

Truncation errors in many-body perturbation theory and inference of three-nucleon couplings from neutron-star data

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TECHNISCHE
UNIVERSITÄT
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Crash course in nuclear theory workflow

To go from (physics) model parameters—low-energy constants/couplings (LECs)—to observables, we:

- ➊ Input LECs into χ EFT, construct an interaction potential
- ➋ Input the potential into a many-body method and solve the Schrödinger equation
- ➌ Output: scattering cross sections, nuclear binding energies, radii, equation of state (EOS) ...

Steps 1 and 2 both introduce *separate* truncation errors!

(Also, the parameters/couplings/LECs are unknown and inferred from data)

Part one: assessing truncation errors in many-body methods

arXiv > nucl-th > arXiv:2507.09079

Nuclear Theory

[Submitted on 11 Jul 2025]

A Bayesian approach for many-body uncertainties in nuclear structure: Many-body perturbation theory for finite nuclei

Isak Svensson, Alexander Tichai, Kai Hebeler, Achim Schwenk

A comprehensive assessment of theoretical uncertainties defines an important frontier in nuclear structure research. Ideally, theory predictions include uncertainty estimates that take into account truncation effects from both the interactions and the many-body expansion. While the uncertainties from the expansion of the interactions within effective field theories have been studied systematically using Bayesian methods, many-body truncations are usually addressed by expert assessment. In this work we use a Bayesian framework to study many-body uncertainties within many-body perturbation theory applied to finite nuclei. Our framework is applied to a broad range of nuclei across the nuclear chart calculated from two- and three-nucleon interactions based on chiral effective field theory. These developments represent a step towards a more complete and systematic quantification of uncertainties in *ab initio* calculations of nuclei.

Based on arXiv:2507.09079

All code and data: https://github.com/svisak/manybody_uncertainties

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Accepted by Phys. Rev. C last night :)

Motivation - errors in chiral effective field theory (χ EFT)¹

χ EFT calculations of (e.g.) nuclei have four main sources of error:

- Uncertainty in the determination of the χ EFT model parameters
- Truncation of the EFT expansion (See Hannah's talk yesterday)
- [Truncation of the many-body method](#)
- Limited model spaces

Goal:

Rigorous treatment of uncertainties arising from truncating the many-body perturbation theory (MBPT) expansion at finite order, replacing ad-hoc/expert assessments

Model is heavily inspired by the BUQEYE model for EFT truncation errors, in particular Wesolowski, IS *et al.*, Phys. Rev. C **104** (2021)

¹Weinberg, van Kolck, Kaplan, Savage, Wise, Bernard, Epelbaum, Kaiser, Meißner, . . .

Inference framework

Ground-state energy E in MBPT:

$$E = E_{\text{HF}} + \text{MBPT}(2) + \text{MBPT}(3) + \dots$$

We assume that the ratios of contributions are (roughly) constant, i.e.:

$$\frac{\text{MBPT}(2)}{E_{\text{HF}}} \approx \frac{\text{MBPT}(3)}{\text{MBPT}(2)} \approx \frac{\text{MBPT}(4)}{\text{MBPT}(3)} \approx \dots \approx \text{constant}$$

Similar to EFT, where each order is suppressed by $\approx Q!$

MBPT data and input nuclear interaction models

Our inference data: binding energies² for 37 nuclei from ^{14}O to ^{208}Pb

Use three different χEFT interaction models (sets of LECs):

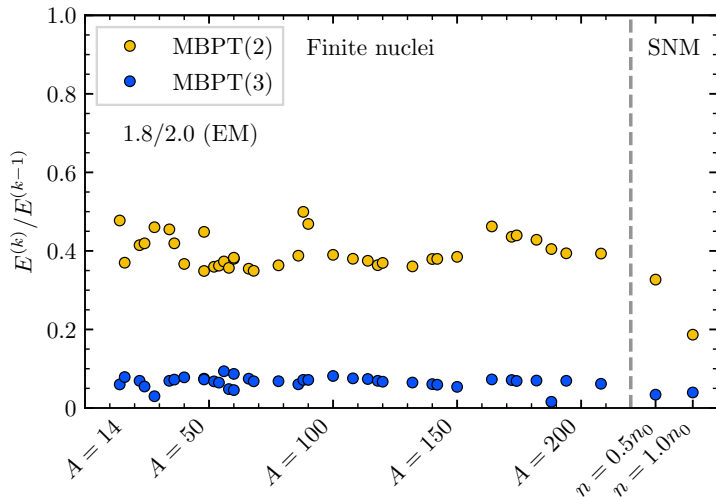
- 1.8/2.0 (EM) (“Magic”)³
- $\Delta\text{N}^2\text{LO}_{\text{GO}}$ ⁴
- 1.8/2.0 (EM7.5)²

²P. Arthuis *et al.*, arXiv:2401.06675

³K. Hebeler *et al.*, Phys. Rev. C **83** (2011)

⁴W. Jiang *et al.*, Phys. Rev. C **102** (2020)

MBPT ratios



Calculated [1.8/2.0 (EM)] ratios of MBPT corrections. Gives an idea of the convergence of the expansion as well as the correlation structure across nuclei. Symmetric nuclear matter (SNM) results are not used in the main inference.

Inference framework – EFT inspiration

BUQEYE model for EFT errors:

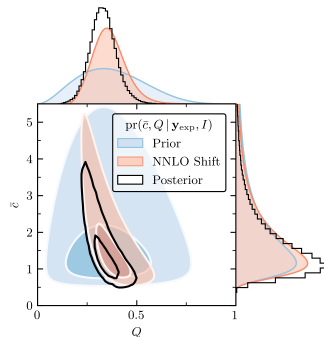
$$y = y_{\text{ref}} \sum_{i=0}^{\infty} c_i Q^i, \quad Q \approx \frac{1}{3}, \quad \text{pr}(c_i) = \mathcal{N}(0, \bar{c}^2), \quad \bar{c} \approx 1$$

Yields a truncation error⁵:

$$\delta y = \mathcal{N} \left(0, y_{\text{ref}}^2 \bar{c}^2 \frac{Q^{2(\nu+1)}}{1 - Q^2} \right) \quad (\nu \text{ chiral order})$$

Q and $\bar{c}^2$ can be learned from data (calculations)
via:

$$c_i = \frac{y_i - y_{i-1}}{y_{\text{ref}} Q^i}$$



Wesolowski, IS *et al.*, Phys. Rev. C **104** (2021)

⁵S. Wesolowski *et al.*, J. Phys. G **46**, 045102 (2019)

We assume that the **MBPT expansion** can be expressed as

$$E = E_{\text{ref}} \sum_{n=0}^{\infty} \gamma_n R^n$$

where $n = k - 1$ and k is the MBPT order (counting HF as $k = 1$)

Yields an **MBPT truncation error**: $\delta E = \mathcal{N}\left(0, E_{\text{ref}}^2 \bar{\gamma}^2 \frac{R^{2(n+1)}}{1-R^2}\right)$

Assumes $R < 1$ (i.e., a convergent series). If not, replace variance with ∞ !

R and $\bar{\gamma}^2$ can be learned from order-by-order calculations, just like Q and $\bar{c}^2$

⁶“BUQEYMBM”: Bayesian Uncertainty Quantification: Errors in Your Many-Body Method

Finding an expression for $\text{pr}(R, \bar{\gamma}^2)$

By the product rule:

$$\text{pr}(R, \bar{\gamma}^2 | \vec{\gamma}, I) = \text{pr}(\bar{\gamma}^2 | R, \vec{\gamma}, I) \times \text{pr}(R | \vec{\gamma}, I) \quad (1)$$

$\vec{\gamma} = \vec{\gamma}(R)$ is input data from order-by-order calculations. Assuming $\vec{\gamma} \sim \mathcal{N}$, placing a conjugate prior

$$\text{pr}(\bar{\gamma}^2 | I) = \mathcal{IG}(\alpha, \beta)$$

yields

$$\text{pr}(\bar{\gamma}^2 | R, \vec{\gamma}, I) = \mathcal{IG}(\alpha', \beta')$$

with

$$\alpha' = \alpha + \frac{N_{\text{nuclei}} N_{\text{orders}}}{2},$$
$$\beta' = \beta + \frac{\bar{\gamma}^2}{2}$$

Downside: does not account for correlated data. $\rightarrow$ only use 3 nuclei in inference

Q: How do we verify $\vec{\gamma} \sim \mathcal{N}$ with ~ 5 coefficients?

Finding an expression for $\text{pr}(R, \bar{\gamma}^2)$

For R , we take a uniform prior $\mathcal{U}(0, 2)$ (allowing for divergent series'!)

With these priors and $\text{pr}(\bar{\gamma}^2|R, \vec{\gamma}, I)$ in place, we get the posterior for R :

$$\text{pr}(R|\vec{\gamma}, I) \propto \frac{\text{pr}(R|I)}{\left(\frac{\beta'}{\alpha'}\right)^{\alpha'} \prod_k R^{N_{\text{nuclei}}(k-1)}}.$$

We now have every ingredient for $\text{pr}(R, \bar{\gamma}^2|\vec{\gamma}, I)$ and **sample it with MCMC**

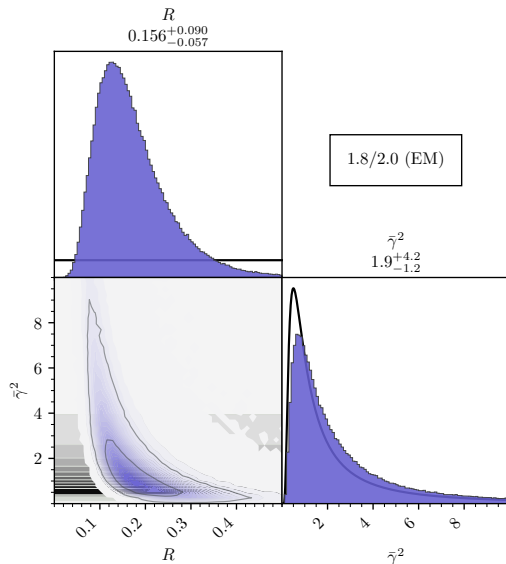
Posterior for the hyperparameters – 1.8/2.0 (EM)

We find the most likely value for $R \approx 0.15$ (with rather large uncertainty)

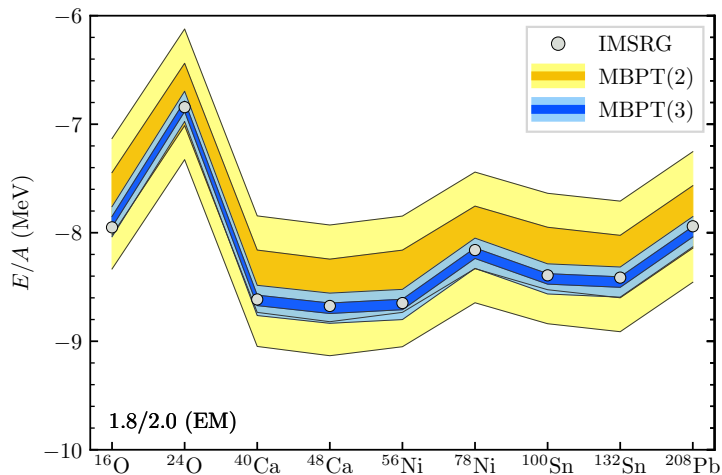
Most likely value for $\bar{\gamma}^2 \approx 1$

Naturally, R and $\bar{\gamma}^2$ are correlated (larger R can compensate for smaller $\bar{\gamma}^2$ etc.)

Each new MBPT order contributes $\approx 15\%$ of the previous order

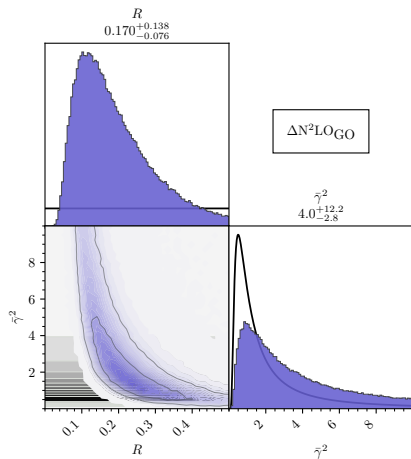


Posterior predictive distributions for nuclei

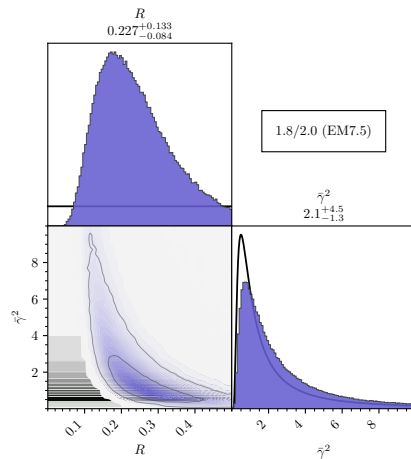


Uncertainty bands for selected nuclei, scaled by the mass number A . IMSRG(2) results for comparison as gray circles. Credibility intervals shown at the 68% and 90% levels.

Interaction sensitivity – hyperparameter posteriors



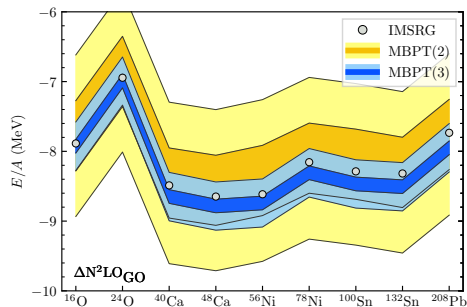
$\Delta N^2\text{LO}_{\text{GO}}$



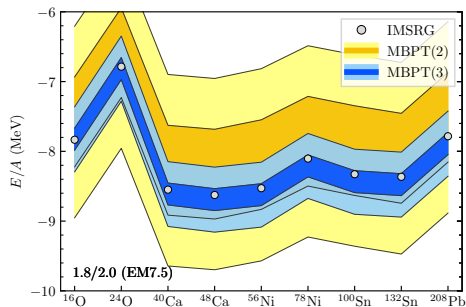
1.8/2.0 (EM7.5)

Note that R is larger than for 1.8/2.0 (EM) – **slower convergence**

Interaction sensitivity – PPDs



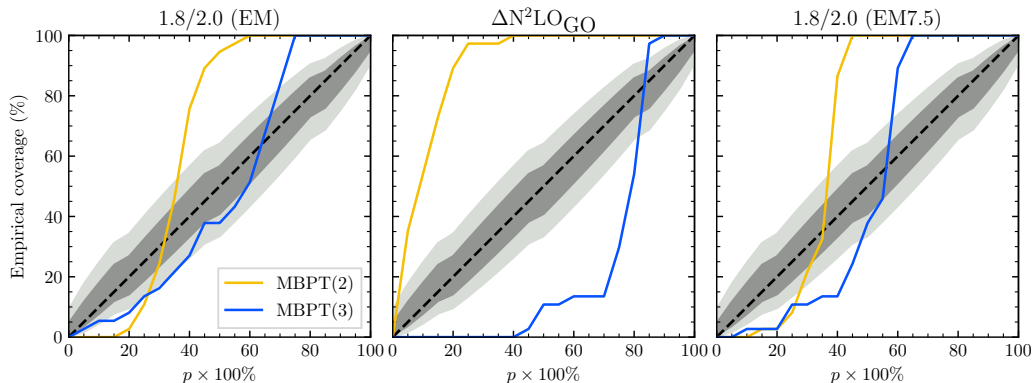
PPDs with $\Delta N^2 LO_{GO}$...



... and 1.8/2.0 (EM7.5)

These interactions are harder (converge slower), hence **larger uncertainties**

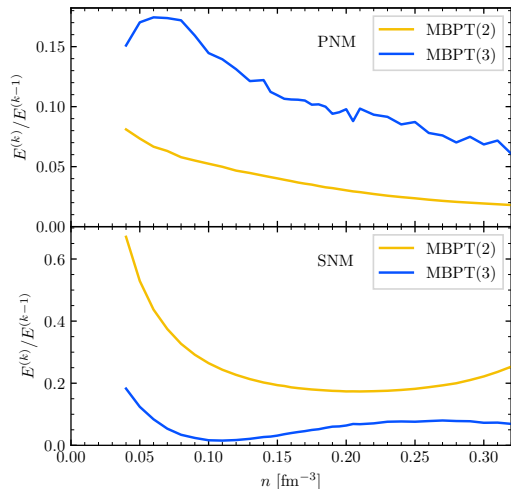
Empirical coverage of MBPT bands with respect to IMSRG data



Empirical coverages. Measures the **observed** (y -axis) vs **expected** (x -axis) coverage of the credibility intervals. Ideal result is a diagonal line. Gray areas are confidence intervals that measure whether the observed result is compatible with the ideal.

Q: How to model check when error is mostly a systematic offset?

Future work: including nuclear matter



Data from F. Alp, Y. Dietz *et al.*,
arXiv:2504.18259

For **symmetric nuclear matter** (bottom), ratios behave similarly to those of finite nuclei. We have tested the inference with two density points (0.5 and 1.0 n_0), with similar results to before.

Pure neutron matter (top), on the other hand, behaves quite differently: the MBPT(3)/MBPT(2) ratio is **larger** than the MBPT(2)/ E_{HF} ratio.

In the future, we would like to model this kind of data using **Gaussian processes**

Part two: Inferring three-nucleon couplings from multi-messenger neutron-star data

nature communications



Article

<https://doi.org/10.1038/s41467-025-64756-6>

Inferring three-nucleon couplings from multi-messenger neutron-star observations

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Achim Schwenk^{3,4,5} & Ingo Tews²

Based on Nature Commun. **16** (2025) 1, 9819

Code and data: https://github.com/svisak/multimessenger_3N_constraints

Inferring three-nucleon couplings from neutron-star (NS) data

χ EFT: Low-momentum-scale (Q) expansion

New orders introduce **unknown low-energy constants** (LECs) that need to be fit to data:

- NN LECs fit to NN scattering data
- $3N$ LECs fit to properties of light nuclei
- πN (pion-nucleon) LECs fit to πN scattering data

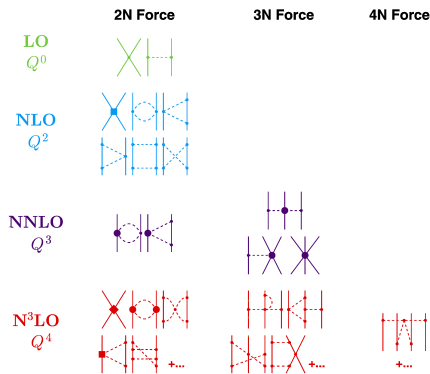


Figure adapted from Entem *et al.*, Phys. Rev. C **96**.2 (2017).

Inferring three-nucleon couplings from neutron-star (NS) data

χ EFT: Low-momentum-scale (Q) expansion

New orders introduce **unknown low-energy constants** (LECs) that need to be fit to data:

- Two-nucleon (2N) LECs fit to 2N scattering data
- 3N LECs fit to properties of light nuclei
- Pion-nucleon (πN) LECs fit to πN scattering data
- This work: fit πN LECs (governing 3N forces) to multimessenger NS data

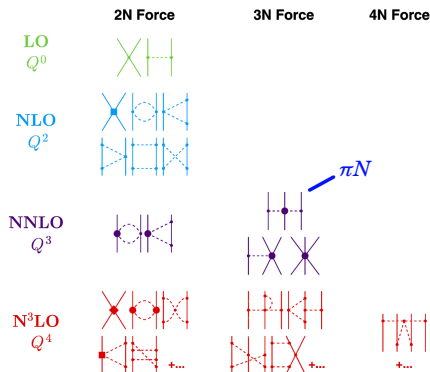


Figure adapted from Entem *et al.*, Phys. Rev. C **96.2** (2017).

Bayesian inference

χ EFT calculations of neutron matter depend on πN LECs c_1, c_3

→ In principle, neutron-star observables can constrain c_1, c_3

From LECs to NS observables:

- ➊ Input LECs into χ EFT
- ➋ Compute neutron-matter EOS using many-body perturbation theory
- ➌ Solve TOV and quadrupolar tidal perturbation equations
- ➍ Output: neutron-star masses, tidal deformabilities

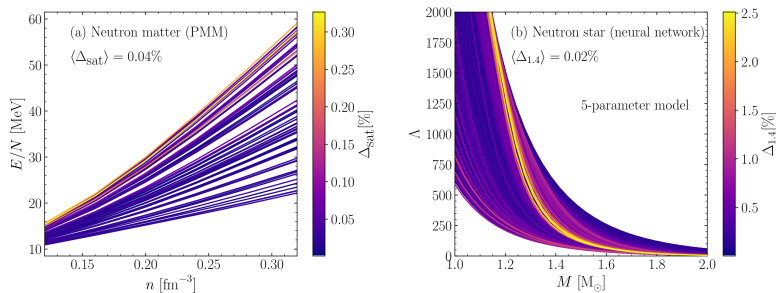
With Bayesian inference, we can go from NS data to LECs

Problem: huge computational cost

Solution: emulators, allow us to calculate $\mathcal{O}(10^8)$ samples

Emulators for the EOS (energy per particle): parametric matrix models (PMM)⁷, trained on 30 MBPT curves (+70 for validation)

Emulators for NS observables: neural networks⁸



Very good accuracy in both cases ($< 0.05\%$ on average)

Use a metamodel⁹ to provide smooth interpolation of EOS and extrapolation to matter in beta equilibrium

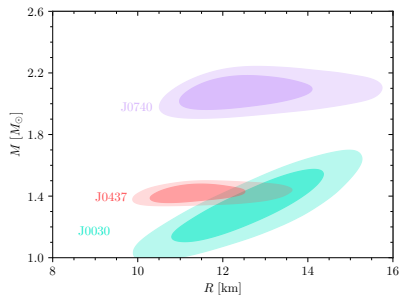
⁷Cook *et al.*, arXiv:2401.11694 (2024), Somasundaram *et al.*, arXiv:2404.11566 (2024).

⁸Reed *et al.*, arXiv:2405.20558 (2024)

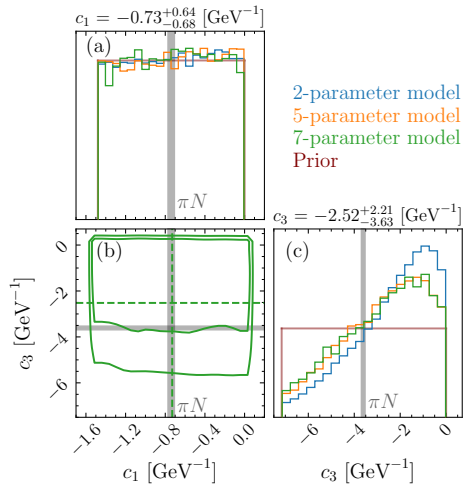
⁹Margueron *et al.*, Phys. Rev. C **97** (2018)

LEC posteriors using currently available data

We use NICER mass-radius data¹⁰ and
GW170817 gravitational wave event¹¹



No constraints on c_1 , but
clear preference for less negative c_3
(less repulsive $3N$ force)



(πN result from Hoferichter *et al.*, Phys. Rept. **625** (2016))

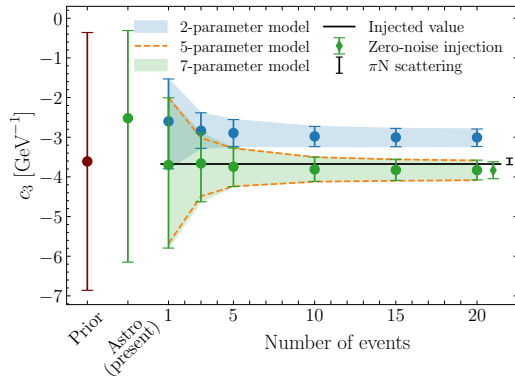
¹⁰Riley *et al.*, ApJ Lett. **887** (2019), Salmi *et al.*, ApJ **941** (2022), Choudhury *et al.*, ApJ Lett. **971** (2024)

¹¹Abbott *et al.*, PRL **119** (2017)

Can we improve this with more&better GW data?

Next, use **simulated** next-generation GW data from Einstein Telescope¹² and Cosmic Explorer¹³, ~ 1 year of observation

- Select 20 highest-SNR events, perform Bayesian inference
- c_3 converges quickly with number of observed events
- Final constraints almost comparable with πN scattering constraints
- Must marginalize over high-density parameters; 2-parameter model has large systematic uncertainty



Uncertainties given as 90% credibility intervals.

¹²Punturo *et al.*, Class. Quant. Grav. **27** (2010)

¹³Reitze *et al.*, Bull. Am. Astron. Soc. **51**, (2019)

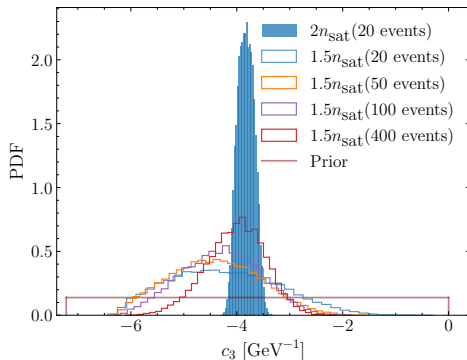
Future work: determining the EFT breakdown scale for nuclear matter

Before we used χ EFT up to $2n_0$

If we instead trust χ EFT only to $1.5n_0$
then **constraints on c_3 become much weaker**

Demonstrates the importance of learning
the breakdown scale

Distributions appear to **converge to the same value** – use this to infer
breakdown scale?



Posterior for c_3 with different upper limit for χ EFT.

Summary and outlook (MBPT UQ)

- BUQEYE-style Bayesian error model for many-body perturbation theory
- Tested on three interactions with varying convergence properties, appears to work quite well
- Gaussian processes for nuclear matter
- Handle correlated input data for finite nuclei
- Further validation of the error model – does it do what it's supposed to?
- Does the assumption of normality for $\vec{\gamma}$ hold?
- Refinements to the model, maybe make R vary with order?

Collaborators:

Alex Tichai, Kai Hebeler, Achim Schwenk

Also thanks to Dick Furnstahl, Zhen Li, Pierre Arthuis, Matthias Heinz, Takayuki Miyagi, Yannick Dietz, and Faruk Alp for discussions and input

Summary and outlook (3N inference)

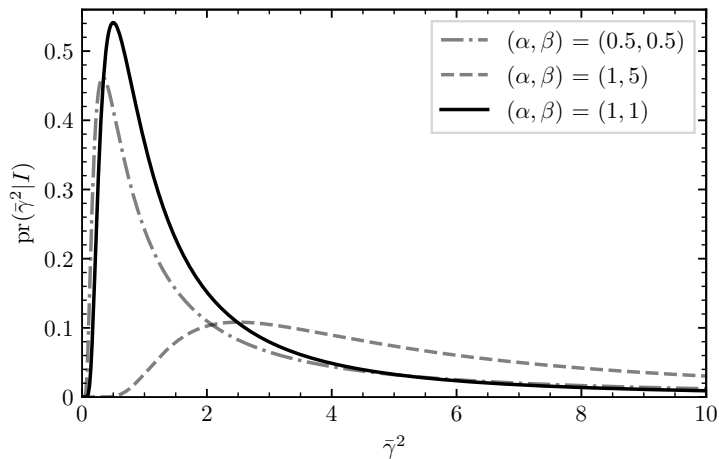
- We have developed a framework to infer 3N couplings from multi-messenger NS data
- Current and future data can provide constraints on c_3
- Provides constraints complementary to πN scattering, enables consistency checks for χ EFT
- Infer χ EFT breakdown scale for nuclear matter?

Collaborators:

Rahul Somasundaram, Soumi De, Andrew E. Deneris, Yannick Dietz, Philippe Landry, Achim Schwenk, Ingo Tews

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Prior for the hyperparameter $\bar{\gamma}^2$



Conjugate inverse-gamma prior for $\bar{\gamma}^2$. Enables analytic calculation of the posterior. Solid black line is our chosen prior. The prior for R is uniform in the range $[0,2]$.