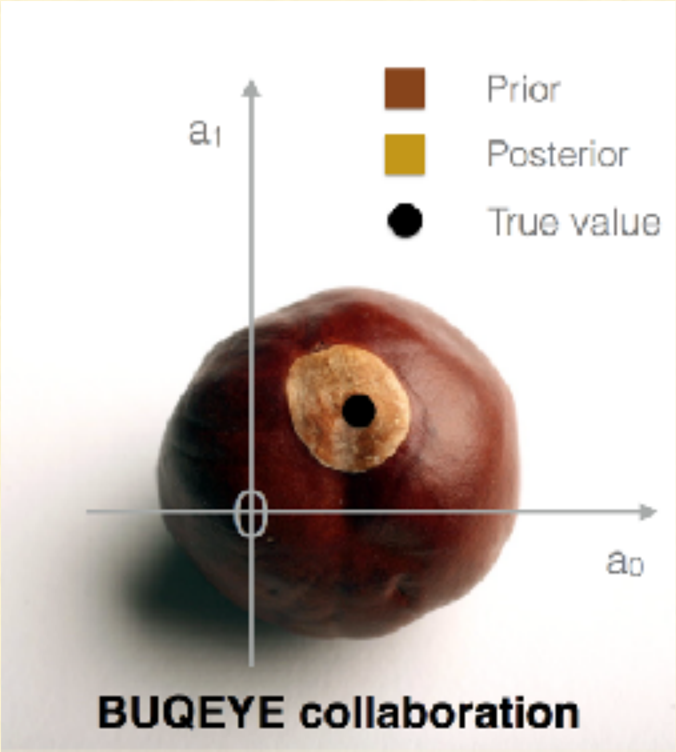
BAYESIAN PARAMETER ESTIMATION FOR NUCLEAR FORCES

Daniel Phillips
Institute of Nuclear and Particle Physics
Ohio University

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

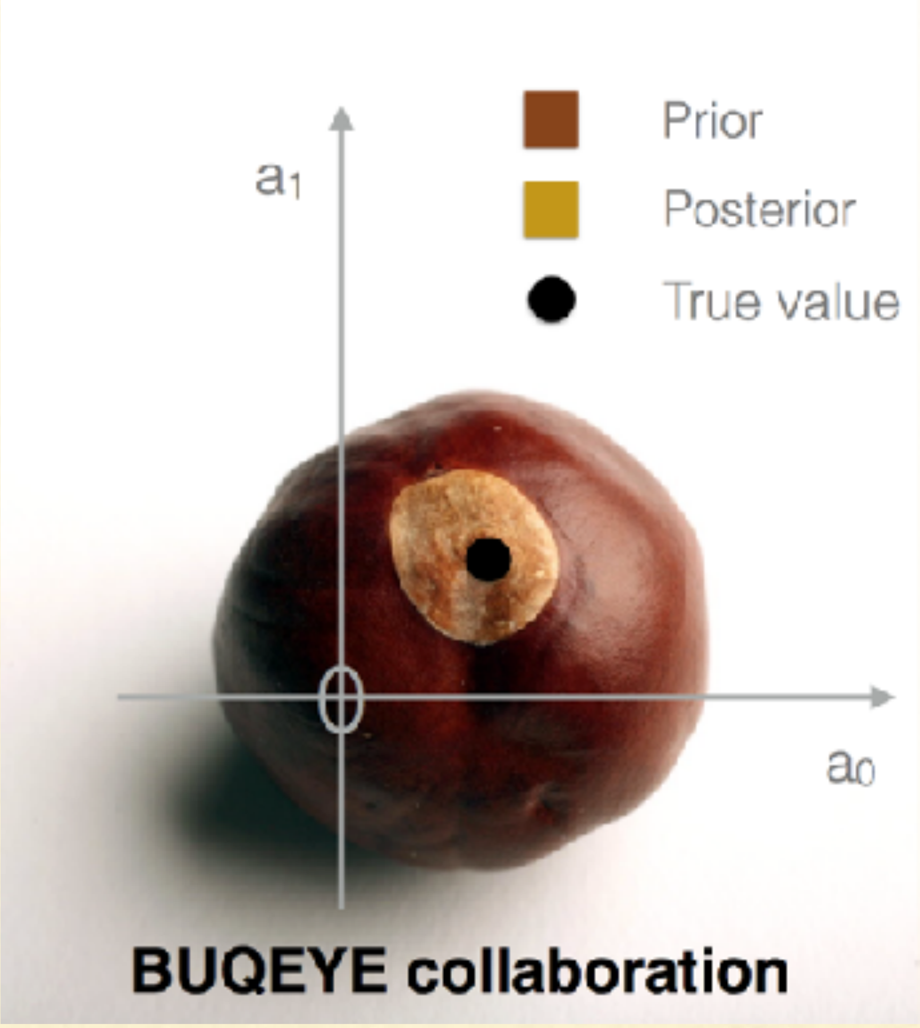
R. J. Furnstahl, J. Melendez, M. Pratola (Ohio State University)
DP (Ohio University)
S. Wesolowski (Salisbury University)



RESEARCH SUPPORTED BY THE US DOE AND NSF

Outline

- Nucleon-nucleon scattering
  - Goal
  - Data
  - Incorporating theory errors
  - Results
- Parameter estimation for the 3N force
- Modeling correlations in EFT truncation errors (cf. Jordan Melendez's talk on Th.)
- Summary



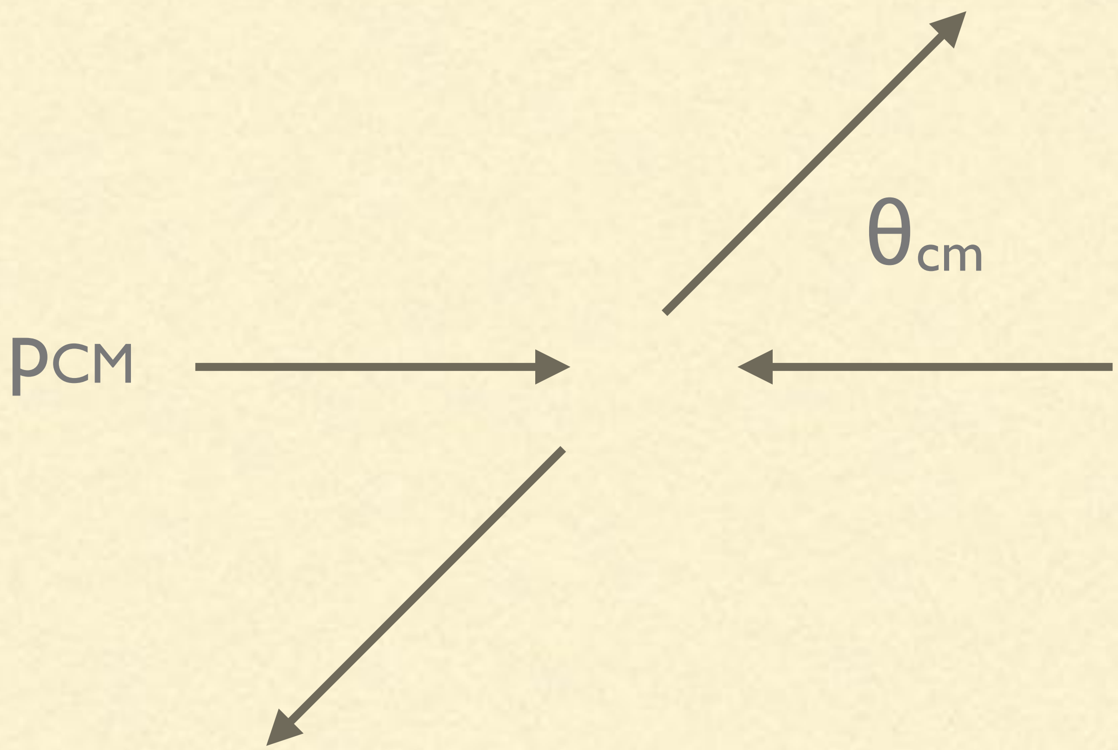
R. J. Furnstahl, N. Klco, DP, and S. Wesolowski, Phys. Rev. C **92**, 024005 (2015)

S. Wesolowski, N. Klco, R. J. Furnstahl, DP, and A. Thapaliya, J. Phys. G. **43,** 074001 (2016)

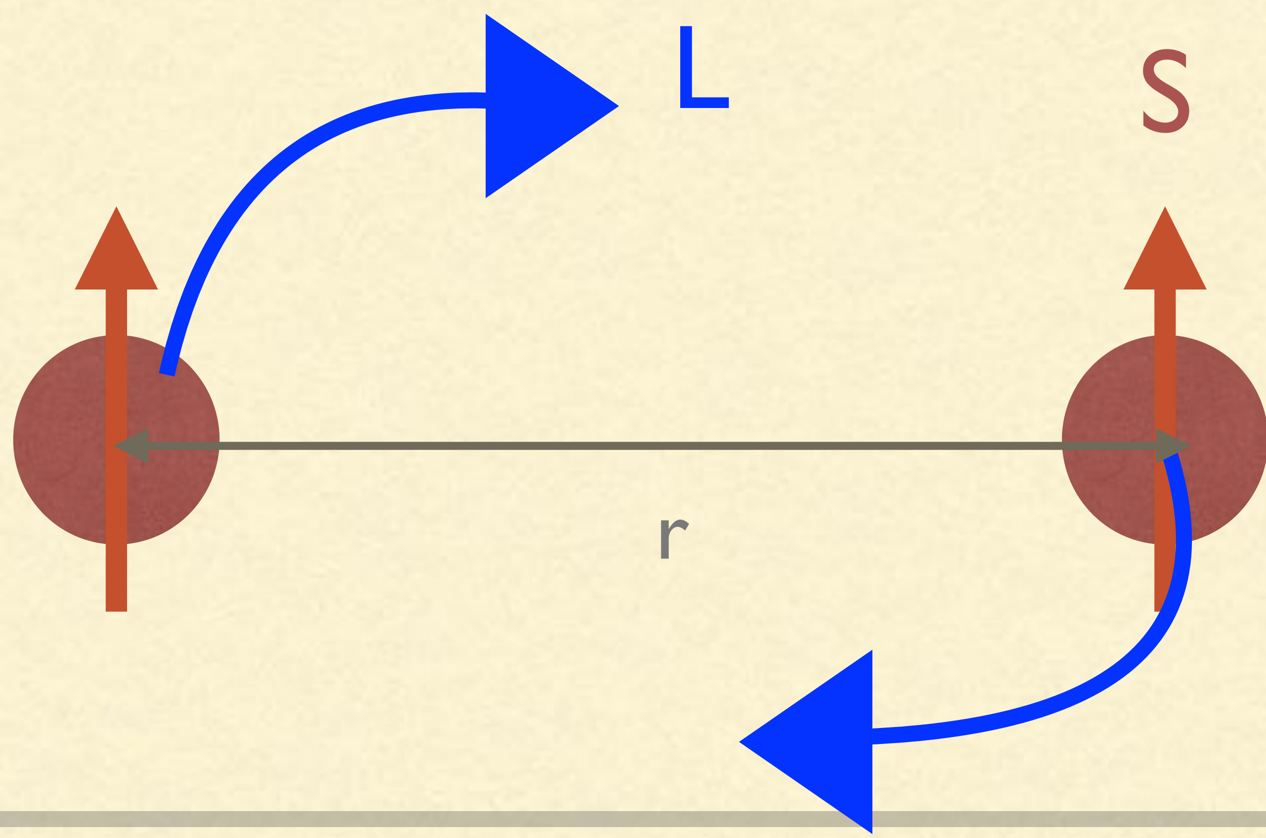
S. Wesolowski, R. Furnstahl, J. Melendez, DP, J. Phys. G **46**, 045102 (2019)

J. Melendez, R. Furnstahl, DP, M. Pratola, S. Wesolowski, Phys. Rev. C, to appear

NN scattering



Goal: infer force between nucleons, parameterized in terms of V(r)

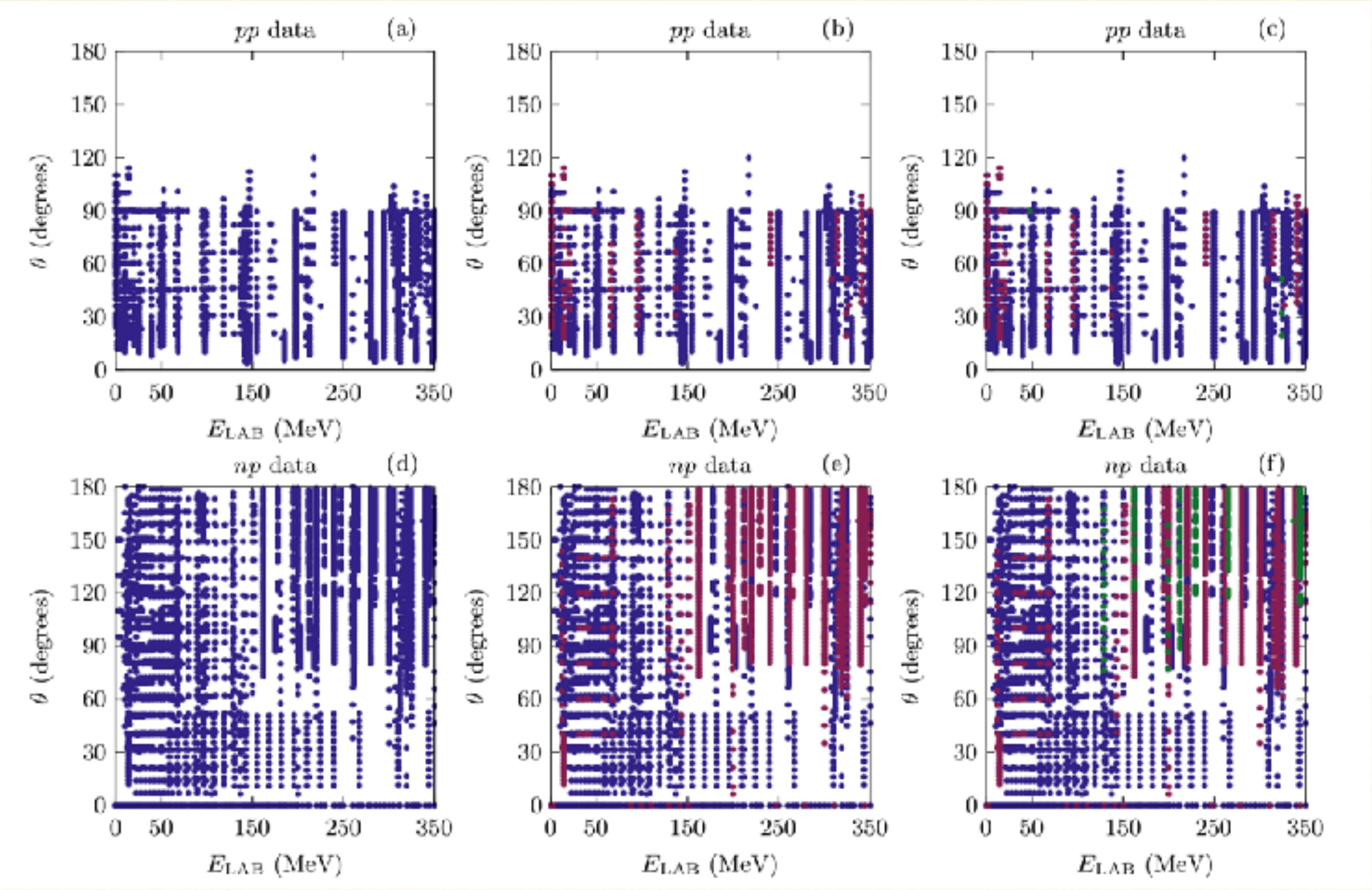


V depends on angular momentum (L), spin (S), and way these add together (J), too.

$^{2S+1}L_J$

NN data

$\frac{d\sigma}{d\Omega}, A_y, D, A, A_{xx}, A_{yy}$ all as a function of angle and energy



6700 data that form a 3σ consistent data base; 8100 data in all

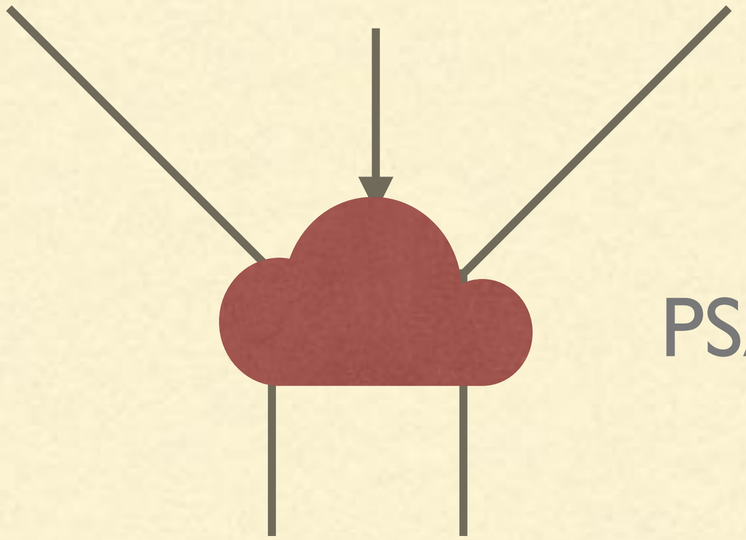
Navarro Perez, Amaro, Ruiz Arriola, PRC (2014)

The energy range

- Higher momentum means shorter de Broglie wavelength ($\lambda = h/p$), so higher energy allows us to resolve shorter-distance features of the potential
- Here data up to E_{lab}=300 MeV
- Corresponds to p_{CM}=266 MeV⇒don't resolve r less than about 1 fm
- If we are willing to fit all the data to 300 MeV there is more statistical power. But, for that to be meaningful, the model will need to be more sophisticated than if we only fit to, say, 100 MeV because fine details of NN system matter more and more as E_{lab} increases

Phase-shift analysis

$\boxed{\frac{d\sigma}{d\Omega}, A_y, D, A, A_{xx}, A_{yy}}$ all as a function of angle and energy



PSA

$$\psi_E(r) \to j_L(pr) + (-i)^L \frac{e^{i\delta} \sin\delta}{p} \frac{e^{ipr}}{r} \text{ as } r \to \infty$$

$$p = \sqrt{\frac{2\mu E}{\hbar^2}}$$

$\delta_{^1S_0}, \delta_{^3P_0}, \delta_{^3P_1}, \delta_{^3P_2}, \ldots$ each as a function of energy

$$\left[-\frac{1}{r^2}\left(\frac{d}{dr}\left(r^2\frac{d}{dr}\right)\right) + \frac{L(L+1)}{r^2} + \frac{2\mu V(r)}{\hbar^2}\right] \psi_E(r) = p^2 \psi_E(r)$$

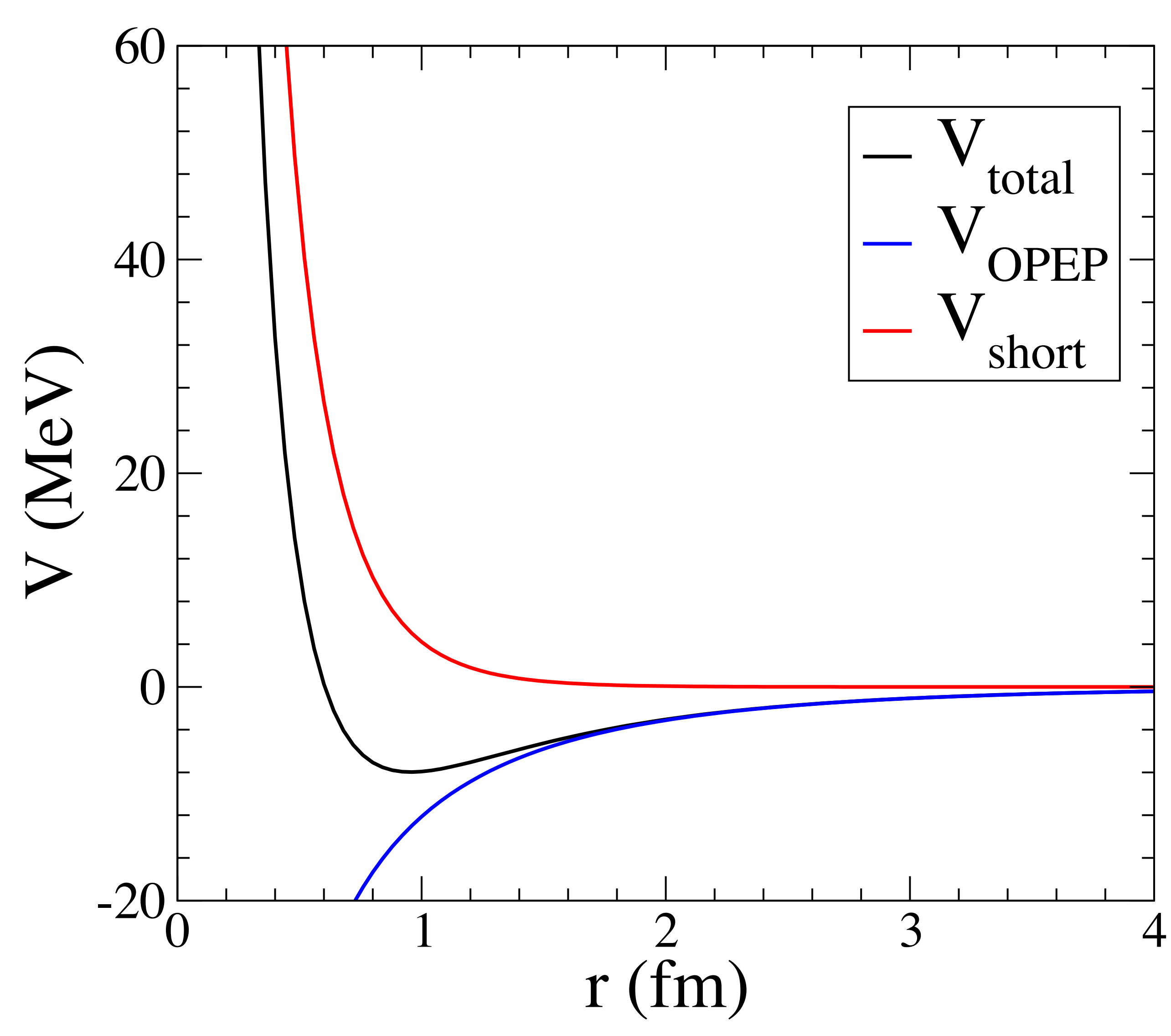
The object of inference: V(r)

$$V(r) \rightarrow \psi_E(r) \rightarrow \delta_{^{2S+1}L_J} \leftarrow \text{actual data}$$

- Long-range part generated by one-pion exchange

$$V_{^{2S+1}L_J}(r) = C_{LSJ} \frac{g^2_{\pi NN}}{4\pi} \frac{e^{-m_\pi r}}{r}$$

- Intermediate ranges: multiple pion exchange
- Short ranges: stuff happens
- "Stuff" needs to be parameterized, then fit to data



ChiEFT organization of V

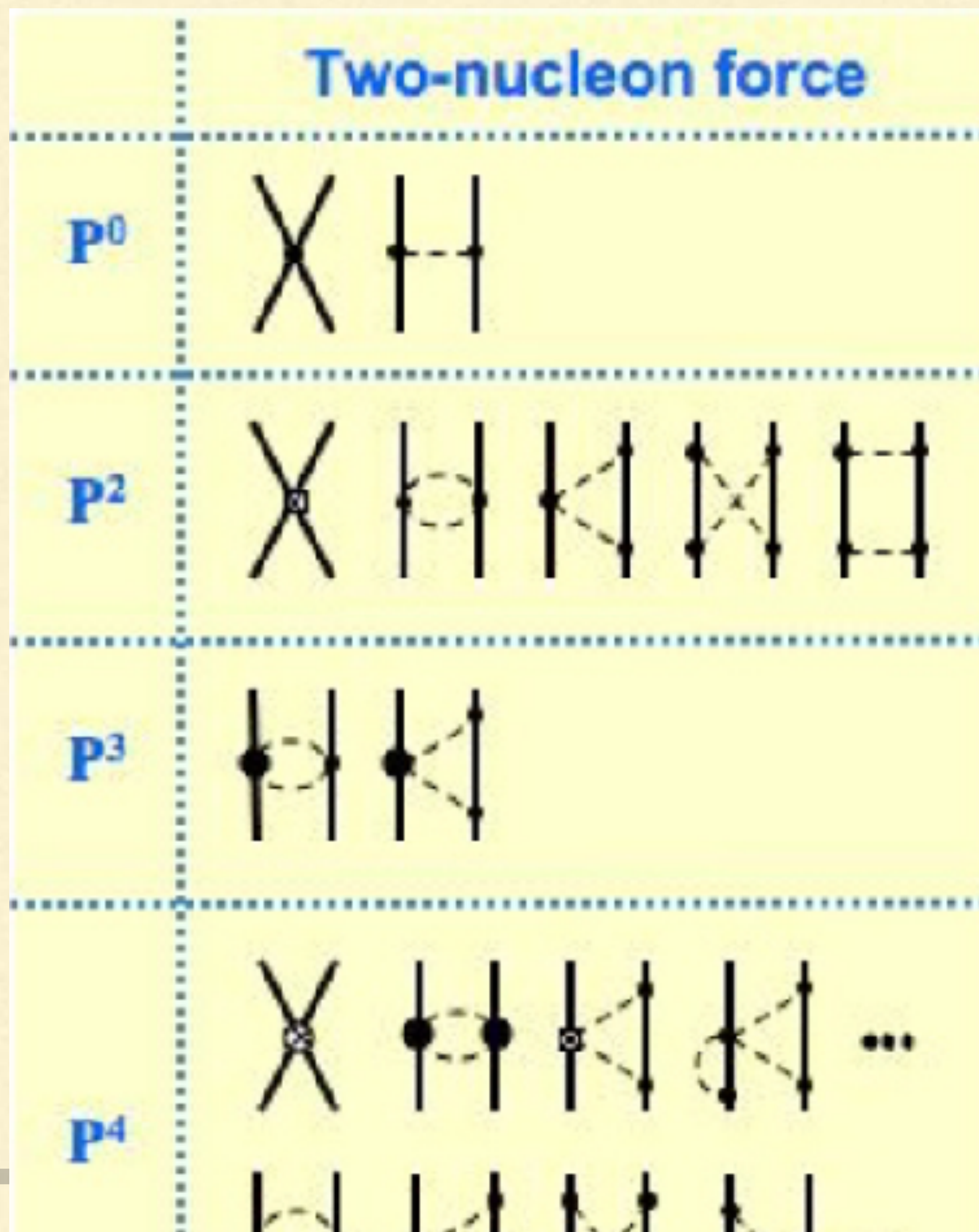
Ordonez, Ray, van Kolck (1996); Epelbaum, Meissner, Gloeckle (1999); Entem, Machleidt (2001)

$$V = V^{(0)} + V^{(2)} + V^{(3)} + V^{(4)}$$

Which details matter at some accuracy?

Expansion in $Q = \dfrac{p, m_\pi}{\Lambda_b}$

$$m_\pi = 139 \text{ MeV}; \Lambda_b \approx 600 \text{ MeV}$$



ORDER	SHORT-DISTANCE PARAMETERS
Q^0	2
Q^2	2+7
Q^3	2+7
Q^4	2+7+12

Discrepancy model

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

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

δy_{exp}: we take normally distributed, uncorrelated errors

$$Q = \frac{p, m_\pi}{\Lambda_b}$$

- $\delta y_{\mathrm{th}} = y_{\mathrm{ref}}(p)[c_{k+1}Q^{k+1} + c_{k+2}Q^{k+2} + \ldots]$
- Predictions for model discrepancy size AND growth with p
- How much do “fine details matter” as we go to higher energy?
- Avoid unintended spurious precision from assumption that model is arbitrarily precise to arbitrarily high energy/short distances

Bayesian EFT parameter estimation

- $\delta y_{\rm th} = y_{\rm ref}(p)[c_{k+1} Q^{k+1} + \ldots]$ $\qquad y_{\rm exp} = y_{\rm th} + \delta y_{\rm exp} + \delta y_{\rm th}$
- Posterior for parameters **a**={$a_0,\ldots,a_k$} by marginalizing:

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

and Bayesing $$= \int dc_{k+1}\ldots dc_{k_{\max}} \frac{\mathrm{pr}(D|\mathbf{a},c_{k+1},\ldots,c_{k_{\max}},k,k_{\max})\mathrm{pr}(\mathbf{a}|\bar{a}_{\rm fix})\prod_{j=k+1}^{k_{\max}}\mathrm{pr}(c_j|\bar{c}_{\rm fix})}{\mathrm{pr}(D|k,k_{\max})}$$

- Marginalization over c's produces revised correlation matrix in standard likelihood, accounts for uncertainties (and correlation structure) induced by omitted terms

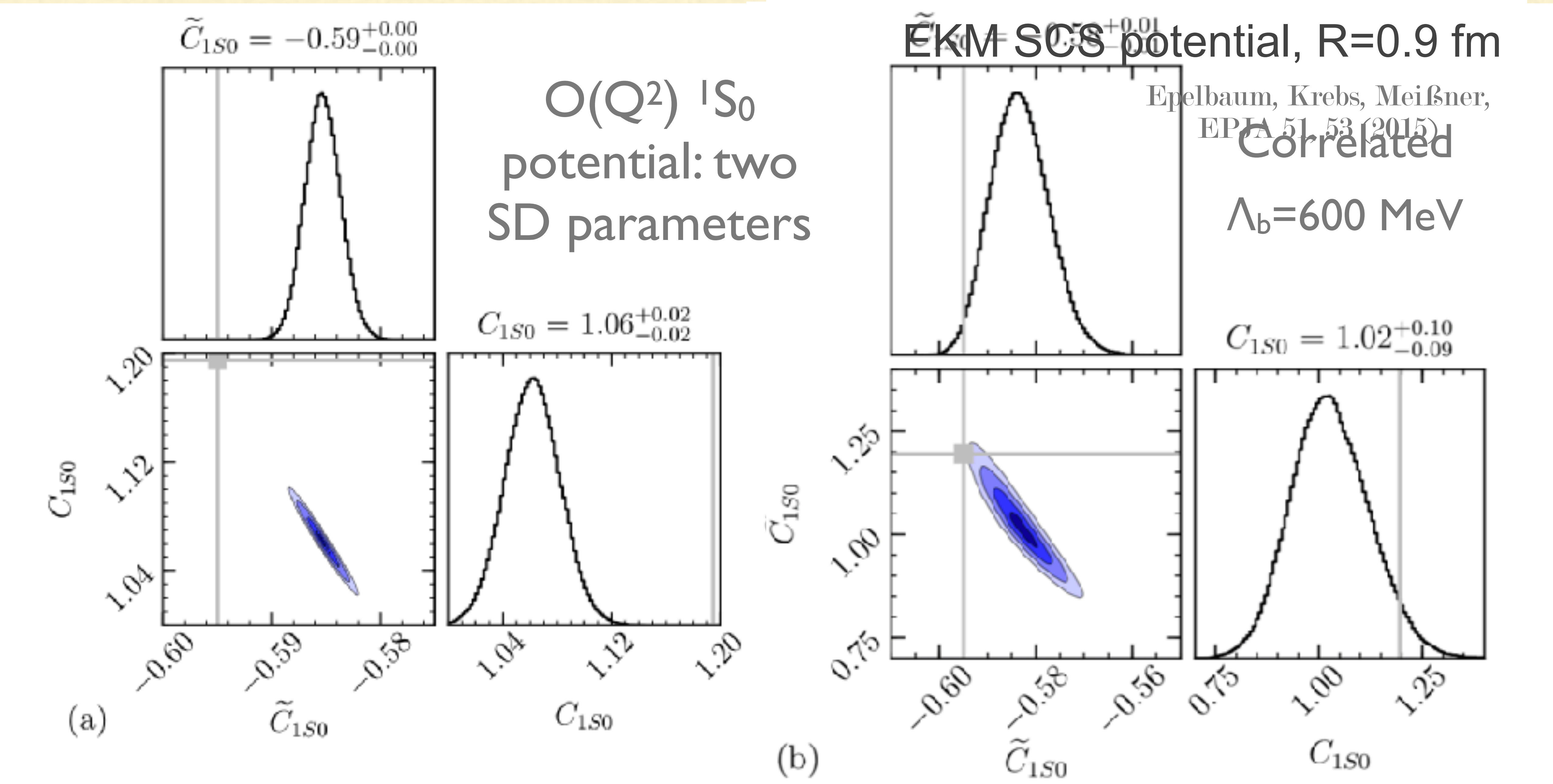
$$\mathrm{pr}(\mathbf{a}\,|\,D,k,k_{\max}) \propto \exp\left(-\frac{1}{2}\mathbf{r}^T(\mathbf{\Sigma}_{\rm exp}+\mathbf{\Sigma}_{\rm th})^{-1}\mathbf{r}\right)\exp\left(-\frac{\mathbf{a}^2}{2\bar{a}^2}\right) \qquad \mathbf{r} \equiv \mathbf{y}_{\rm exp} - \mathbf{y}_{\rm th}$$

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

- Naturalness prior for LECs (maximum entropy given a width and mean). Here we take a fixed $\bar{a}$, could also marginalize over it.

Parameter estimates: $^1S_0$

Wesolowski et al., JPG 46, 045102



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

EKM SCS potential, R=0.9 fm

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

Correlated

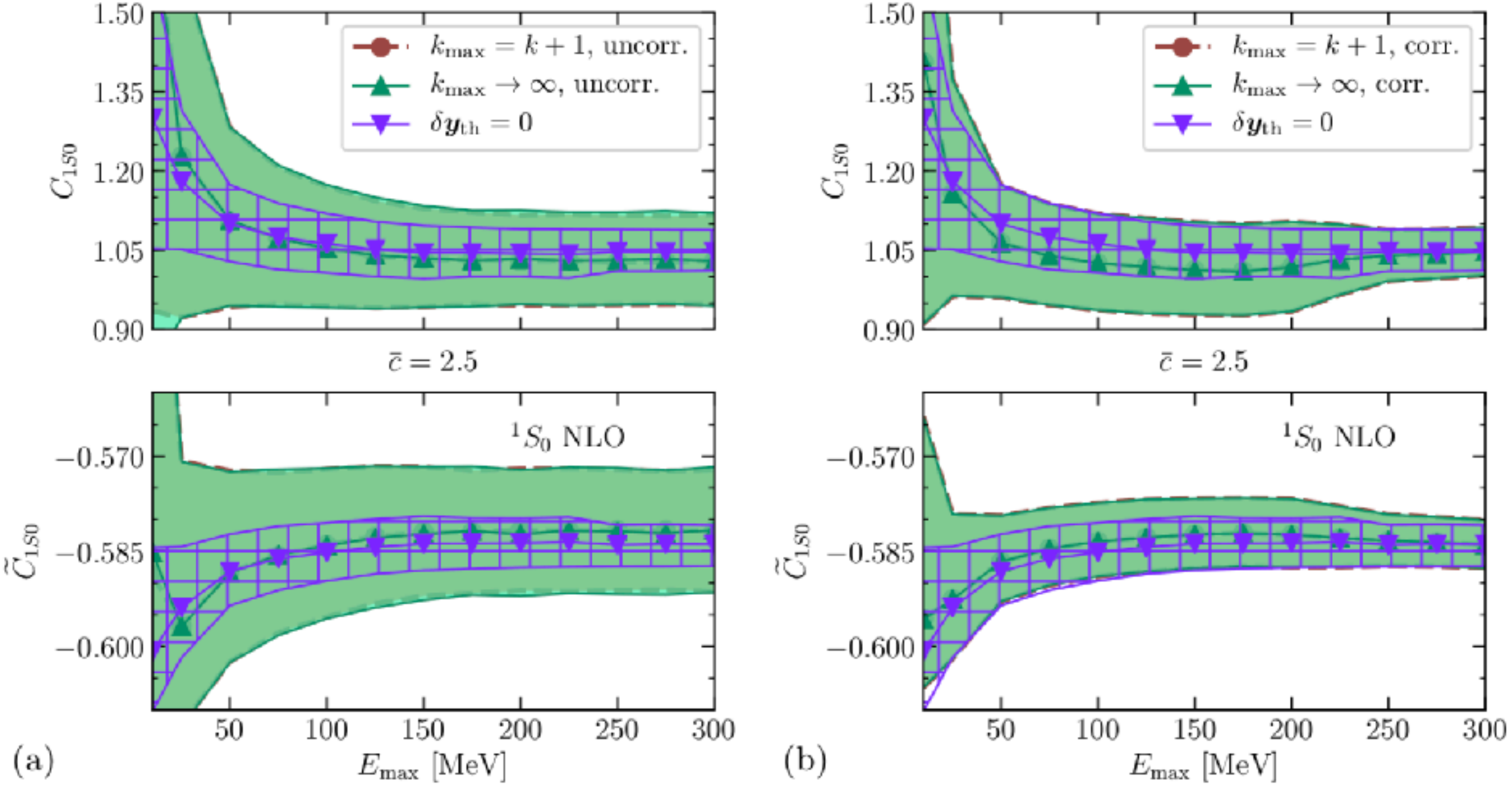
Λ_b=600 MeV

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

$$(\Sigma_{\rm th,corr})_{ij} = (y_{\rm ref})_i (y_{\rm ref})_j \bar{c}^2 \sum_{n=k+1}^{k_{\rm max}} Q_i^n Q_j^n$$

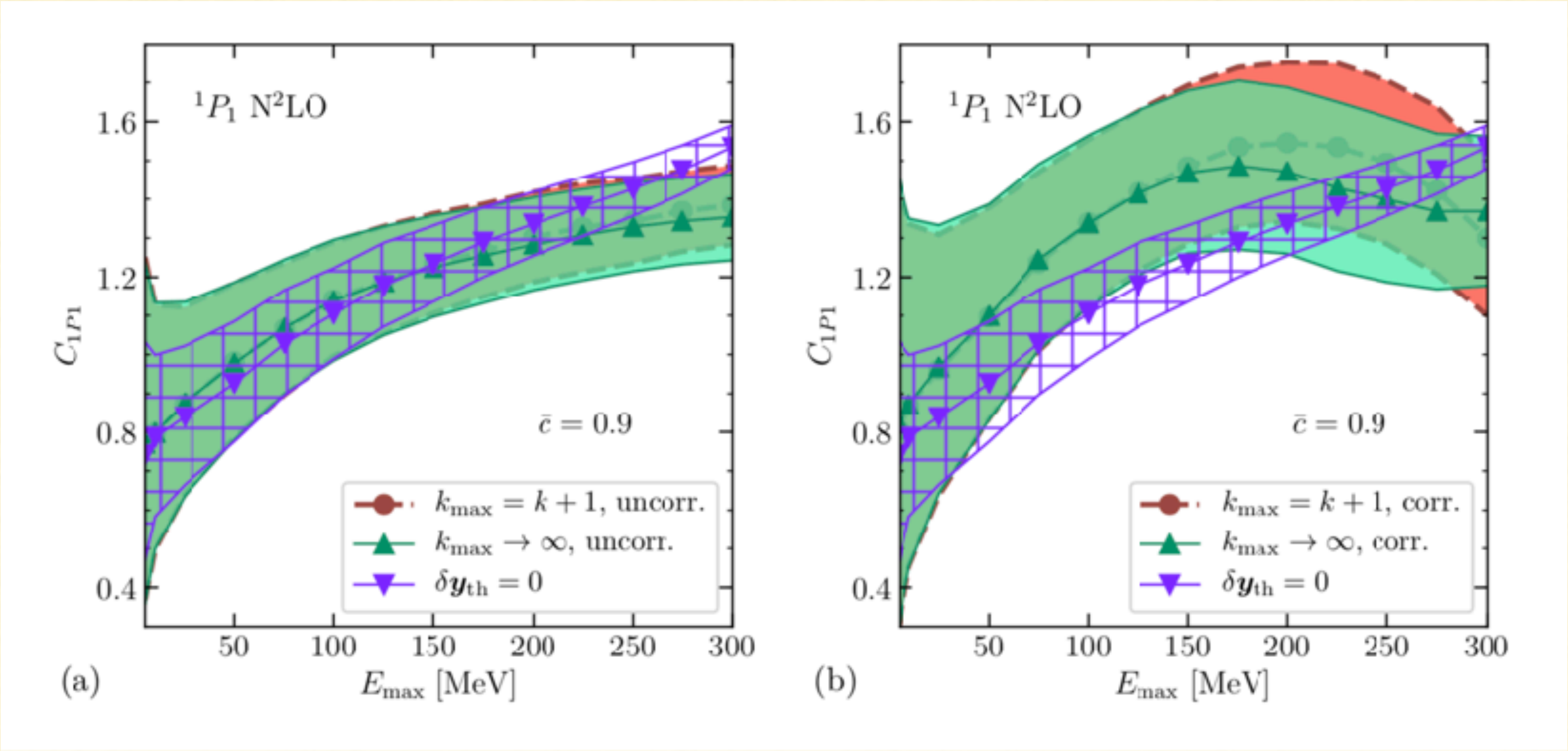
E_{max} plot in the $^1S_0$ at $O(Q^2)$

E_{max} plots: are parameter estimates stable with maximum energy of data?



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

Wesolowski et al., JPG 46, 045102

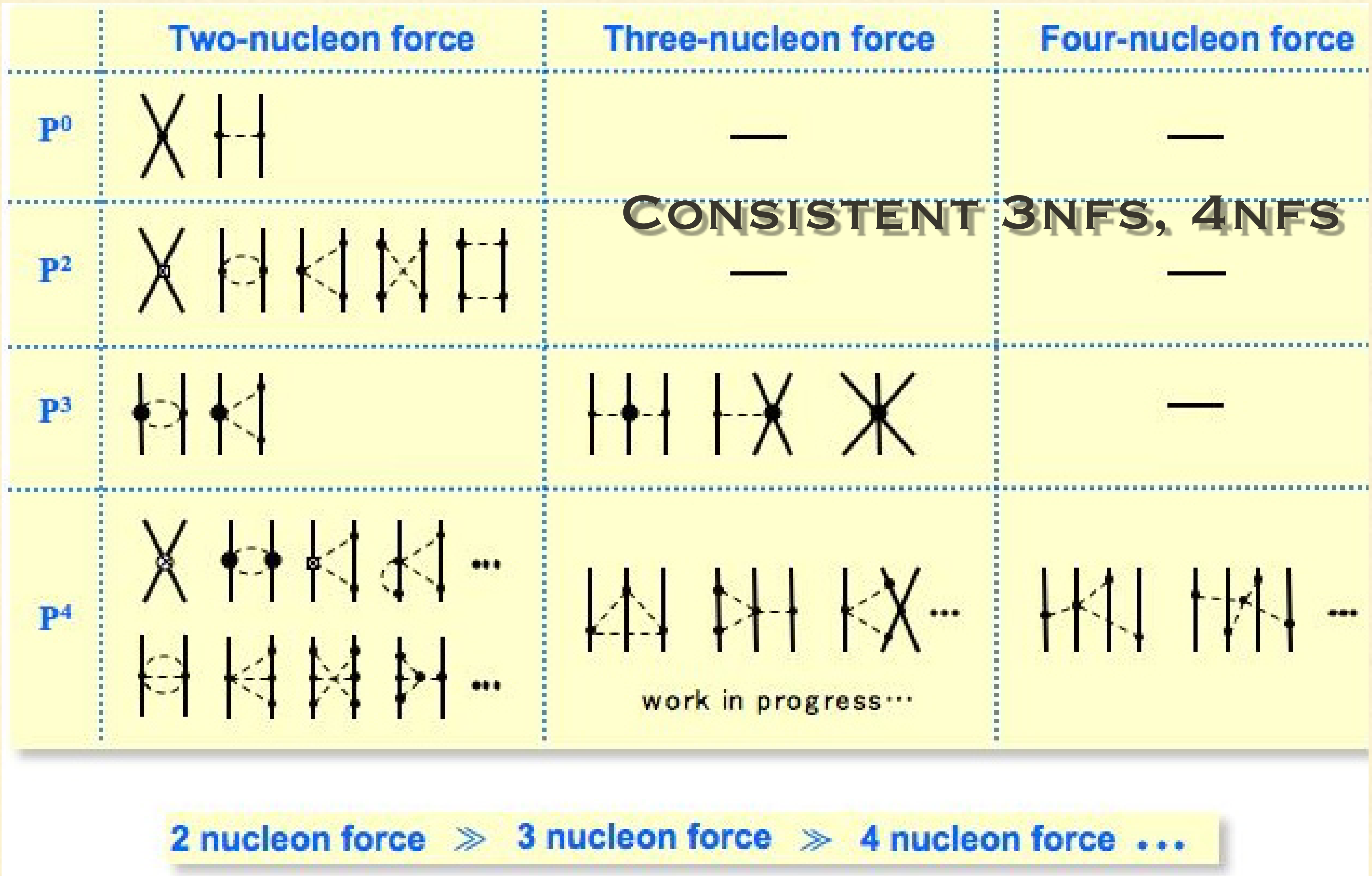


$$(\Sigma_{\rm th,uncorr})_{ij} = (\mathbf{y}_{\rm ref})^2 \bar{c}^2 \delta_{ij} \sum_{n=k+1}^{k_{\max}} Q_i^{2n} \qquad (\Sigma_{\rm th,corr})_{ij} = (\mathbf{y}_{\rm ref})_i (\mathbf{y}_{\rm ref})_j \bar{c}^2 \sum_{n=k+1}^{k_{\max}} Q_i^n Q_j^n$$

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

Next target: 3N potential

van Kolck (1994); Epelbaum et al. (2002)



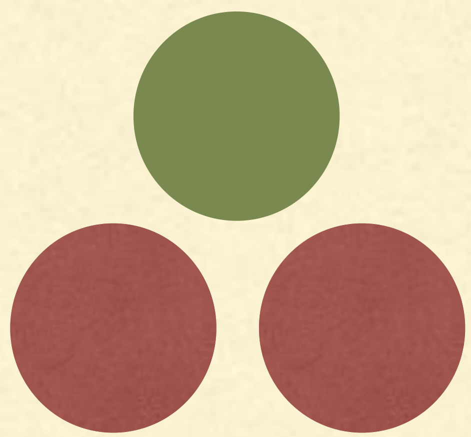
Two 3N potential parameters at $O(Q^3)$: c_D and c_E

3N data

Wesolowski, Ekström, Forssén, Melendez, Furnstahl, DP

For the moment we stick to bound-state observables

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



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

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

3N error model

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

All five observables have been measured to better than 1% precision: δy_{exp} is negligible compared to δy_{th}

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

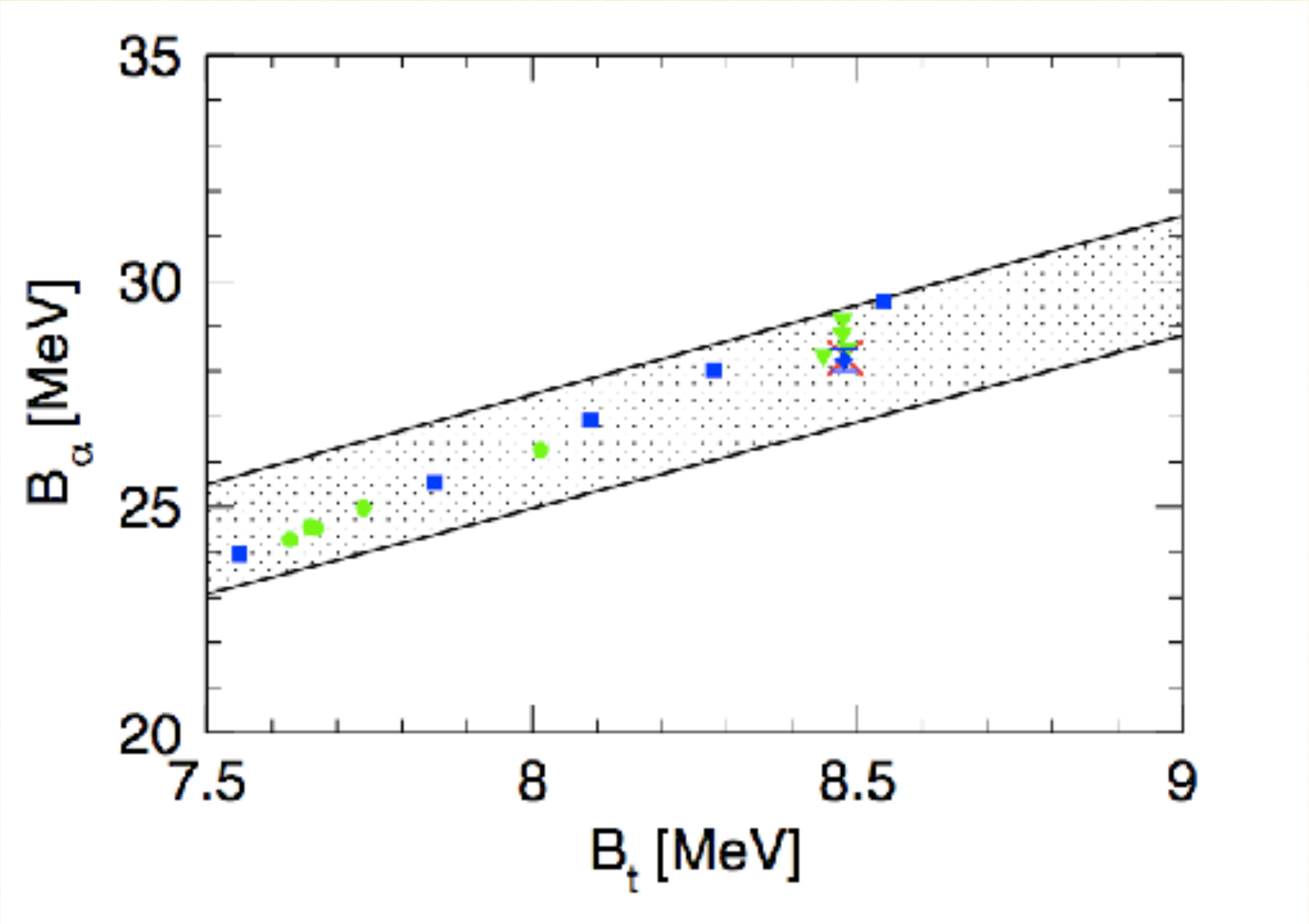
- This time Q is not obvious: we could infer it from convergence pattern of each observable. We will try $Q = m_\pi/\Lambda_b$ and see if it gives reasonable results
- To start take NN force as fitted separately: use two-body NNLO_{sim} or NNLO_{sep} [both $O(Q^3)$] with πN LECs from Roy-Steiner analysis
- Propagate uncertainties from NN and πN LECs to final result for c_D and c_E

Correlation structure

We want $\mathrm{pr}(c_D, c_E \,|\, \mathrm{3N\ data, NN\ posterior}, I)$ I: EFT error structure

Correlation structure of EFT errors may again be important

- Uncorrelated? $(\boldsymbol{\Sigma}_{\mathrm{th,uncorr}})_{ij} = (\mathbf{y}_{\mathrm{ref}})^2 \bar{c}^2 \delta_{ij} \sum_{n=k+1}^{k_{\max}} Q_i^{2n}$
- Different $\bar{c}$ for each observable?
- Correlations from universality?
- Correlations from cutoff variation in $O(Q^3)$ calculation?

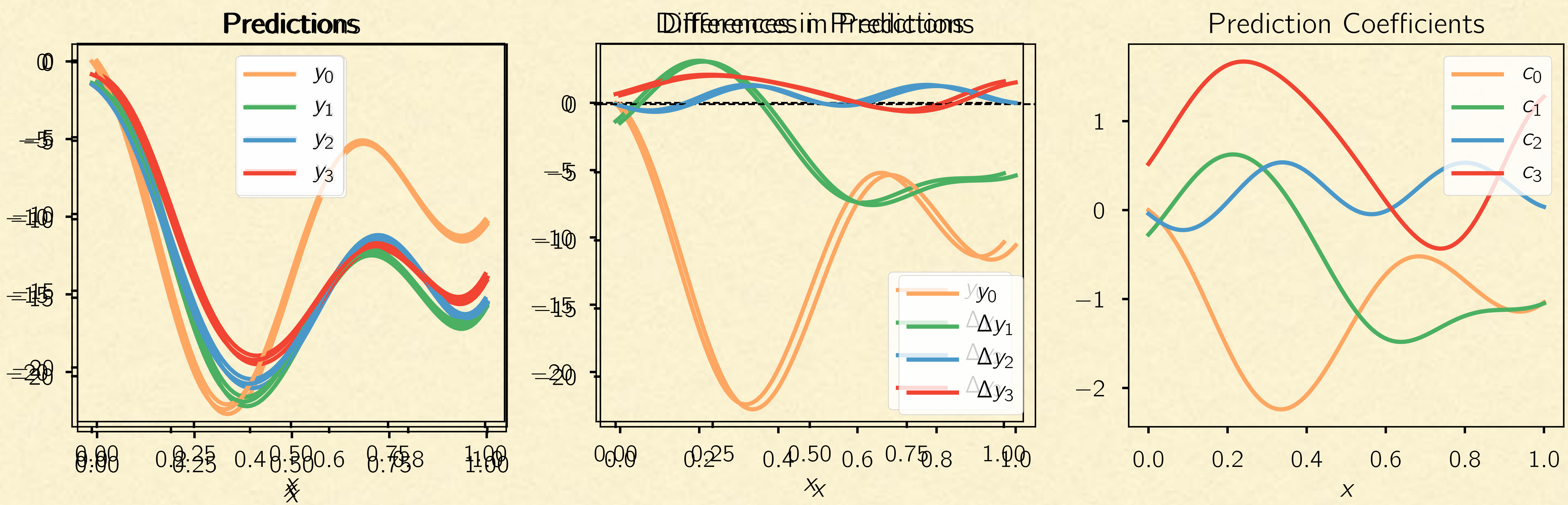


Platter, Hammer, Meißner (2005)

An EFT expansion in pictures

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

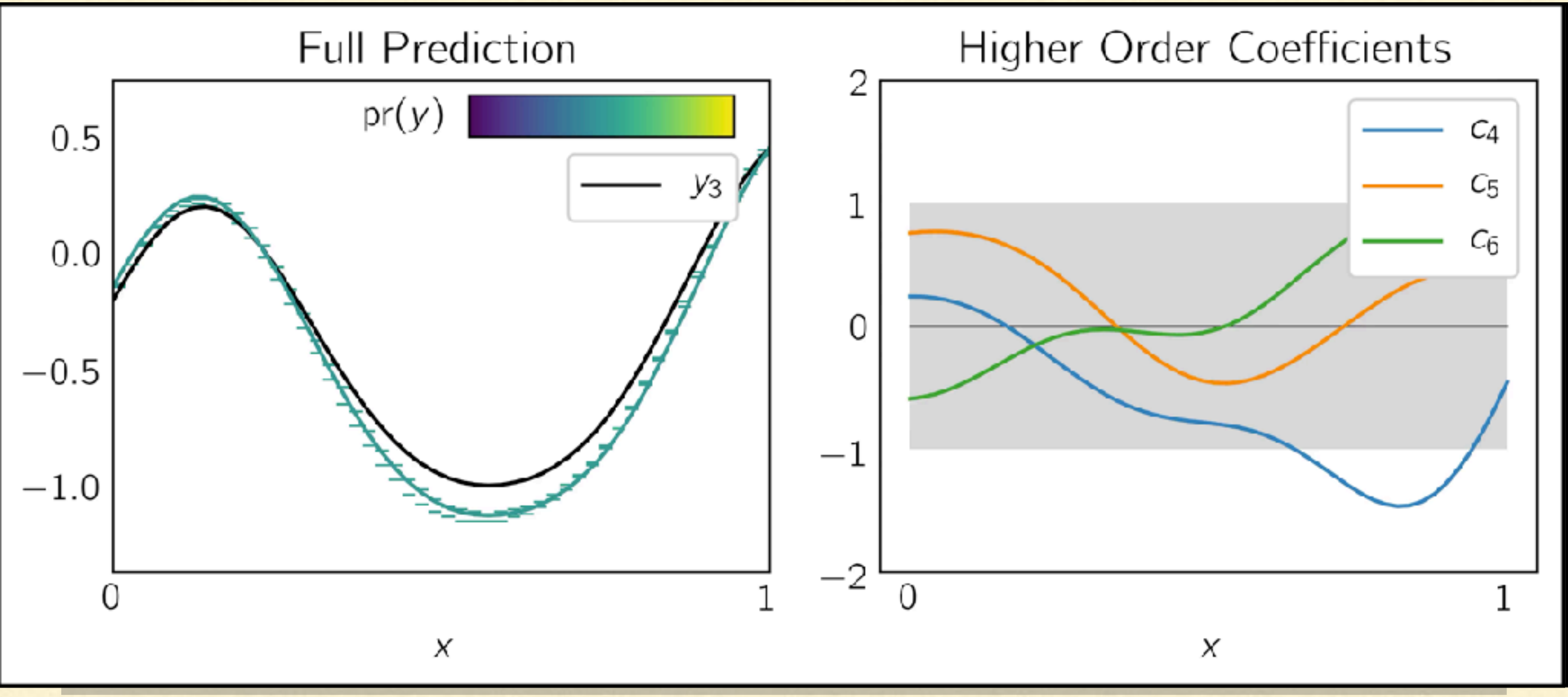
- General EFT series for observable to order k: $y = y_{\rm ref} \sum_{n=0}^{k} c_n Q^n$
- In ChiEFT $Q = \dfrac{(p, m_\pi)}{\Lambda_b}$; $\quad \Lambda_b \approx 600$ MeV



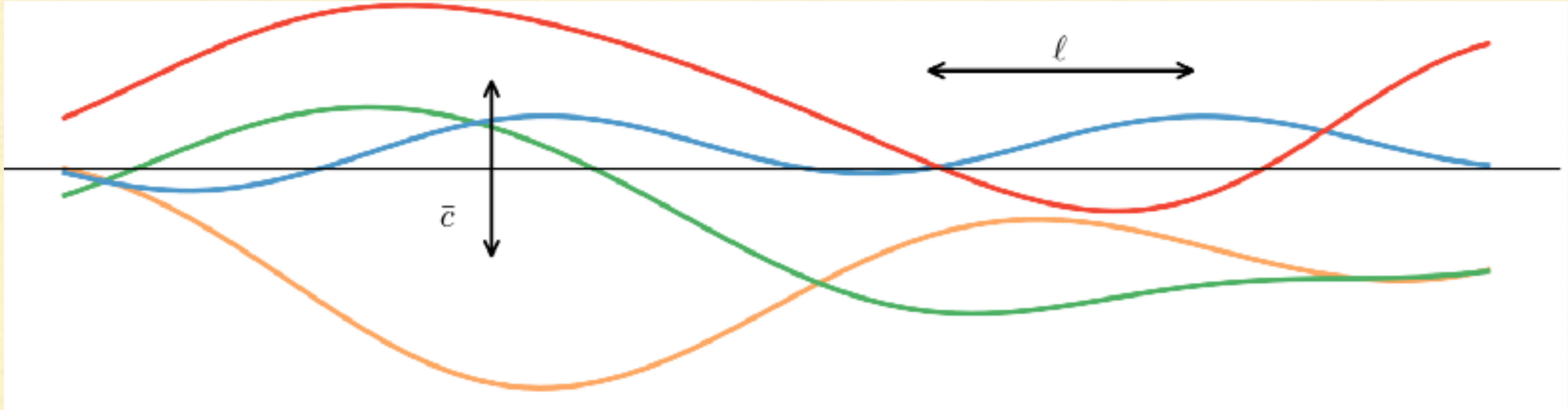
This is what a healthy observable expansion looks like: bounded coefficients, that do not grow or shrink with order.

Why GPs?

Assumptions about correlation structure have significant impact on parameter estimation, NN model assessments, physics extraction, ….



Hypothesis: the c_n's are a GP



GP describes "functional data" as

- Gaussian distribution at each point.
- With specified correlation structure.

Our hypothesis:

EFT coefficients at different orders can be modeled as:

- independent but identical realizations of one Gaussian Process;
- with a correlation structure; here we use a "squared exponential" (Gaussian) kernel, but we test it

Summary

- Bethe (Scientific American, 1953): "…in the past quarter century physicists have devoted a huge amount of experimentation and mental labor to [the NN] problem–probably more man-hours than have been given to any other scientific question in the history of mankind."
- Until recently most theory efforts did not account for theory uncertainty
- Including model discrepancy, i.e. EFT truncation errors, stabilizes and improves parameter estimates
- Simple modification to likelihood can account for this in two limits: uncorrelated or completely correlated truncation errors
- Need to understand how EFT truncation errors are correlated across kinematics: GP models of EFT-truncation errors for continuous data.
- Analysis of 3N observables needed for inference on 3N force. Interesting issues regarding expansion parameter and correlation structure.

ISNET 2.0 JPG focus issue

Focus on further enhancing the interaction between nuclear experiment and theory through information and statistics (ISNET 2.0)

Guest Editors

Dick Furnstahl Ohio State University

David Ireland University of Glasgow

Daniel Phillips Ohio University

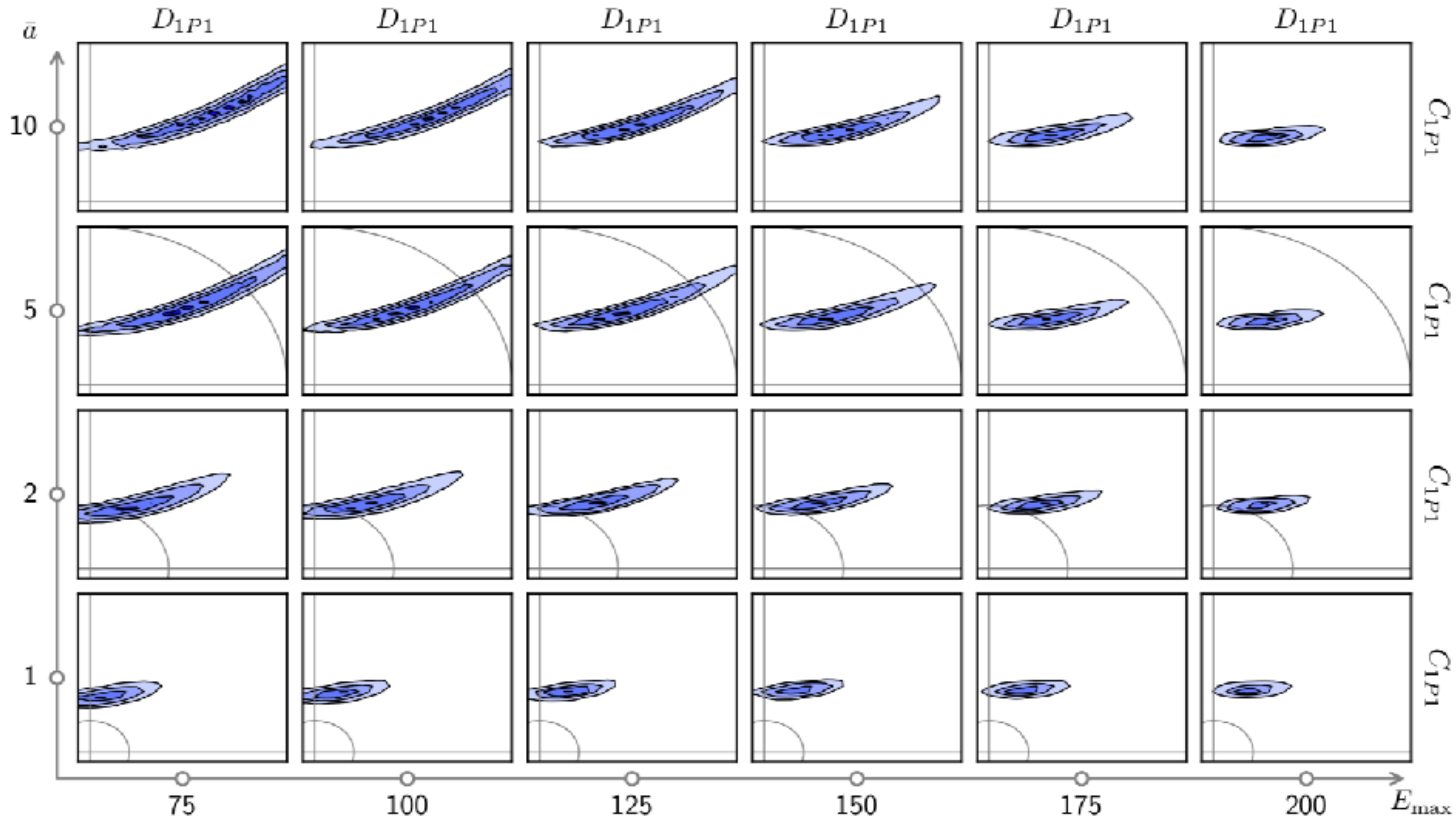
Following on from the hugely successful first edition in 2015, Journal of Physics G: Nuclear and Particle Physics is delighted to announce a second focus issue inspired by the ISNET workshops (Information and Statistics in Nuclear Experiment and Theory).

Two articles already published!

Please send more!

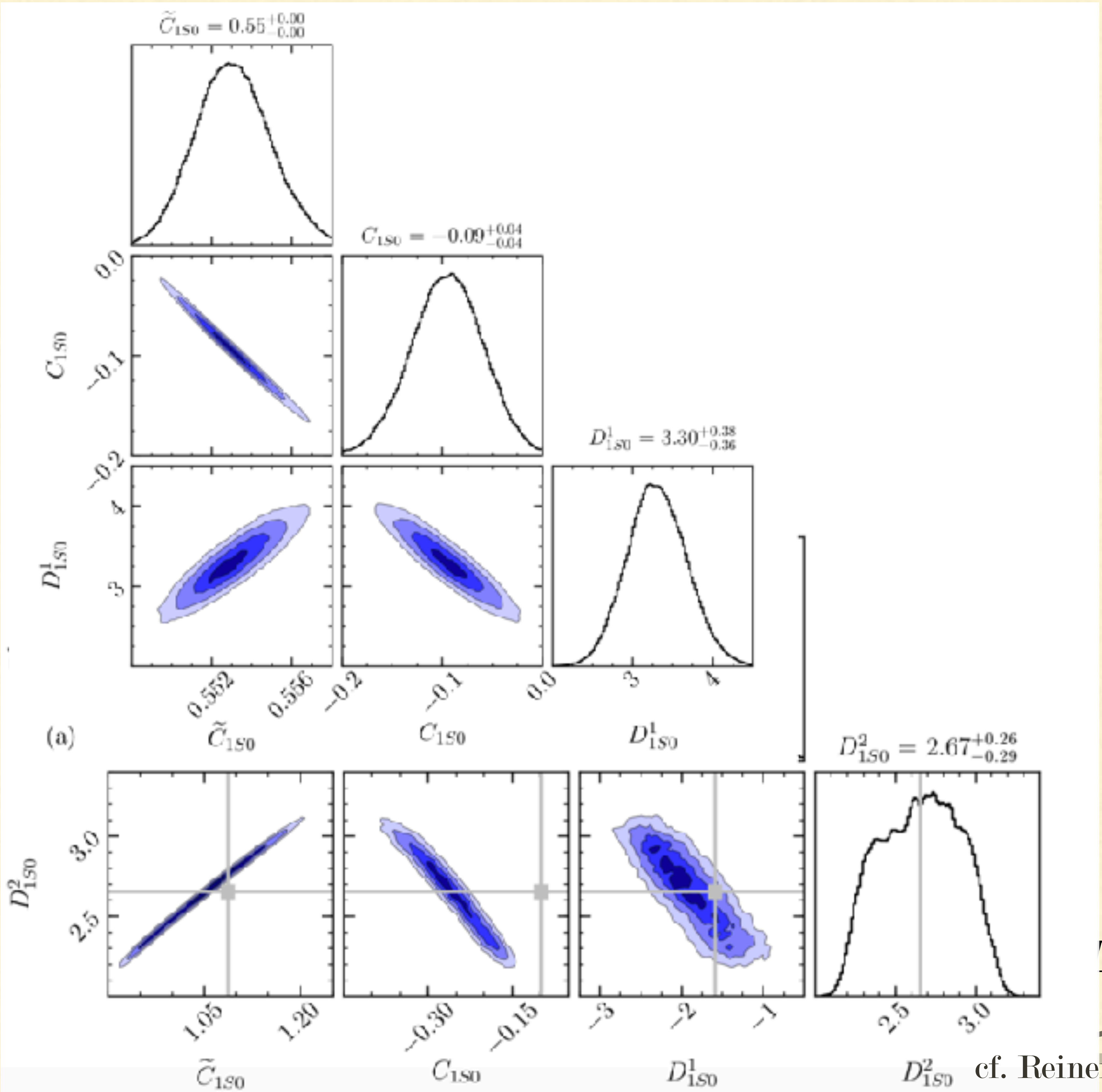
E_{max}-prior Tradeoffs

$^1P_1$ channel at $O(Q^4)$: two SD parameters



O(Q⁴): parameter degeneracy

Wesolowski et al., JPG 46, 045102



- Parameter estimation for NN potential in the $^1S_0$ channel at N3LO in the chiral EFT expansion
- Posterior plot allows diagnosis of parameter degeneracy $D^1{}_{(1S0)}$-$D^2{}_{(1S0)}$
- Which we also understand analytically

On-shell

$$D^1_{(1S0)} - 2D^2_{(1S0)})(p^2 - p'^2)^2 \,, \xrightarrow{\quad} 0$$

cf. Reinert, Krebs, Epelbaum, EPJA, 54, 86 (2018)