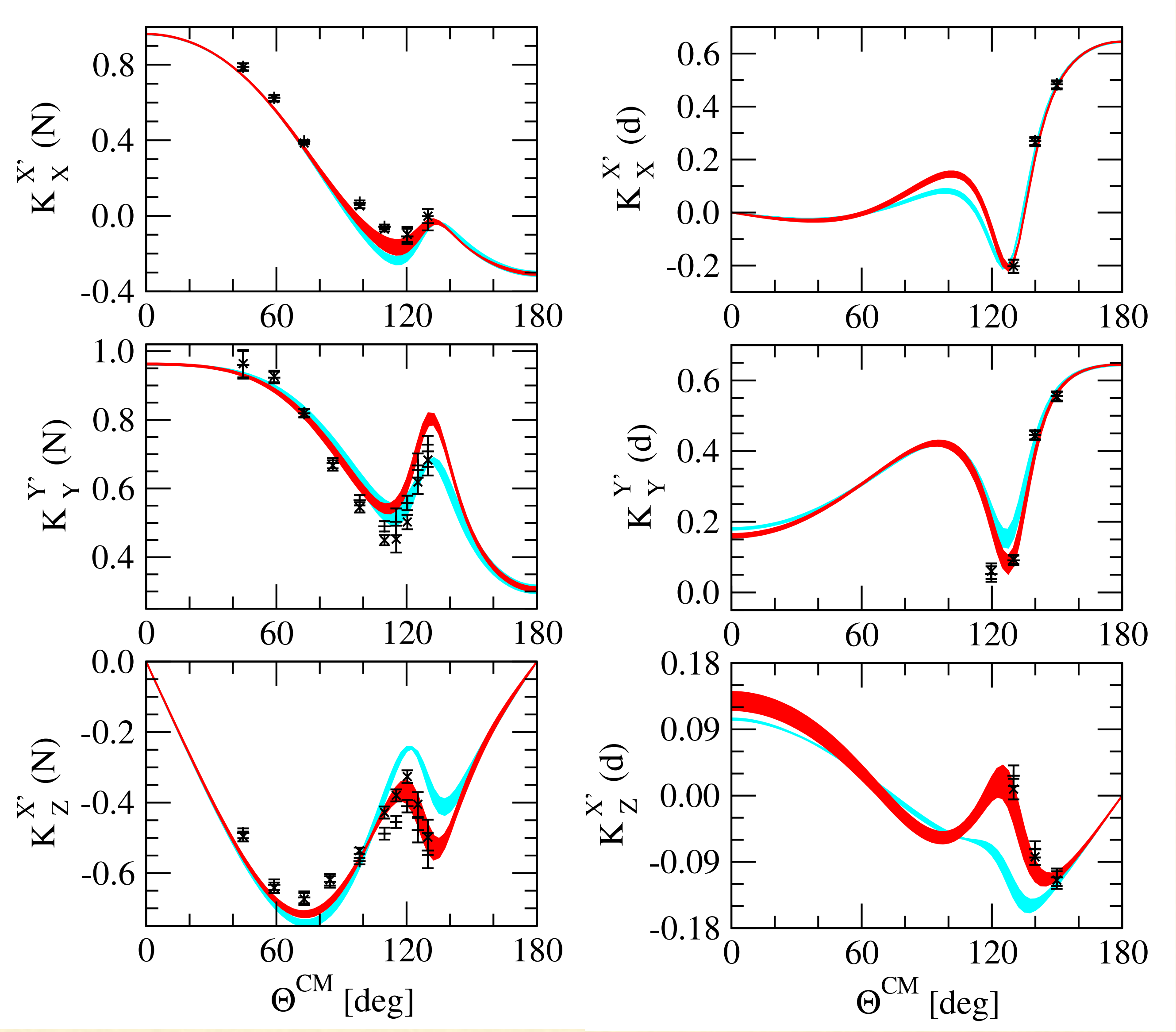
1. If the authors claim high accuracy, or improvements on the accuracy of previous work.
2. If the primary motivation for the paper is to make comparisons with present or future high precision experimental measurements.
3. If the primary motivation is to provide interpolations or extrapolations of known experimental measurements.

- Realizing full promise of χEFT requires quantification of theory uncertainties.
- These arise from: truncation of H at finite order in EFT expansion, computational/many-body technique, input parameters in H.
- Multiple sources of theory uncertainty that are connected in complicated ways.
- Goal: ability to propagate uncertainties to predictions.

UNCERTAINTY QUANTIFICATION IN χEFT

Chiral EFT predictions for p-d spin observables with theory errors from cutoff variation

Epelbaum, Hammer, Meissner, RMP, 2009



This talk: truncation errors

Standard technique in few-nucleon χEFT calculations had been to vary cutoff in reasonable range.

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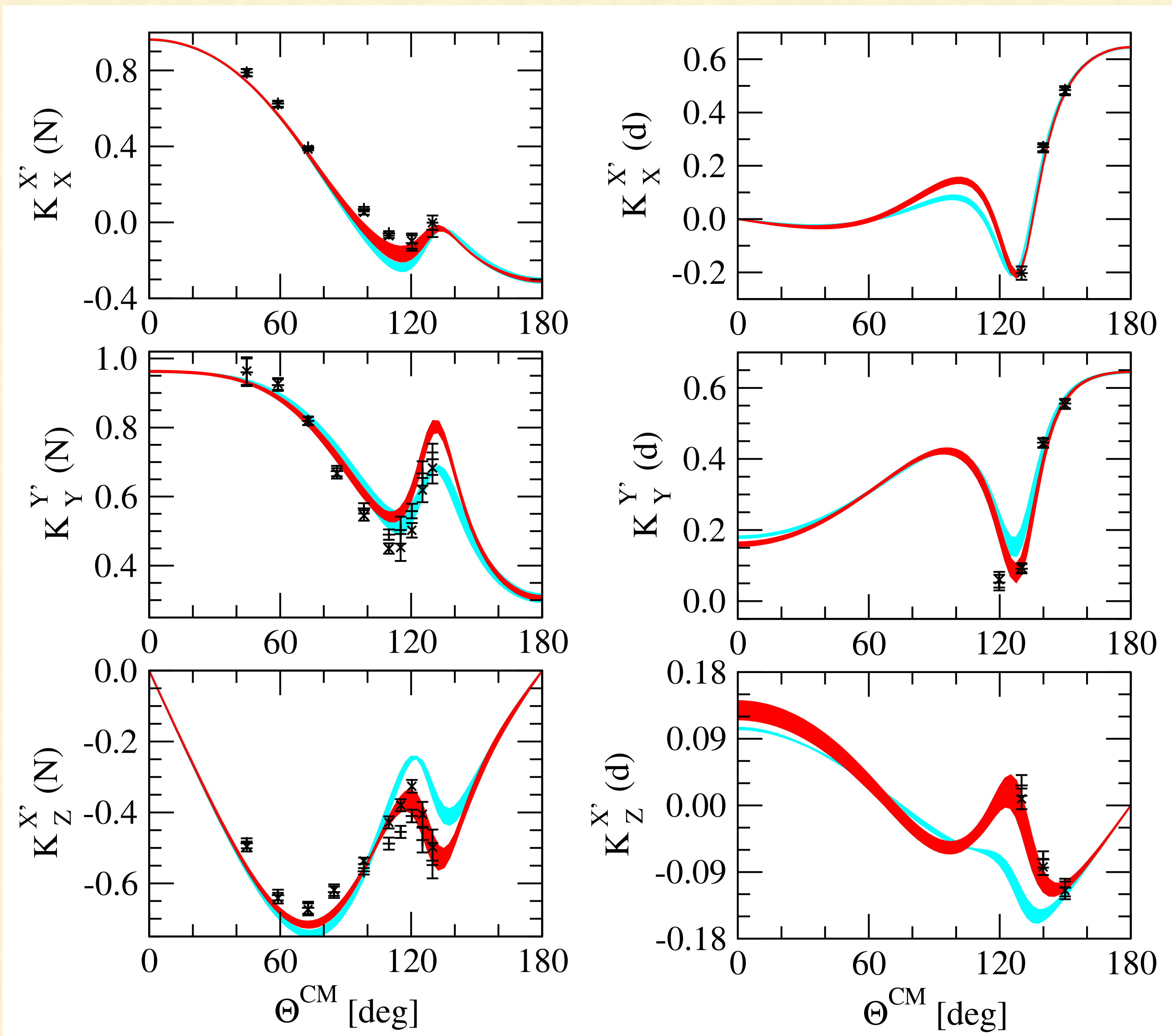

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PROBLEMS WITH CUTOFF VARIATION

- Size of error depends on how smart you are choosing regulator function;
- Depends on range of cutoffs chosen;
- Error does not necessarily decrease order-by-order;
- Only captures errors from even orders in the EFT;
- Statistical interpretation is not clear.

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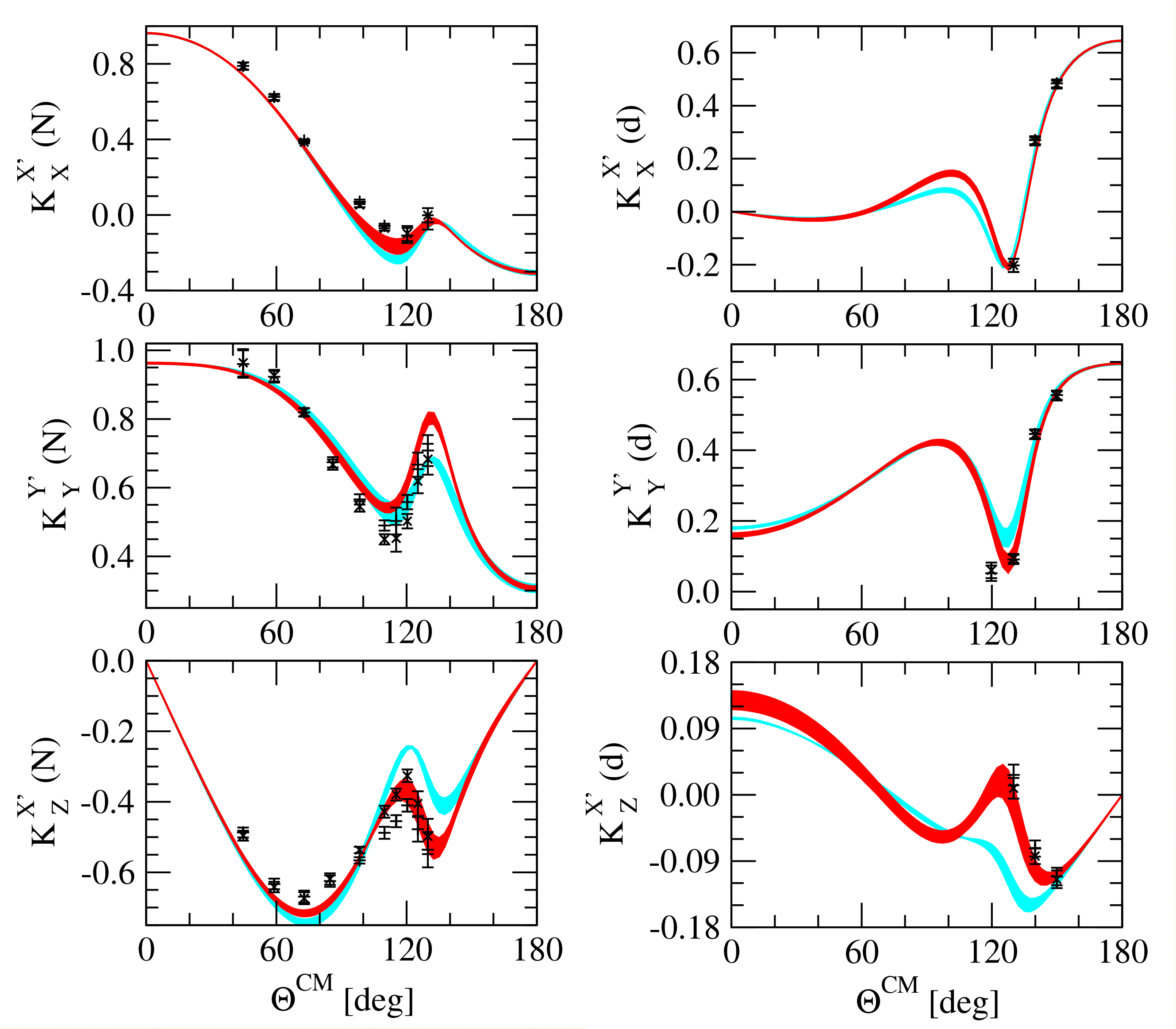

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Cutoff variation is a regulator artefact which may or may not reflect full size of theory uncertainty

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- One possibility: $c_3=\max\{c_0,c_1,c_2\}$.

Epelbaum, Krebs, Meissner (2014)
cf. McGovern, Griesshammer, Phillips (2013); many others.

PROBABILITY FOR EFT COEFFICIENTS

Furnstahl, Klco, Phillips, Wesolowski, arXiv:1506.03143

after Cacciari and Houdeau, JHEP, 2011

- General EFT series to order k: $X = X_0 \sum_{n=0}^{k} c_n Q^n$
- Compute conditional probability distribution: pr(c_{k+1}|c_0,…,c_k,I).
- I=information about χEFT, e.g. naturalness.
- "Prior A": $\mathrm{pr}(c_n|\bar{c}) = \frac{1}{2\bar{c}}\theta(\bar{c} - c_n);\ \mathrm{pr}(\bar{c}) = \frac{1}{2\ln(\epsilon)\bar{c}}\theta\left(\frac{1}{\epsilon} - \bar{c}\right)\theta(\bar{c} - \epsilon)$
- Uniformly distributed coefficients up to maximum, maximum distributed uniformly in its logarithm. ϵ→0+ at end.
- Prior expectations will guide result, but they are not be all and end all.
- Maximum of coefficients informed by known coefficients.

BAYES → RESULT

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- Bayes' theorem: $\mathrm{pr}(\bar{c}|c_0, c_1, \ldots, c_k) = \dfrac{\mathrm{pr}(c_0, c_1, \ldots, c_k|\bar{c})\mathrm{pr}(\bar{c})}{\mathrm{pr}(c_0, c_1, \ldots, c_k)}$

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- Marginalization:

$$\mathrm{pr}(c_{k+1}|c_0, c_1, \ldots, c_k) = \int_0^\infty d\bar{c}\,\mathrm{pr}(c_{k+1}|\bar{c})\mathrm{pr}(\bar{c}|c_0, c_1, \ldots c_k)$$

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- This is generic, but the integrals are simple in the case of "Prior A"

$$\mathrm{pr}(\bar{c}|c_0, c_1, \ldots, c_k) \propto \begin{cases} 0 & \text{if } \bar{c} < \max\{c_0, \ldots, c_k\} \\ 1/\bar{c}^{k+2} & \text{if } \bar{c} > \max\{c_0, \ldots, c_k\} \end{cases}$$

$$\mathrm{pr}(c_{k+1}|c_0, c_1, \ldots, c_k) \propto \begin{cases} 1 & \text{if } c_{k+1} < c_{\max} \\ \left(\frac{c_{\max}}{c_{k+1}}\right)^{k+2} & \text{if } c_{k+1} > c_{\max} \end{cases}$$

THE CANONICAL PROCEDURE

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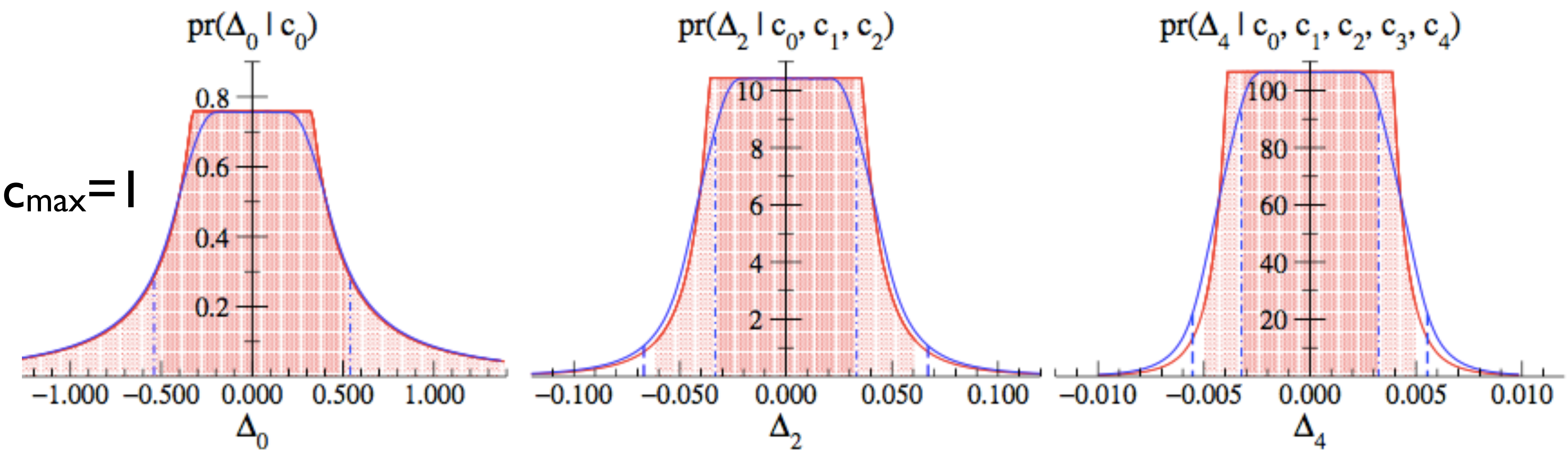
- pr (Δ_k) α X_0 Q^{k+1} $pr(c_{k+1})$
- 68%, 95% DOB intervals from integration of probability distribution

Q=0.33; c_{max}=1



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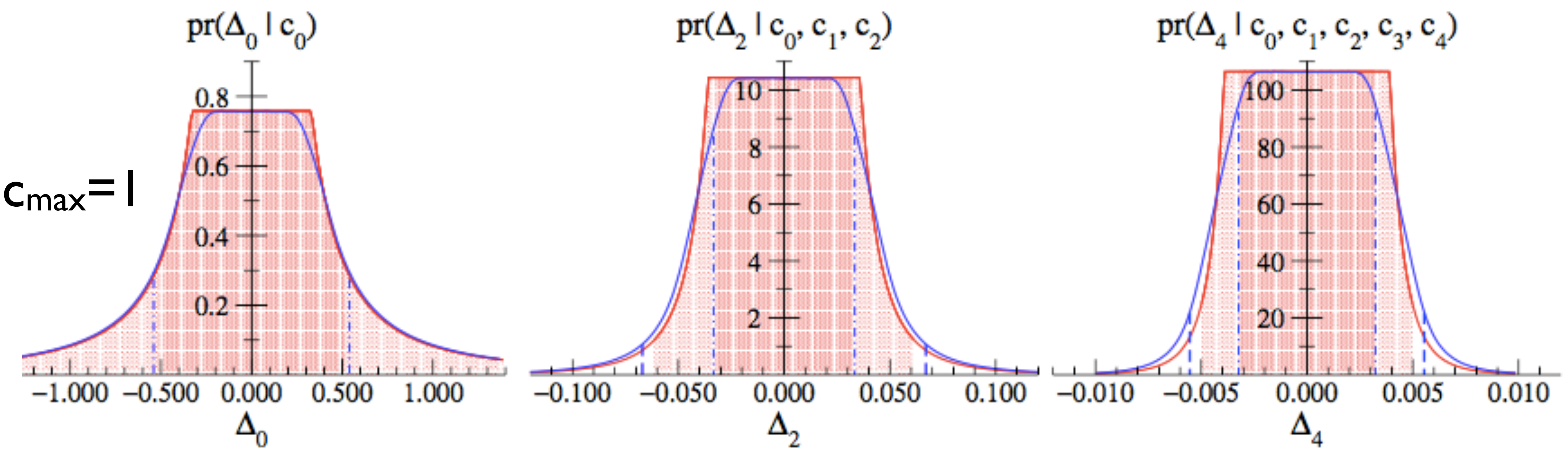

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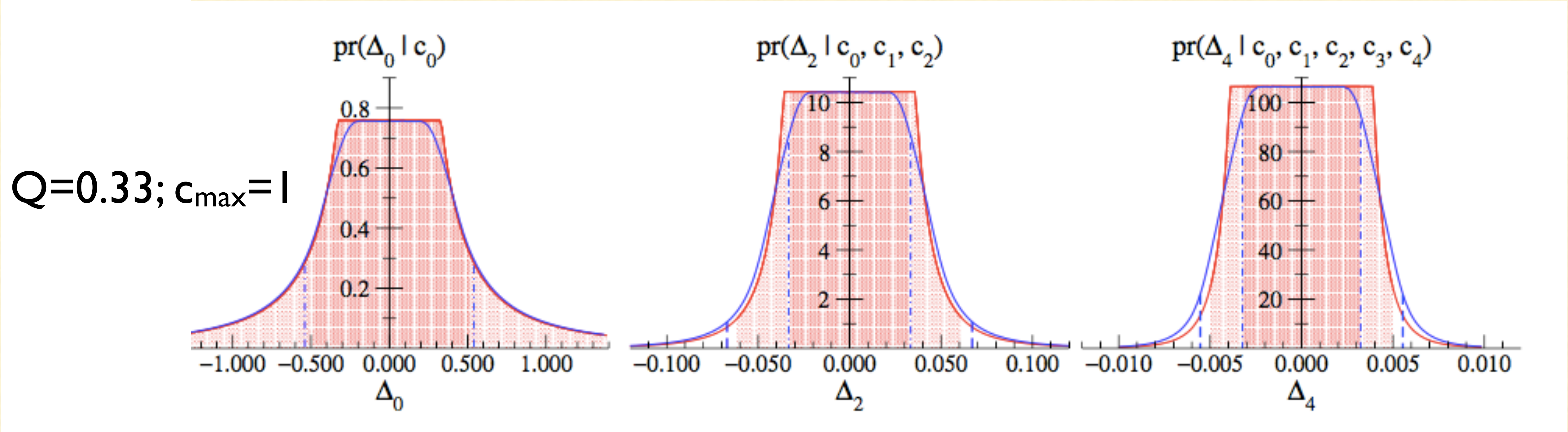


- Main feature is reduction by factor of Q for each order; but tails also become steeper as more information on coefficients acquired
- Not Gaussian!
- [-c_{max} X_0 Q^{k+1},c_{max} X_0 Q^{k+1}] is a $\frac{k+1}{k+2} * 100\%$ DOB interval

I DON'T LIKE THAT PRIOR!

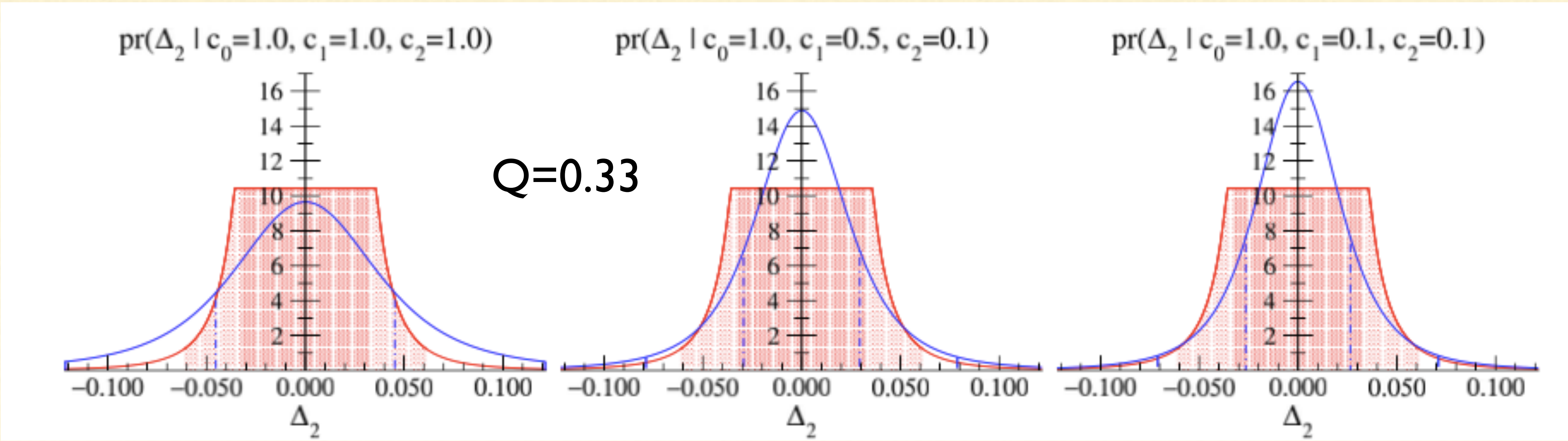
- Modify Set A to restrict cbar to a finite range, e.g. $A_{[0.25,4]}$
- Set B: give cbar a log-normal prior: $\mathrm{pr}(\bar{c}) = \frac{1}{\sqrt{2\pi}\bar{c}\sigma} e^{-(\log \bar{c})^2/2\sigma^2}$
- Set C: $\mathrm{pr}(c_n|\bar{c}) = \frac{1}{\sqrt{2\pi}\bar{c}} e^{-c_n^2/2\bar{c}^2}$; $\mathrm{pr}(\bar{c}) \propto \frac{1}{\bar{c}} \theta(\bar{c} - \bar{c}_<)\theta(\bar{c}_> - \bar{c})$
- Same formulas as before can be invoked. Now numerical.

$$\mathrm{pr}(c_{k+1}|c_0, c_1, \ldots, c_k) = \int_0^\infty d\bar{c}\, \mathrm{pr}(c_{k+1}|\bar{c})\mathrm{pr}(\bar{c}|c_0, c_1, \ldots c_k)$$

$$\mathrm{pr}(\bar{c}|c_0, c_1, \ldots, c_k) = \mathcal{N} \mathrm{pr}(\bar{c}) \Pi_{n=0}^k \mathrm{pr}(c_n|\bar{c})$$

- You don't like these? Pick your own and follow the rules…
- First omitted term approximation

REPRESENTATIVE EXAMPLES



- Set C differs from Set A in that entire distribution of $\{c_n\}$ matters.
- Set A_ϵ and Set C_ϵ DOB intervals closest for most uniform $\{c_n\}$.
- Choice of prior matters less and less at higher orders. At and beyond k=2 different choice of priors affect 68% DOB interval by at most 10-15%.
- Updating refines knowledge of coefficients: Bayesian convergence.
- Bigger effect on 95% DOB interval.

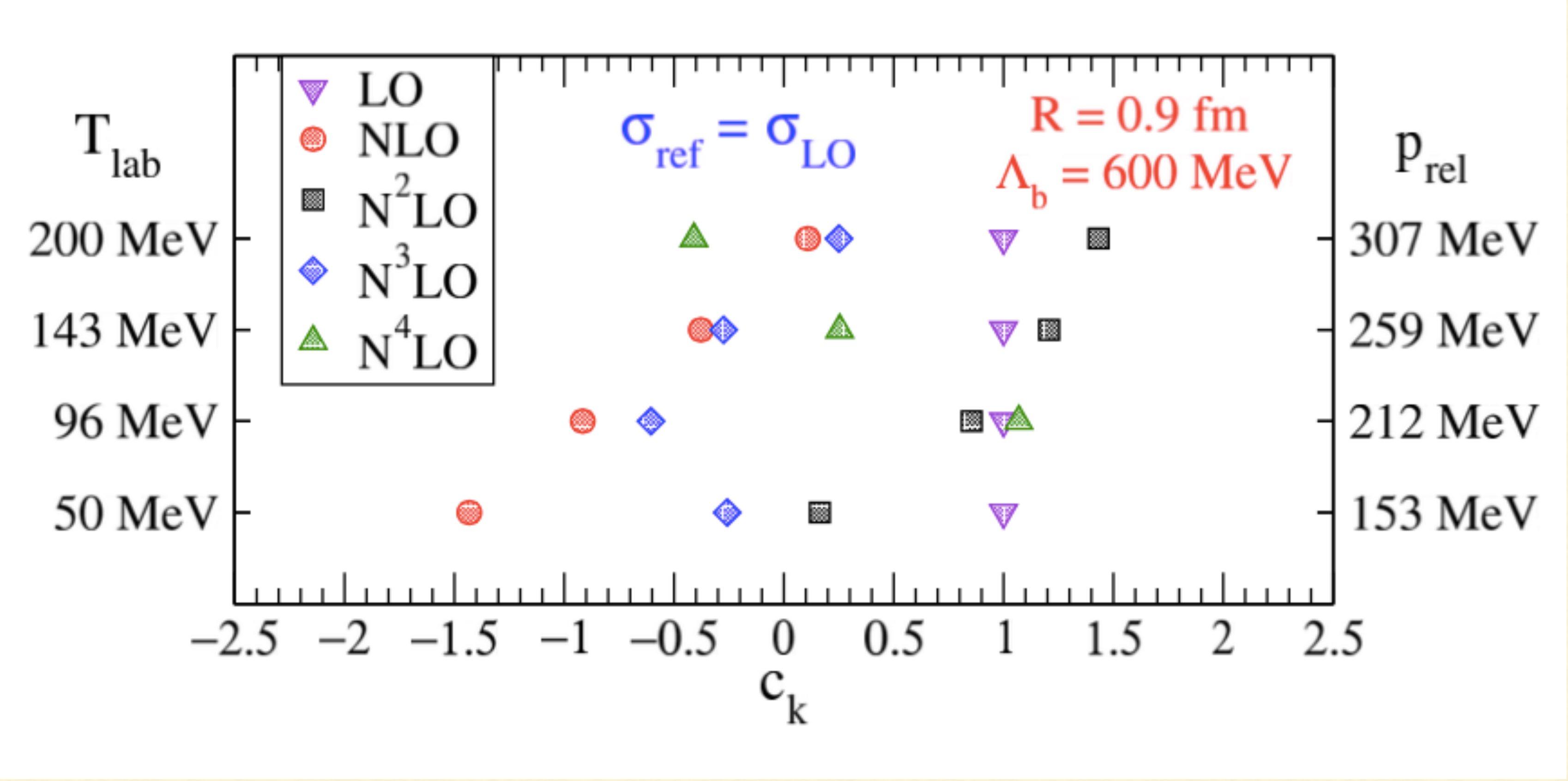
EKM'S NN SCATTERING ANALYSIS

Epelbaum, Krebs, Meissner, arXiv:1412,0412; arXiv:1412.4623

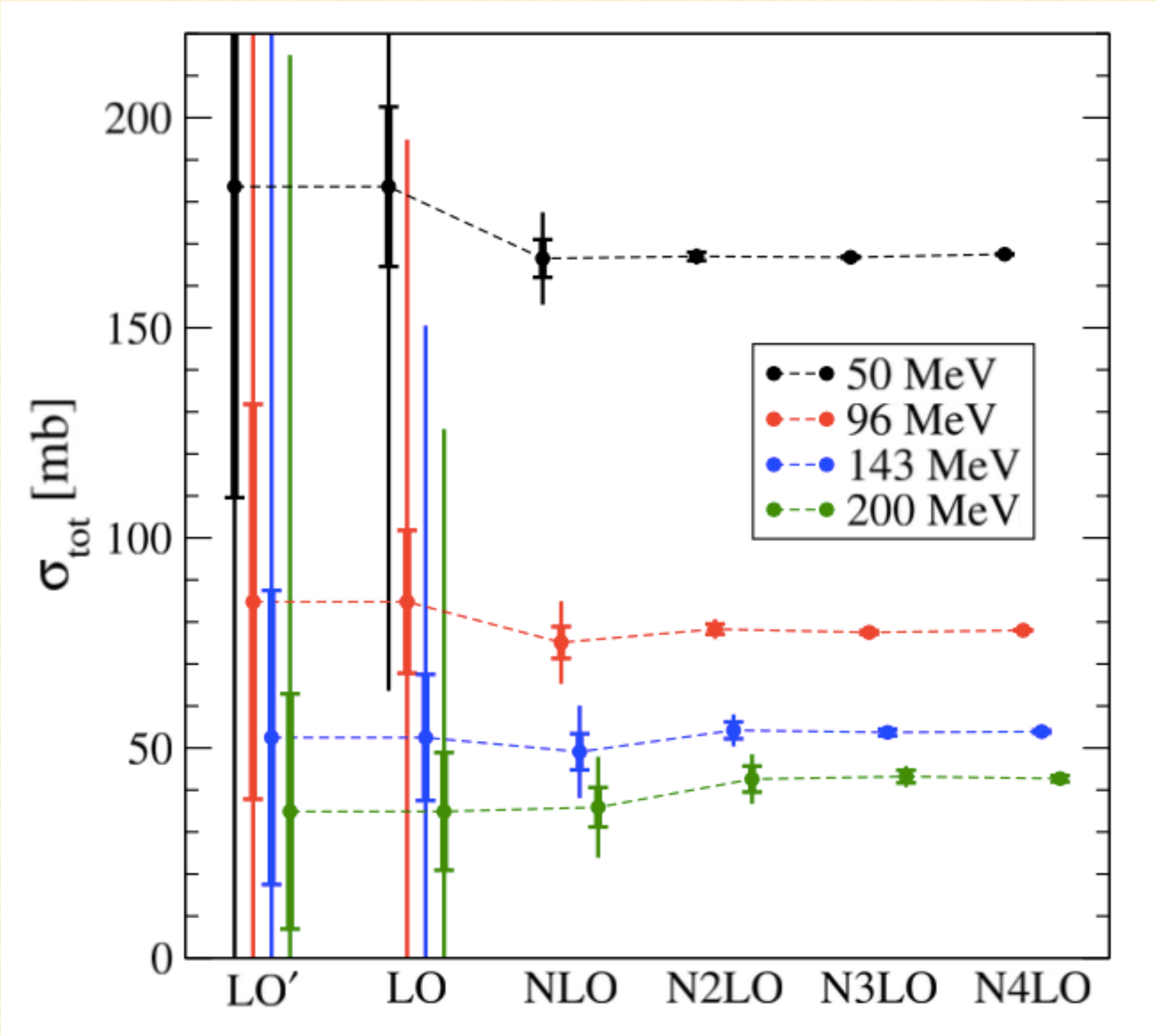
- NN cross section at T_{lab}=50, 96, 143, 200 MeV
- Local regulator, parameterized by R.
- EKM identify Λ_b=600 MeV for smaller R values.
- Here I examine R=0.9 fm data.
- Results at LO, NLO, N^2LO, N^3LO, N^4LO (k=0, 2, 3, 4, 5).
- One outlier. Fitting procedure?

$$\sigma_{np}(E_{\rm lab}) = \sigma_{\rm LO} \sum_{n=0}^{k} c_n(p_{\rm rel}) \left(\frac{p_{\rm rel}}{\Lambda_b}\right)^n$$

$$Q = \frac{p_{\rm rel}}{\Lambda_b}$$

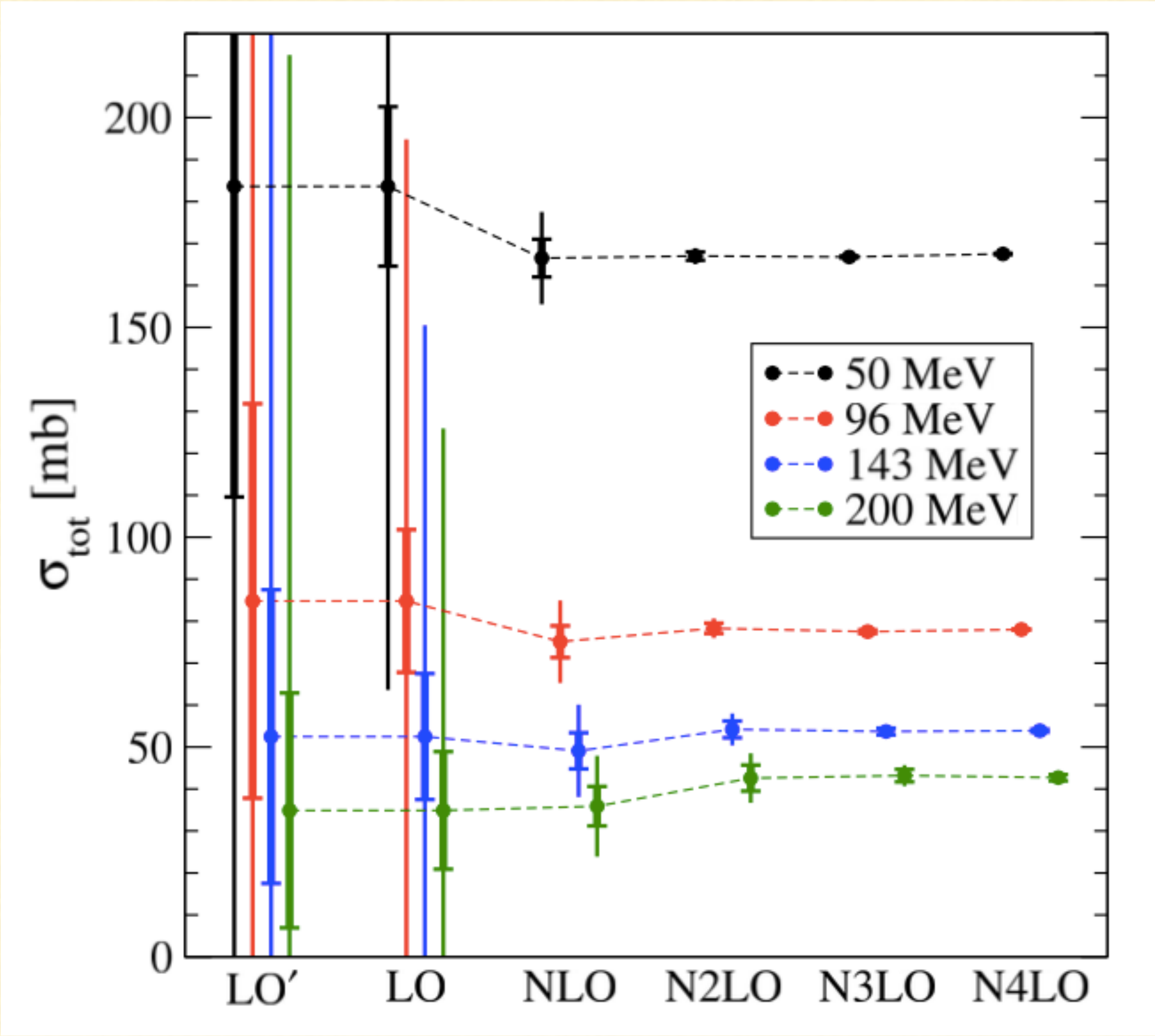


RESULTS



200
150
100
50
0
σ_{tot} [mb]
LO′
LO
NLO
N2LO
N3LO
N4LO
50 MeV
96 MeV
143 MeV
200 MeV

RESULTS



σtot [mb]
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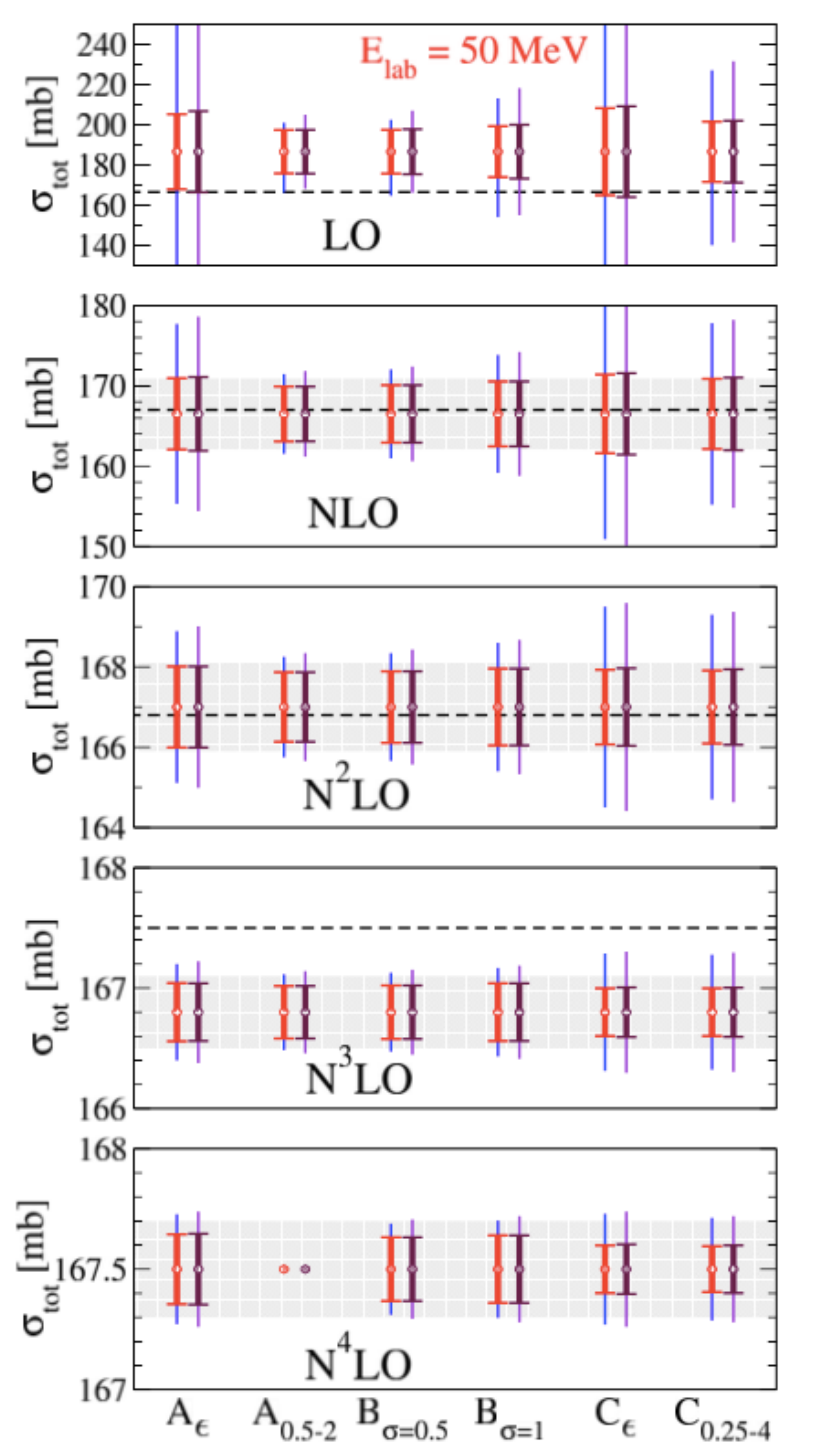
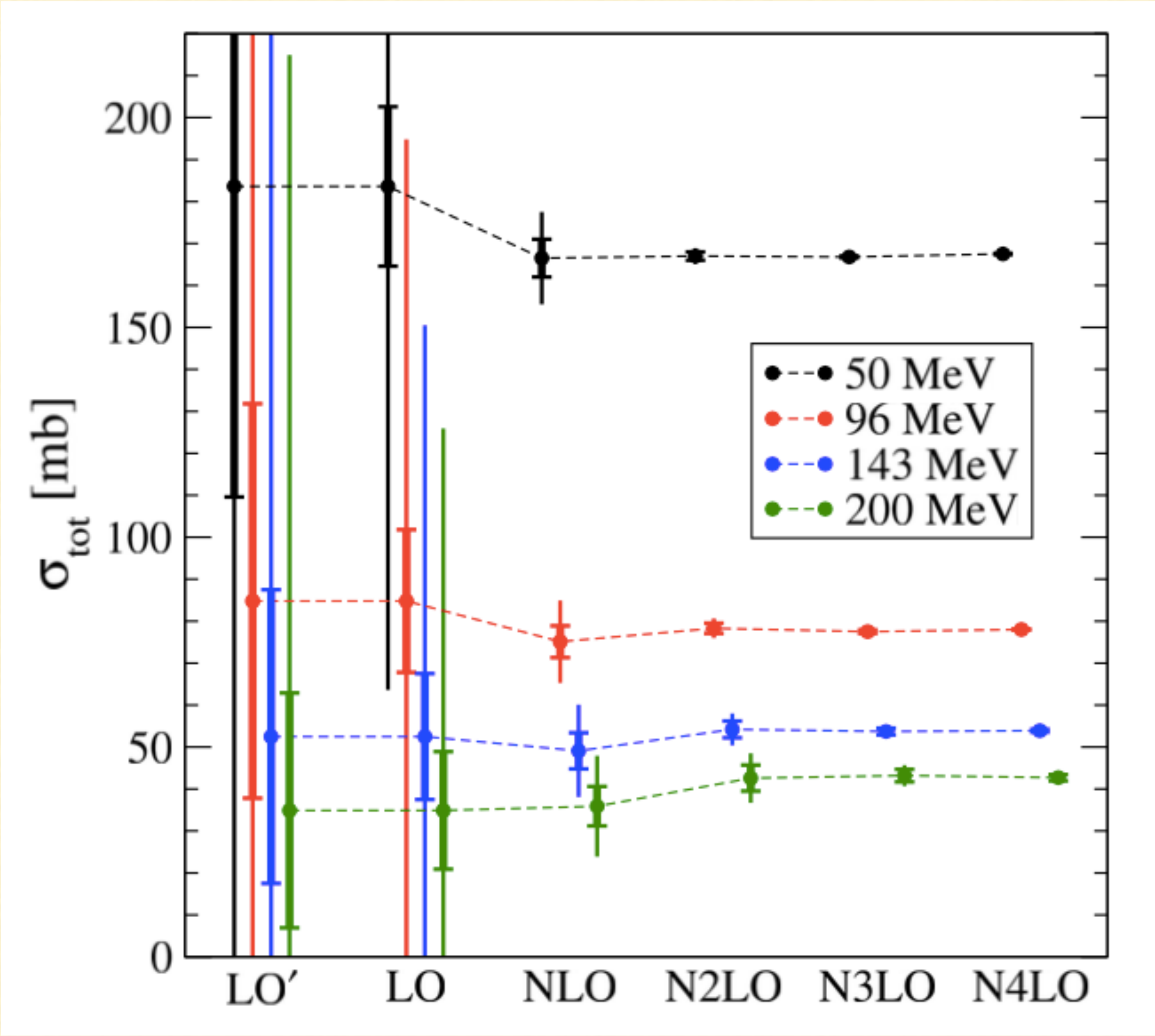


Elab = 50 MeV
σtot [mb]
LO
NLO
N2LO
N3LO
N4LO
Aϵ
A0.5-2
Bσ=0.5
Bσ=1
Cϵ
C0.25-4

RESULTS



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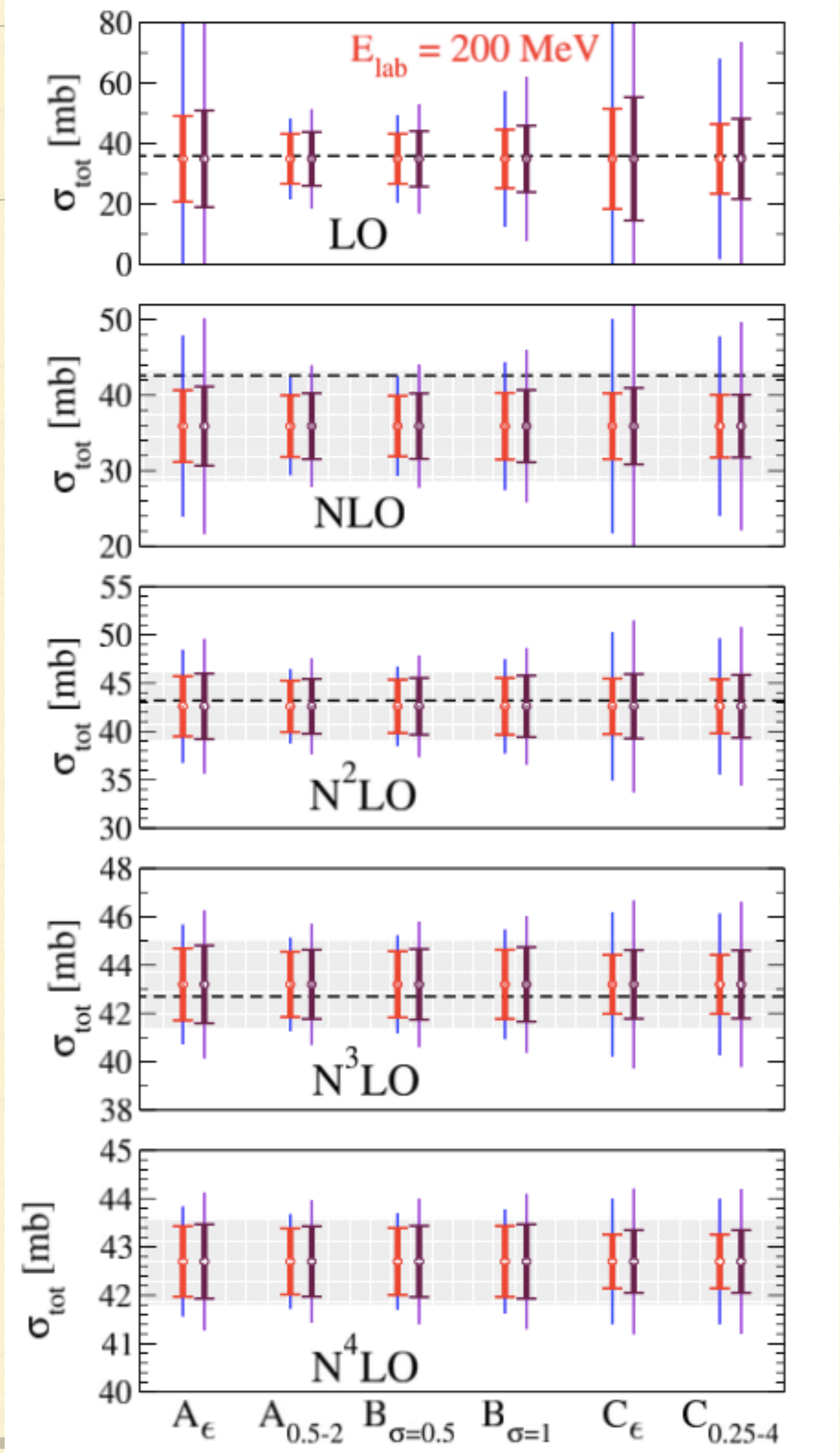

Elab = 200 MeV
σtot [mb]
LO
NLO
N2LO
N3LO
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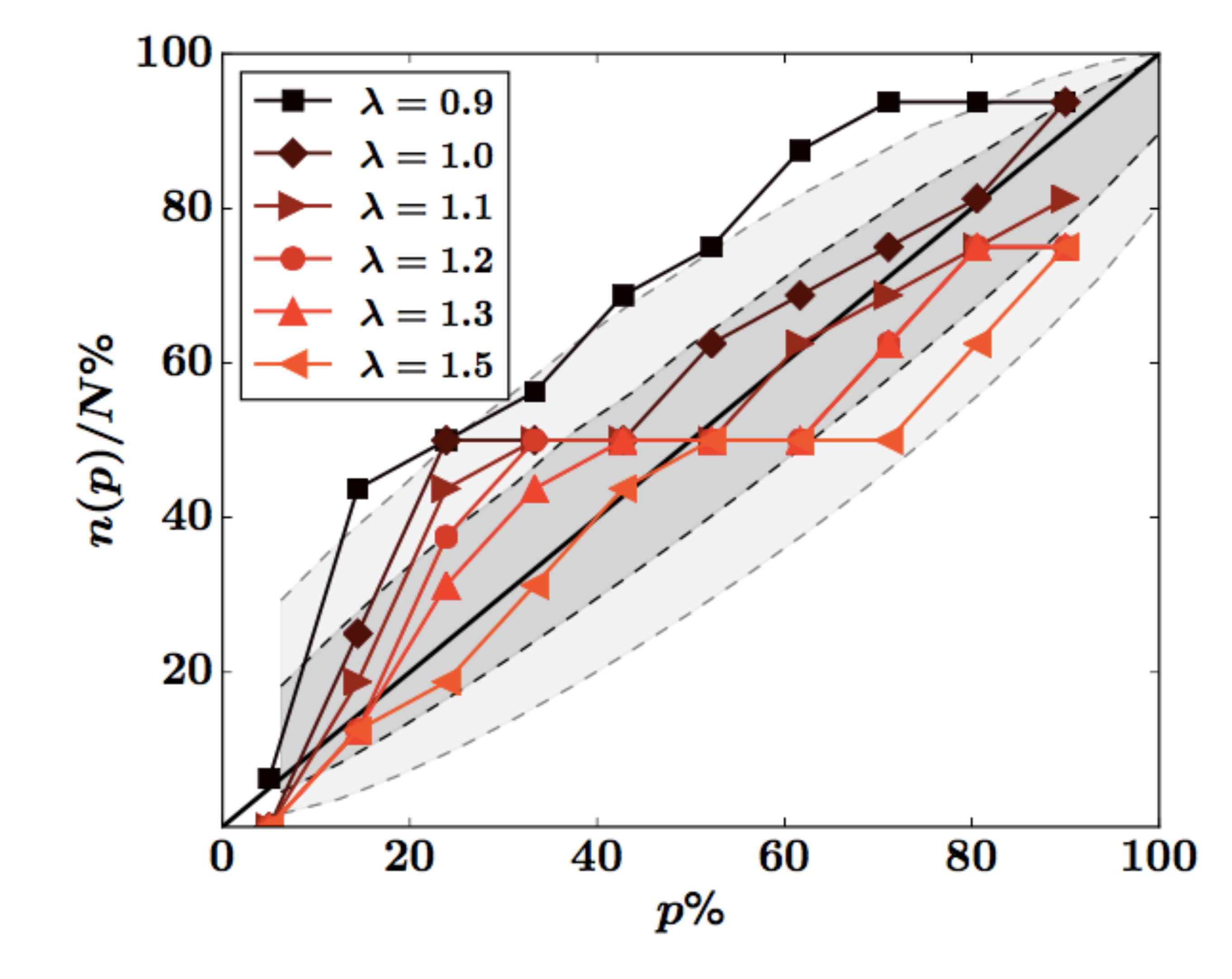
Aϵ
A0.5-2
Bσ=0.5
Bσ=1
Cϵ
C0.25-4

CONSISTENCY?

Furnstahl, Klco, Phillips, Wesolowski, arXiv:1506.03143

after: Bagnaschi, Cacciari, Guffanti, Jenniches, 2015



- Now we consider predictions at each order, with their error bars, as data and test them to see if the procedure is consistent.
- Fix a given DOB interval, compute actual success ratio and compare.
- Look at this over EKM predictions at four different orders and four different energies.
- Interpret in terms of rescaling of Λ_b by a factor λ.

No evidence for significant rescaling of Λ_b

NORMAL NATURALNESS?

- Treat 19 coefficients as data and test for naturalness.
- Approach 1: coefficients should be normally distributed around a mean μ with a variance σ^2.

Forte, Isgro, Vita, PLB, 2014

- Approach 2: see if χ^2 has size expected, assuming μ=0 and a particular σ.

$$\chi^2 = \sum_{i=1}^{N_O} \sum_{n=0}^{k} \left(\frac{|c_n^{(i)}|\lambda^n - \mu}{\sigma} \right)^2$$

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- Approach 1 (σ^2=1): $\lambda = 1.01^{+0.18}_{-0.19}$
- Approach 2 (σ^2=1): λ=1.09 gives χ^2=19. λ=1.01→1.15 consistent.

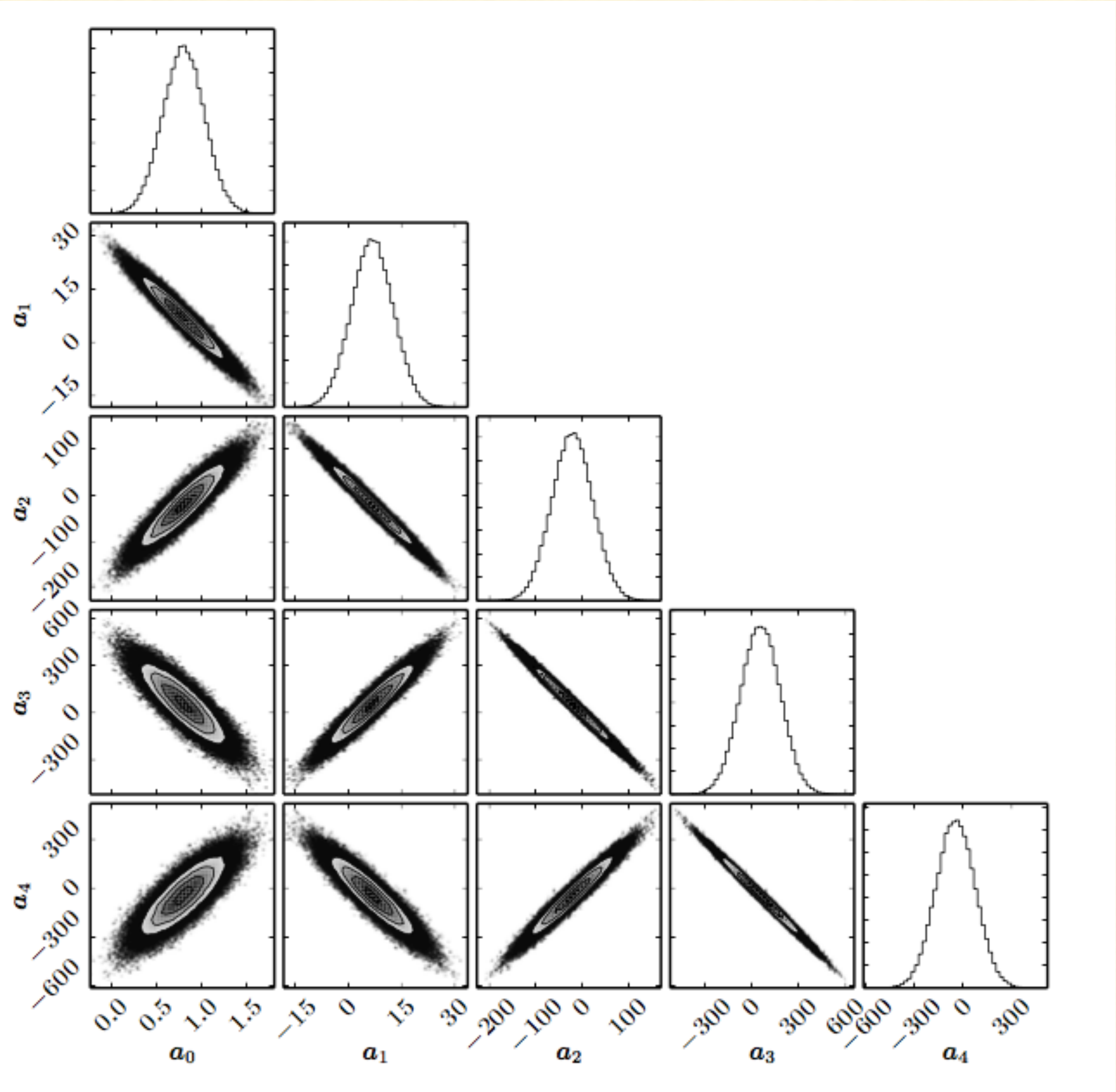
No evidence for significant rescaling of Λ_b

CAVEATS

- Naturalness of coefficients in Q-expansion for NN cross section assumed. Justified for perturbative process, but justification not so clear for NN.
- m_π not included in Q (anticipate this is only a small effect).
- We looked at results only for one R; at larger Rs the regulator effects dominate and:
  - The distribution $\{c_n\}$ is qualitatively different;
  - Λ_b is identified as lower by EKM. Cutoff artefact, not true EFT breakdown scale.
- We took EKM's LECs as given. LECs themselves have statistical errors, but we did not incorporate those in our analysis.
- LECs also have truncation errors, which should be included in their quoted errors.

IN PROGRESS: LEC EXTRACTION

with A. Thapaliya



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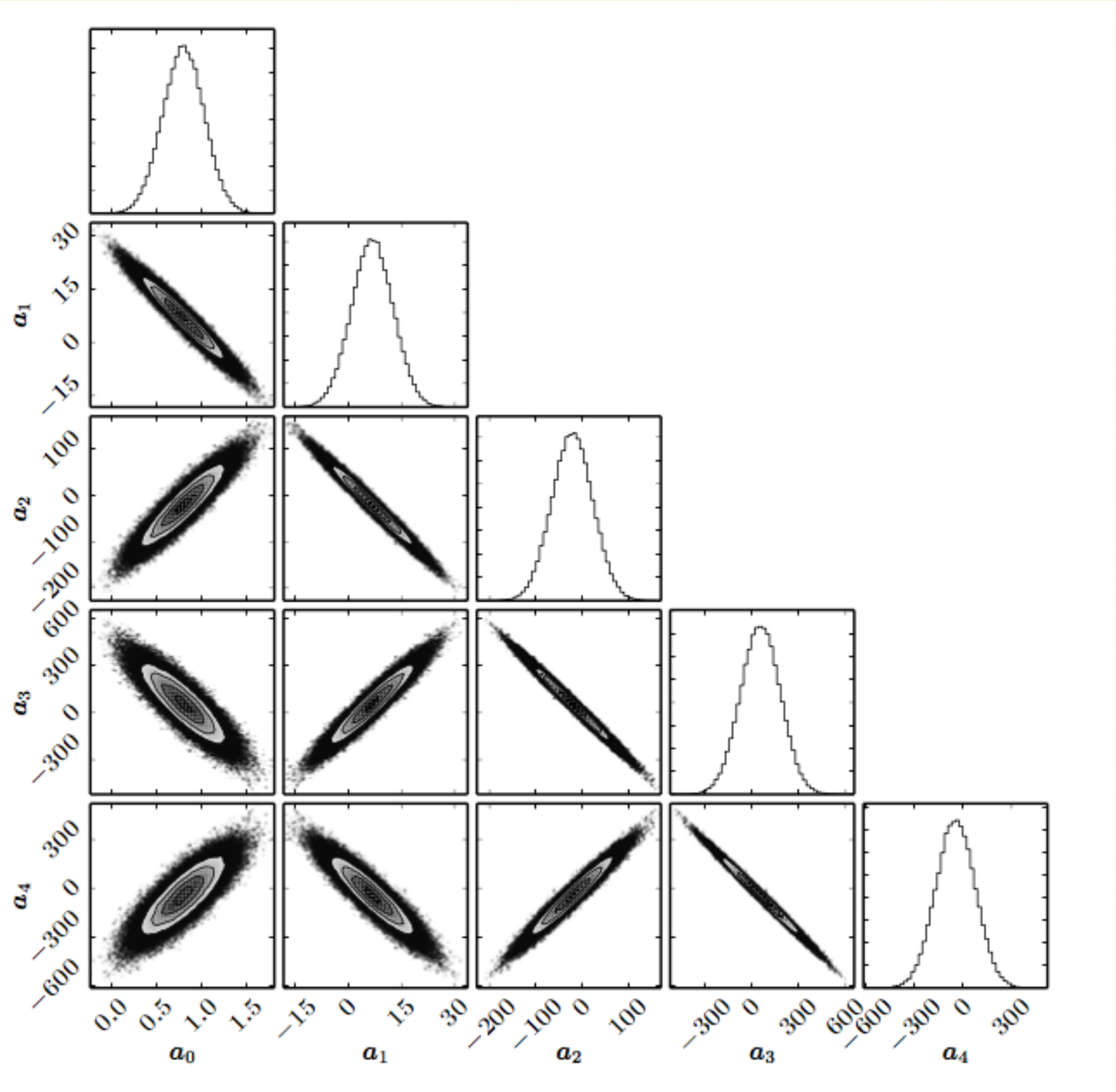

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Schindler and Phillips (2009)

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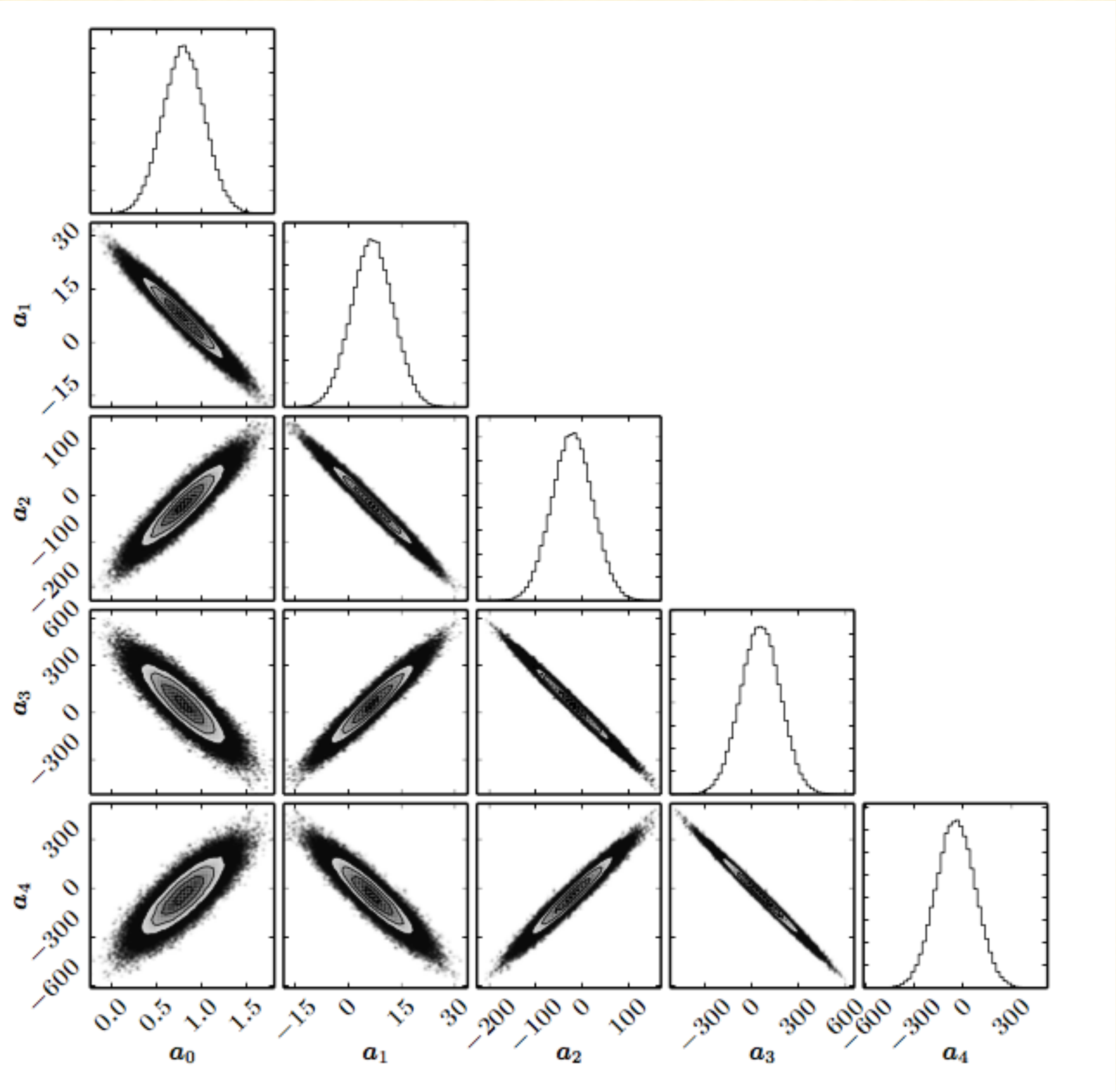

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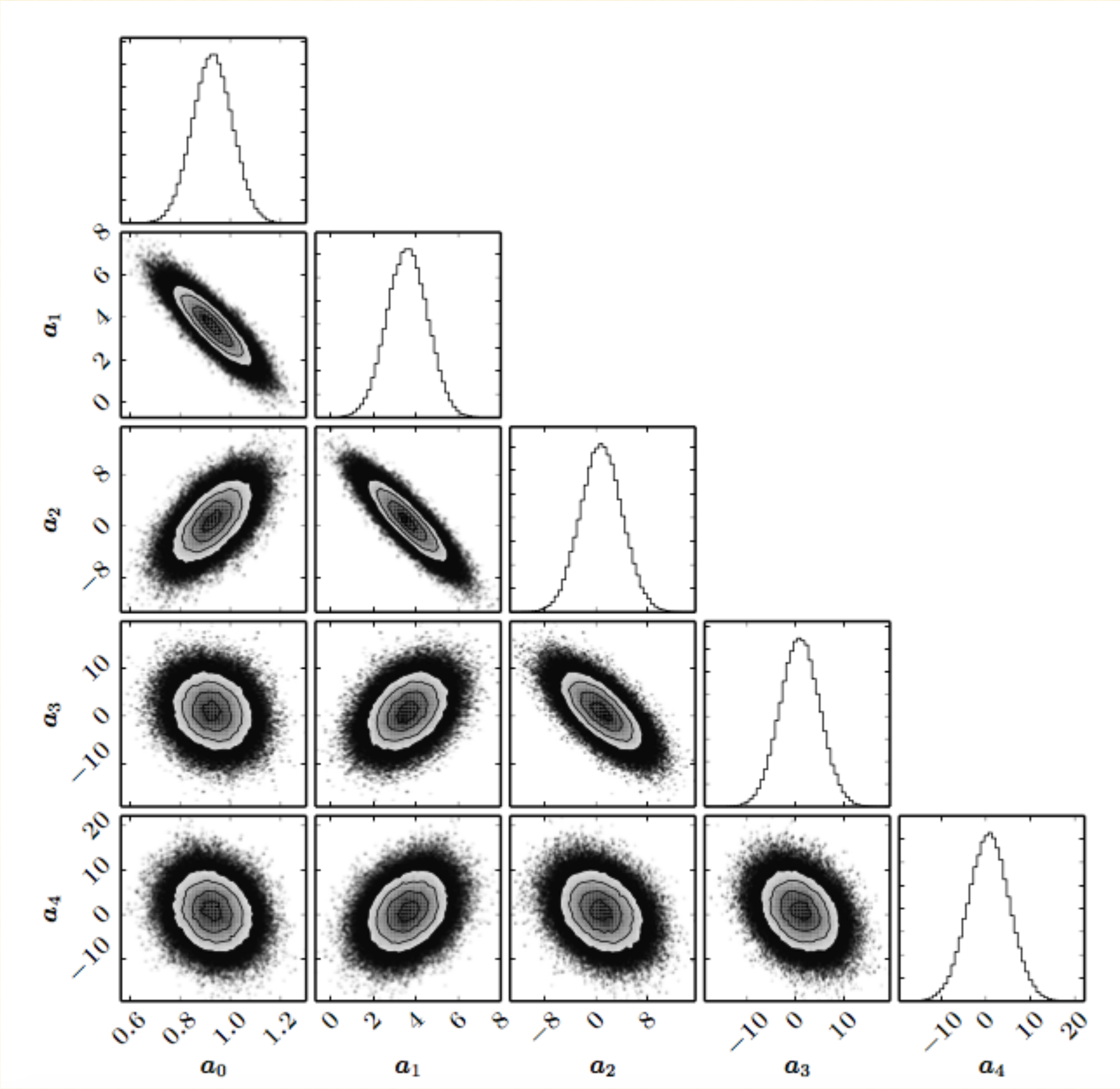

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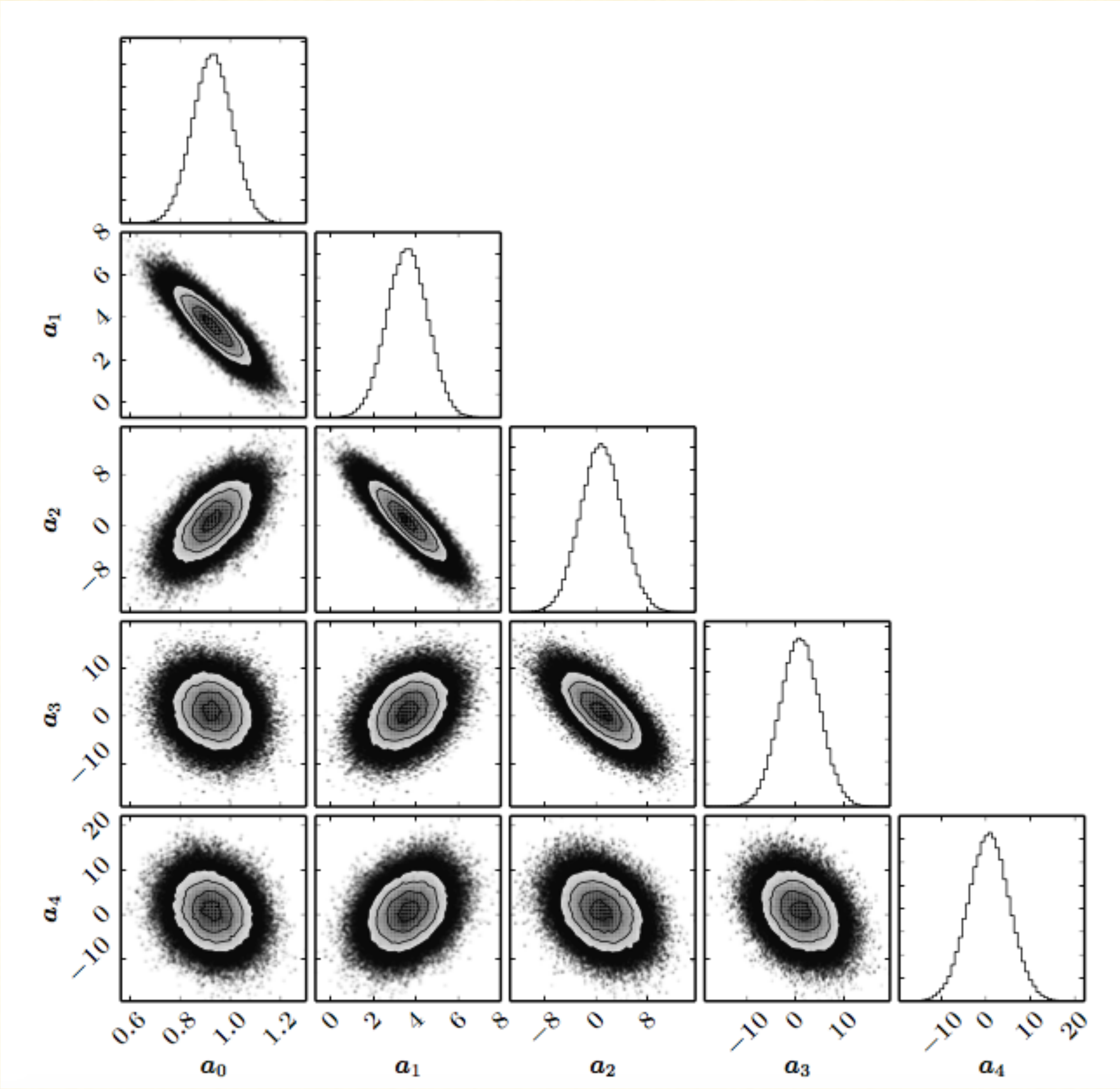

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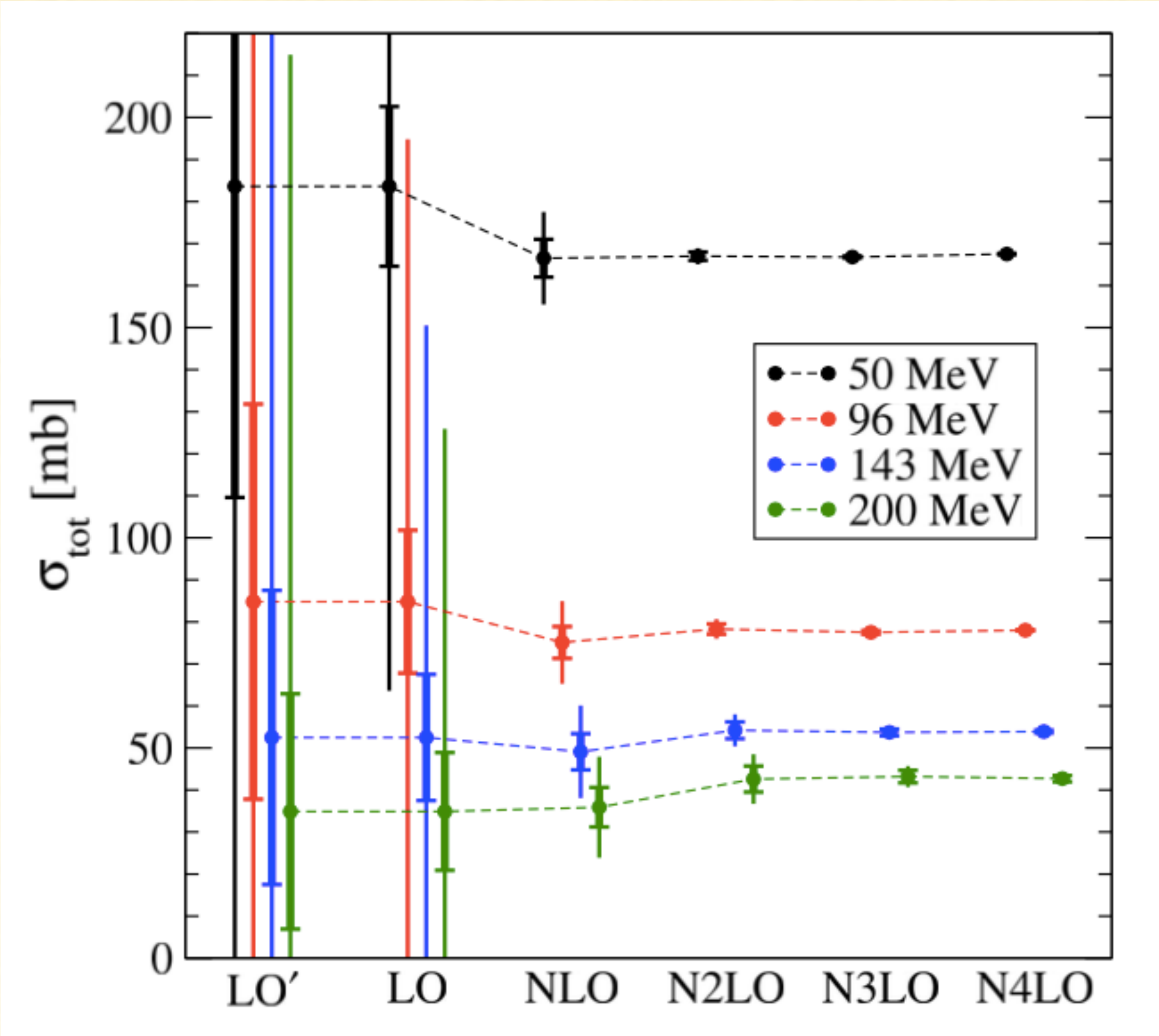
- Impose prior on higher-order terms in EFT expansion, via, e.g. augmented χ^2: remedies over-fitting.
- Numerous diagnostics developed to ensure that prior does not bias final result for LECs.

CONCLUSION

- A Bayesian analysis of truncation error makes explicit assumptions about the pattern of EFT LECs, allowing rigorous consequences to be derived.
- The "Set A_ϵ" prior justifies the standard EFT error estimation procedure.
- Theory uncertainties quite stable under choice of other (reasonable) priors.
- Resulting error bars have a statistical interpretation.
- Permits to combine errors in a consistent way.



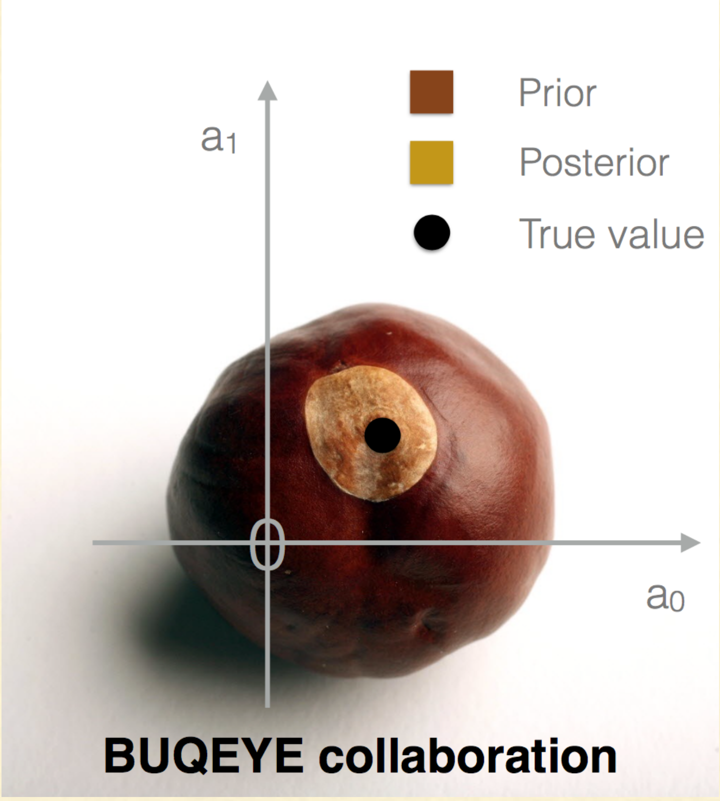
OUTLOOK

Goal 1: provide clear guidance on how to extract χEFT parameters;

Goal 2: facilitate tests of whether χEFT is working as advertised;

Goal 3: theory predictions with well-understood and motivated error bars that incorporate ALL sources of uncertainty in the calculation.

Robust guidance regarding new measurements that refine and test the theory



ON THE MENU:

- Understanding truncation errors
- LEC extractions with truncation errors included
- Analyze systematics of residuals: Bayesian model selection for EFT testing
- Theory predictions with full error bars