Fast & rigorous constraints on chiral three-nucleon forces from few-body observables

Sarah Wesolowski
Department of Mathematical Sciences
Salisbury University

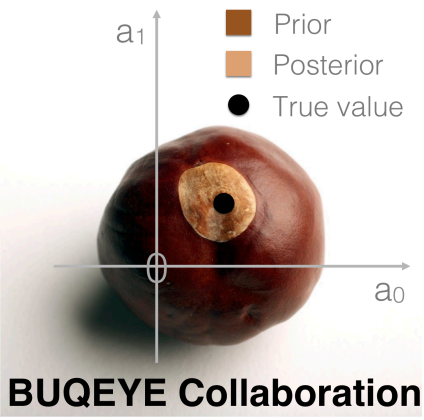
Institute for Nuclear Theory Program 21-1b

April 27th, 2021

Thanks to my collaborators

Presenting work today from [arXiv:2104.04441]

Bayesian uncertainty quantification: errors for your EFT



Andreas Ekström
Dick Furnstahl
Christian Forssén
Jordan Melendez
Daniel Phillips
Isak Svensson

Visit us online at buqeye.github.io for Jupyter notebooks and software

Fast & rigorous constraints on chiral 3NFs from few-body observables

Estimate constraints on c_D and c_E from few-body data

sw et al. [arXiv:2104.04441]

- Explore different combinations of $A = 3,\ 4$ bound-state observables
- Exemplify statistical best practices for EFT parameter estimation
  sw et al. 2019 JPhysG **46** 045102
- Include EFT truncation error— and estimate it
- Implement eigenvector continuation (EC) emulators for fast evaluations
  Frame et al. 2018 PRL **121** 032501
  König et al. 2020 PLB **810** 135814
- DIY: Train your own emulators using your interaction
  OR use our emulators

This is a particular example, but the points are more general

The three nucleon force in chiral EFT

Chiral EFT (χEFT) nuclear forces

Delta-less, Weinberg power counting

Three-body forces emerge at NNLO

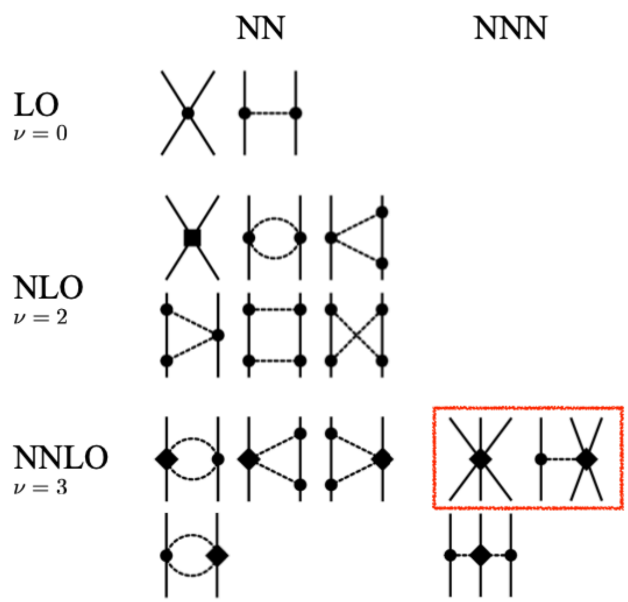
Expected size of next order: Q^4

Contribute on-shell to $A \geq 3$ systems

Estimated from $A \geq 3$ observables

Three terms

- Pure contact: contains c_E
- 2N-1π: contains c_D
- Fujita-Miyazawa
  Fujita+Miyazawa 1957



Carlsson et al. 2016 PRX **6** 011019

Our pdf for c_D and c_E

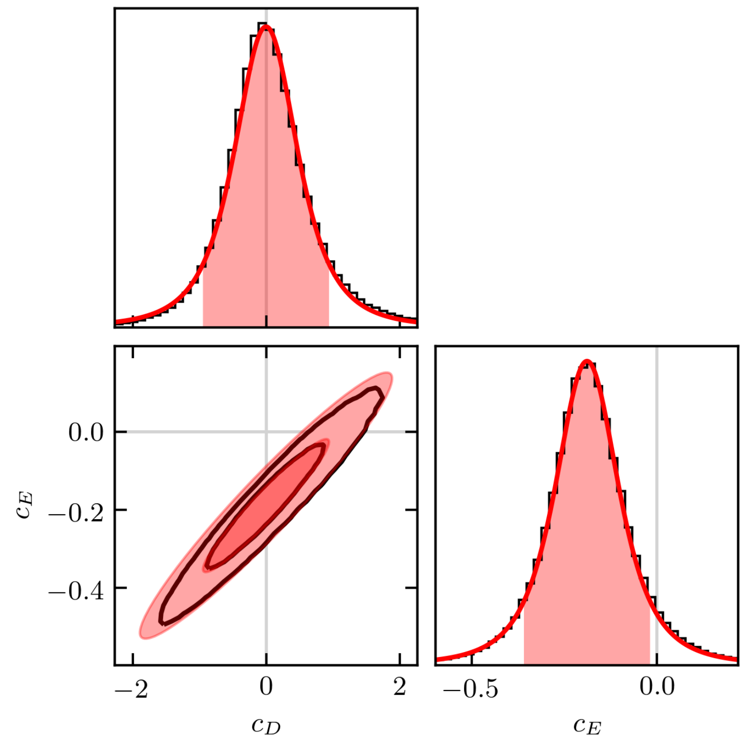
MCMC samples of the probability distribution (pdf) $\mathrm{pr}(c_D, c_E | \mathbf{y}_{\rm exp}, I)$

The data $\mathbf{y}_{\rm exp}$ are

- ^{3}H ground state energy
- ^{3}H β-decay half-life
- ^{4}He ground state energy
- ^{4}He charge radius

Background information I includes

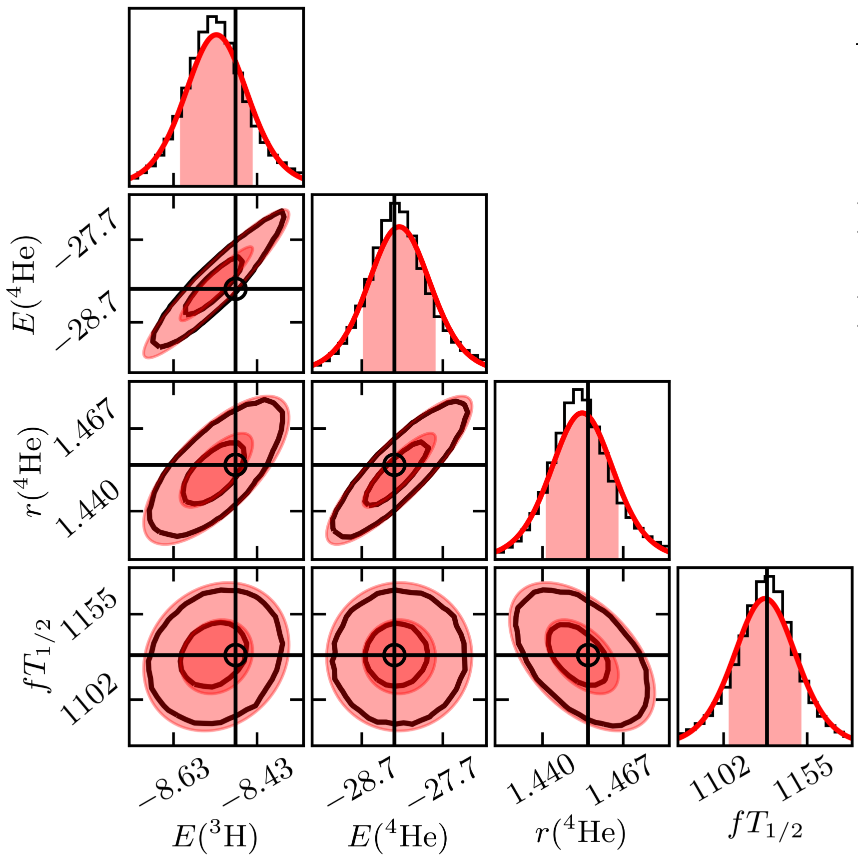
- truncation error [CRUCIAL]
- input NN LECs and covariance
- fixed πN LECs
- data and method errors



sw et al. [arXiv:2104.04441]

Posterior predictive distribution

Propagate errors from pdf for c_D and c_E to fit observables



Analysis is statistically consistent

Some observables highly correlated

But some are less correlated!

Not necessary to have perfect "bulls-eyes"- these are pdfs!

So what was all that "background information", really?

And how do our results depend on those assumptions?

The full pdf we estimated

$$\mathrm{pr}(\vec{a}, Q, \bar{c}^2 \,|\mathbf{y}_{\mathrm{exp}}, I)$$

The LEC vector $\vec{a}$ includes 13 entries:

- Vector of 9^* NN LECs $\vec{a}_{\mathrm{NN}}$
  (11 including isospin breaking)
- 3N LECs $c_D, \ c_E$

The full pdf we estimated

$$\mathrm{pr}(\vec{a}, Q, \bar{c}^2 \,|\mathbf{y}_{\exp}, I)$$

The LEC vector $\vec{a}$ includes 13 entries:

- Vector of 9* NN LECs $\vec{a}_{\mathrm{NN}}$
  (11 including isospin breaking)
- 3N LECs $c_D,\ c_E$

The random variables Q and $\bar{c}^2$ parametrize EFT truncation error

A few-body observable computed order-by-order in EFT is assumed to follow

$$y_{\mathrm{k}} = y_{\mathrm{ref}} \sum_{n=1}^{k} c_n Q^k$$

$\bar{c}^2$ is a variance that describes the size of c_n's
y_{ref} is dimensionful characteristic observable size

If the EFT is well-behaved we expect $\bar{c} \sim 1$ and $0 < Q < 1$

Melendez, sw, et al. 2019 PRC **100** 044001

The likelihood and sources of error

$$\mathrm{pr}(\vec{a}, Q, \bar{c}^2 | \mathbf{y}_{\mathrm{exp}}, I) \propto \mathrm{pr}(\mathbf{y}_{\mathrm{exp}} | \vec{a}, \Sigma, I)\, \mathrm{pr}(\vec{a}|I)\;\; \mathrm{pr}(\bar{c}^2 | Q, \vec{a}, I)\;\; \mathrm{pr}(Q|\vec{a}, I)$$

Likelihood: $\mathrm{pr}(\mathbf{y}_{\mathrm{exp}} | \vec{a}, \Sigma, I) \sim \mathcal{N}(\mathbf{y}_{\mathrm{th}}(\vec{a}),\; \Sigma_{\mathrm{exp}} + \Sigma_{\mathrm{method}} + \Sigma_{\mathrm{th}})$

Gaussian likelihood (looks like χ^2) but different variance

Method and experimental error matrices $\Sigma_{\mathrm{exp}} + \Sigma_{\mathrm{method}}$ are diagonal

Theory error matrix Σ_{th} includes truncation error

- Diagonal here
  means truncation error of different FB observables independent
- Depends explicitly on EFT expansion parameter Q
- Variance estimation problem!
  EFT parameter estimation helps us estimate EFT expansion parameter!

The likelihood and sources of error

$$\mathrm{pr}(\vec{a}, Q, \bar{c}^2 | \mathbf{y}_{\mathrm{exp}}, I) \propto \mathrm{pr}(\mathbf{y}_{\mathrm{exp}} | \vec{a}, \Sigma, I)\, \mathrm{pr}(\vec{a}|I)\;\; \mathrm{pr}(\bar{c}^2|Q, \vec{a}, I)\;\; \mathrm{pr}(Q|\vec{a}, I)$$

Likelihood: $\mathrm{pr}(\mathbf{y}_{\mathrm{exp}}|\vec{a}, \Sigma, I) \sim \mathcal{N}(\mathbf{y}_{\mathrm{th}}(\vec{a}),\; \Sigma_{\mathrm{exp}} + \Sigma_{\mathrm{method}} + \Sigma_{\mathrm{th}})$

Gaussian likelihood (looks like χ^2) but different variance

Method and experimental error matrices $\Sigma_{\mathrm{exp}} + \Sigma_{\mathrm{method}}$ are diagonal

Theory error matrix Σ_{th} includes truncation error

- Diagonal here
  means truncation error of different FB observables independent
- Depends explicitly on EFT expansion parameter Q
- Variance estimation problem!
  EFT parameter estimation helps us estimate EFT expansion parameter!

Now let's discuss the priors

Development of priors

$$\mathrm{pr}(\vec{a}, Q, \bar{c}^2 \,|\, \mathbf{y}_{\mathrm{exp}}, I)$$

The priors on the LECs in $\vec{a}$

- 11 NN LECs $\vec{a}_{\mathrm{NN}}$ the input prior includes
  - the NN optimum from fitting to 2B data
    our fit was new but roughly follows Carlsson et al. 2016 PRX **6** 011019
  - the covariance matrix from this optimization
- This tightly constrains the NN LECS from leaving their optimum

Development of priors

$$\mathrm{pr}(\vec{a}, Q, \bar{c}^2 | \mathbf{y}_{\mathrm{exp}}, I)$$

The priors on the LECs in $\vec{a}$

- 11 NN LECs $\vec{a}_{\mathrm{NN}}$ the input prior includes
    - the NN optimum from fitting to 2B data
      our fit was new but roughly follows Carlsson et al. 2016 PRX **6** 011019
    - the covariance matrix from this optimization
- This tightly constrains the NN LECS from leaving their optimum
- The 3N LECs $c_D,\ c_E$ are assumed to be naturally sized
- Loose prior parametrized by a Gaussian mean 0 with std. dev. $\bar{a} = 5$

Development of priors

$$\mathrm{pr}(\vec{a}, Q, \bar{c}^2 \,|\, \mathbf{y}_{\mathrm{exp}}, I)$$

The priors on the truncation error parameters Q and $\bar{c}^2$
Melendez, sw, et al. 2019 PRC **100** 044001

- Start with order-by-order calculations of these few-body observables
  - ^{3}H binding energy, ^{4}He binding energy and radius
    3He excluded as an isospin mirror: its convergence pattern is highly correlated
  - Exclude the triton half-life $fT_{1/2}$ due to irregular convergence
  - Deuteron can be used, but doesn't make much difference + $A < 3$
- Use the NLO to NNLO observable shift only
  The weak binding of these nuclei makes the LO to NLO shift large, so this is excluded
- Assume $0 < Q < 1$
- For χEFT, additionally expect $Q < 1/2$
  The possibility that Q > 1/2 is not completely excluded
- Q also plays a role in Σ_{th} in the likelihood [sensitive dependence on $(Q^4)^2$]

Sampling of the pdf

$$\mathrm{pr}(\vec{a}, Q, \bar{c}^2 \,|\mathbf{y}_{\mathrm{exp}}, I)$$

The priors on the truncation error parameters Q and $\bar{c}^2$

The entire pdf is sampled with MCMC over 13 + 2 dimensions

A few more notes of interest

- The NLO to NNLO shift is recalculated every time $\vec{a}$ changes
- Doable on a laptop in a few hours because eigenvector continuation (EC)
- NN LECs part of $\vec{a}$ with prior values+covariance from optimization = propagation of uncertainty from the NN sector!
  This lets you propagate error from NN without doing the NN fit simultaneously

Why didn't you include πN LECs in this?

A trivial extension of $\vec{a}$ to include the three NNLO LECs

$$c_1,\ c_3,\ c_4$$

is possible given optimum and covariances from e.g., Roy-Steiner analysis
Hoferichter et al. 2015 PRL **115** 192301
Hoferichter et al. 2016 Physics Reports **625** 1

Our input optimization of the NN force was not simultaneous with πN sector
In principle this can be done as NNLOsim was in the future

We fixed these using RS analysis values and have covariance available

BUT we do not have crucial covariance between the NN and πN LECs

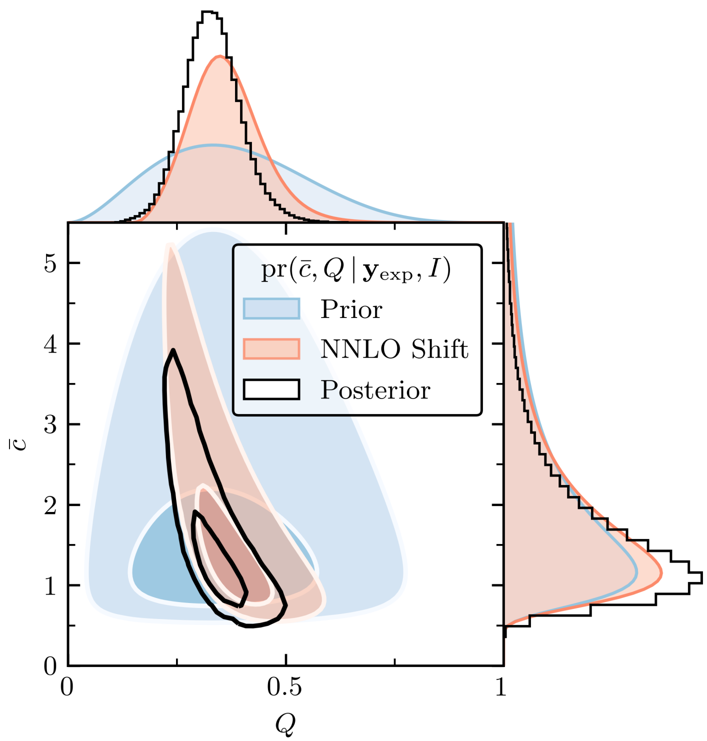
If we do it anyway, the NN optimum becomes distorted in sampling

This distorts the results for $c_D,\ c_E$

Results for Q and $\bar{c}^2$

$$\mathrm{pr}(\vec{a}, Q, \bar{c}^2 | \mathbf{y}_{\mathrm{exp}}, I) , \qquad y_{\mathrm{k}} = y_{\mathrm{ref}} \sum_{n=1}^{k} c_n Q^k , \quad \bar{c}^2 \text{ variance for } c_n\text{'s}$$

Integrate out $\vec{a}$: in MCMC this just means plotting only Q, $\bar{c}^2$ dimensions



Prior: loose starting assumptions

NNLO shift (recalculated at each $\vec{a}$)

Posterior: $Q \sim 1/3$

Since this is simultaneous with estimation of $\vec{a}$, this is what the data prefer for size of N^{3}LO uncertainty

EC for fast observable evaluations

MCMC sampling is facilitated by eigenvector continuation (EC)

We are solving the A-body problem

$$H(\vec{a})|\psi(\vec{a})\rangle = E(\vec{a})|\psi(\vec{a})\rangle$$

many times as we sample $\vec{a}$

Solution: train EC emulators on a sampling of N_{EC} points in $\vec{a}$ space

Project Hamiltonian (and other observables) into $N_{\mathrm{EC}} \times N_{\mathrm{EC}}$ subspace

Our Hamiltonians are in a HO basis computed in NCSM
Similar to König et al. 2020 PLB **810** 135814

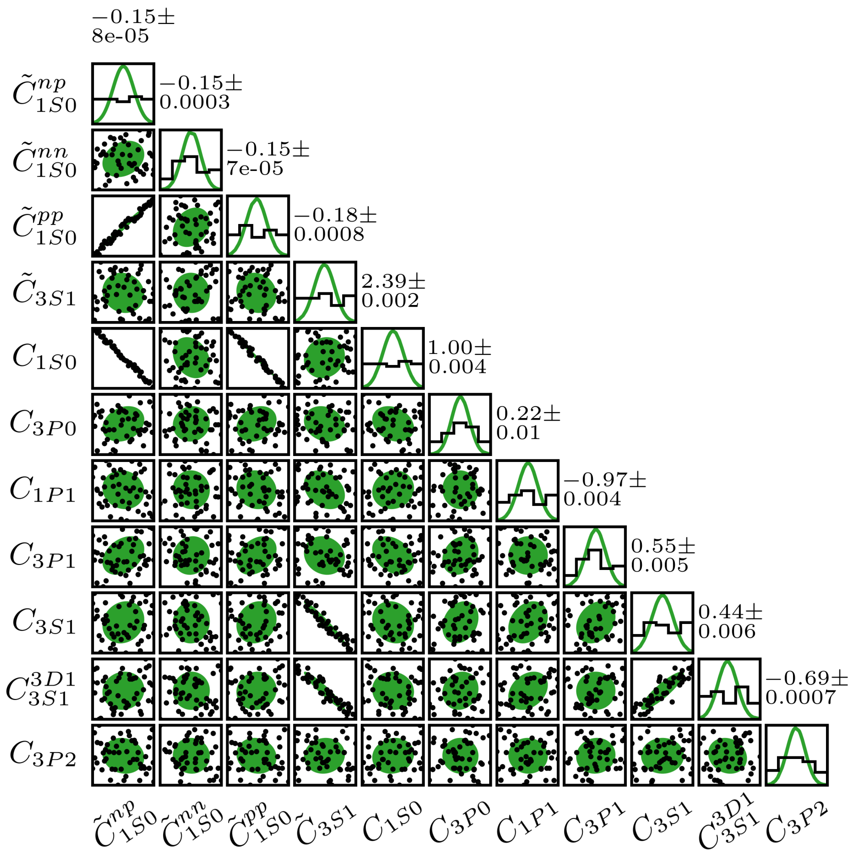
Observable evaluations go from ~ 1 minute to 10 ms

The emulator training only needs to be done once at the beginning

Emulators take up little disk space making them portable and easy to share

Training our EC emulators

We use $N_{\mathrm{EC}} = 50$ training points in this work



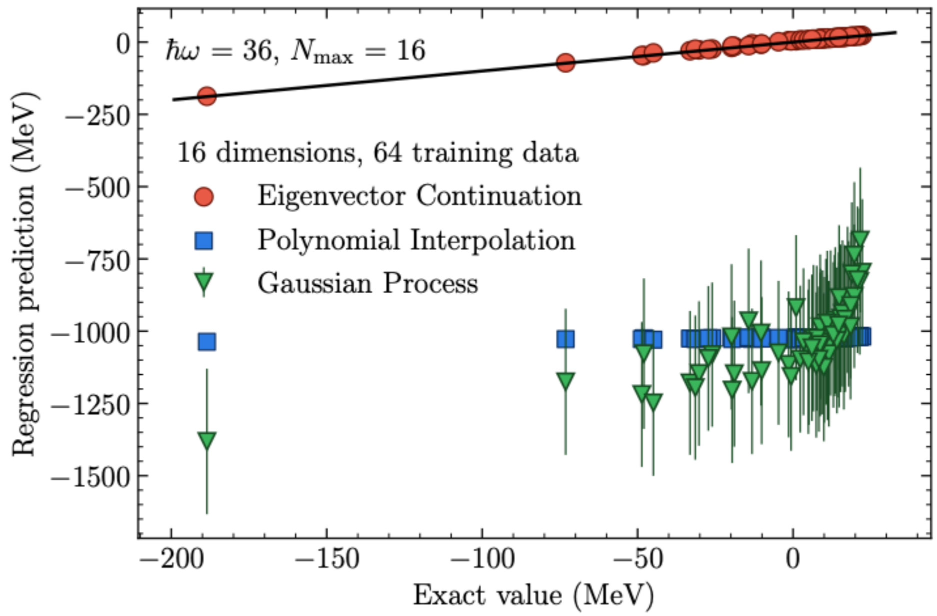
NN training points near optimum

c_D and c_E both spread over $[-5, 5]$

We are generally interpolating

Accuracy of emulators

This was explored in detail by König et al.
König et al. 2020 PLB **810** 135814

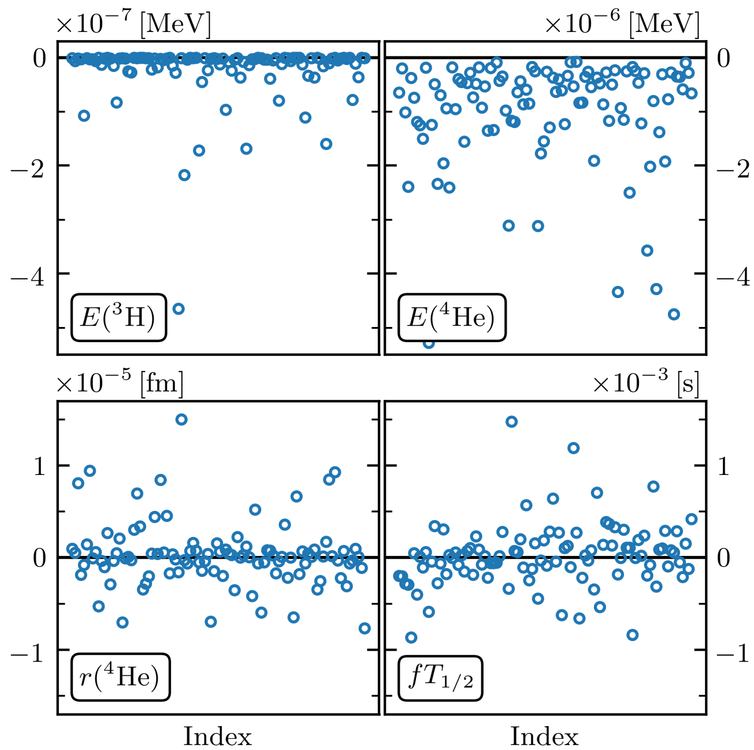


Comparison of results for ^{4}He binding energies

Interpolation with 64 training points in the full 16 LEC dimensions

Accuracy of emulators

Our emulators give very accurate results for observables



Residuals between exact and emulator

Validation points shown

Error negligible compared to NCSM/expt. ("adopted errors")

Emulator provides upper bounds for energies

Again: Our pdf for c_D and c_E

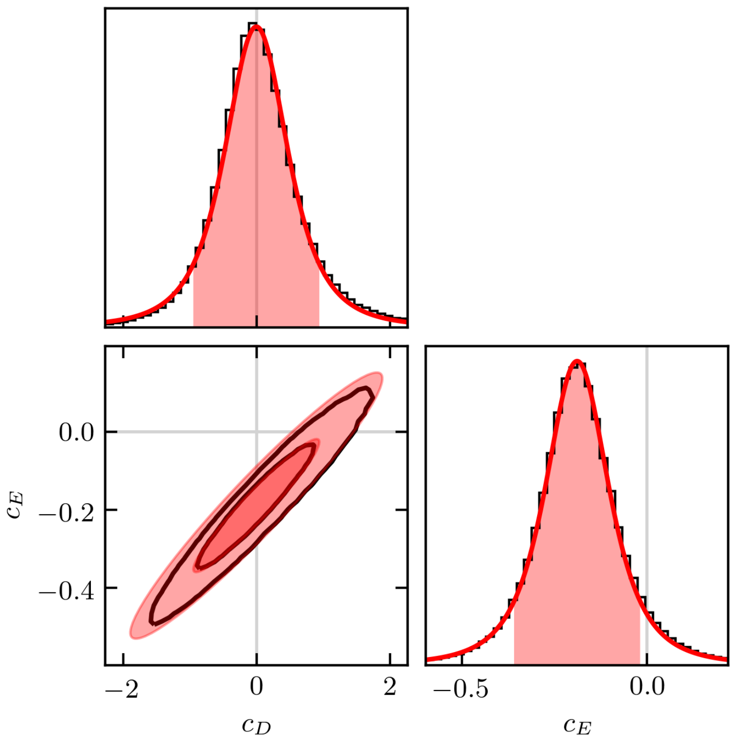
MCMC samples of the probability distribution (pdf) $\mathrm{pr}(c_D, c_E | \mathbf{y}_{\rm exp}, I)$

The data $\mathbf{y}_{\rm exp}$ are

- ^{3}H ground state energy
- ^{3}H β-decay half-life
- ^{4}He ground state energy
- ^{4}He charge radius

Background information I includes

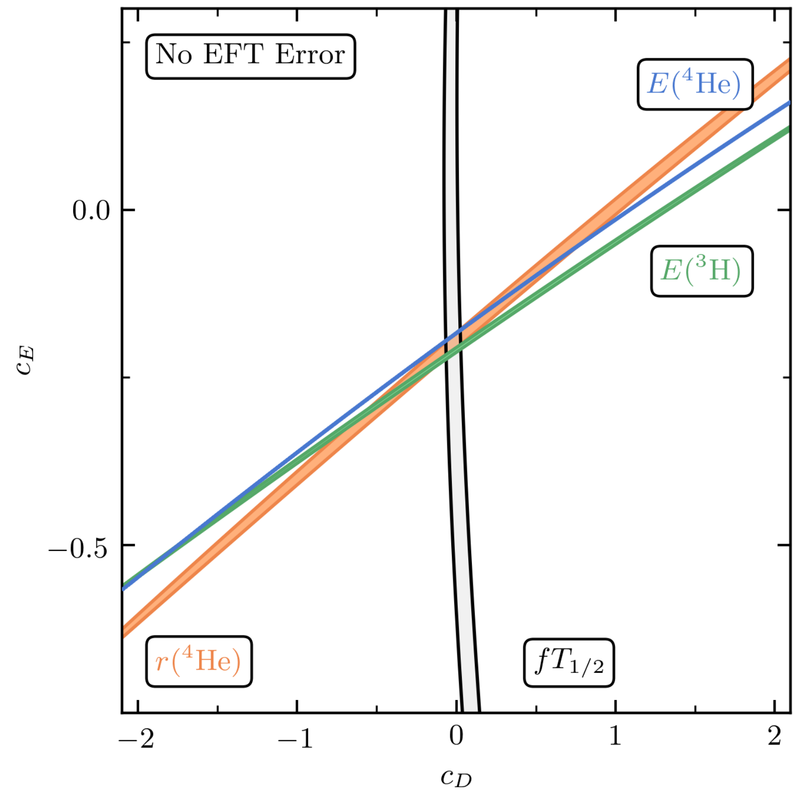
- truncation error [CRUCIAL]
- input NN LECs and covariance
- fixed πN LECs
- data and method errors



sw et al. [arXiv:2104.04441]

One-by-one observable analysis

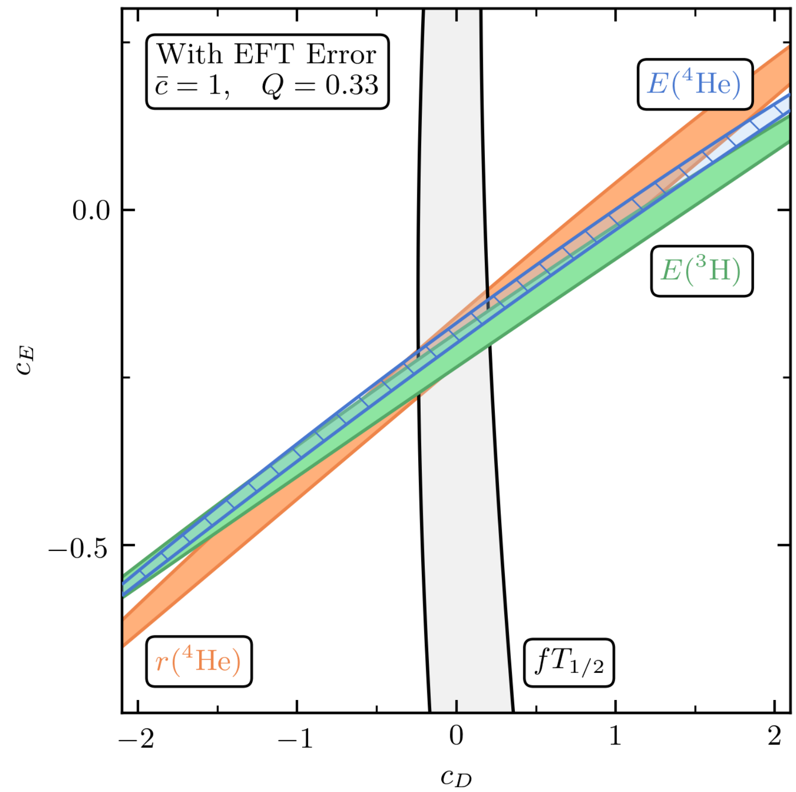
What constraints are provided by each of our available observables?
no truncation error included here



Note: no mutual overlap is possible without truncation error!

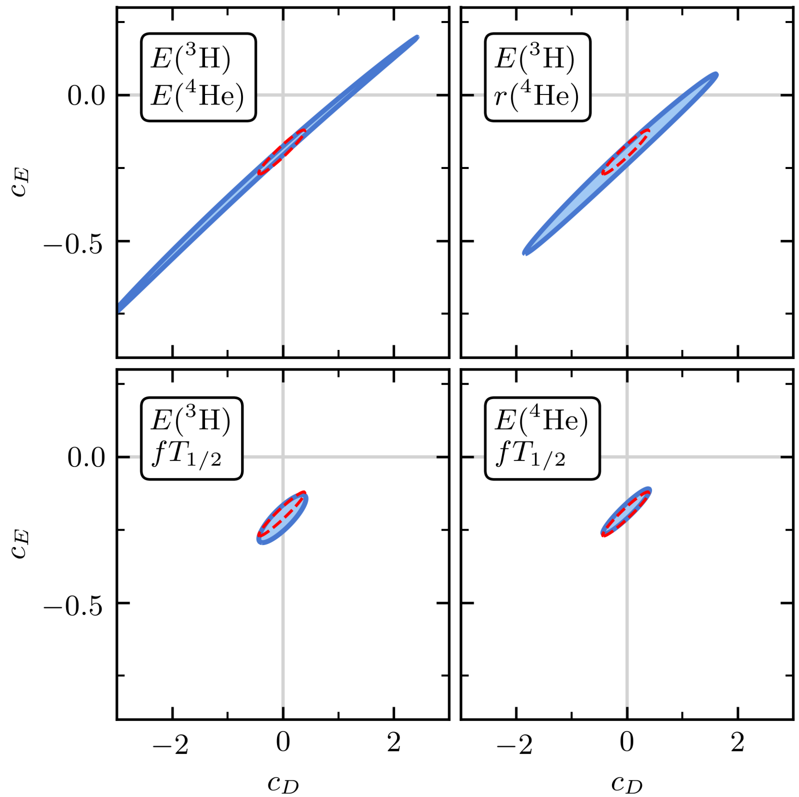
One-by-one observable analysis

What constraints are provided by each of our available observables?
Now include truncation error but $Q = 0.33$ and $\bar{c} = 1$



Truncation error parameters must be fixed: single datum doesn't provide enough constraint

Observable pairs analysis



Truncation error included but fixed

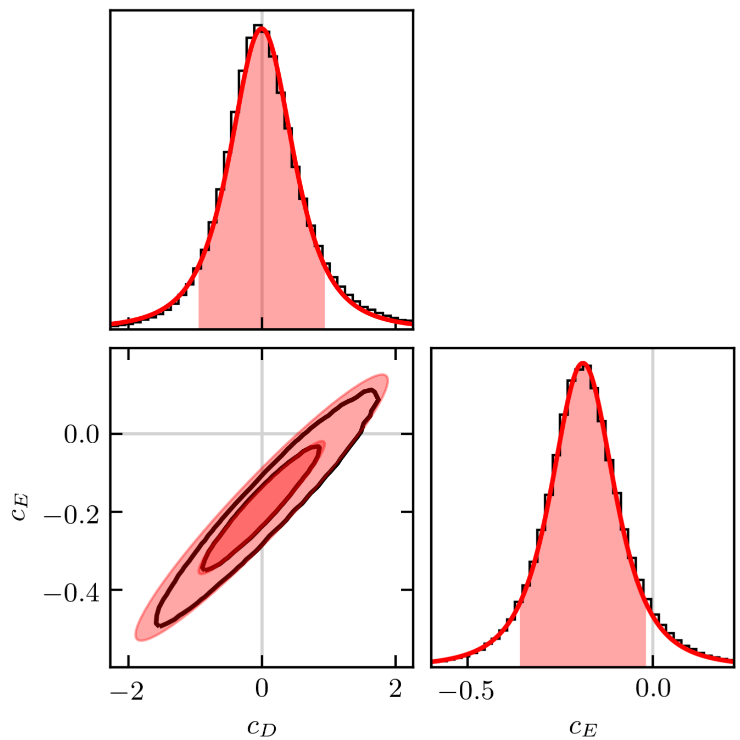
Fixing EFT error makes pdfs Gaussian!

We STILL need truncation error marginalization to get the tails right!

Use all observables possible, but not only degenerate observables!

The pdf for c_D and c_E is t-distributed

Those contours might not mean what you think they mean...



Observables are approximately linear in c_D and c_E

$Q, \bar{c}^2$ enter likelihood variance and are marginalized over

Without this marginalization, we lose the t shape

Takeaway points

sw et al. [arXiv:2104.04441]

- For 3NF parameter estimation, don’t only use observables that are related by universality

Takeaway points

sw et al. [arXiv:2104.04441]

- For 3NF parameter estimation, don't only use observables that are related by universality
- The LECs c_D and c_E are strongly correlated

Takeaway points

sw et al. [arXiv:2104.04441]

- For 3NF parameter estimation, don't only use observables that are related by universality
- The LECs c_D and c_E are strongly correlated
- Truncation errors must be included for complete UQ

Takeaway points

sw et al. [arXiv:2104.04441]

- For 3NF parameter estimation, don't only use observables that are related by universality
- The LECs c_D and c_E are strongly correlated
- Truncation errors must be included for complete UQ
- Impact of including NN LEC uncertainties on the c_D-c_E posterior is small

  That of π N LECs remains to be assessed

Takeaway points

sw et al. [arXiv:2104.04441]

- For 3NF parameter estimation, don't only use observables that are related by universality
- The LECs c_D and c_E are strongly correlated
- Truncation errors must be included for complete UQ
- Impact of including NN LEC uncertainties on the c_D-c_E posterior is small

  That of π N LECs remains to be assessed
- The EFT expansion parameter is $Q \approx 1/3$ for these observables

Takeaway points

sw et al. [arXiv:2104.04441]

- For 3NF parameter estimation, don't only use observables that are related by universality
- The LECs c_D and c_E are strongly correlated
- Truncation errors must be included for complete UQ
- Impact of including NN LEC uncertainties on the c_D-c_E posterior is small

  That of π N LECs remains to be assessed
- The EFT expansion parameter is $Q \approx 1/3$ for these observables
- χEFT gives a statistically consistent description of these FB observables

Takeaway points

sw et al. [arXiv:2104.04441]

- For 3NF parameter estimation, don't only use observables that are related by universality
- The LECs c_D and c_E are strongly correlated
- Truncation errors must be included for complete UQ
- Impact of including NN LEC uncertainties on the c_D-c_E posterior is small

  That of π N LECs remains to be assessed
- The EFT expansion parameter is $Q \approx 1/3$ for these observables
- χEFT gives a statistically consistent description of these FB observables
- Not all distributions are Gaussian!

Takeaway points

sw et al. [arXiv:2104.04441]

- For 3NF parameter estimation, don't only use observables that are related by universality
- The LECs c_D and c_E are strongly correlated
- Truncation errors must be included for complete UQ
- Impact of including NN LEC uncertainties on the c_D-c_E posterior is small

  That of π N LECs remains to be assessed
- The EFT expansion parameter is $Q \approx 1/3$ for these observables
- χEFT gives a statistically consistent description of these FB observables
- Not all distributions are Gaussian!

Thanks again to Andreas Ekström, Dick Furnstahl, Christian Forssén, Jordan Melendez, Daniel Phillips, and Isak Svensson!