Case studies in Bayesian parameter estimation for chiral effective field theory

Sarah Wesolowski
Department of Mathematics and Computer Science
Salisbury University

Dick Furnstahl

Daniel Phillips

BUQEYE Collaboration

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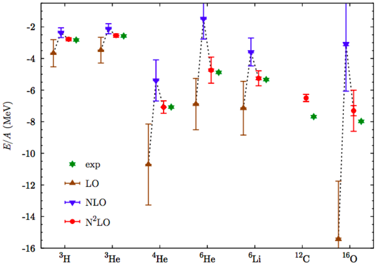
Uncertainty quantification in *ab initio* calculations

Are we there yet?



Recent QMC result for binding energy per nucleon
Lonardoni et. al, [arXiv:1709.09143], cf. Ingo's talk
Two types of error bars: method and truncation errors

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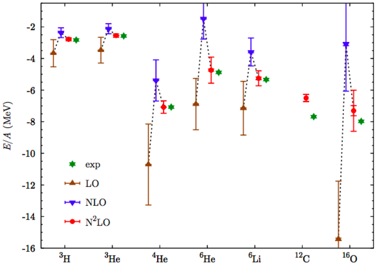

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  - Regulator artifacts
  - Convergence
  - LEC fitting in NN and 3N
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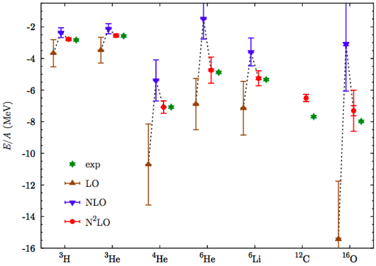

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- Issues remain in χEFT:
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  - LEC fitting in NN and 3N
  - What degrees of freedom?
- Need full, statistically meaningful UQ!
  I.e., only as successful as the p% interval predicts

Focus on low-energy constant (LEC) estimation.

(which is entangled with other uncertainties in the calculation)

The Bayes Way

EFTs are special because they have a convergence *pattern*:

$$X(p) = X_0 \sum_{n=0}^{k} c_n \, Q^n, \qquad \Delta_k = \sum_{n=k+1}^{k_{\rm max}} c_n Q^n$$

$$Q = \max(p, m_\pi)/\Lambda_b$$

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  naturalness of LECs/observable expansion, truncation errors, breakdown scale.

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  - χ^2 optimization procedures vs. Bayesian posteriors.
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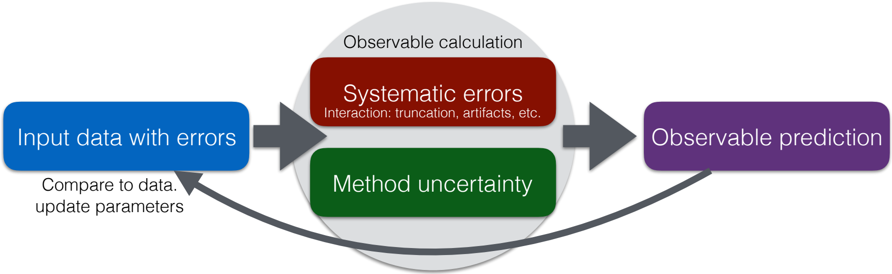
- Parameter estimation framework for LEC estimation.
  Furnstahl et. al, J. Phys. G (2015) and sw et al., J. Phys. G (2016)
- Can combine LEC + truncation error consistently.
  Coming soon: sw, Furnstahl, and Phillips

Sources of error in parameter estimation

What goes into the parameter estimation procedure?



- Parameter estimation procedure entangles sources of error.
- Data + priors $\rightarrow$ sampling $\rightarrow$ LEC posterior distribution
- Focus on semi-local (coordinate-space) interaction of Epelbaum, Krebs, and Meißner (EKM) for case studies.
  NN contact terms in partial waves.
  Epelbaum, Krebs, and Meißner, Eur. Phys. J. A **51** (2015)
  Epelbaum, Krebs, and Meißner, PRL **115** (2015)

How does truncation error enter into the parameter estimation procedure?

χ^2-likelihood depends on observable calculation

$$\chi^2(\mathbf{a}) = \sum_{i=1}^{N} \left(\frac{d_i - X^k(p_i, \mathbf{a})}{\sigma_i^2} \right)$$

- Full observable $X(p) = X^k(p; \mathbf{a}) + X_0(p) \sum_{k+1}^{k_{\max}} c_n Q^n$

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Marginalize to introduce higher-order c_n's into likelihood

$$\mathrm{pr}(D|\mathbf{a}, I) = \int \mathrm{d}c_{k+1} \cdots \mathrm{d}c_{k_{\max}}$$

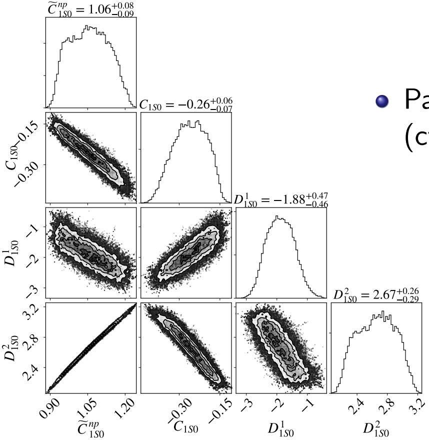
Stump *et al* Phys. Rev. D **65** (2001)

$$\mathrm{pr}(D|c_{k+1}, \cdots, c_{k_{\max}}, \mathbf{a}, I) \times \mathrm{pr}(c_{k+1}, \cdots, c_{k_{\max}}|I)$$

The final posterior $\mathrm{pr}(\mathbf{a}|D, I) \propto$ likelihood $\times$ prior

NN problem:
Numerous, high-precision data: what more do we learn?

posterior for $^1S_0$ terms at N^{3}LO



- Parameter posteriors: *s*-wave redundancy. (cf. Christian and Hermann's talks)

Learning physics from Bayesian posteriors

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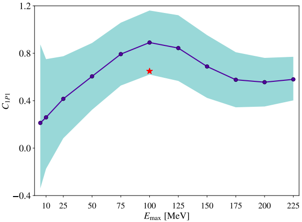

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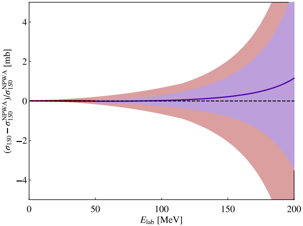

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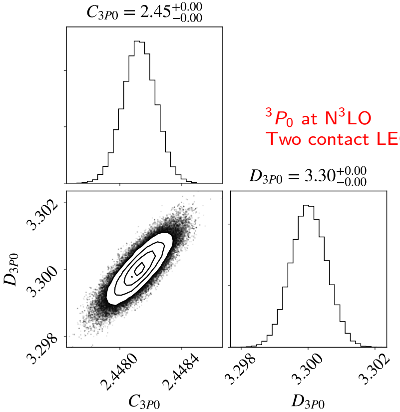
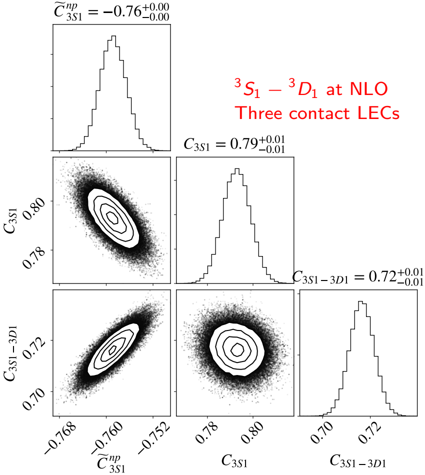
- What range of data to use? $E_{\max}$ plots.
- Formalism: combine truncation and parameter errors to make predictions.
- Briefly demonstrate these without getting into too much formalism.

Case study 1: parameter posterior for NN contact LECs

- Prior input information: naturalness and truncation errors.
- Framework outputs (LEC) parameter posteriors with uncertainties consistently included:



$^3P_0$ at N^{3}LO
Two contact LECs



$^3S_1$ – $^3D_1$ at NLO
Three contact LECs

Case study 1: redundancy in the s-waves

The operators in the s-wave sat N^{3}LO (Q^4) may be rewritten as:

$$
\begin{aligned}
D^1_{(1S0)} p^2 p'^2 + D^2_{(1S0)} (p^4 + p'^4) \\
&= \frac{1}{4}(D^1_{(1S0)} + 2D^2_{(1S0)})(p^2 + p'^2)^2 \\
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\end{aligned}
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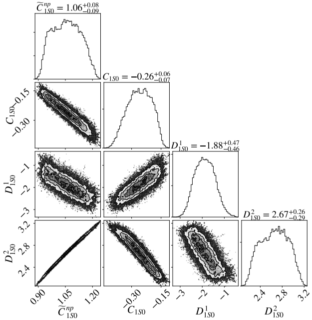
The LEC posterior is non-Gaussian behavior with large correlations:



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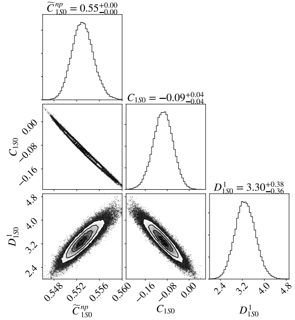
But becomes more Gaussian with restriction of parameters $D^2_{1S0} = 0$:

and equivalent description of data!



Case study 2: what range of data to use?

EFT convergence

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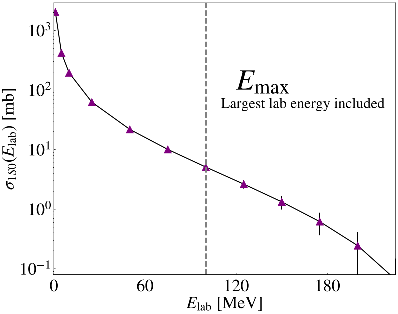
As we go to higher E_{max}, more terms contribute in the expansion.



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As we go to higher $E_{\max}$, more terms contribute in the expansion.

- Including truncation error in fit procedure avoids overfitting.
- $E_{\max}$ plots: how high to make $k_{\max}$ to absorb UV physics?
- Bayesian model selection makes quantitative statements about how many terms are constrained by data.
- $E_{\max}$ plots serve as simpler proxy to model selection.

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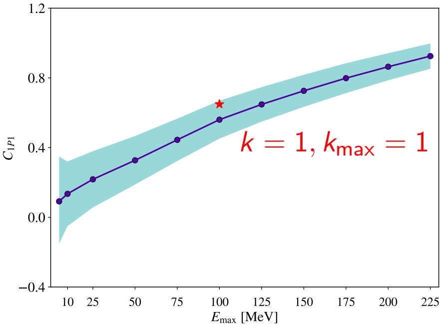

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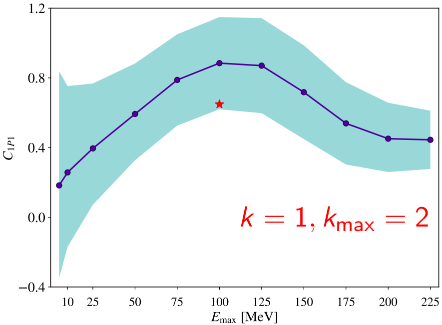
With enough terms, LEC saturates as function of E_{max}.



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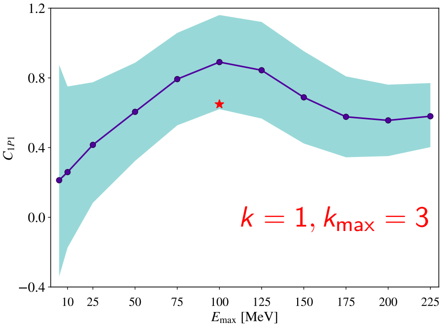

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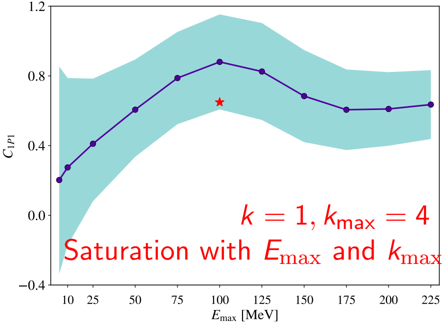
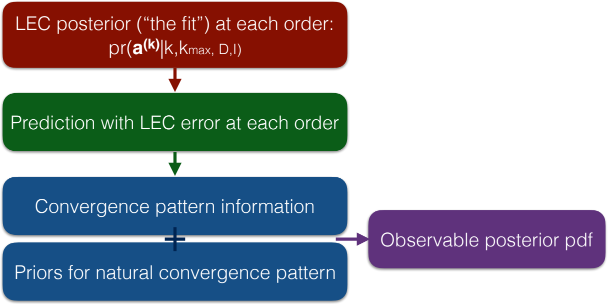


Case study 3: combining LEC and truncation uncertainty

How to make predictions with combined uncertainties?

Using Bayesian methods, can derive a posterior for observables:

$$\mathrm{pr}(X(p)|D, k, k_{\mathrm{max}}, I)$$



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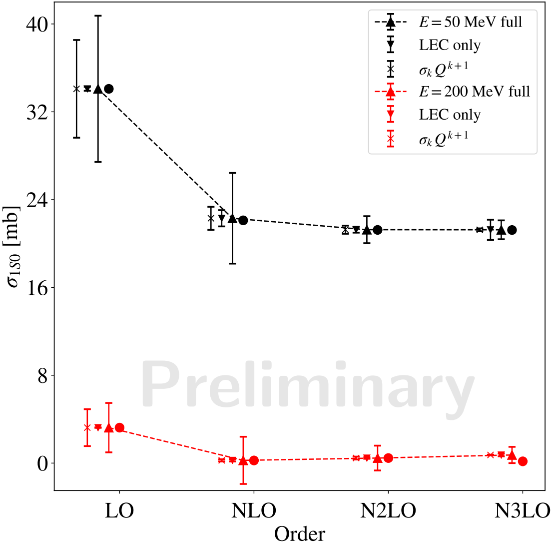

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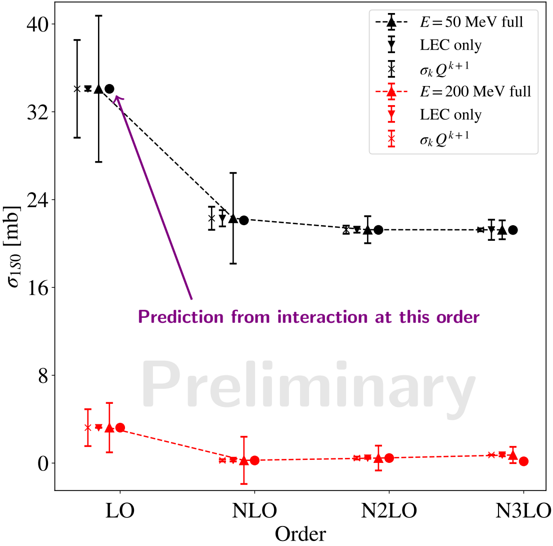

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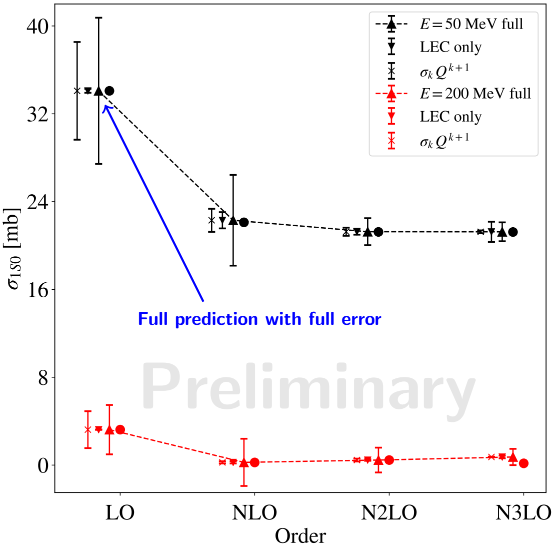

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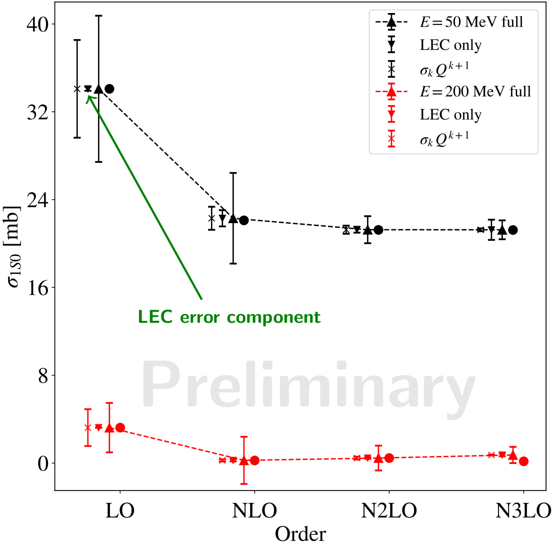

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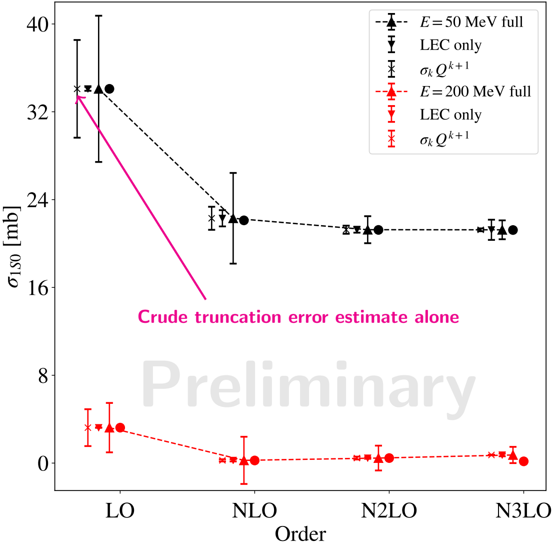
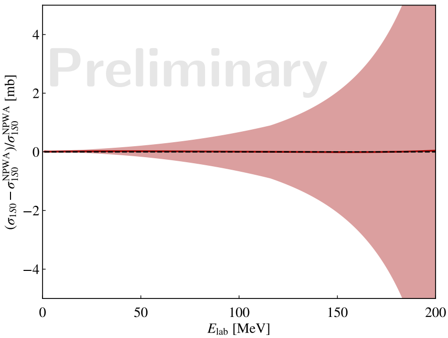


Combining LEC and truncation uncertainty: results

Plot relative uncertainty

$$\sigma_{\text{res}} = (\sigma_{\text{pred.}} - \sigma_{\text{NPWA}})/\sigma_{\text{NPWA}}$$

Note: this is singlet s component only!



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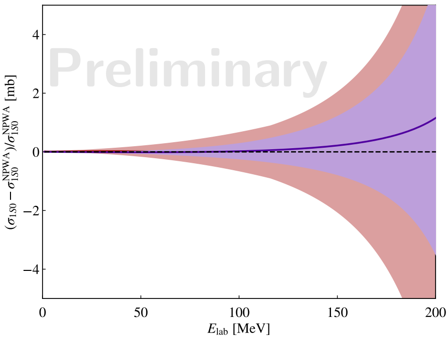

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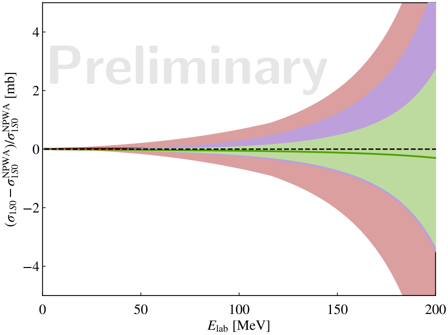

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- Next-to-leading order (Q^2) starts to know about convergence
- N^2LO (Q^3) includes even more convergence information
- Finally, N^3LO (Q^4) has converged even further.

Summary and outlook

Summary

- Bayes $\rightarrow$ consistent analysis of error in *ab initio* calculations
- Here: EFT truncation error + LEC error/correlations.
- Model checking and validation possible!
- Can extract physics insight based on data
(cf. *s*-wave redundancy)

Outlook

- Extend to 3N and problems with few data.
- Bayesian model selection for deciding between formulations.
- Working on model selection for nd scattering in pionless EFT.
- Make code accessible for interaction practitioners.