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

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with Sarah Wesolowski, Isak Svensson, Andreas Ekström, Christian Forssén, Dick Furnstahl, and Jordan Melendez

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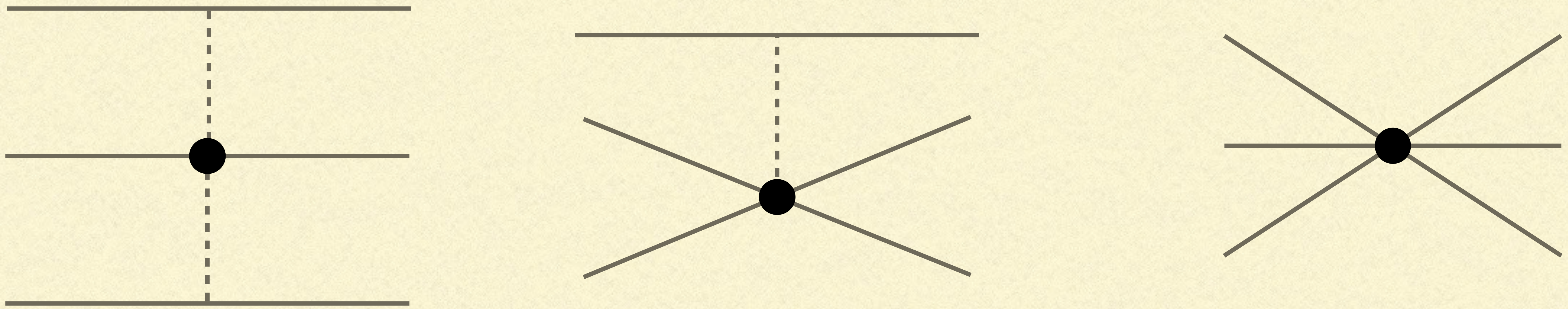
The importance of the three-nucleon force in Chiral Effective Field Theory

- In EFTs three-body forces inevitably arise because degrees of freedom are integrated out
- In χEFT without an explicit $\Delta(1232)$ three-nucleon forces (3NFs) appear at $O(Q^3)$ (NNLO)

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



- Depends on two parameters, c_D and c_E, once πN low-energy constants (LECs) are fixed
- This 3NF has small but important effects in light nuclei and helps drive saturation in heavier systems and symmetric nuclear matter
- <u>Goal here:</u> estimate c_D and c_E from few-nucleon data **including χEFT truncation error**

Few-nucleon physics implementation

- No-Core Shell Model calculations of A=3 and A=4 bound-state observables
- Binding energy of ^{3}H, ^{4}He, Charge radius of ^{4}He, β-decay half-life of ^{3}H, aka "GT matrix element"
- Fully converged for A=4 with $\hbar\omega = 36$ MeV, N_{max}=18 due to use of relatively soft interaction
- New fit to np and pp scattering data for $0 \leq E_{lab} \leq 290$ MeV. Truncation error included
- πN LECs fixed at central values of Roy-Steiner analysis of Siemens et al.

	LO	NLO	$\langle$NNLO$\rangle_{ppd}$	Experiment	Adopted uncertainty
$E(^3\mathrm{H})$ [MeV]	−5.65	−8.38	−8.52	−8.482 [40]	0.015
$E(^4\mathrm{He})$ [MeV]	−24.08	−30.21	−28.19	−28.296 [41]	0.005
$r(^4\mathrm{He})$ [fm]	1.27	1.33	1.45	1.4552(62) [42]	0.0062
$fT_{1/2}$ [s]			1127.3	1129.6(3.0) [43]	3.0

3N error model

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

$$y_{\rm th} = y_{\rm ref} \sum_{i=0}^{k} c_i(\{a_j\}) Q^i \qquad Q = \frac{p_{\rm typ}}{\Lambda_b} \qquad y_{\rm ref} = y_{\rm LO} \text{ here}$$

- Assume c_i's are Gaussian random variables with mean zero $\Rightarrow \delta y_{\rm th} = y_{\rm ref} \bar{c} \frac{Q^{k+1}}{\sqrt{1-Q^2}}$
- Q is not obvious: we will actually make it a parameter and sample it. We will also sample $\bar{c}^2$, the mean-square value of the higher-order coefficients
- $\bar{c}^2$ and Q are also constrained by information from the lower-order calculations
- As a first go we will take the uncertainties in the different observables to be uncorrelated

Posterior and priors

$$\mathrm{pr}(c_D, c_E, \bar{c}^2, Q \,|\, D, I) \propto \exp\left(-\frac{1}{2}\mathbf{r}^T(\boldsymbol{\Sigma}_{\mathrm{exp}} + \boldsymbol{\Sigma}_{\mathrm{th}})^{-1}\mathbf{r}\right) \exp\left(-\frac{c_D^2 + c_E^2}{2\bar{a}^2}\right) \mathrm{pr}(\bar{c}^2 \,|\, Q, \bar{a}, I)\mathrm{pr}(Q \,|\, c_D, c_E, I)$$

$$\mathbf{r} = \mathbf{y}_{\mathrm{exp}} - \mathbf{y}_{\mathrm{th}}$$

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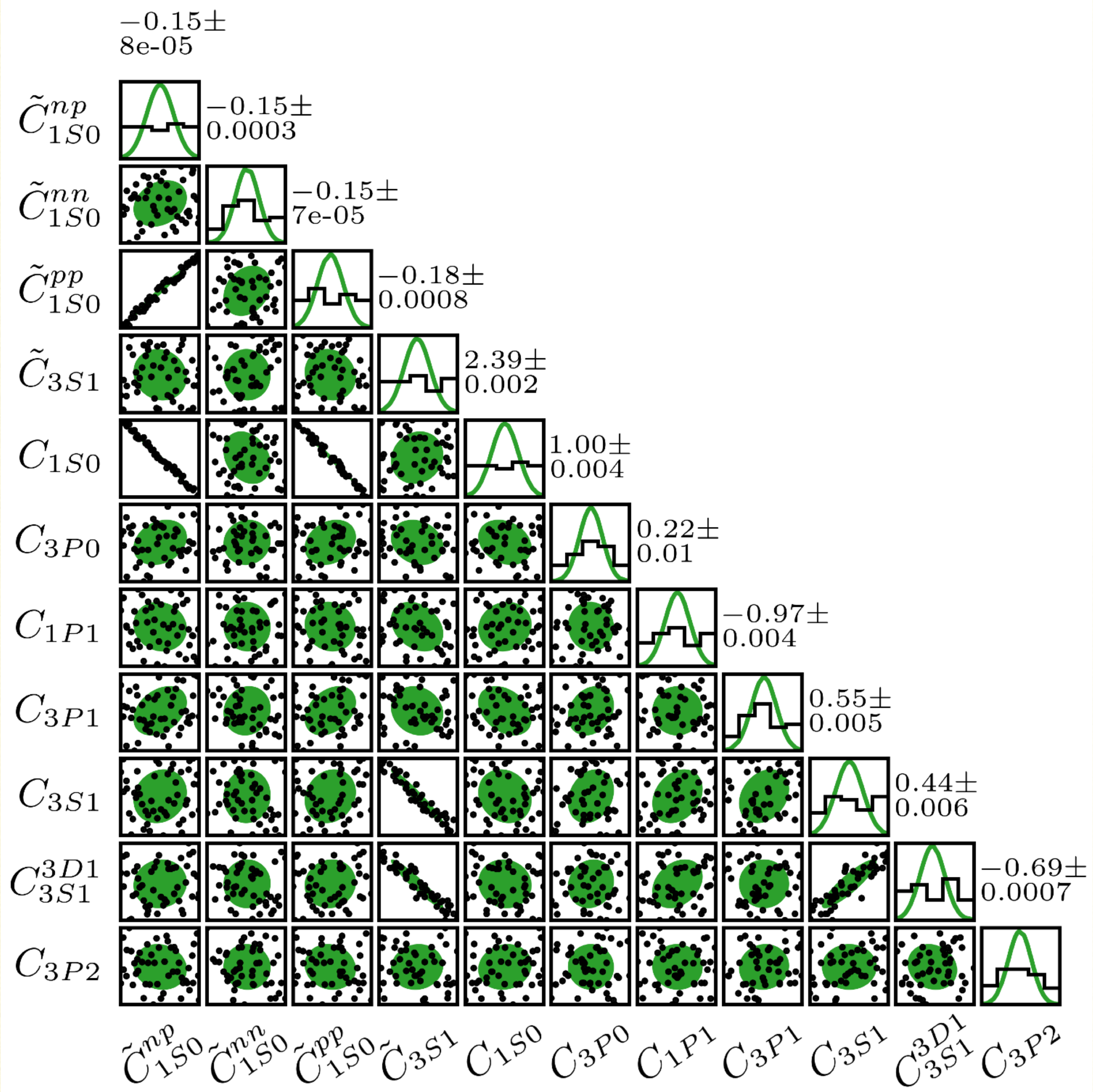
- $\mathrm{pr}(Q \,|\, \mathbf{a}, I)$ then also affected by that information. Starts as weakly informative Beta distribution.

Emulation using Eigenvector Continuation

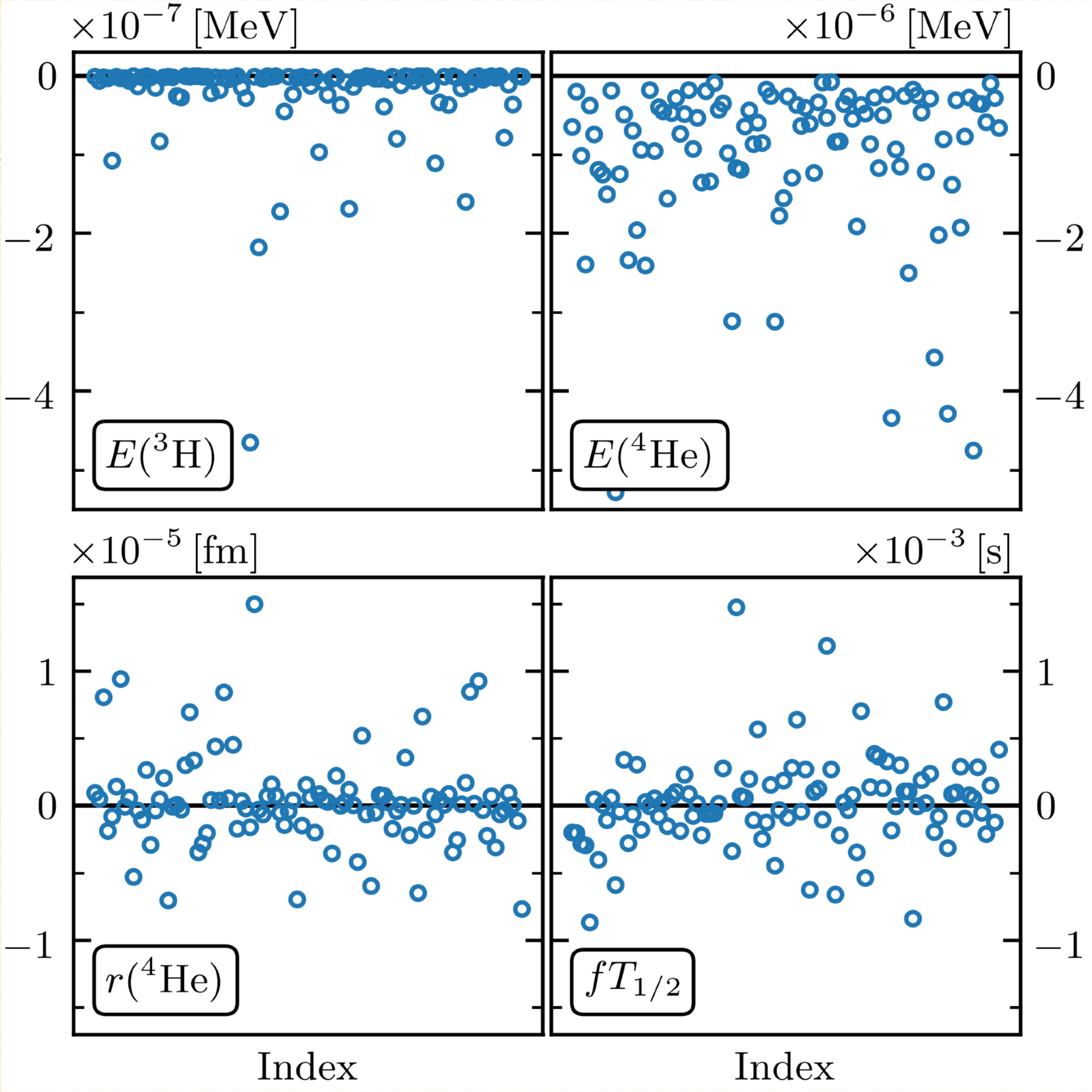
Frame et al., Phys. Rev. Lett. 121, 032501 (2018); König et al., Phys. Lett. B 810, 135814 (2020)

- We use Eigenvector Continuation to emulate few-nucleon observables
- Emulator is built in 13-dimensional parameter space: $\vec{a}$ includes c_D and c_E and 11 NN parameters at NNLO: "$\vec{a}_{NN}$"
- Solve $H(\vec{a})|\psi(\vec{a})\rangle = E(\vec{a})|\psi(\vec{a})\rangle$ at N_{EC} points in parameter space
- Project $H(\vec{a})$ onto subspace spanned by these N_{EC} wave functions; solve generalized eigenvalue problem in subspace
- Eigenvector at $\vec{a}$ obtained as linear combination of N_{EC} vectors in subspace. Denote coefficients of linear combination by $\beta(\vec{a})$
- Observables at $\vec{a}$ then reconstructed from $\beta(\vec{a})$ and projection of observable to subspace



Emulation results

- First EC emulation of transition matrix element
- Eigenvector continuation with N_{EC}=50 training points is very accurate for all observables considered.



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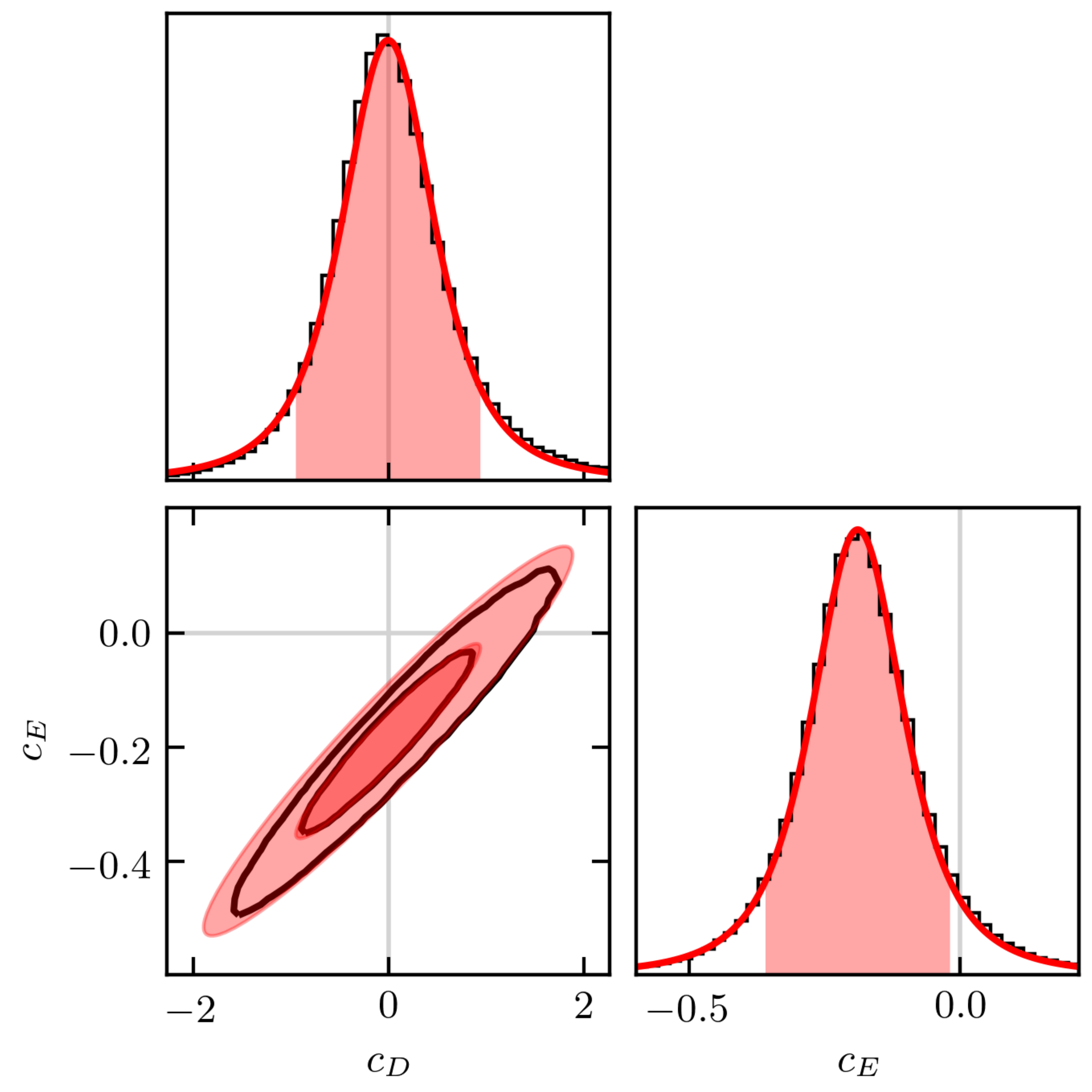

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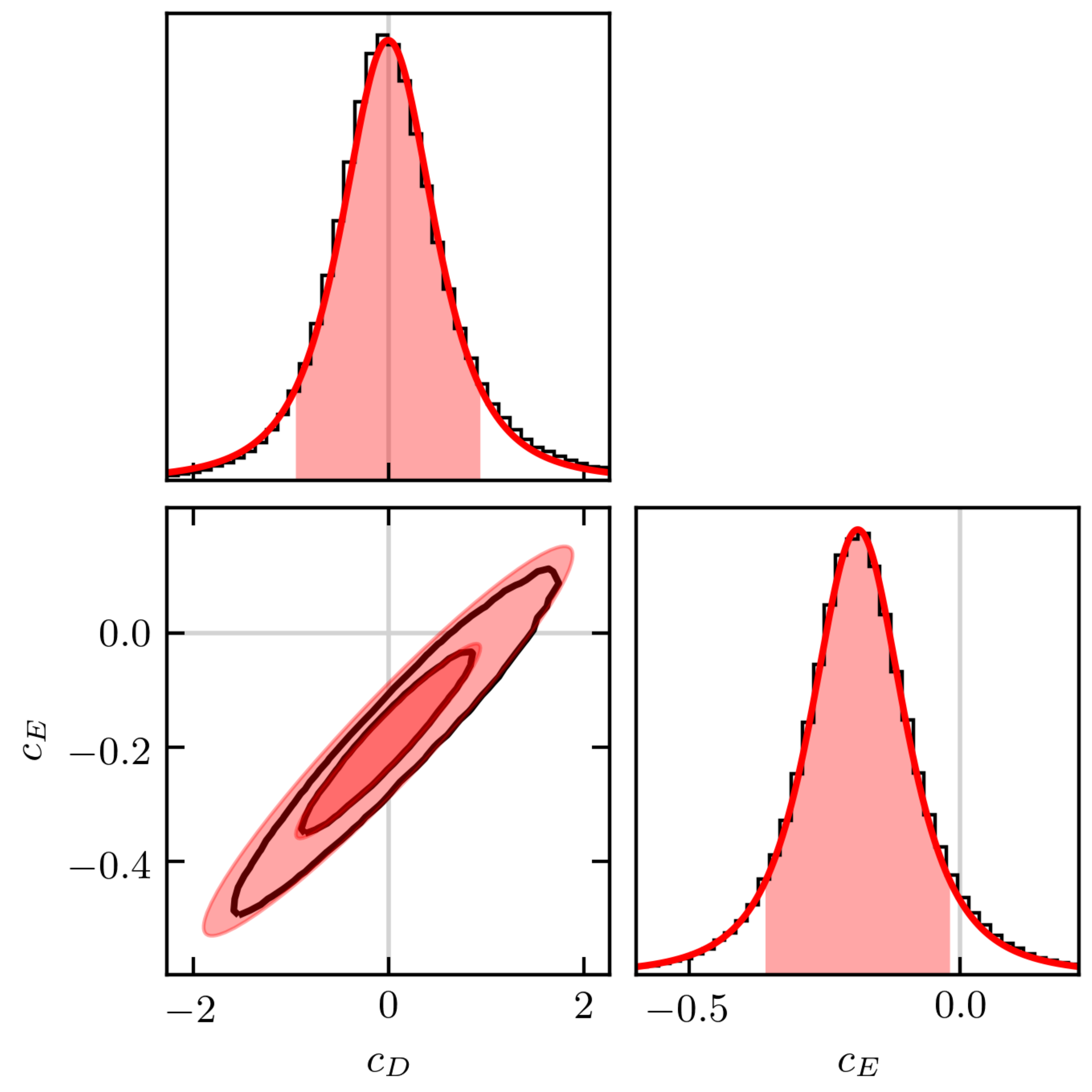

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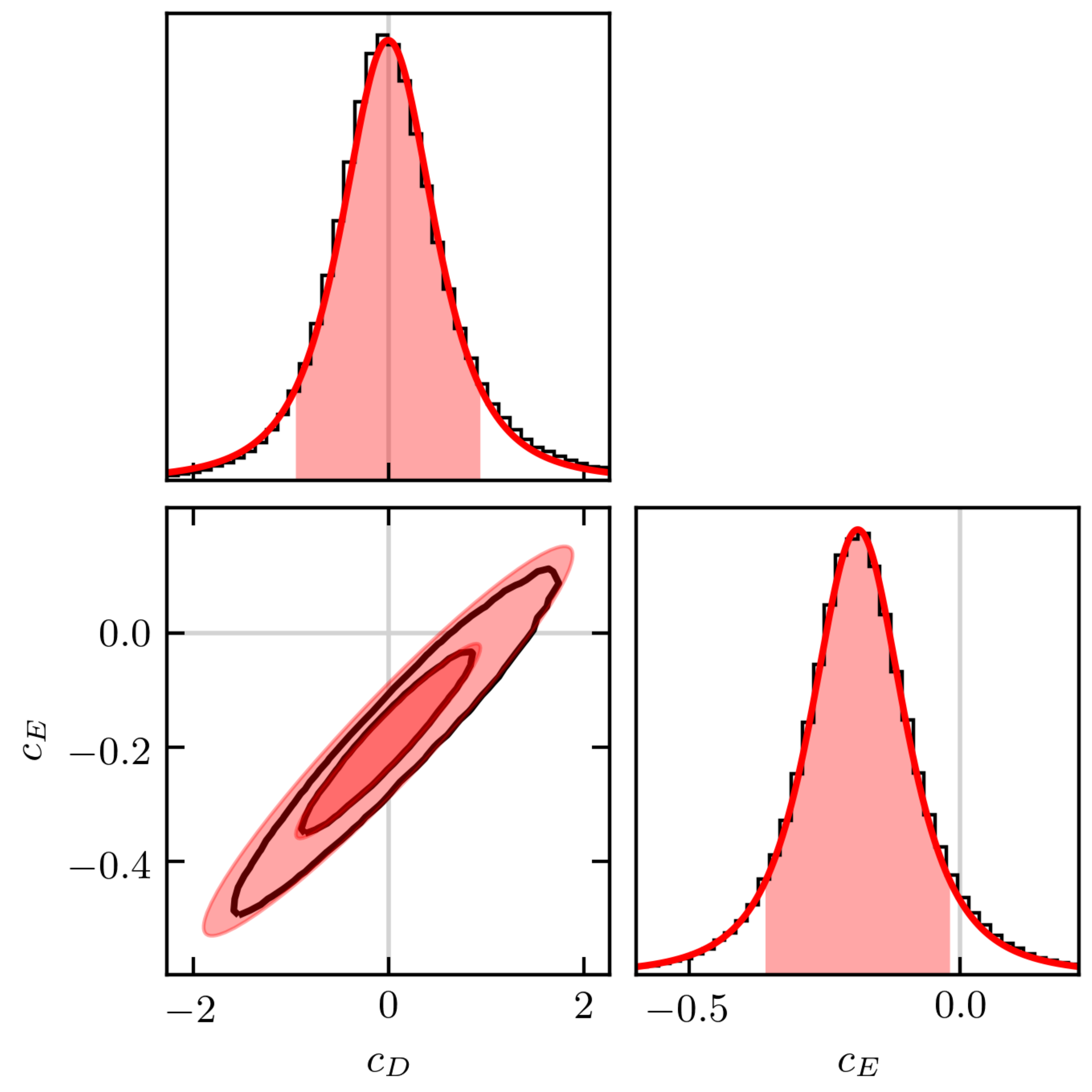

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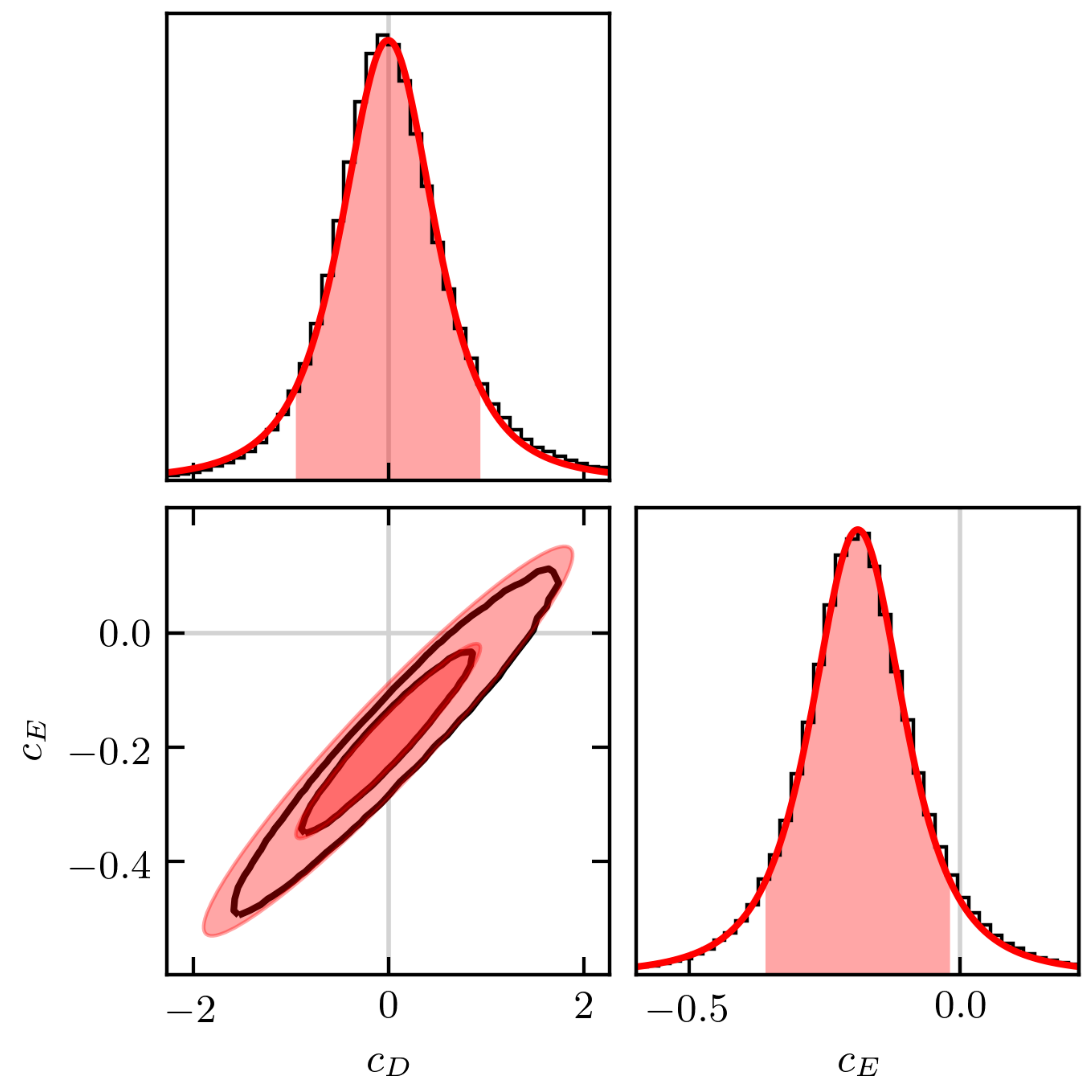
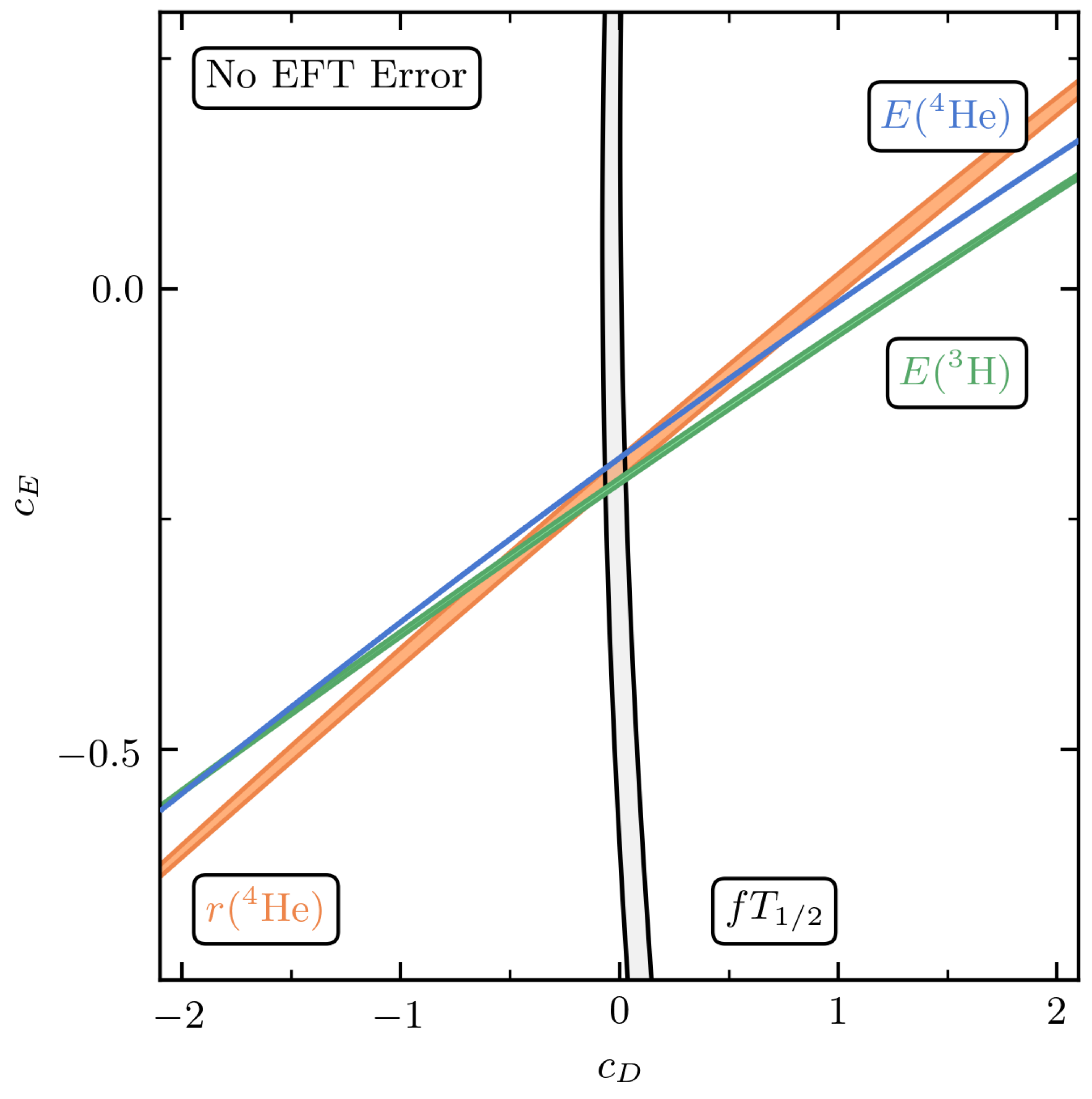
- Not Gaussian! t-distribution with ν=2.6 degrees of freedom



The role of truncation errors & different data



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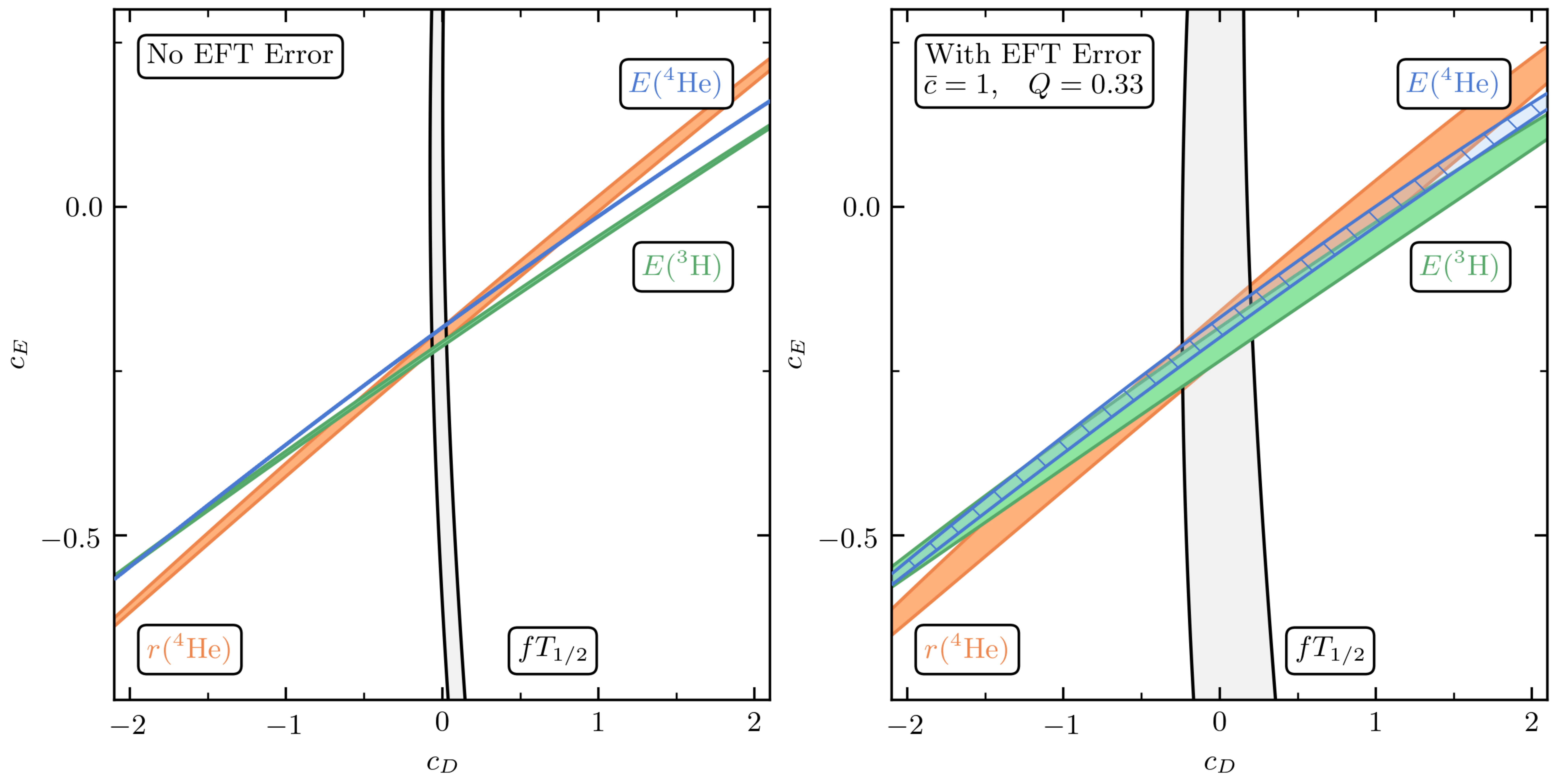

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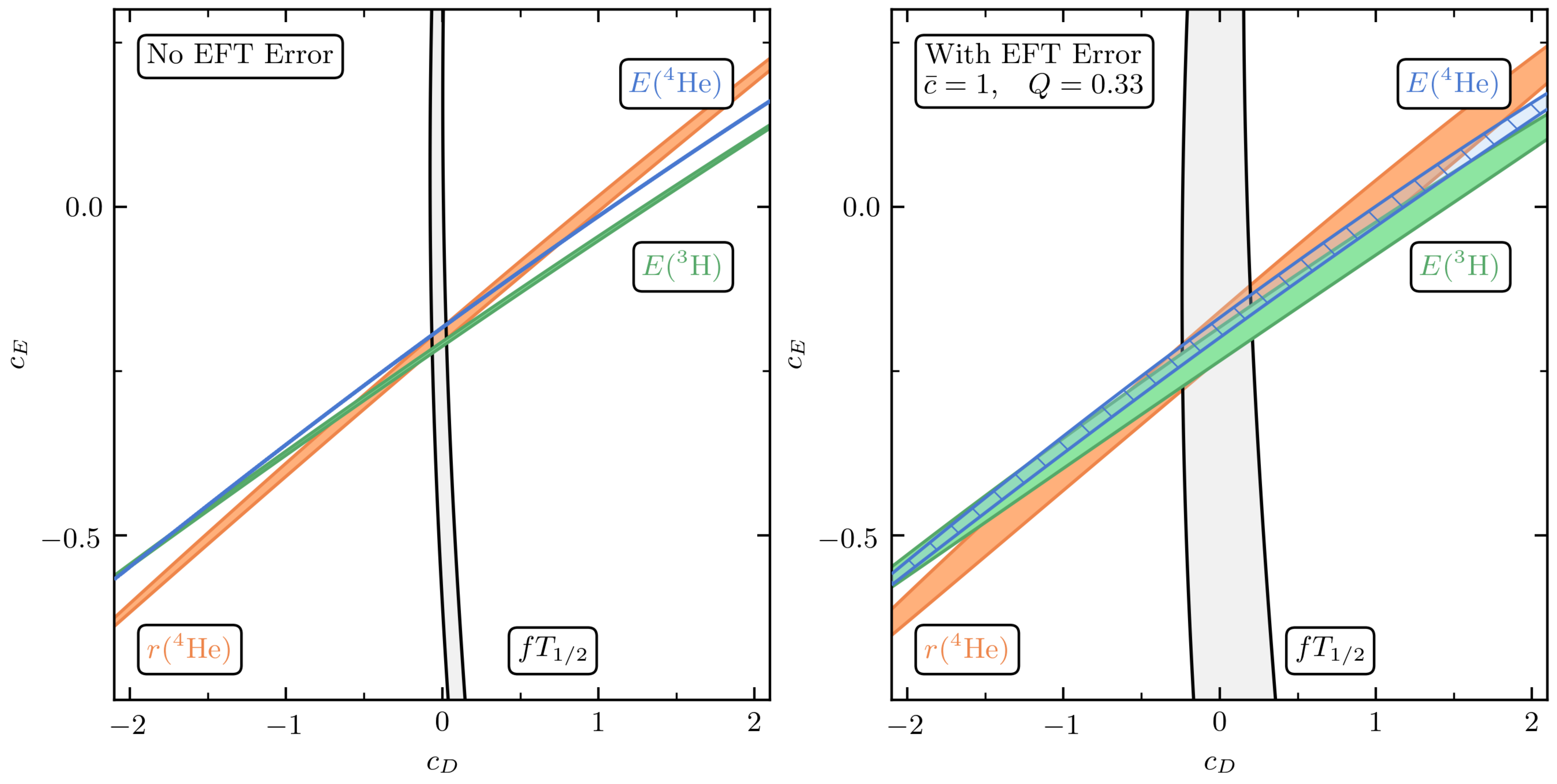

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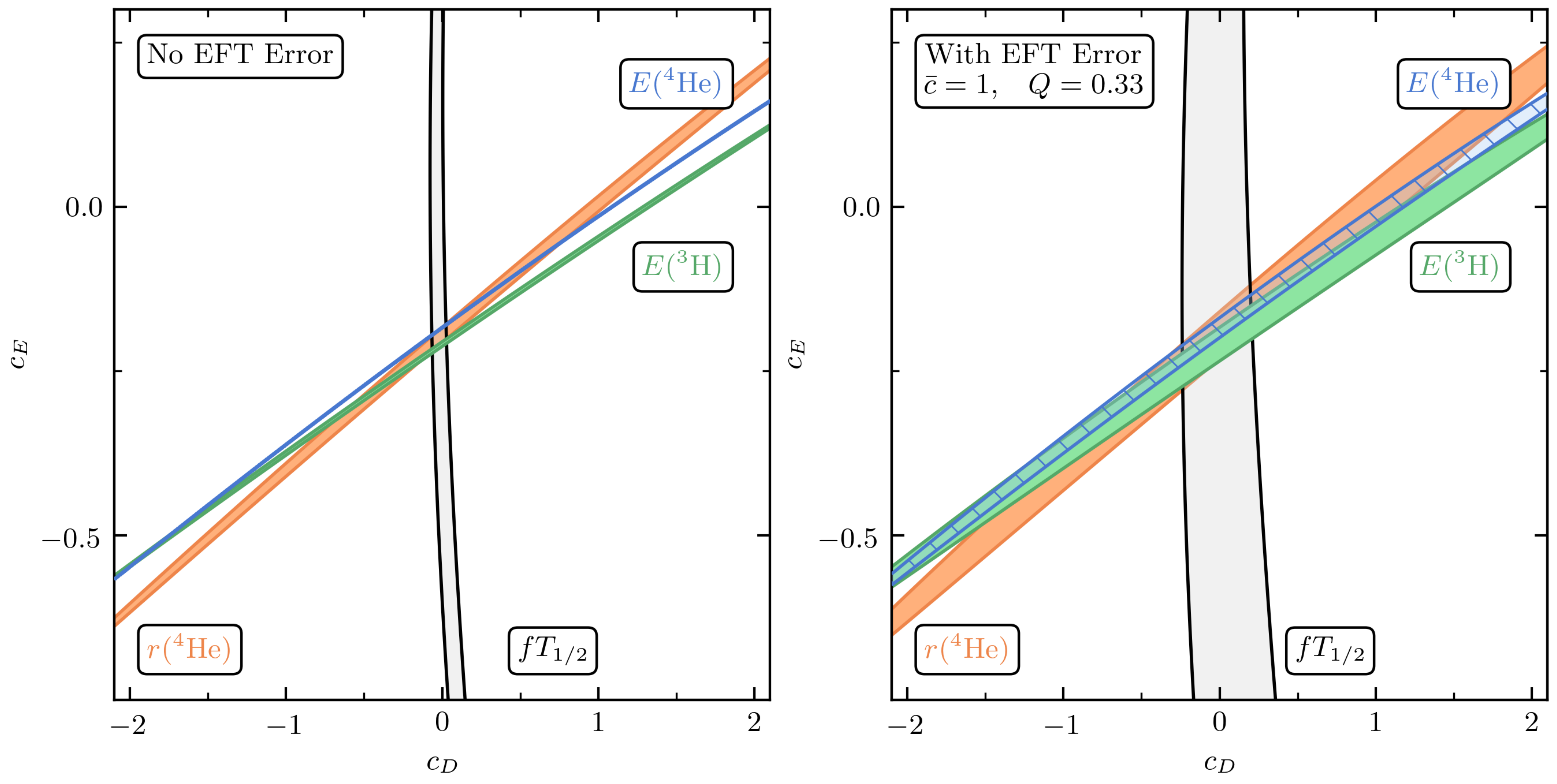

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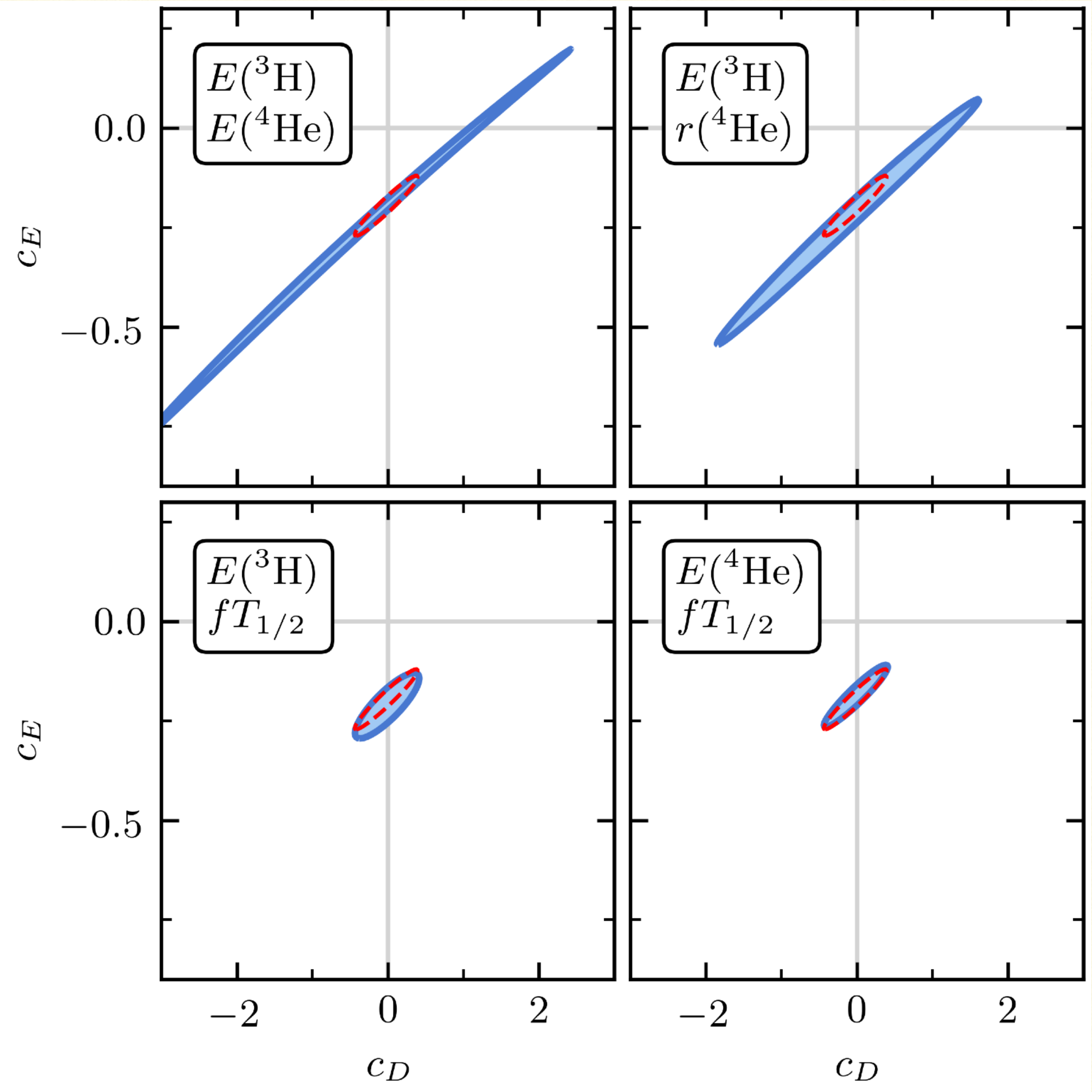
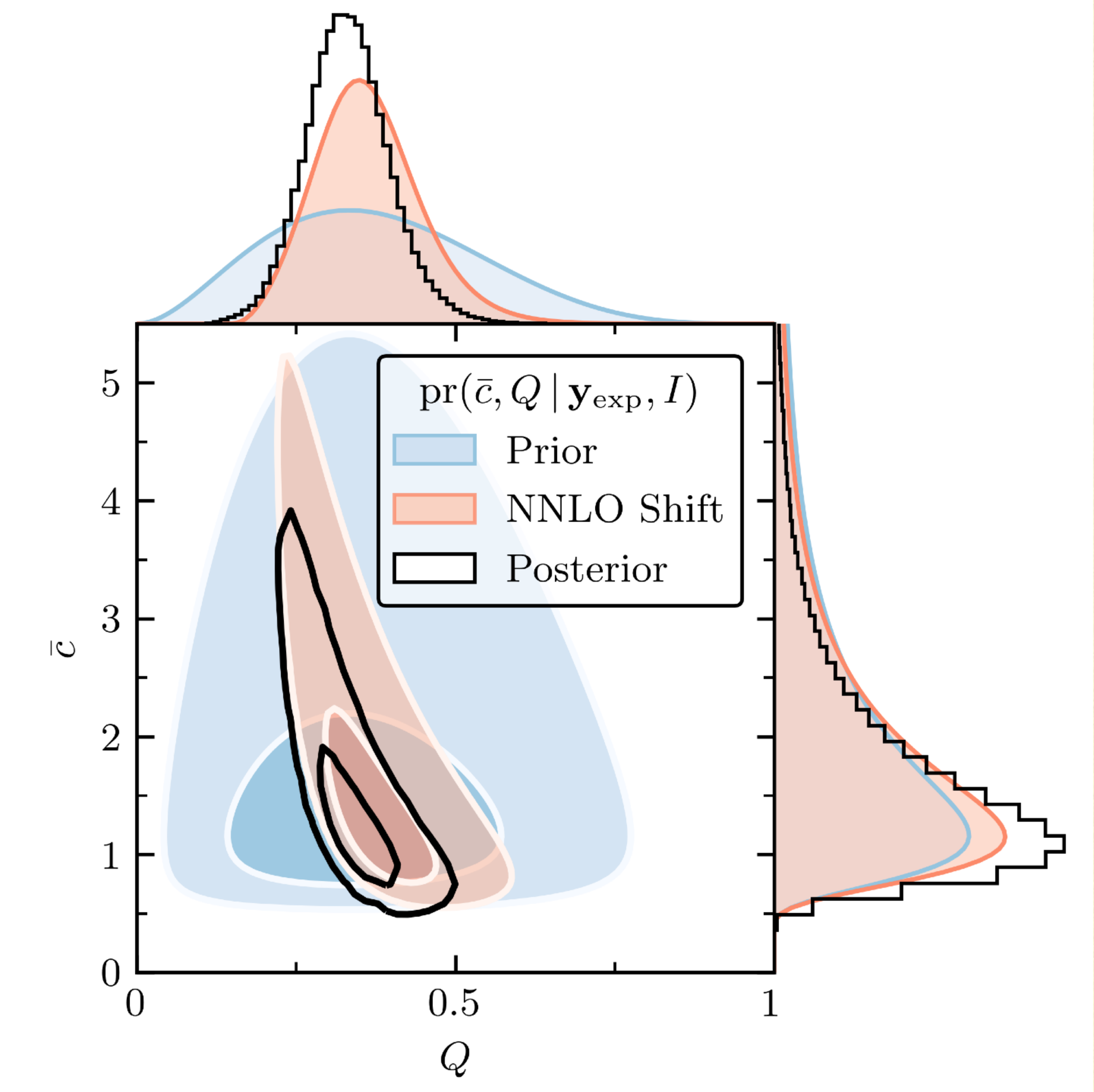


- Truncation errors essential to get consistency
- Constraints other than GT matrix element essentially degenerate
- Posterior almost obtained with just $fT_{1/2}$ and $E(^4\mathrm{He})$

Results for Q, $\bar{c}$

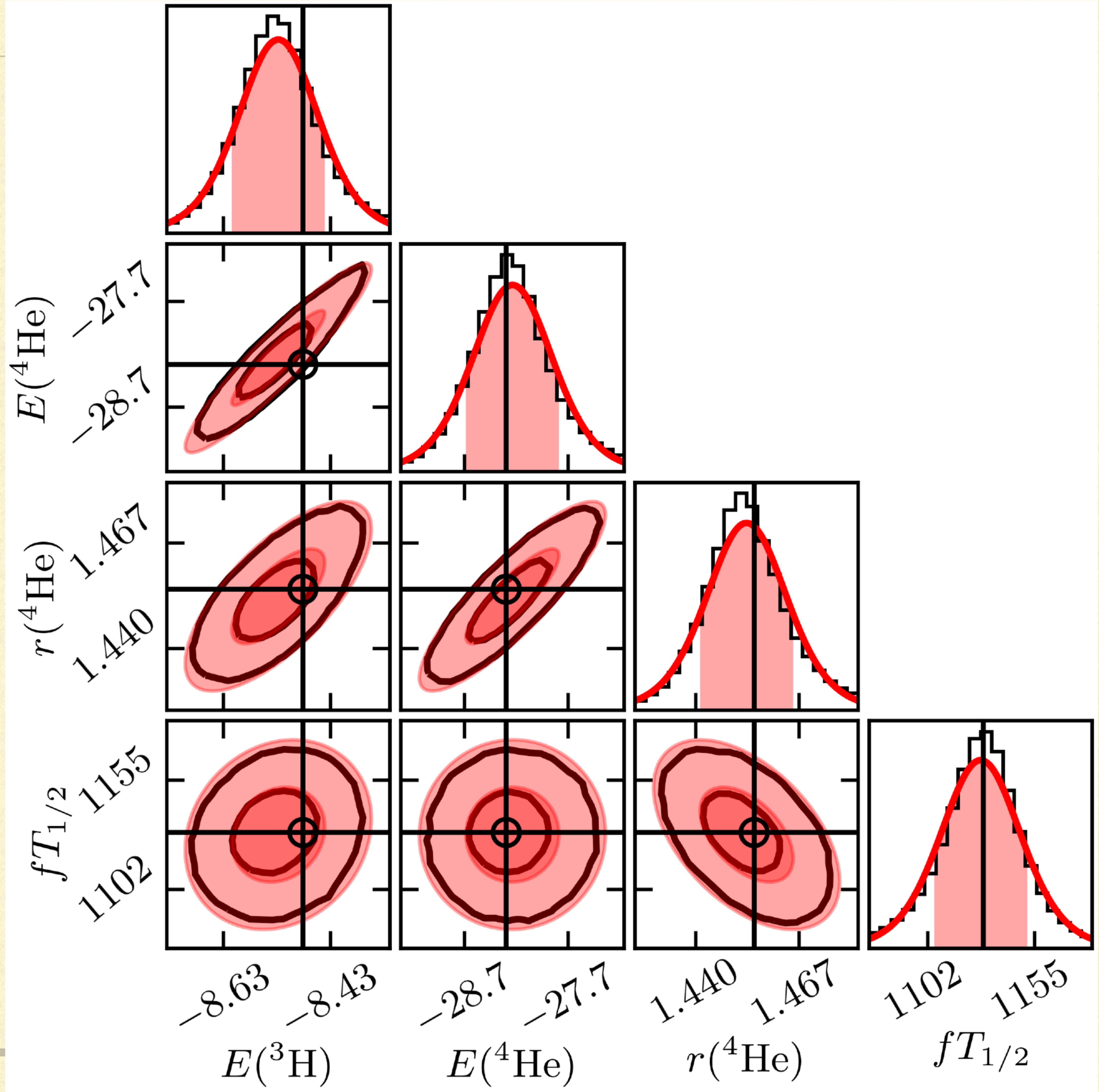
- $\mathrm{pr}(Q\,|\,\vec{a}, I)$ starts as a weakly informative Beta distribution
- Can use information on size of c_3 (NNLO-NLO shift) to update Q posterior (and $\bar{c}$ posterior too)
- But then we sample the likelihood (times the prior) allowing size of theory errors (i.e. $\bar{c}$ and Q) to vary
- Q and $\bar{c}$ then include information on how far NNLO result is from experiment
- $\bar{c}$ natural; $Q = 0.33(6)$



Posterior predictive distribution

Chiral Effective Field Theory can describe all these data at NNLO [O(Q^3)] once truncation errors are accounted for

These are also t-distributions



Linear models with variance estimation: time for t

- This problem is linear in c_D and c_E in the region that matters for the final posterior
- So posterior for c_D and c_E would be Gaussian if we kept $\bar{c}$ and Q fixed
- By sampling $\bar{c}$ and Q we end up doing "variance estimation" in our statistical model
- If $\mathscr{V} = \bar{c}^2 Q^{2(k+1)}$ we have (approximately):

$$\mathrm{pr}(\vec{a}\,|\,D, \mathscr{V}) \propto \frac{1}{\sqrt{V}} \exp\left(-\frac{(y_{\mathrm{exp}} - y_{\mathrm{th}}(\vec{a}))^2}{2\mathscr{V}}\right) \qquad \mathrm{pr}(\mathscr{V}) \propto \frac{1}{\mathscr{V}^{n/2+1}} \exp\left(-\frac{ns^2}{2\mathscr{V}}\right)$$

- Since $y_{\mathrm{th}}(\vec{a})$ is linear in $\vec{a}$ marginalizing over $\mathscr{V}$ then yields a t-distribution

Summary and Outlook

- Part of an ongoing effort to develop, apply, and evaluate Bayesian statistical methods for EFTs of nuclei

  See also: P. Maris et al., Phys. Rev. C (2021)

- Truncation errors are included in extraction of c_D and c_E from few-nucleon observables

  See also: K. Kravvaris et al., Phys. Rev. C (2020)

- Parameters of statistical model of truncation errors estimated simultaneously: $Q = 0.33(6), \bar{c} \in [0.87, 1.44]$

- The LECs c_D and c_E are strongly correlated. Joint pdf best represented by a multivariate *t* distribution

- For 3NF parameter estimation you should not only use observables that are related by universality

  Lupu, Barnea, Gazit, arXiv:1508.05654

- Impact of NN uncertainties in the posterior is small; that of πN uncertainties remains to be assessed

- Future work: comparing χEFT Hamiltonians with different regulators and with Δ(1232) degrees of freedom; different assumptions for correlations of theory uncertainties

- Extending the results is straightforward via open-source Python package fit3bf