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

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arXiv:2104.04441 and Phys. Rev. C (in press)

BAND Bayesian Analysis of Nuclear Dynamics

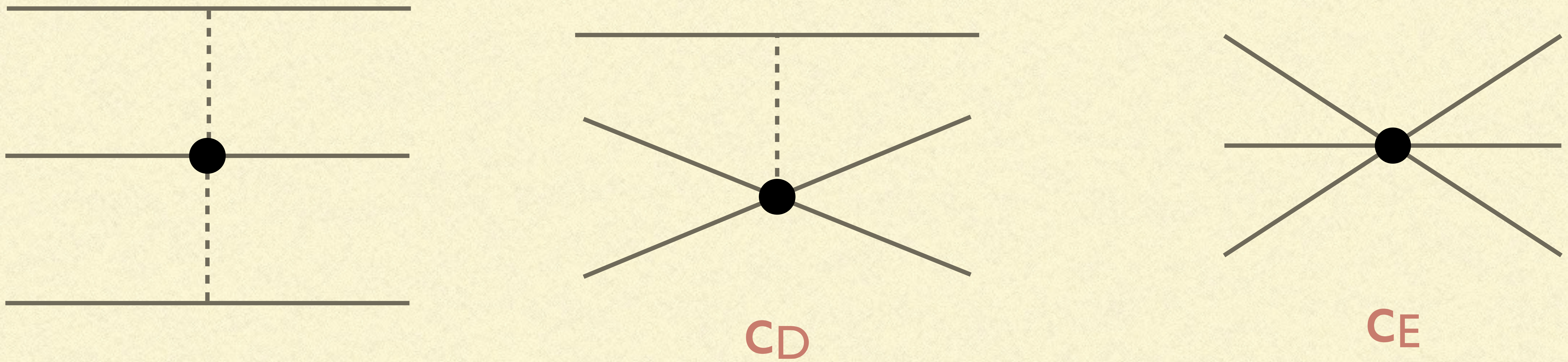
RESEARCH SUPPORTED BY THE DOE OFFICE OF SCIENCE, THE NSF MPS DIVISION AND OFFICE OF ADVANCED CYBERINFRASTRUCTURE, THE SWEDISH RESEARCH COUNCIL, AND THE ERC HORIZONS INITIATIVE

BUQEYE Collaboration

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	$\langle\text{NNLO}\rangle_{\text{ppd}}$	Experiment	Adopted uncertainty
$E(^3\text{H})$ [MeV]	−5.65	−8.38	−8.52	−8.482 [40]	0.015
$E(^4\text{He})$ [MeV]	−24.08	−30.21	−28.19	−28.296 [41]	0.005
$r(^4\text{He})$ [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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- $(\boldsymbol{\Sigma}_{\mathrm{th,uncorr}})_{ij} = (\mathbf{y}_{\mathrm{ref}})^2 \bar{c}^2 \delta_{ij} \sum_{n=k+1}^{\infty} Q^{2n}$; experimental errors are negligible in comparison

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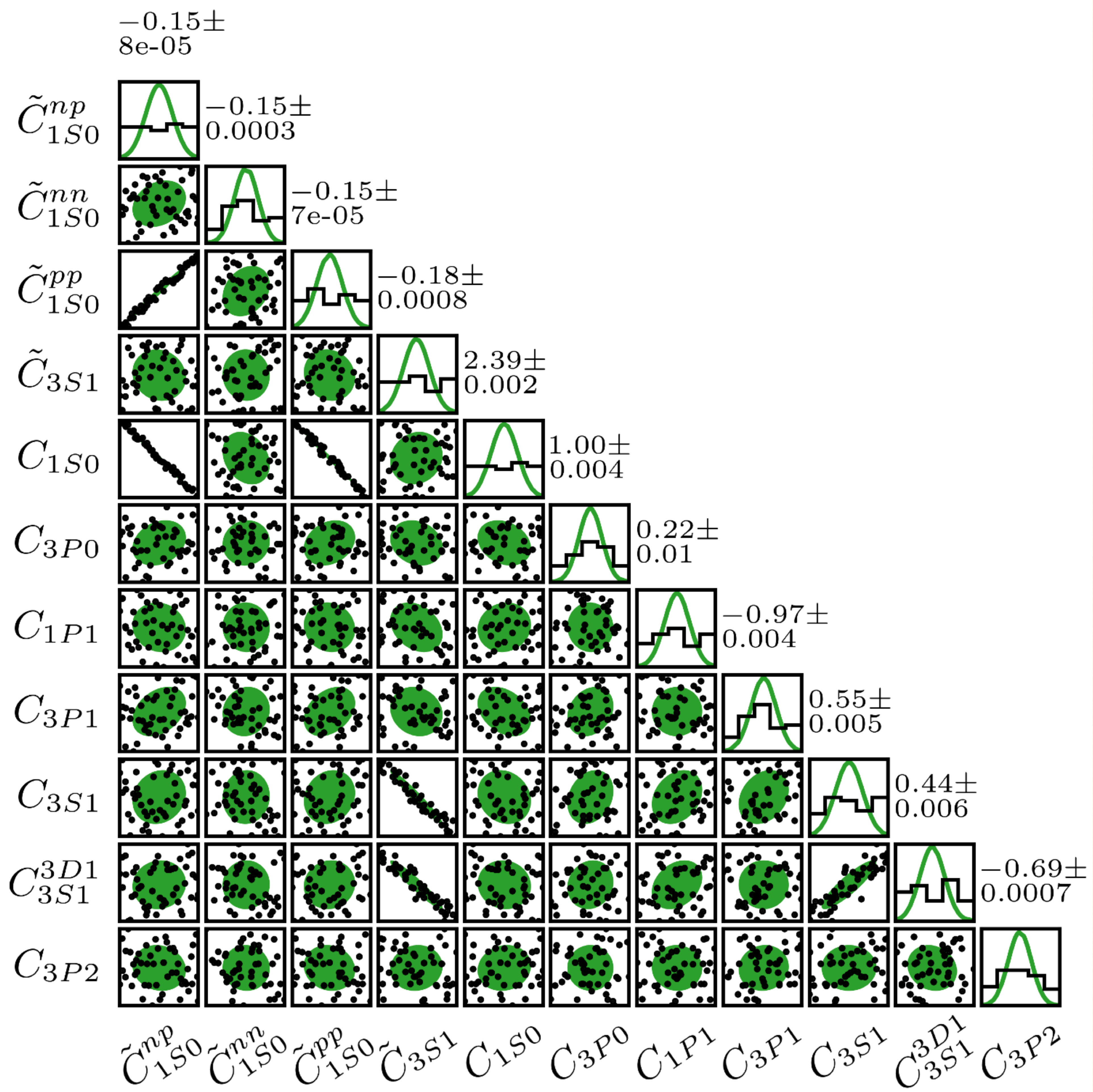
- $\mathrm{pr}(Q \,|\, \mathbf{a}, I)$ then also affected by that information. Starts as weakly informative Beta distribution.

Emulation using Eigenvector Continuation

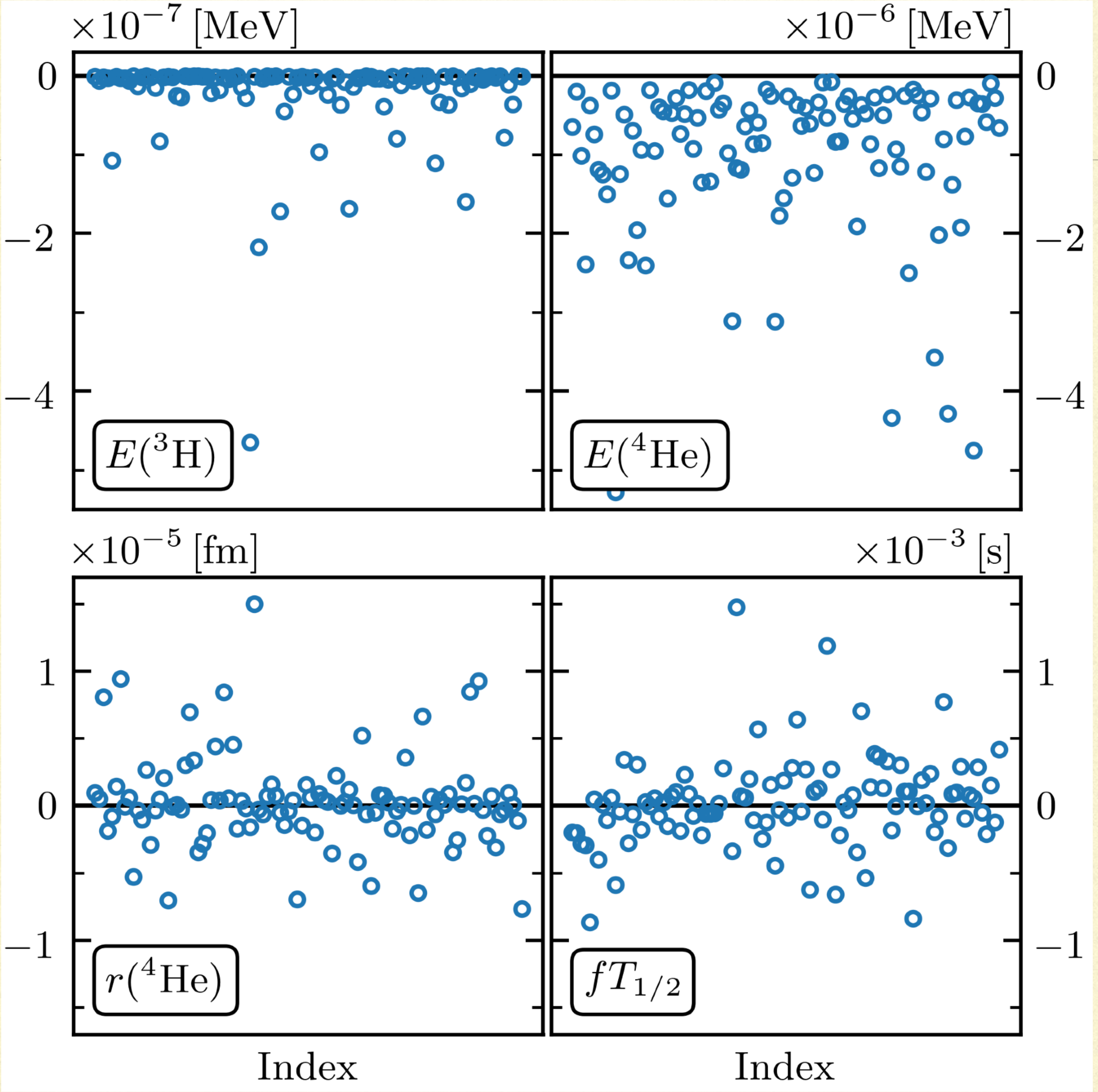
Frame et al., Phys. Rev. Lett. 121, 032501 (2018); König et al., Phys. Lett. B 810, 135814 (2020)

- We use Eigenvector Continuation to emulate few-nucleon observables
- Emulator is built in 11-dimensional parameter space: $\vec{a}$ includes c_D and c_E and 9 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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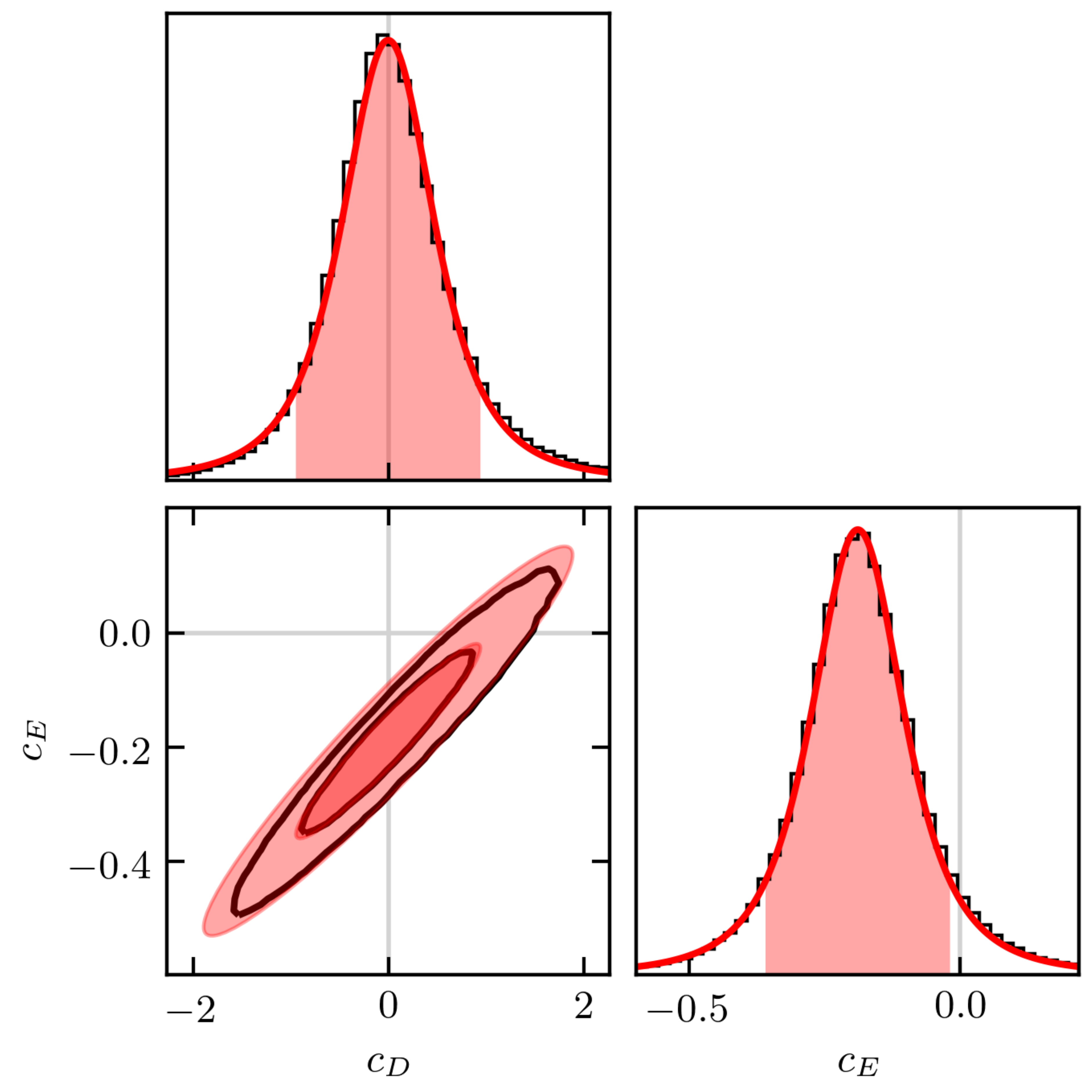

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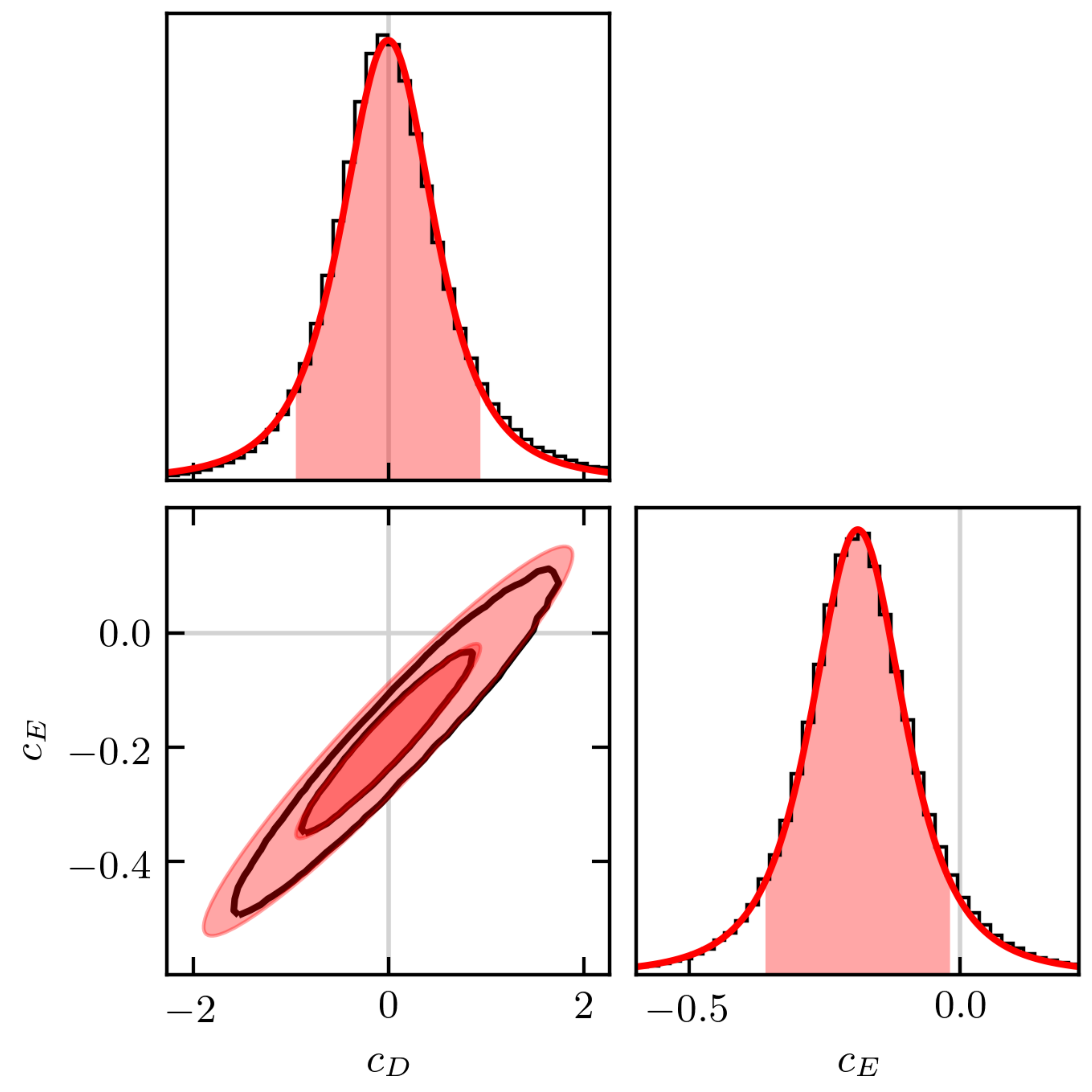

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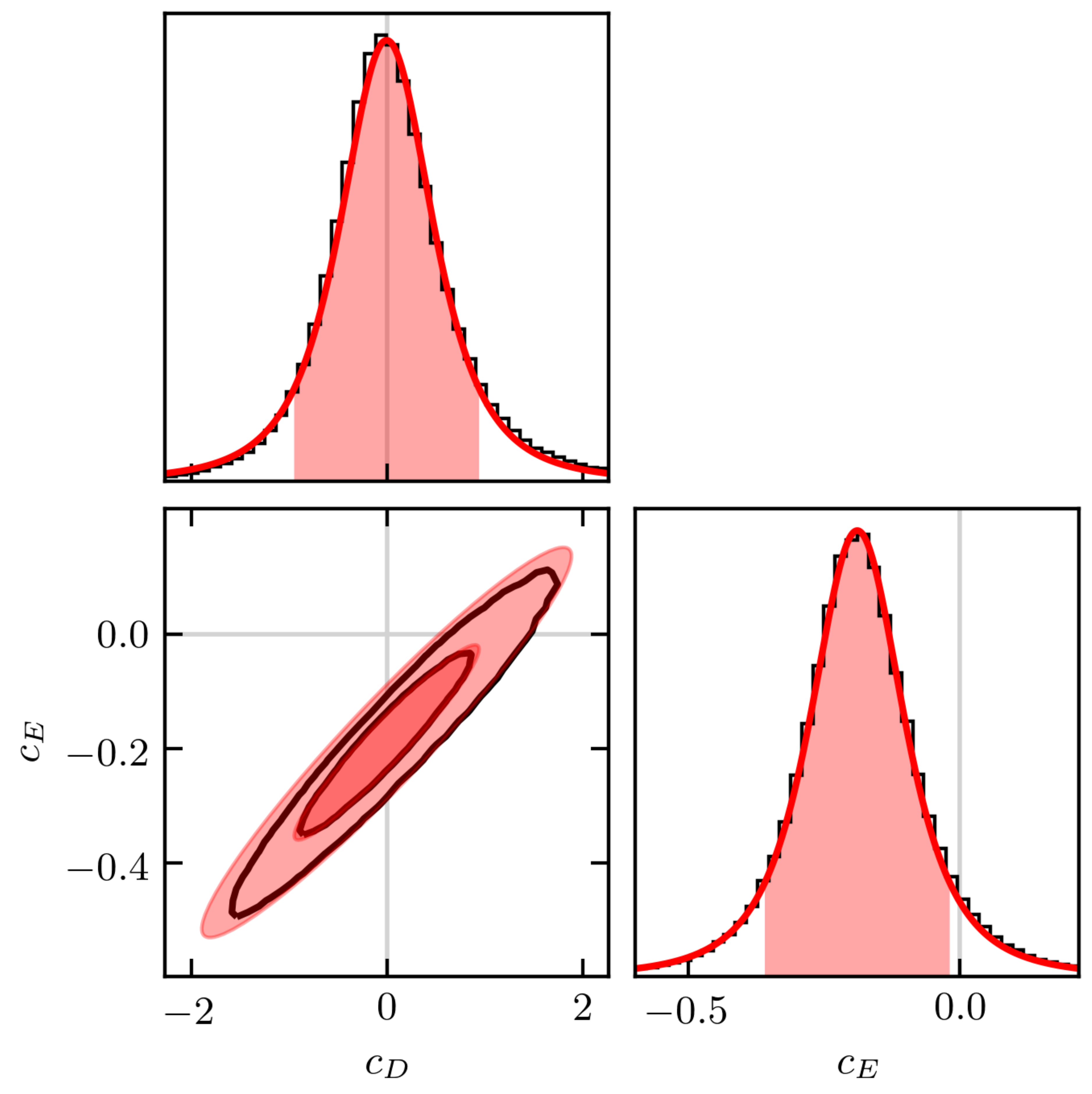

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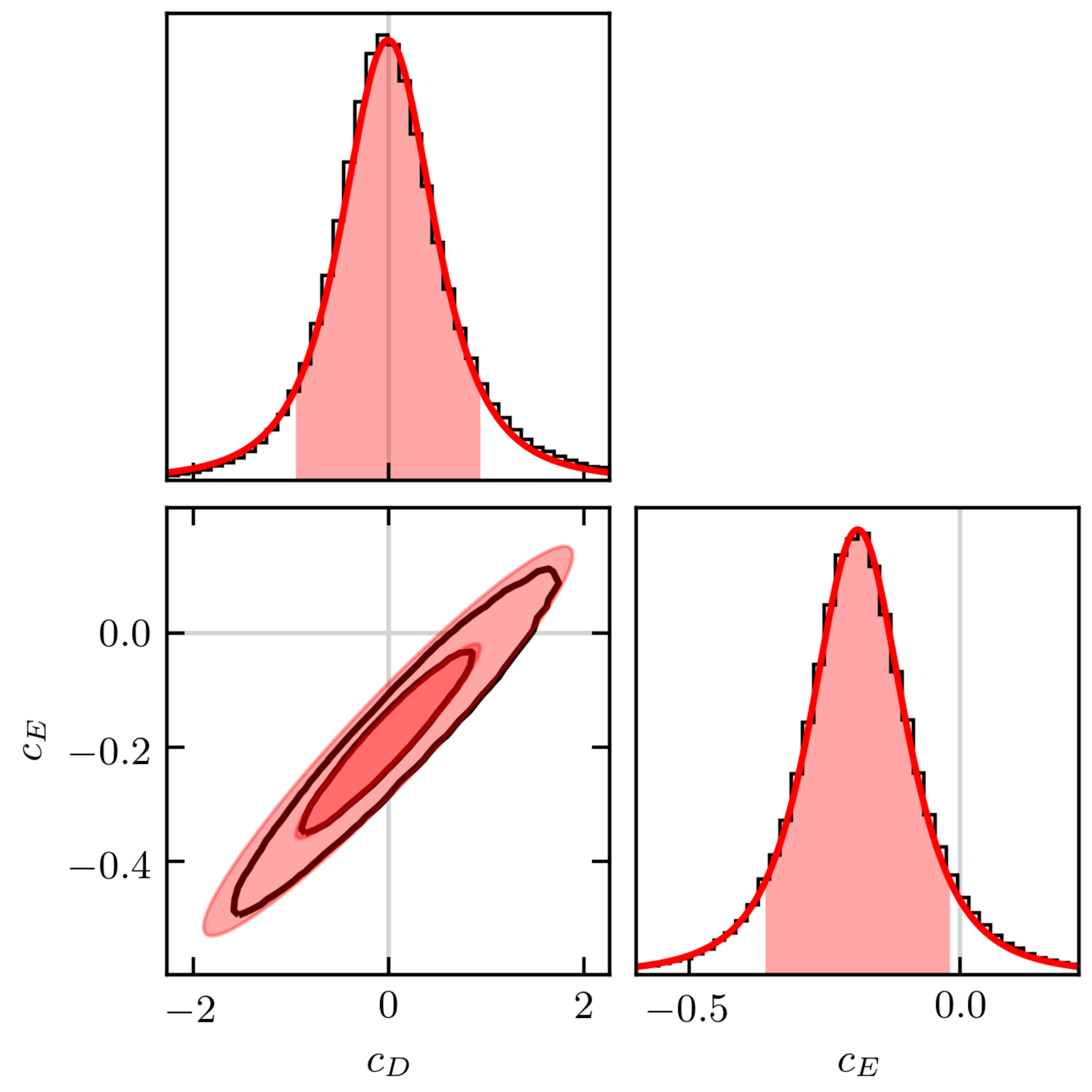
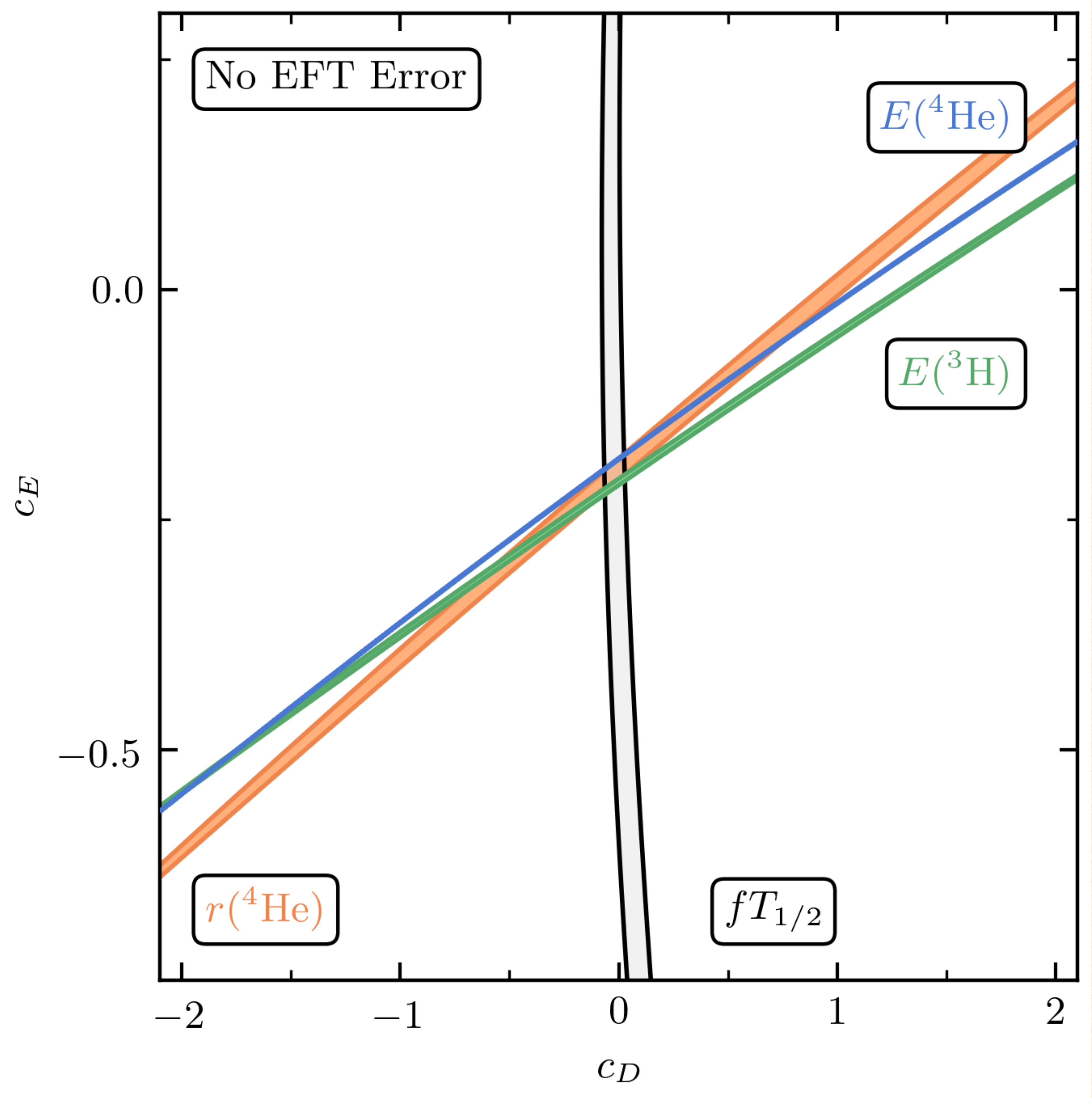
- Not Gaussian! t-distribution with ν=2.6 degrees of freedom



The role of truncation errors & different data



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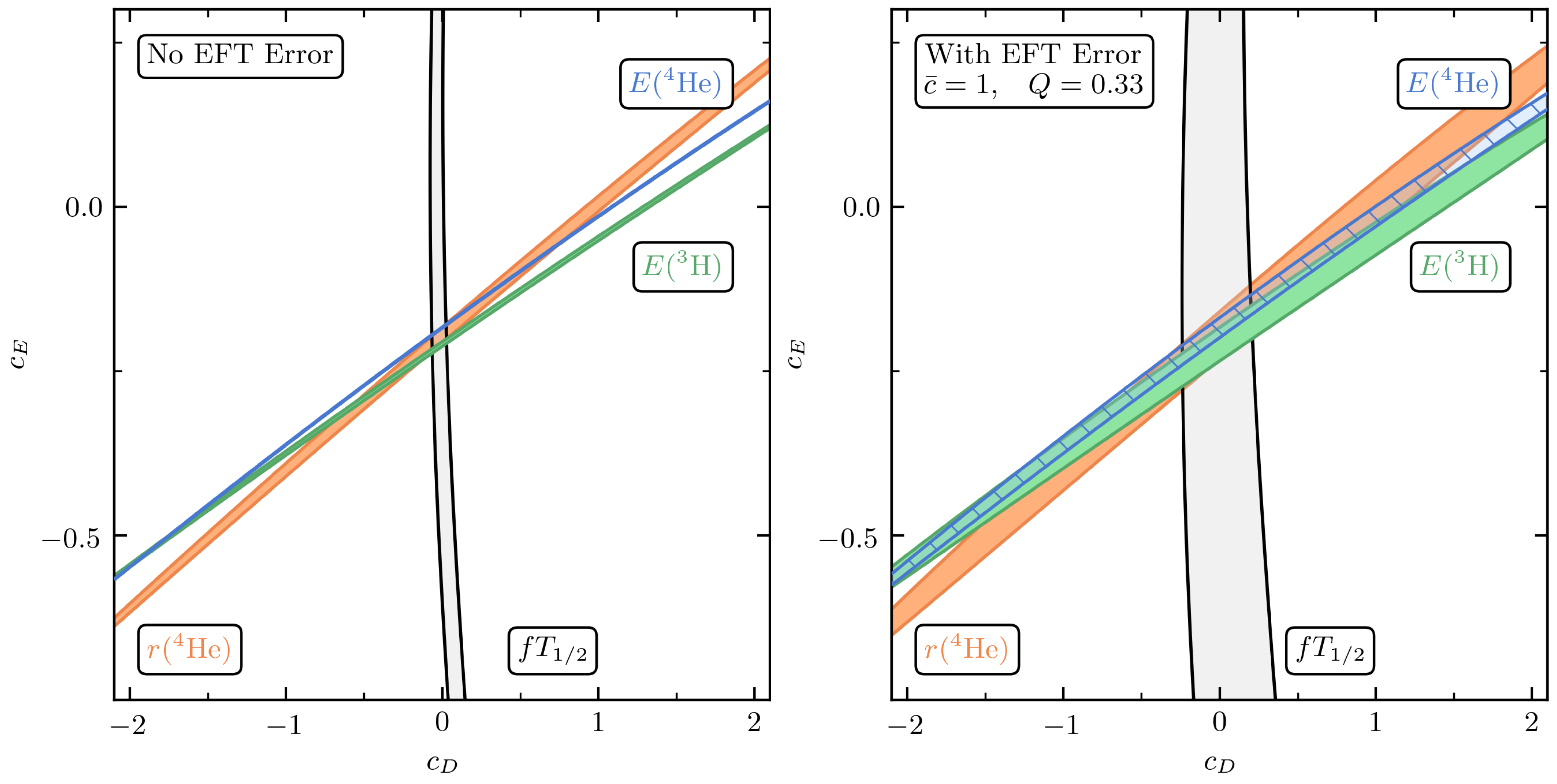

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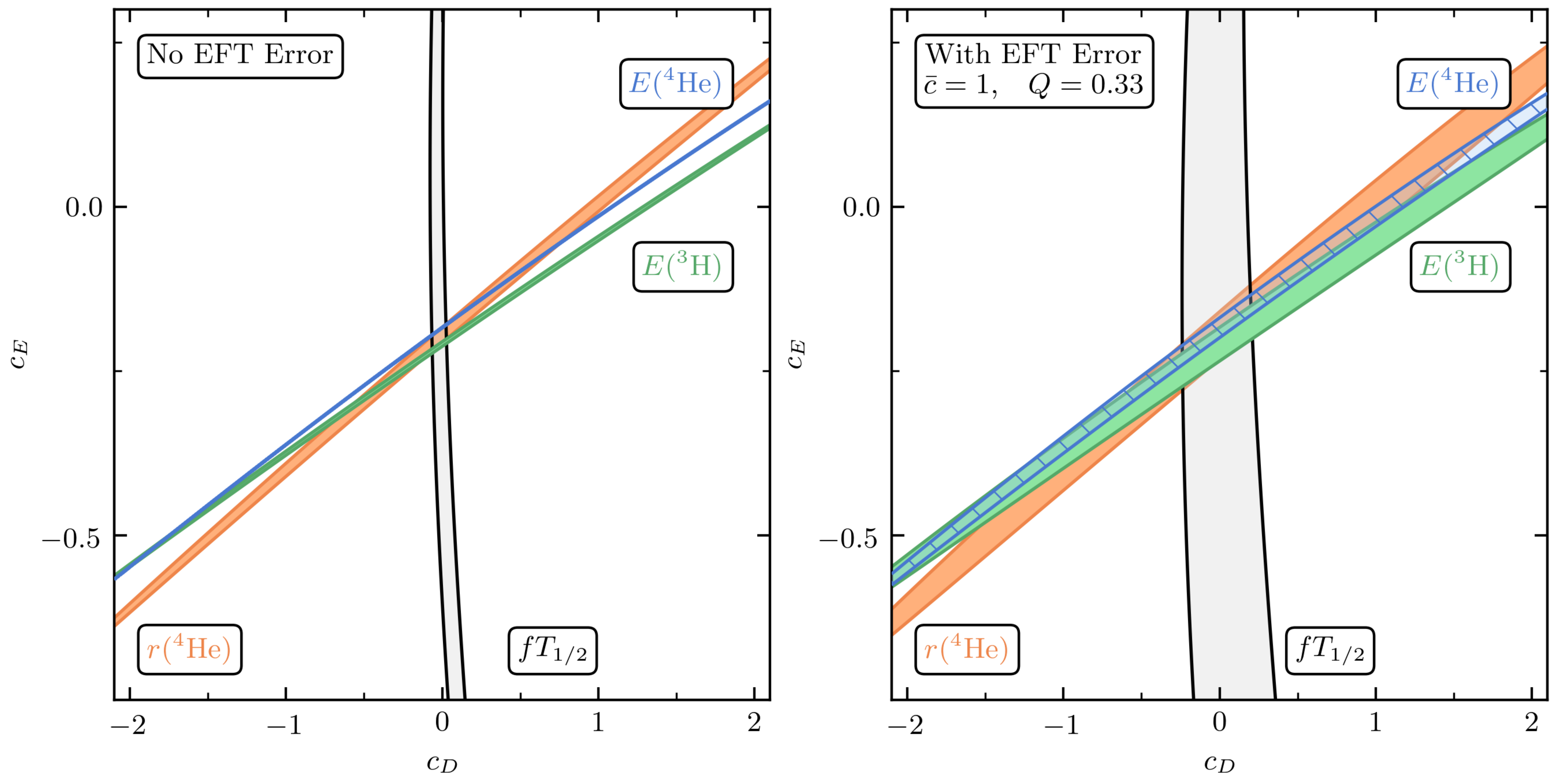

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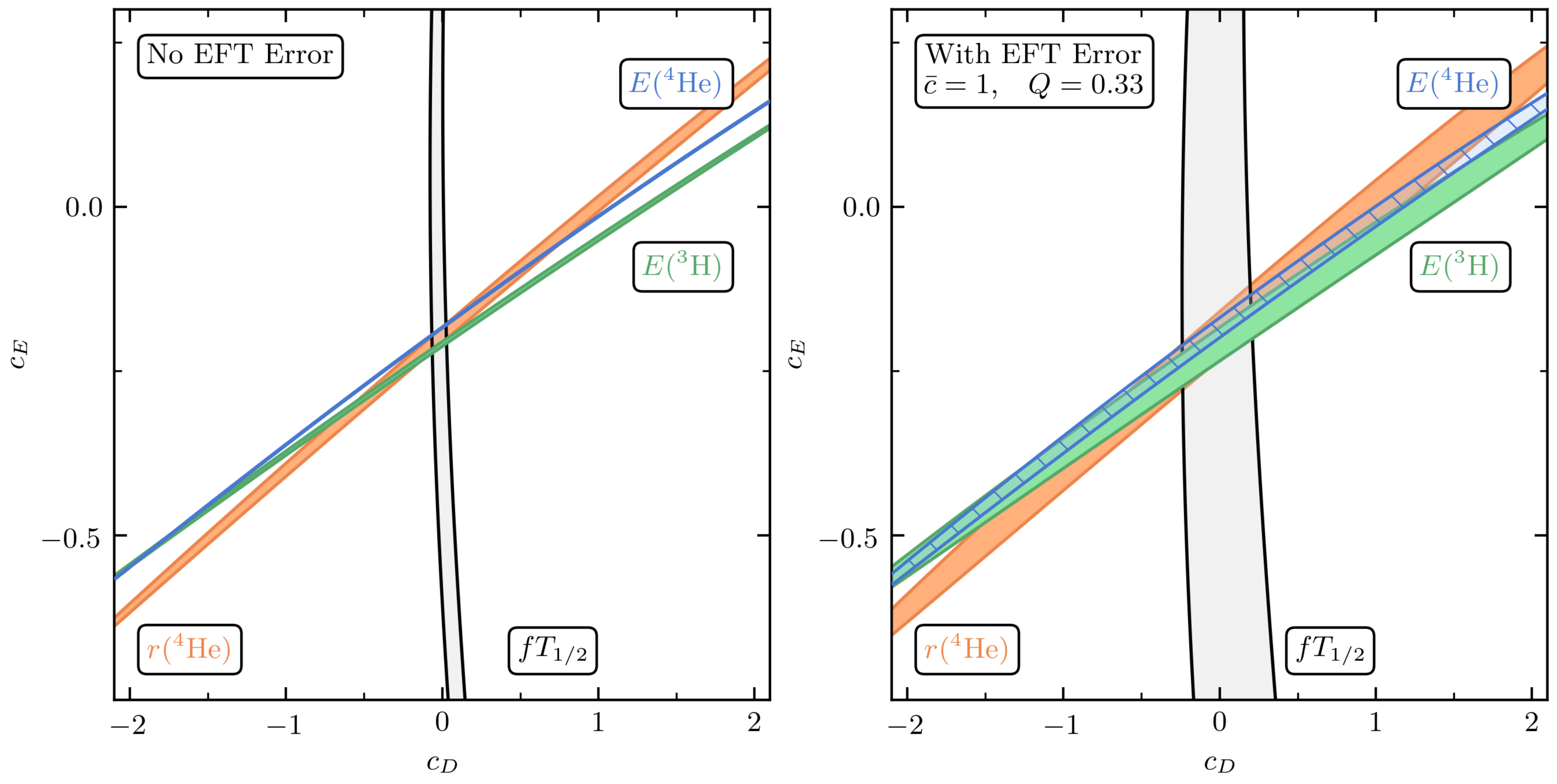

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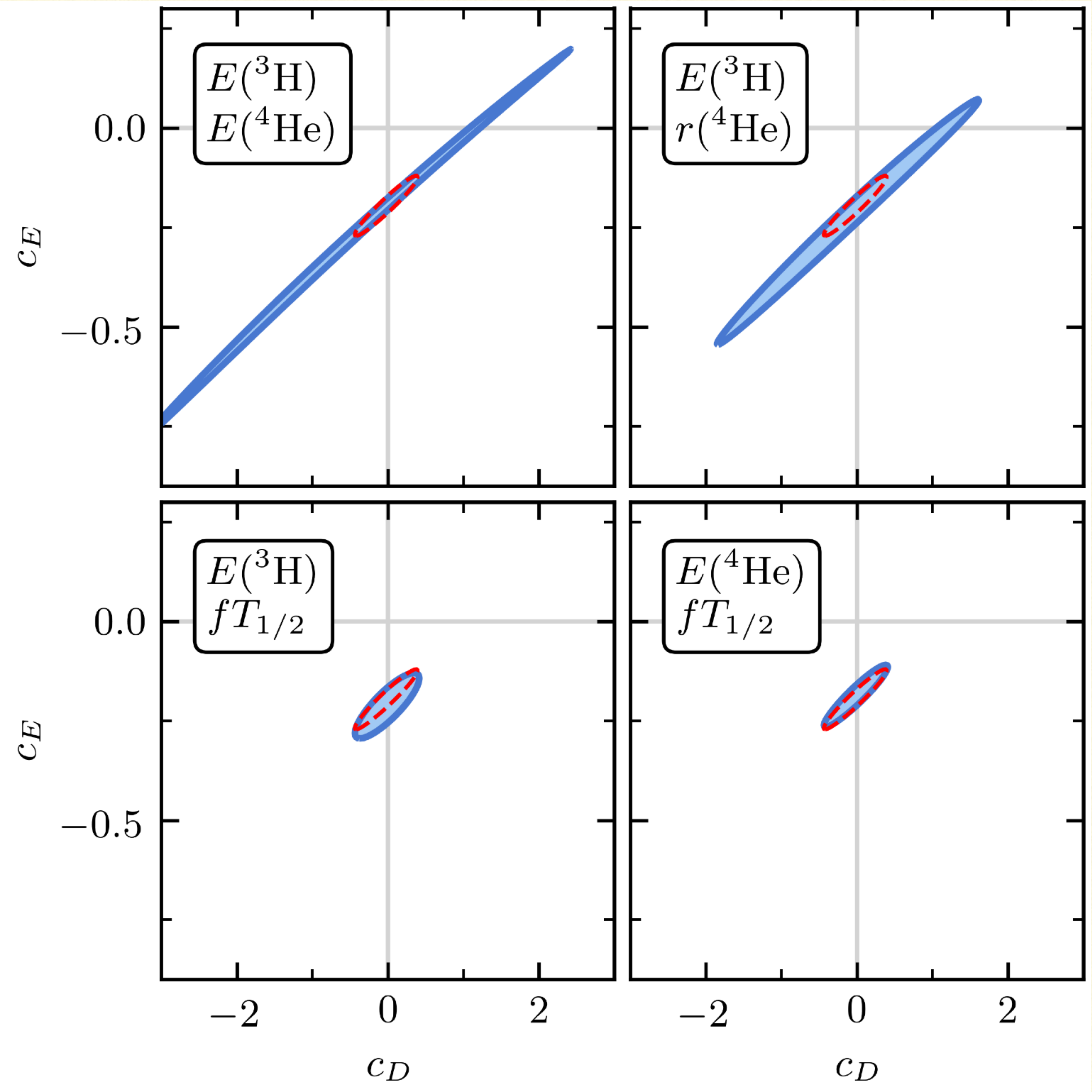
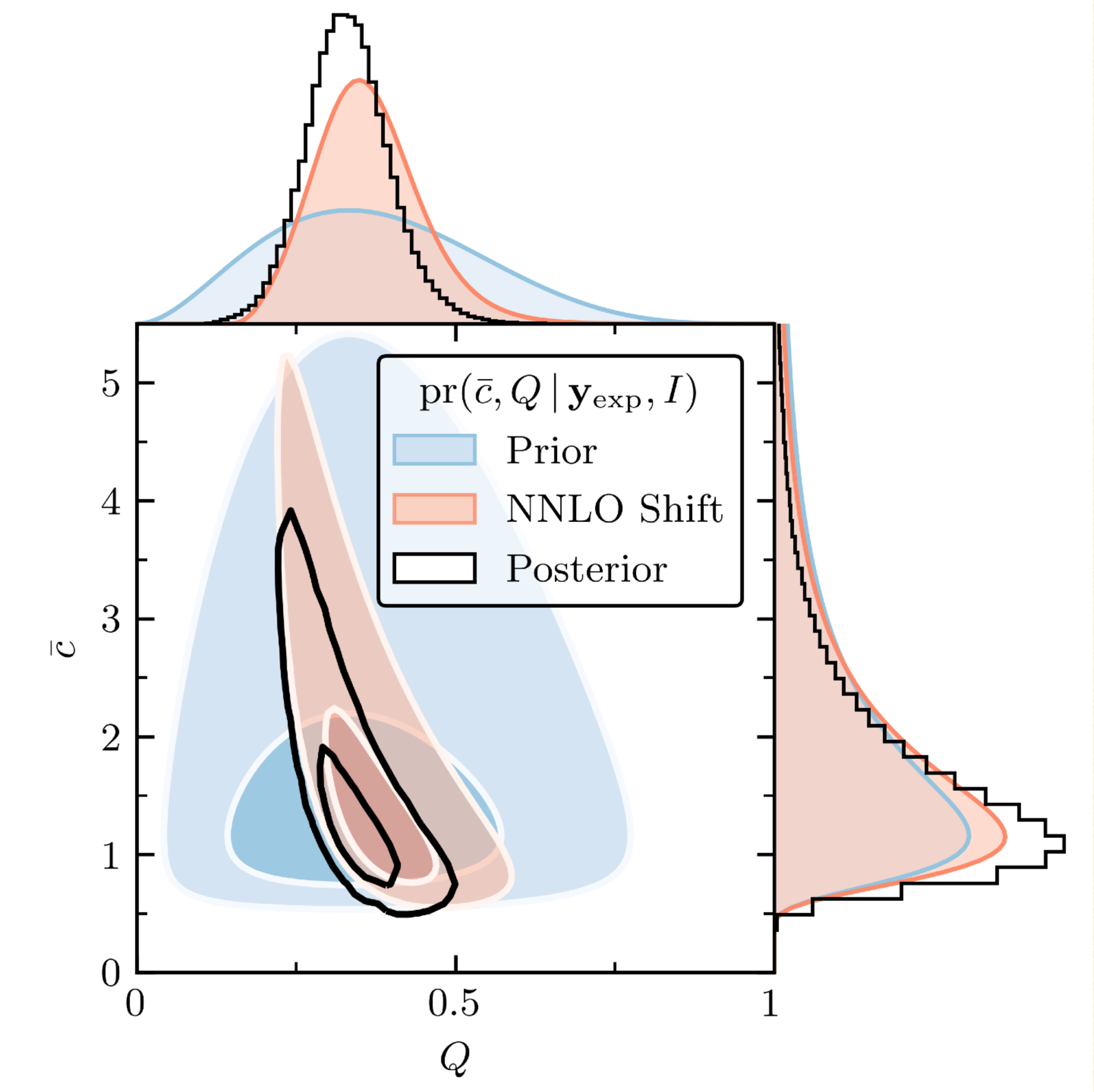


- Truncation errors essential to get consistency
- Constraints other than GT matrix element essentially degenerate
- Posterior almost obtained with just $fT_{1/2}$ and $E(^4\mathrm{He})$

Results for Q, $\bar{c}$

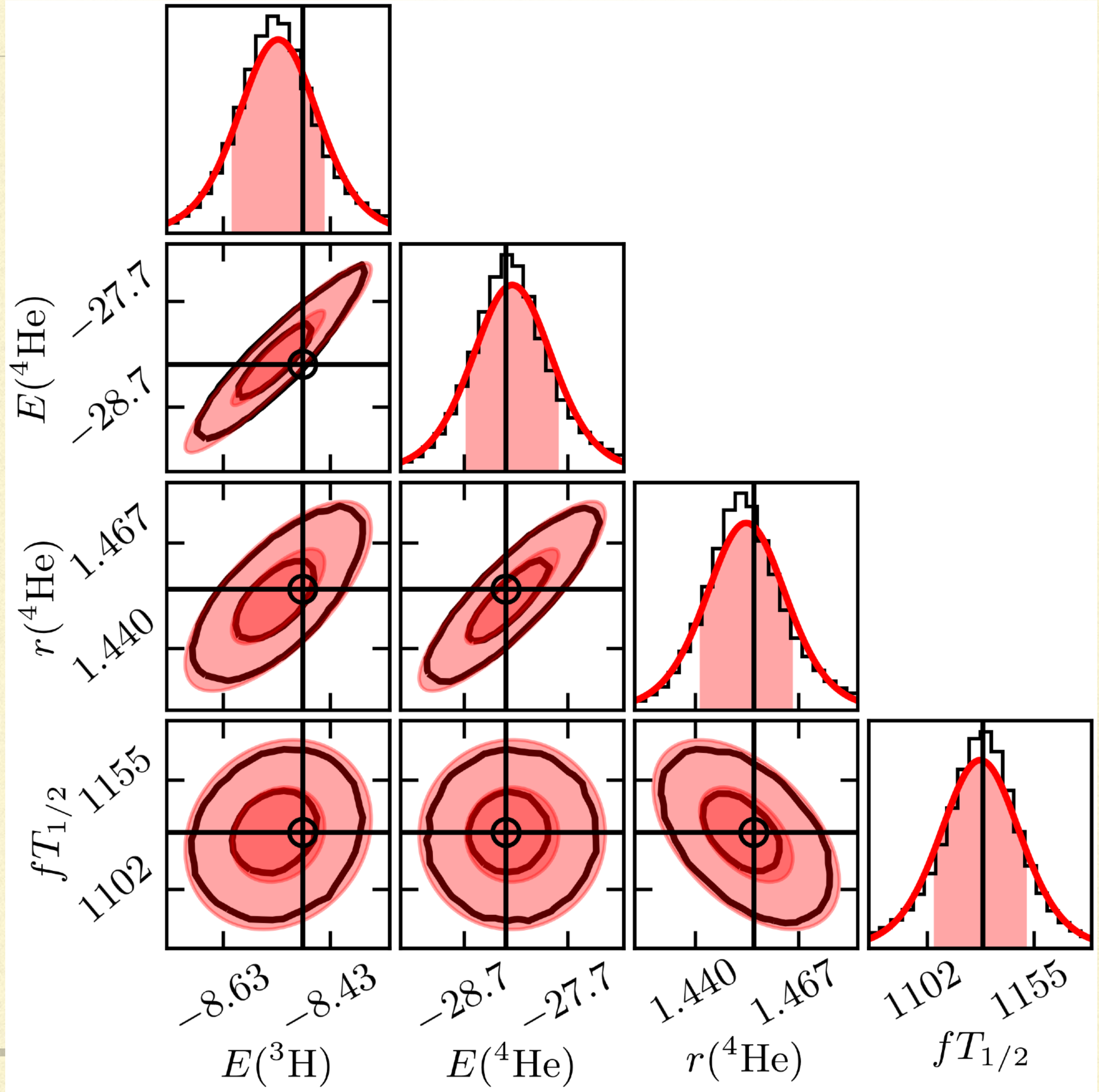
- $\mathrm{pr}(Q \,|\, \vec{a}, I)$ starts as a weakly informative Beta distribution
- Can use information on size of c_3 (NNLO-NLO shift) to update Q posterior (and $\bar{c}$ posterior too)
- But then we sample the likelihood (times the prior) allowing size of theory errors (i.e. $\bar{c}$ and Q) to 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 $\mathcal{V} = \bar{c}^2 Q^{2(k+1)}$ we have (approximately):

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

- Since $y_{\mathrm{th}}(\vec{a})$ is linear in $\vec{a}$ marginalizing over $\mathcal{V}$ 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