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Uncertainties with Low-Resolution Nuclear Forces



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Introduction

Uncertainty quantification is a key aspect of modern nuclear theory. Theories of nuclear forces and most many-body methods are approximate, and the uncertainties associated with these approximations must be quantified. Chiral effective field theory (EFT) provides a systematically improvable description of nuclear forces rooted in quantum chromodynamics. Such forces have several sources of uncertainty, due to the truncation of the EFT, how the forces are regularized, and how they are fit to data. Recent advances in Bayesian uncertainty quantification have enabled systematic approaches to quantifying theoretical uncertainties from various sources and propagating them to nuclear observables. A notable gap in this body of work is uncertainty quantification for low-resolution Hamiltonians from chiral EFT, which have been successful in providing accurate predictions for nuclear structure. An interaction that stands out in the accurate description of binding energies and spectra across the nuclear chart is the 1.8/2.0 (EM) interaction. Despite this remarkable accuracy, the uncertainties of this Hamiltonian are notoriously difficult to quantify. Recent works have significantly advanced the quality of uncertainty estimates for nuclear structure observables. We aim to do the same for low-resolution Hamiltonians, combining their historical success with modern uncertainty quantification methods.

Methods

A key barrier to performing Bayesian inference and robust uncertainty quantification for low-resolution Hamiltonians is the lack of an explicit operator basis. Low-resolution Hamiltonians

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are produced through nonlinear renormalization group (RG) transformations. The RG transformations make them amenable to manybody calculations but destroy the underlying analytic structure of the potentials that is typically leveraged for uncertainty quantification. While EFT truncation uncertainty estimates for such potentials are possible in some prescriptions, a complete treatment of uncertainties, going from few-body observables to Bayesian inference for low-energy constants (LECs) to posterior predictive distributions for nuclear structure, is still missing. We overcame this barrier by leveraging data-driven singular value decompositions (SVDs) of nuclear forces. Such decompositions have been demonstrated to precisely reproduce the input Hamiltonians using only a few terms, meaning such decompositions effectively expose a low-rank operator basis for nuclear Hamiltonians. Based on such decompositions, we are able to use state-of-the-art Bayesian uncertainty quantification approaches to account for EFT truncation uncertainties when using low-resolution Hamiltonians. We applied these developments to study the structure of neutron-rich oxygen and calcium isotopes. In order to obtain distributions for medium mass observables we have to repeadeatly solve the many-body Schrödinger equation with the use of the in-medium similarity renormalization group (IMSRG). This computationally heavy task would be infeasible without the use of supercomputers like the lichtenberg HPC. We have developed a framework to quantify EFT truncation uncertainties for lowresolution interactions. We obtained a linear operator structure for SRG-evolved NN interactions through singular value decompositions. We used the sensitivity of lowenergy phase shifts to identify relevant low-energy operators. With a parametric description of the interaction at hand, we performed Bayesian inference for the underlying singular values. We constructed the likelihood for the inference from predictions for NN scattering phase shifts in S- and P-waves and for the triton energy and comparative half life. For NN phase shifts, we considered two likelihoods, both using phase shifts at energies up to 200 MeV. Phase shifts at different energies are treated as uncorrelated quantities, a simplification that can be improved in future work through the construction of correlated EFT truncation models using Gaussian processes. One likelihood, E_2, is more conservative than the other E_1, including less information about low-energy phase shifts in the construction.

Results

Based on the combined NN and 3N likelihoods, we performed Bayesian inference for the singular values in our NN potentials and for c_D and c_E in our 3N potentials. We performed model checking for the inferred parameter distributions. We found that the input 3N likelihood is accurately reproduced by our posterior Hamiltonian distributions. On the other hand, we found that for the NN phase shifts they did not exactly reproduce the likelihood as expected for unconstrained uniform priors. We concluded that the limited amount of independent operators in each partial wave and untreated correlations in phase shifts are responsible for these shortcomings. Finally, we propagated the Hamiltonian uncertainties to medium-mass nuclei through IMSRG calculations

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using Hamiltonians sampled from our posterior distribution. We calculated PPDs for the ground-state energies of ^{24}O, ^{28}O, and the difference $\Delta E(^{28,24}O)$. We found that our more conservative distribution based on the E_2 likelihood is compatible with experiment for $\Delta E(^{28,24}O)$. We also calculated PPDs for the energy, charge radius, and neutron skin thickness of ^{48}Ca. We compared our distributions to existing estimates of uncertainties for these observables. Our uncertainties were significantly smaller than the more conservative history matching results.

Discussion

Our work focuses on capturing EFT truncation uncertainties in the distribution of underlying parameters in our Hamiltonian, commonly called parametric uncertainty. Through the inclusion of EFT truncation uncertainties in the Bayesian inference, the parametric uncertainty is closely related to the actual EFT truncation uncertainty. For full uncertainty quantification in nuclear structure calculations, the parametric uncertainty must be augmented with additional EFT truncation and many-body method uncertainties. A key challenge here is that these three uncertainties (parametric, EFT truncation, and many-body method) are all correlated, but this correlation is challenging to study quantitatively and needs further work. A systematic study of correlations between truncation uncertainties of observables across nuclei remains an important subject for future research.

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