How well do we know the neutron-matter equation of state at the densities inside neutron stars? A Bayesian approach with correlated uncertainties

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We introduce a new framework for quantifying correlated uncertainties of the infinite-matter equation of state (EOS) derived from chiral effective field theory (χEFT). Bayesian machine learning, via Gaussian Processes with physics-based hyperparameters, allows us to efficiently quantify and propagate theoretical uncertainties of the EOS, such as χEFT truncation errors, to derived quantities. We apply this framework to state-of-the-art many-body perturbation theory calculations with consistent nucleon-nucleon and three-nucleon interactions up to fourth order in the χEFT expansion. This produces the first statistically meaningful uncertainty estimates for key quantities of neutron stars. We give results up to twice nuclear saturation density for the energy per particle, pressure, and speed of sound of neutron matter, as well as for the nuclear symmetry energy and its derivative. At nuclear saturation density the predicted symmetry energy and its slope are consistent with experimental constraints.

Introduction—How well do we know the neutron-matter equation of state (EOS) at the densities inside neutron stars? This is a key question for nuclear (astro)physics in the era of multi-messenger astronomy. To answer this question from nuclear theory requires a systematic understanding of strongly interacting, neutron-rich matter at densities several times the typical density in heavy nuclei, i.e., well beyond nuclear saturation density, \( n_0 \approx 0.16 \text{ fm}^{-3} \) \( (\rho_0 \approx 2.7 \times 10^{14} \text{ g cm}^{-3}) \). The dominant microscopic approach to describing nuclear forces at low energies is chiral effective field theory (χEFT) with nucleon and pion degrees of freedom [1–4]. It has made great progress in predicting the EOS of infinite (nuclear) matter and the structure of neutron stars at densities \( \lesssim n_0 \) [5–18] (see also Refs. [19–21] for recent reviews). But the truncation errors inherent in χEFT grow dramatically with density [22–25]. Existing predictions only provide rough estimates for them, and do not account for correlations within or between observables.

In this Letter we use a novel Bayesian approach to quantify the truncation errors in χEFT predictions for pure neutron matter (PNM) at zero temperature [26, 27]. The EOS is obtained from state-of-the-art many-body perturbation theory (MBPT) calculations with consistent nucleon-nucleon (NN) and three-nucleon (3N) interactions up to fourth order in the χEFT expansion (i.e., next-to-next-to-next-to-leading order, N^3LO) [28]. Our algorithm accounts for EOS truncation errors that are correlated—both across densities and between observables—enabling us to obtain reliable uncertainties for physical properties derived from the EOS, e.g., the pressure and the speed of sound. This significant advance in uncertainty quantification (UQ) is timely given the need for statistically meaningful comparisons between nuclear theory and recent observational constraints [29].

These include the joint mass-radius measurement of the millisecond pulsar PSR J0030+0451 by NASA’s Neutron star Interior Composition ExploreR (NICER) [30–33] and tidal deformabilities of neutron stars inferred from direct detection of gravitational waves by the LIGO-Virgo collaboration [34–36].

χEFT is a systematic expansion in powers of a typical momentum scale, \( p \), over the EFT breakdown scale, \( \Lambda_b \). For infinite matter, \( p \) will be of order the nucleon Fermi momentum \( k_F \). χEFT then enables improvable calculations of strongly interacting matter up to any desired accuracy (provided \( k_F < \Lambda_b \)). But in practice there is always a discrepancy between the χEFT result and reality, because observables are only ever calculated at a finite order in the expansion, leaving a residual error that must be quantified [37–39].

Melendez et al. [26] developed a Bayesian model for EFT truncation errors that accounts for uncertainties which vary smoothly with the independent variable(s)—in this case \( k_F \) or the nucleon density \( n \). A machine learning algorithm is trained on the computed orders in the χEFT expansion, from which it learns the magnitude of the truncation error and how it is correlated in density. In a companion publication [27], we apply this new approach to infinite matter. This provides, for the first time, estimates of in-medium EFT breakdown scales and nuclear saturation properties with correlated EFT truncation errors. We also uncover a strong correlation between PNM and symmetric nuclear matter (SNM) for the χEFT Hamiltonians of interest. This is crucial to the UQ of the nuclear symmetry energy we present here.

This Letter focuses on PNM and, together with its companion paper [27], sets a new standard for UQ in infinite-matter calculations. We first review definitions relevant to our study: the energy per particle, pressure,
and speed of sound, along with the symmetry energy and its slope. Next we explain how machine learning algorithms can estimate statistically meaningful uncertainties for these observables along with their correlations. We then provide the results of our analysis. Our predictions for the symmetry energy and its slope at saturation density are shown to be in accord with experimental and theoretical constraints. The annotated Jupyter notebooks used to perform the UQ of infinite-matter observables and their derivatives are publicly available [40].

Equation of State—We consider the standard (quadratic) expansion of the infinite-matter EOS as a function of the total density $n = n_n + n_p$ and isospin asymmetry $\beta = (n_n - n_p)/n$,

$$
\frac{E}{A}(n, \beta) \approx \frac{E}{A}(n, \beta = 0) + \beta^2 S_2(n),
$$

about SNM ($\beta = 0$); with the neutron (proton) density given by $n_n$ ($n_p$). Microscopic asymmetric matter calculations based on chiral NN and 3N interactions at $n \lesssim n_0$ have shown that this commonly used expansion works reasonably well [41, 42] (see also Refs. [43, 44]). The density-dependent symmetry energy $S_2(n)$ is then given by the difference between the energy per particle in PNM ($\frac{E}{N}$) and SNM ($\frac{E}{A}$),

$$
S_2(n) \approx \frac{E}{N}(n) - \frac{E}{A}(n) \equiv S_v + \frac{L}{3} \left( \frac{n - n_0}{n_0} \right) + \ldots
$$

We focus our analysis on four key quantities for PNM and neutron stars. The first two are $S_2(n)$ and its (rescaled) density-dependent derivative $L(n) \equiv 3n \frac{d}{dn} S_2(n)$. When evaluated at $n_0$ these become, respectively, $S_v \equiv S_2(n_0)$ and $L \equiv L(n_0)$. The other two quantities are the pressure

$$
P(n) = n^2 \frac{d}{dn} \frac{E}{N}(n),
$$

and the speed of sound squared,

$$
c_s^2(n) = \frac{\partial P(n)}{\partial \varepsilon(n)} = \frac{\partial P(n)}{\partial n} \left[ 1 + n \frac{\partial}{\partial n} \frac{E}{N}(n) + m_n \right]^{-1}.
$$

[Note that the energy density $\varepsilon(n) = n \left( \frac{E}{N}(n) + m_n \right)$ includes the neutron rest mass energy $m_n$ (with $c^2 = 1$).]

The central many-body inputs of our analysis are $\frac{E}{N}(n)$ and $\frac{E}{A}(n)$ as obtained in MBPT. We extend the neutron-matter calculations in Ref. [28] to $2n_0$ and use the results reported in Refs. [22, 28] for SNM. The high-order MBPT calculations are driven by the novel Monte Carlo framework introduced by Drischler et al. [28]. It uses automatic code generation to efficiently evaluate arbitrary interaction and many-body diagrams, enabling calculations with controlled many-body uncertainties (see the reference for technical details).

Reference [28] also constructed a family of order-by-order chiral NN and 3N potentials up to $N^3$LO. The NN potentials by Entem, Machleidt, and Nosyk [45] with momentum cutoffs $\Lambda = 450$ and $500$ MeV were combined with consistent 3N interactions, where the two 3N low-energy couplings $c_D$ and $c_E$ were fit to the triton and the empirical saturation point of SNM. These intermediate- and short-range 3N interactions, respectively, do not contribute to $\frac{E}{N}(n)$ with nonlocal regulators [46]. There is consequently only one neutron-matter EOS determined for each cutoff and chiral order [28]. Our results for a given cutoff do not differ significantly for the different 3N fits. We restrict the discussion here to the $\Lambda = 500$ MeV potentials of Ref. [28] with $c_D = -1.75 (-3.00)$ and $c_E = -0.64 (-2.22)$ at $N^2$LO ($N^3$LO) and refer to the Supplemental Material for results with the other cutoff. More details on these Hamiltonians can be found in Refs. [27, 28].

Uncertainty Quantification—Our truncation error model relies on Gaussian processes (GPs), a machine-learning algorithm, to uncover the size and smoothness properties of the EFT uncertainty [47]. We train physically motivated GPs from our UQ framework to the order-by-order predictions of $\frac{E}{N}(n)$ and $\frac{E}{A}(n)$, leading to smooth regression curves. Training refers here to both estimating the GP hyperparameters (e.g., $\alpha_0$ and the GP correlation length) and finding the regression curve. Note that this approach requires choices for the functional form of the EFT expansion parameter and a reference scale for each observable, as discussed in Refs. [26, 27]. The resulting curves also include an interpolation uncertainty that accounts for many-body uncertainties in the training data. Reference [28] showed that the residual many-body uncertainty is much smaller than the $\chi$EFT truncation error for the interactions considered here. Nevertheless, to be conservative, we set this additional interpolation uncertainty to 0.1% of the total energy per particle (but $\geq 20$ keV) and check that the results are insensitive to that choice.

An important byproduct of finding the optimal regression curves is a Gaussian posterior—that includes correlations in density—for the truncation error. Combining the respective regression curve with the interpolation and EFT truncation uncertainties produces a GP for each EOS from the to-all-orders EFT. Furthermore, GPs are closed under differentiation. It is then straightforward to compute a joint distribution that includes correlations between the EOS and its derivatives [48–51].

But assessing the uncertainty in $S_2(n)$ requires an additional step. We have found that $\frac{E}{N}(n)$ and $\frac{E}{A}(n)$ converge in a similar fashion [27]; given an EFT correction of $\frac{E}{N}(n)$, it is likely that the correction to $\frac{E}{A}(n)$ will have the same sign. This additional correlation between observables implies that the truncation error in $S_2(n)$ is less than the in-quadrature sum of errors from PNM and SNM. Our truncation framework naturally extends to this case via multi-task machine learning (for details see...
Results—Figure 1 shows our order-by-order χEFT predictions, up to N^3LO, for \( F(n) \), \( P(n) \), and \( S_2(n) \) in PNM, as well as \( S_2(n) \), \( L(n) \), and \( E(n) \) in SNM. We find an EFT breakdown scale \( \Lambda_s \) consistent with 600 MeV, and optimized truncation error correlation lengths \( \ell = 0.97 \text{fm}^{-1} \) (0.48 \text{fm}^{-1}) for PNM (SNM). The correlation between the truncation errors of \( F(n) \) and \( E(n) \) is \( \rho = 0.94 \). These hyperparameters are only tuned to the derivative-free quantities \( E(n) \) and \( F(n) \); derivatives and their uncertainties are thus pure predictions of our framework, as are \( S_2(n) \) and \( L(n) \). The bands in Fig. 1 account for both the EFT truncation error and the overall interpolation uncertainty. Our Bayesian 1σ uncertainties for derivative-free quantities have been shown [38] to be broadly similar to those obtained with the “standard EFT” error prescription [56, 57]; e.g., as it was applied to the UQ of the EOS in Ref. [28]. But only our correlated approach can reliably propagate these meaningful uncertainties to \( P(n) \), \( S_2(n) \), \( L(n) \), and \( c_s^2(n) \).

We observe an order-by-order EFT convergence pattern for the observables at low densities, \( n \lesssim 0.1 \text{fm}^{-3} \). However, at N^2LO and beyond, 3N interactions enter the chiral expansion with repulsive contributions—especially at densities \( n \gg n_0 \). Their N^2LO and N^3LO EFT corrections then have a markedly different density dependence, as indicated by our model checking diagnostics [26] for each energy per particle [27]. This leads to bands that do not appear to encapsulate higher-order predictions. Nevertheless, we stress caution when critiquing the consistency of the uncertainty bands; due to the strong correlations, statistical fluctuations can occur over large ranges in density. Our credible interval diagnostics show that the bands are consistent up to these fluctuations [27].

The distributions of all observables follow a multivariate Gaussian, except for \( c_s^2(n) \), which requires sampling. The strong correlation between \( S_v \) and \( L \) produces narrow constraints at \( n_0 \): \( S_v = 31.7 \pm 1.1 \text{MeV} \) and \( L = 59.8 \pm 4.1 \text{MeV} \) at the 1σ-level. Our results for \( c_s^2(n) \) are below the asymptotic high-density limit predicted by perturbative quantum chromodynamics calculations, \( c_s^2(n \gg 50n_0) = \frac{1}{3} \) [58]. The uncertainties, however, are sizeable at the maximum density: \( c_s^2(2n_0) \simeq 0.14 \pm 0.08 \) (N^2LO) and \( c_s^2(2n_0) \simeq 0.10 \pm 0.07 \) (N^3LO). Precise measurements of neutron stars with mass \( \gtrsim 2M_\odot \) [59–62] indicate that the limit has to be exceeded in some density regime beyond \( n_0 \) [63]. Our 2σ uncertainty bands are consistent with this happening slightly above \( 2n_0 \)—especially since the downward turn of \( c_s^2(n \gtrsim 0.28 \text{fm}^{-3}) \)
Comparison with Experiment—Figure 2 depicts constraints in the $S_v$–$L$ plane. The allowed region we derive from χEFT calculations of infinite matter is shown as the yellow ellipses (dark: 1σ, light: 2σ) and denoted “GP–B” (Gaussian Process–BUQEYE collaboration). Also shown are several experimental and theoretical constraints compiled by Lattimer et al. This region is in excellent agreement with our prediction.

Our yellow ellipses in Fig. 2 represent the posterior $\text{pr}(S_v, L \mid D)$, where the training data $D$ are the order-by-order predictions of $\langle E(n) \rangle$ and $\langle S(n) \rangle$ up to $2n_0$. The distribution is accurately approximated by a two-dimensional Gaussian with mean and covariance

$$\begin{bmatrix} \mu_{S_v} \\ \mu_L \end{bmatrix} = \begin{bmatrix} 31.7 \\ 59.8 \end{bmatrix} \quad \text{and} \quad \Sigma = \begin{bmatrix} 1.24 & 3.27 \\ 3.27 & 16.95 \end{bmatrix}.$$ (5)

We consider all likely values of $n_0$ via $\text{pr}(S_v, L \mid D) = \int \text{pr}(S_v, L \mid n_0, D) \text{pr}(n_0 \mid D) \text{d}n_0$. Here, $\text{pr}(S_v, L \mid n_0, D)$ describes the correlated to-all-orders predictions at a particular density $n_0$, and $\text{pr}(n_0 \mid D) \approx 0.17 \pm 0.01 \text{fm}^{-3}$ is the Gaussian posterior for the saturation density, including truncation errors, determined in Ref. [27]. If the canonical empirical saturation density, $n_0 = 0.164 \text{fm}^{-3}$, is used instead then the posterior mean shifts slightly downwards: $S_v \rightarrow S_v - 0.8 \text{MeV}$ and $L \rightarrow L - 1.4 \text{MeV}$. This shift is well within the uncertainties computed using our internally consistent $n_0$. In contrast to experiments, which extract $S_v$–$L$ from measurements over a range of densities, our theoretical approach predicts directly at saturation density, thereby removing artifacts induced by extrapolation.

Our 2σ ellipse falls completely within constraints derived from the conjecture that the unitary gas is a lower limit on the EOS [73] (solid black line). The same work also made additional simplifying assumptions to derive an analytic bound—only our 1σ ellipse is fully within that region (dashed black line). Figure 2 also shows the allowed regions obtained from microscopic neutron-matter calculations by Hebeler et al. [71] (based on χEFT NN and 3N interactions fit to few-body data only) and Gandolfi et al. [72] (where 3N interactions were adjusted to a range of $S_v$). The predicted ranges in $S_v$ agree with ours, but we find an $L$ that is $\approx 10 \text{MeV}$ larger, corresponding to a stronger density-dependence of $S_2(n_0)$. References [71, 72] quote relatively narrow ranges for $S_v$–$L$, but those come from surveying available parameters in the Hamiltonians and so—unlike our quoted intervals—do not have a statistical interpretation.

Summary and Outlook—We presented a novel framework for EFT truncation errors that includes correlations within and between observables. It enables the efficient, reliable evaluation of derived quantities. We then constrained multiple key observables for neutron-star physics based on cutting-edge MBPT calculations with consistent chiral NN and 3N interactions up to N³LO. Correlations in the EFT truncation error—both across densities...
and between different observables—must be accounted for in order to obtain honest credible intervals. In several cases (e.g., $S_m$) the result is a much smaller uncertainty than one might naïvely expect. Our narrow predictions for $S_m - L$ are in excellent agreement with the joint experimental constraint.

A rigorous comparison between empirical constraints on the EOS and our knowledge of the underlying microscopic dynamics of strongly interacting nuclear matter is particularly important in the era of multimessenger astronomy, because new empirical constraints on the neutron-star EOS are anticipated from NASA’s NICER [30–33] as well as the LIGO-Virgo collaboration [34–36]. Nuclear physics experiments, such as the California Nuclear Physics Experiment (CREX) [76] and those at The Facility for Rare Isotope Beams (FRIB) [77], will also contribute important information to this overall picture.

Our Bayesian framework can be straightforwardly adapted and used in future studies that will more firmly establish this comparison. A full Bayesian analysis can be performed via Markov Chain Monte Carlo sampling over GP hyperparameters and the low-energy couplings in the nuclear interactions [39, 78, 79]. This will require the development of improved chiral NN and 3N forces up to N$^3$LO [80]. Extensions of our analysis to arbitrary isospin asymmetry and finite-temperature are also an important avenue for future study. Work in all these directions will be facilitated by the public availability of the tools presented here as Jupyter notebooks [40].

We thank S. Reddy for fruitful discussions. We are also grateful to the organizers of “Bayesian Inference in Subatomic Physics – A Marcus Wallenberg Symposium” at Chalmers University of Technology, Gothenburg, for creating a stimulating environment to learn and discuss the use of statistical methods in nuclear physics. CD acknowledges support by the Alexander von Humboldt Foundation through a Feodor-Lynen Fellowship and between different observables—must be accounted for in order to obtain honest credible intervals. In several cases (e.g., $S_m$) the result is a much smaller uncertainty than one might naïvely expect. Our narrow predictions for $S_m - L$ are in excellent agreement with the joint experimental constraint.

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