B. Project Description

1 Overview

This proposal is to support in part the individual research efforts of the PI (Furnstahl) and associated students and postdocs. Current NSF support is from Sept. 1, 2016 to Aug. 31, 2019 through NSF Grant PHY–1614460, *Research in Strong-Interaction Theory*, which is a group grant with Profs. Sabine Jeschonnek and Robert Perry.

a. Overview of Nuclear Theory Group Personnel

The Nuclear Theory Group (NTG) at Ohio State does research on a wide range of nuclear systems. The faculty members based at the Columbus campus are Profs. Furnstahl, Perry, Ulrich Heinz, and Yuri Kovchegov, while Prof. Jeschonnek teaches at the Lima Campus. Profs. Heinz and Kovchegov, whose research is on relativistic heavy-ion physics, are supported by a joint grant from DOE. Prof. Scott Bogner of MSU is an Adjunct Professor at OSU and is a frequent visitor.

We have a long-established record of strong nuclear theory postdocs at Ohio State. Postdocs mentored by the PI who were supported in the past by group NSF grants and are now in faculty positions include Scott Bogner (MSU), Joaquin Drut (UNC), Hans-Werner Hammer (U. Bonn), Heiko Hergert (MSU), Derek Leinweber (U. Adelaide), Tom Mehen (Duke), Lucas Platter (U. Tennessee), Sunethra Ramanan (IIT Madras), Achim Schwenk (TU Darmstadt), and Mike Strickland (Kent State U.). Other talented postdocs have gone on to success outside of physics, such as Werner Koepf (Senior VP of Engineering, Live Nation), Jim Steele (VP of Engineering, Knowles Corporation), Huabin Tang (Aerospace Engineer at NASA), and most recently, Nathan Parzuchowski (Staff Scientist, Riverside Research Institute). Recent postdocs Kai Hebeler (Research Scientist, soon to be Privatdozent) and Sebastian Koenig (five-year Herzberg Fellow) are now both at TU Darmstadt, and CSC-FRIB Fellow Yinu Zhang has just started a postdoc at WMU. New postdoc Xilin Zhang, formerly at the University of Washington, will continue at OSU into the next grant period.

We have found that the mix of analytical and numerical computation our undergraduate and graduate students must employ is excellent preparation for both academic and industrial research. The most recent PhD's are Alex Dyhdalo, who graduated in Spring 2018 and is working at the Johns Hopkins Applied Physics Lab; Sarah Wesolowski, who graduated in Summer 2017 and has just accepted a tenure-track Assistant Professor offer from Salisbury University; and Sushant More, who graduated in Summer 2016, did a postdoc at MSU, and is now working for Chase Bank. Kyle Wendt, who graduated in 2013, is currently a Lawrence Fellow at LLNL.

There are two advanced graduate students working on projects described in this proposal. Jordan Melendez started research in 2016 and will continue into the next grant period working on Bayesian statistical methods for effective field theories (EFTs). Anthony Tropiano started research in 2017 and will join the current grant in January, 2019. His research so far has been on renormalization group methods; he is likely to next pick up the optical potential project described below.

b. Intellectual Merit of Proposed Research

We are now in the era of precision calculations of nuclear structure and reactions, which seek to address the full table of nuclides and astrophysical systems such as neutron stars. The precision era has been enabled by advances in theoretical methods, both conceptual and algorithmic, computational capabilities, and enhanced confrontation with experiment. Past grants supporting the PI have made significant contributions to this progress; particular contributions from the current grant are detailed in section 2. We propose to build on the insights, tools, diagnostics, and collaborations described there to address how to make credible predictions of a wide variety of nuclear phenomena, with quantified uncertainties, and to further validate our theoretical models.

Projects are proposed in three major categories: Bayesian statistical methods for EFT uncertainty quantification (UQ), EFT for finite density nuclear systems, and calculation/extraction of process-independent quantities. The Bayesian methods have been under development since 2014 and have a wide scope: they will be extended and applied to inter-nucleon interactions, few- and many-body systems, and electroweak probes. Our recent studies of the density matrix expansion and phase-space contributions to many-body calculations motivate further work on finite-density power counting and a renewed look at EFT for nuclear density functional theory. Finally, we will build on recent progress in understanding knock-out reactions from a renormalization group perspective, which highlights scale and scheme dependence in these interactions and raises questions about how to best analyze experiments that rely on factorization assumptions. Applications range from optical potentials to alternative treatments of short-range-correlation (SRC) physics (e.g., the nuclear contact). These projects all contribute to the goal of microscopic, model-independent calculations of nuclei. They will impact forefront problems in low-energy nuclear physics as outlined in the Long Range Plan [1], such as the physics of nuclei far from stability, which is relevant for astrophysics and to FRIB, and they will contribute to the SciDAC-4 NUCLEI project.

As in all past grants involving the PI, we expect that there will be projects not anticipated in this proposal that arise from the initiative of supported postdocs and students. This is natural, as the PI has always provided postdocs and students with a large measure of intellectual freedom, which is essential if they are to have the chance to demonstrate their independence.

c. Broader Impacts of the Proposed Work

The training and mentoring received by undergraduates, graduate students, and postdoctoral research associates in carrying out the proposed activities contributes directly to the building of a diverse scientific workforce. The mix of analytical and numerical computation our students and postdocs must employ is excellent preparation for both academic and industrial research. This is validated by the strong track record of past members of the group.

Other impacts listed here and in the section on Results from Prior NSF Support are either directly tied to research projects or arise indirectly through the activities of the co-PIs. Examples: i) The PI will continue to actively involve undergraduates in research, which benefits them *and* the group. A new initiative on visualization for advanced physics in Python will involve a large number of students at Ohio State and beyond. Ongoing curriculum developments are listed in section 2b. ii) The PI is Director of the TALENT initiative to provide Training in Advanced Low-Energy Nuclear Theory. Furnstahl and Achim Schwenk are actively writing a textbook based on a past TALENT course and on current courses given at their institutions, to be released online during the new grant cycle. iii) Use of Bayesian methods is spreading rapidly in nuclear physics and the PI will continue to facilitate this dissemination. He was a co-organizers of an INT program for summer, 2016 entitled “Bayesian Methods in Nuclear Physics” and of an EMMI workshop in 2018 on "Uncertainty Quantification at the Extremes" (both part of the ISNET series), which brought together statisticians and nuclear practitioners to explore how Bayesian inference can enable progress on the frontiers of nuclear physics and open up new directions for the field. iv) Many projects proposed here directly tie into the SciDAC-4 NUCLEI-2 project.

2 Results from Prior NSF Support

Projects funded by the NSF in the PI's group have helped push reliable nuclear calculations to new domains and have attacked important open questions. Most of these developments are in close synergy with the efforts of the NUCLEI projects; NUCLEI has funded travel for the PI and the postdocs and students to collaboration meetings, and for some visitors to OSU, and partially supported the postdocs and some students. In this section we highlight results from NSF research projects funded from 2016 to the present that have been published [2–21]. Further details on projects that are ongoing or will lead to new proposed projects are given in subsequent sections.

a. Intellectual Merit

A major theme in the current grant is the development of tools for uncertainty quantification (UQ) based on Bayesian statistics. Most projects are part of the BUQEYE collaboration to apply Bayesian methods to UQ for EFT, which was initiated by the PI and then-grad-student Sarah Wesolowski with Daniel Phillips and students at Ohio University in 2014. Wesolowski's PhD work included a detailed framework for parameter estimation in EFTs [3] and specific applications to chiral EFT [21] (completed after her move to Salisbury University). Current grad student Jordan Melendez, Wesolowski, and the PI extended previous work on truncation errors for chiral EFT in an Editor's Suggestion paper [10]. Some results from the latter are shown in Fig. 1 and were also featured as the March picture on the 2018 APS wall calendar. Ongoing projects and new extensions are outlined in section 3, with an emphasis on physics *discovery* and model checking, not just error assessment.

Uncertainty quantification is also a major theme of the LENPIC collaboration. LENPIC is focused on applying a new generation of consistent chiral EFT interactions and operators with semi-local regulators, which are designed to reduce regulator artifacts. The PI's contributions to LENPIC in Refs. [2, 6, 19] included a Weinberg eigenvalue analysis of the new potentials and explorations of an appropriate expansion parameter for UQ. It would be natural to adapt our advanced Bayesian methods to the LENPIC efforts in the next grant cycle, but this is not yet planned. Weinberg eigenvalues have been used by the PI and collaborators for many years as a diagnostic tool. Recently the PI and colleagues at TU Darmstadt made an independent Weinberg eigenvalue analysis of a wide range of potentials [11]. This work provided many insights into the perturbativeness and scheme dependencies of these interactions.

Postdoc Sebastian König (or Koenig) brought particular expertise on so-called "pionless" EFT, which describes processes at low energies to high precision, without needing explicit dynamical pions. His work under the prior grant included systematic calculations of the proton-deuteron system including long-range Coulomb effects [22, 23], the consistent renormalization of three-body systems [24], and constraints on a possible dineutron state [25]. His work under the current grant included a treatment of ^{3}He and pd scattering in pionless EFT in second-order perturbation the-

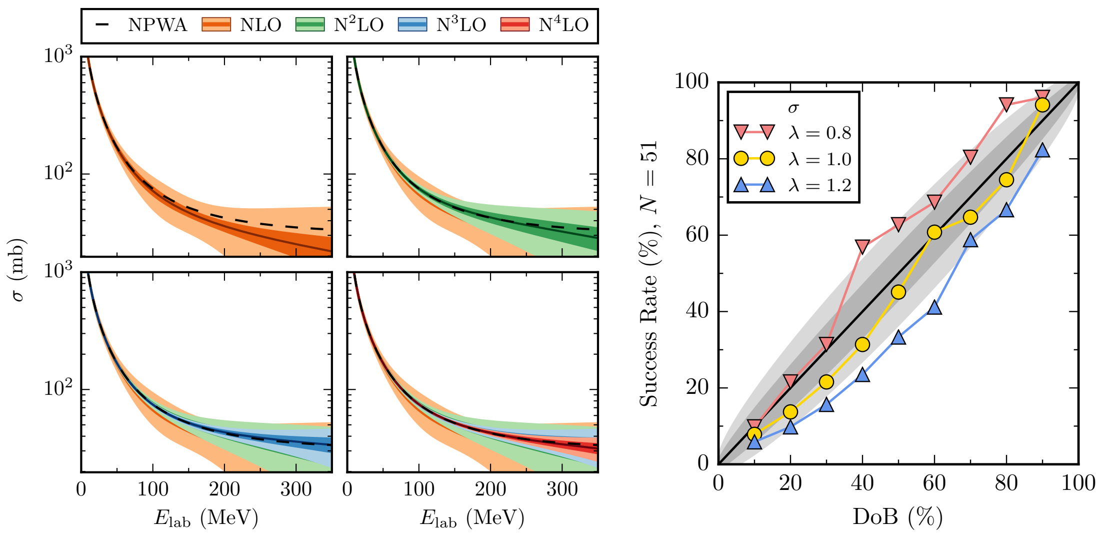

Figure 1: Left: order-by-order credible interval bands (68% and 95%) for the neutron-proton (np) cross section as a function of energy [10]. Right: Credible interval diagnostic for the np cross section with three choices of the breakdown scale $\Lambda_b = \lambda \times 600\,\text{MeV}$. (See section 3 for further details.)

ory [8] and a perturbative effective theory of ^{3}H and ^{3}He [5], leading to a treatment of nuclear physics for light nuclei and possibly higher as an expansion about the unitarity limit [12]. With Hans-Werner Hammer he wrote a timely review article on “General aspects of effective field theories and few-body applications” [7]. All these calculations are of direct experimental interest, but also important because pionless EFT is a much better understood and controlled framework than chiral EFT, which in its current implementation is plagued with intertwined open issues and controversies of power counting, renormalizability, perturbative versus nonperturbative resummations, and regulator dependence. In section 3 we propose using pionless EFT (in collaboration with König) as a laboratory for confronting issues relevant to chiral EFT in a robust framework, and as a guide to uncertainty quantification and precision calculations.

The thesis work of Alex Dyhdalo explored several different aspects of chiral EFT. As with any quantum field theory, a regularization scheme and scale must be introduced to define the theory. To regulate divergent loops, chiral EFT introduces cutoff regulators, which become an intrinsic part of the nuclear potentials. With the Weinberg power counting scheme, which is used in essentially all microscopic calculations to date, iteration of the potential beyond leading order generates divergences without all the corresponding counterterms. As a result, the EFT is no longer strictly renormalizable and there are significant regulator artifacts. Until recently, almost all calculations used potentials with similar non-local regulators. However, now there are fully local regulators for use with quantum Monte Carlo calculations [26] and semi-local regulators designed for improved power-counting behavior [27]. Dyhdalo led an investigation of the impact of different regulators, with help from the PI, former postdoc Hebeler, and Ingo Tews, a postdoc at the INT [4]. The strategy was to use uniform matter as a testbed and work in many-body perturbation theory [28]. A Monte-Carlo sampling method was developed to probe the interaction phase space in energy integrals using a variety of regulators, which revealed some striking differences between different regulators. Another phase-space-based effort by Dyhdalo was to develop and validate a power counting for softened potentials in uniform matter [14]. This power counting completely changes the conventional hole-line-expansion power counting developed for hard potentials. The observed impact of the regulators led to revisiting the implementation of the density matrix expansion (DME), which had stalled in previous attempts that did not include regulators. Dyhdalo, with the PI and Bogner, developed a new formulation with regulators and in coordinate space [9]. This new approach was first implemented by a LLNL team with Dyhdalo, the PI, and Bogner in Ref. [16], with the OSU contributions supported in part by the NUCLEI project. The results are both encouraging and puzzling, as discussed further in section 4 along with follow-up projects.

The development and application of the Similarity Renormalization Group (SRG) [29–31] to low-energy nuclear physics has been a major theme of NSF-supported research at OSU since 2007 (see Refs. [32–34] for reviews). This included early work by Bogner on the in-medium SRG (or IM-SRG) and later major advances spearheaded by Hergert [35–37] as a postdoc at OSU. In the current grant cycle, postdoc Nathan Parzuchowski, a PhD student of Bogner's at MSU who started at OSU in Spring, 2017, worked in particular on the implementation and application of electromagnetic transition operators using the equations-of-motion approach for excited states in the IM-SRG [13, 17, 18]. Parzukowski left OSU early (in March, 2018) for family reasons to take an industry job in Dayton, OH. The ongoing projects, which were largely supported by NUCLEI-2, have been transferred to MSU and will lead to follow-up work credited in part to OSU, but no additional work funded by the NSF is proposed at this time. As his warm-up problem, grad student Anthony Tropiano has been testing the Magnus expansion used for IM-SRG operator evolution on large-cutoff chiral EFT with the SRG [38], with new insights into renormalization issues. This work should be completed and published in the current grant cycle.

Parzukowski had also started work on IM-SRG calculations of the nuclear contact, which will be continued by Bogner and the PI, see section 5. This work ties into complementary efforts to understand the scale and scheme dependence of nuclear observables, which was previously studied for shell structure by Hergert and collaborators [39] and addressed by Furnstahl for RG-evolved systems [40]. In the prior grant cycle, grad student Sushant More and postdoc König (with Furnstahl and former postdoc Hebeler) explored how the ingredients for deuteron electrodisintegration: deuteron wavefunction, interaction current, and final state interactions, intermix with changes in SRG resolution while leaving the observable cross section invariant [41]. A major effort by More (with Bogner and Furnstahl), finished after he became a postdoc at MSU, addresses the scale and scheme dependence of this process [15]. This leads to the general question of how to extract process-independent quantities from experiment, for which several projects are proposed in section 5.

Postdoc Xilin Zhang started at OSU in September, 2018, and is supported in part by the NSF grant and in part by the NUCLEI-2 project. There are two projects he brings with him that will be completed in the current grant cycle. The first, with Prof. Jerry Miller, explores the functional form of the nucleon axial current form factor $G_A(Q)$ in the framework of a quark model quantized on the light front, with the pion cloud contribution explicitly included [42]. The goal is improved theoretical understanding of nucleon form factors used in neutrino-nucleus reactions, which is critical for the success of future long-baseline neutrino oscillation experiments. They are also studying the impact of this form factor on neutrino–nucleus quasi-elastic scattering cross sections and specifically on the DUNE experiment hosted at Fermilab. The second project is on the radiative capture reaction: ${}^3\mathrm{He}\,(\alpha,\gamma)^7\,\mathrm{Be}$. The uncertainty of this reaction's cross section is one of the major uncertainty sources for solar neutrino flux predictions [43]. The current cross section data have energies above 0.1 MeV, so a theory (or model) is needed for extrapolating the cross section down to zero energy (keV in solar environment). Zhang is finishing work with Prof. Ken Nollett and Daniel Phillips to study this reaction in the framework of Halo-EFT [44] by treating the two nuclei in the initial state as point particles and the final state nucleus as a shallow bound state of the former two. The theoretical uncertainty of the NLO calculation is combined with the data uncertainty through Bayesian inference, yielding error bars half the size of the previous recommendation [43]. A new result is that the capture reaction data alone strongly constrain ^{3}He–α elastic scattering parameters.

b. Broader Impacts

The training and mentoring of young scientists by the PI, including three members of underrepresented groups, is a direct contribution to the building of a diverse scientific workforce. Recently supported graduate students and postdocs have already been mentioned. Undergraduates have also been an integral part of the Nuclear Theory group research efforts with REU support from NSF.

The most recent undergraduate students include Yukari Yamauchi, who is in graduate school in physics at the University of Maryland, and Taylor Shaffner, who started in fall, 2018 as a graduate student in physics at Yale University. Yukari and Taylor worked on Bayesian evidence calculations in model problems to simulate EFTs. Matthias Heinz graduated in spring, 2018 and is now studying physics at TU Darmstadt while already working in the group of former postdoc Achim Schwenk, building on his research from OSU. Matthias developed codes for the similarity renormalization group (SRG) in one dimension to study the growth of many-body forces. He was a two-time participant in the DNP/CEU program while at OSU. A large group of current students are participating in a new project initiated this fall by the PI that aims at building visualization tools in Python for upper-level physics classes (in the spirit of the old CUPS simulations) as well as for frontline research.

The PI continued development of a survey course that is part of an FRIB Theory Alliance initiative. He also continued a studio-based computational physics course he originated in 2002 because of the need to train the graduate and undergraduate students supported by the NSF and handed this off to another instructor. Extensive materials for these courses as well as graduate courses on theory for low-energy nuclear physics are freely available online. Furnstahl served as Director of the TALENT initiative. A three-week intensive TALENT course on nuclear forces for structure and reactions, with Furnstahl and Schwenk as lecturers, was given in summer 2013 at the INT. He will be a co-organizer and lecturer at an upcoming course in summer 2019 entitled "Learning from Data: Bayesian Methods and Machine Learning".

3 Bayesian statistics for EFT

There is a widely recognized need for theory uncertainty quantification (UQ) in low-energy nuclear physics. Bayesian statistics offers a compelling alternative to frequentist methods [45] and is ideal for treating systematic theory errors. The Bayesian methodology allows the consistent inclusion of all sources of uncertainty, and allows us to find probability distribution functions (PDFs) for the parameters of the theory by using all the available data, without overfitting, and then to propagate uncertainties to PDFs for observables. The BUQEYE collaboration between OSU and

OU (and now others) revived and extended the application of Bayesian methods to EFTs originated by Schindler and Phillips [46]. For an EFT, the approach makes explicit what is usually implicit, allowing assumptions to be applied consistently, tested, and modified given new information [47]. At OSU this has been the NSF-supported thesis work of Sarah Wesolowski and Jordan Melendez.

The projects proposed here build on our UQ developments since 2015, with an emphasis on validation through Bayesian model checking and exploiting the potential for physics discovery. We will give some brief descriptions of the latest developments as background for the new projects.

The first application to chiral EFT truncation errors [48] was extended recently to a thorough analysis [10] of the potentials of Epelbaum, Krebs, and Meißner (EKM) [27, 49], including a demonstration that their prescription for uncertainty estimates could be embedded in a Bayesian statistical framework. This replaces the conventional use of cutoff variation to estimate errors, which is problematic [27, 47]. The left panel in Fig. 1 shows order-by-order credible intervals (the actual truncation error should lie in the 68% credible interval 68% of the time) for one of the EKM potentials. It is based on a statistical model for the truncation error that treats scaled coefficients in the expansion of observables (not the LECs) as effectively random functions of natural size, whose magnitude provides an estimate of the error incurred by truncating the EFT expansion. The right panel shows a model checking diagnostic, which validates that the predicted credible intervals are consistent with actual truncation errors in cases where higher orders can be calculated. Other figures in Ref. [10] show that this diagnostic detects when the convergence pattern for an EFT with different regulator parameters fails, e.g., when regulator artifacts are severe. Further, the favored value of $\lambda \approx 1$ indicates the conjectured breakdown scale of 600 MeV is consistent within about 20%. Posteriors for the breakdown scale were also given, but it was clear that correlations between calculations at different energies and/or angles needed to be taken into account. This will be addressed with the Gaussian process (GP) statistical model (see below).

Another recent publication looked at two case studies for Bayesian parameter estimation of the low-energy constants (LECs) in chiral EFT that illuminate features which may be obscured or completely missed by conventional fitting protocols [21]. This work builds on an extensive guide to diagnostic tools based on analysis of model problems using synthetic data [3]. Rather than only using best fit values from a likelihood optimization, we advocate sampling and displaying the posterior pdfs when feasible. For the LECs in the NN potential this gives a more complete picture of the uncertainty and correlation structure induced by constraining the LECs using data. The posteriors are computed via simple formulas that follow from explicit, physically motivated assumptions.

A dramatic example of physics discovery enabled by the analysis comes from the posteriors for the fourth-order s-wave LECs, which show strong deviations from normality despite providing a good fit to phase shifts. This uncovered a parameter degeneracy at this order, previously recognized in other contexts [50], but ignored for χEFT fits (see Ref. [51] for how this improves the fits with fewer parameters). The other case study addressed the stability of LEC estimation against the maximum energy of data used in the fit. In non-Bayesian EFT parameter fitting, the choice of energy range can be a challenge: what is the optimal trade-off between including more data to determine LECs more precisely and contamination from the increasing contributions at higher energies of omitted higher-order EFT terms? It was shown that the sensitivity to the choice of $E_{\max}$ is removed with proper Bayesian UQ. The key is to account for truncation errors by adopting a physically motivated model discrepancy function. This stops the LECs being unduly influenced by data at energies where the EFT order is too low to provide an accurate description.

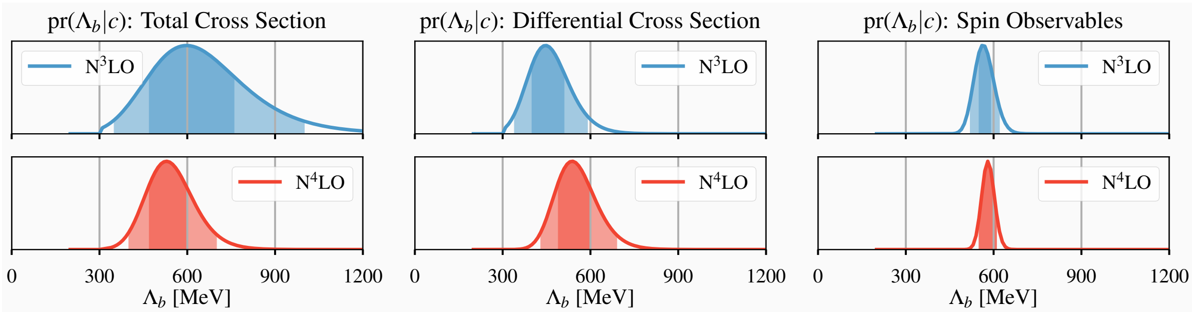

Figure 2: Posteriors for the breakdown scale from three sets of np observables up to N3LO (top) and N4LO (bottom) using a Gaussian process model for the chiral EFT truncation error (*preliminary*).

Melendez spent five months in 2018 at LLNL working with Kyle Wendt and Sofia Quaglioni as part of the DOE SCGSR program (while still funded by the NSF). Elements of this work will spill over into the new grant, as indicated below. The ultimate goal of the project is to perform an in-depth study on UQ for nuclear matrix elements of $0\nu\beta\beta$ and $2\nu\beta\beta$ decay. This has required first developing codes for fitting models of the nuclear forces to low-energy nuclear data to compute neutron-proton (np) and proton-proton (pp) scattering observables, with precise handling of electromagnetic contributions, and *with full uncertainty propagation*. These will be published soon.

The recent work sets the stage for further work in multiple directions. The following projects are proposed, most in collaboration with BUQEYE members or outside collaborators.

Gaussian process model of EFT truncation errors. The truncation of an EFT at a given order creates a systematic bias that must be accounted for when fitting the theory to data. This bias creates *correlated* errors; that is, predictions that are "close" in the input space (energy, scattering angle, etc.) will be biased similarly. Bayesian statistics is uniquely suited to model the error budget based on the convergence pattern: we can build our physical intuition into Bayesian priors, which can be updated to posteriors given the predictions for the system at hand. When χEFT is implemented with the Weinberg power counting scheme, Gaussian processes (GPs)—a machine learning tool for nonparametric regression—are ideal tools to incorporate both naturalness and correlations within an analytic model for truncation errors. Figure 2 shows how including correlations through GPs leads to more consistent posteriors for the EFT breakdown scale Λ_b for the potential of Fig. 1 than found in Ref. [10]. We propose implementing the GP truncation error model for LEC fitting and predictions of observables. We will then incorporate the full spectrum of uncertainties, discern problems in fitting and in EFT construction, and extract new physics such as the EFT correlation length in energy or angle. Several model checking protocols will be implemented for validation.

Other applications of the EFT truncation model. We plan to apply our GP truncation error model and associated model checking to other chiral interactions that are available order-by-order, such as the recent non-local potentials of Entem, Machleidt, and Nosyk in [52] and the fully local potentials of Gerzerlis et al. [26]. This will test the robustness of our statistical approach and complement ongoing analyses of the scheme dependence of chiral EFT through regulator dependence. We will also apply our error model and Bayesian model checking diagnostics to other EFTs, such as pionless EFT (in that case continuing a collaboration with König).

Software development and testing. We will continue development of codes to carry out the Bayesian statistical modeling and make them freely available. For example, the gsum package by Melendez (available on github) is a conjugacy-based Python implementation of the truncation model. The work by Melendez and Wendt will lead to Bayesian parameter estimation codes written in TensorFlow that take into account both the uncertainty in the LECs and the truncation error due to omitted terms in the EFT, which can become interwined in practice. Correlated theory errors have not been considered in fits of χEFT until now. The codes will be precise, well-documented, and user-friendly. As a community service, we also will benchmark alternative MCMC sampling methods (e.g., we are currently using both emcee and PyMC3).

Extensions of parameter estimation for chiral EFT. Follow-ups to Ref. [21] will use NN scattering data instead of extracted partial wave phase shifts for parameter estimation. Other elements to be studied include identifying appropriate priors for incorporating other theoretical expectations such as Wigner $SU(4)$ symmetry [27] and studying how to best parametrize the crossover between the p/Λ_b and m_π/Λ_b expansions. The NN calculations set the stage for the few-body sector, where the 3NF LECs at N2LO are typically only fit to two few-body observables. The BUQEYE team will work with the Chalmers group to study this fitting in a more general context. This will involve propagating all sources of error, including LEC uncertainties, to few-body observables [47], and accounting for correlations between LECs from the πN, NN and few-body sectors [53].

Beta decay. Melendez and Wendt will apply their codes to perform fitting and UQ to a set of χEFT models and then propagate the full uncertainties to $0\nu\beta\beta$ and $2\nu\beta\beta$ matrix elements. The latter will involve writing codes for 2–4 neutrons in a potential trap, which is useful as a model for valence neutrons bound in realistic heavier nuclei, and computing matrix elements for every MCMC sample from the fit, leading to joint pdfs for nuclear matrix elements. This enables study of correlations in a system where all errors are under control. All uncertainties will be propagated in these simple systems as a first step to UQ in the full calculations.

Nuclear matter application. In collaboration with Christian Drischler of LBNL, the core BUQEYE team will apply the GP truncation error model and diagnostics to quantify χEFT truncation errors for the energy/particle of neutron and nuclear matter as a function of Fermi momentum k_F. This includes determining posteriors for the breakdown scale Λ_b and the correlation length in k_F. A physically motivated theory error band for the energy per particle of symmetric nuclear matter will prove useful in comparing to empirical saturation properties and opens the door to using Bayesian optimization to efficiently determine the saturation point for use in fitting nuclear EFTs. The order-by-order calculations will be carried out for different interactions using the many-body perturbation theory (MBPT) infrastructure of Drischler [54, 55].

Compton scattering. Melendez will collaborate with a team extending the latest BUQEYE-developed Bayesian technology to an EFT treatment of Compton scattering [56, 57]. This includes exploiting the flexibility of the GP model to add physical constraints from analytic structure and symmetries (e.g., the cusp structure at the pion production threshold).

Model selection for EFT. We will continue to develop Bayesian model selection for EFT, which is a promising approach to assess longstanding questions. This includes assessing the number of EFT orders that can be constrained by existing (and future) experimental data, which has been demonstrated for model problems [3], but there are many other applications (pionless or chiral EFT? nucleons only versus nucleons and Deltas? which power counting is better? which regulator form is best?). We will further develop software and testing tools for this purpose, extending our experience with the Bayesian evidence in parameter estimation [3]. But we will explore more than just the Bayesian evidence, which was shown to be problematic in model calculations with undergrads Yamauchi and Shaffner working with the PI (e.g, apply methods from Ref. [58]).

Perturbative vs. non-perturbative schemes. The question of how to implement χEFT power counting has been a long-standing dispute. Most commonly used is the Weinberg approach, which constructs an effective potential at each order and then iterates this by solving a Schrödinger or Lippmann–Schwinger equation. Others advocate that any resummation should be done only at leading order (where clearly it is necessary to generate any nuclear bound states at all), and treat all higher-order effects in perturbation theory. The pionless theory can be used as an analog test case where the issue is resumming (or not) the effective range contributions; both are straightforward to implement. We will continue a long-term project with Sebastian König to test i) whether Bayesian model selection distinguishes between them and, ii) the impact of fitting LECs globally to observables versus determining them analytically from counterterm matching.

Model mixing explorations. Bayesian model mixing seeks to combine the predictive power of independent models that have different physics content and limitations (e.g., pionless and chiral EFT). The PI and Phillips will explore strategies for model mixing using as a test problem the predictions from well-known complementary expansions. Examples include the combination of high- and low-temperature expansions and strong- and weak-coupling expansions, which are conventionally interpolated using Padé approximants but could be combined statistically instead. With Drischler, the PI, Phillips, and Schwenk will explore model mixing and the $k_{\rm F}a$ expansion for fermionic matter.

Other breakdown scale analyses. A carry-over project from the current grant is to derive posteriors for the physical breakdown scale of the nucleon mass expansion in χPT constrained by actual lattice calculations. This case is particularly interesting because the breakdown scale Λ_b is not rigorously known.

UQ for extrapolations. Technology for infrared and ultraviolet extrapolations in a harmonic oscillator basis was developed in past grants [59–62], but without uncertainty estimates. The result of an extrapolation still has an uncertainty, which needs to be quantified. We propose using our Bayesian machinery to do so.

4 EFT for finite density nuclear systems

Proposed projects for finite density nuclear systems build from past work in two directions (which also overlap): ab initio and DFT approaches, with the common feature of exploiting phase space constraints. The former extend work by Alex Dyhdalo on understanding many-body power counting in collaboration with Christian Drischler and his infrastructure for diagrammatic calculations in uniform matter [54, 55]. The results from the DME developments mentioned in section 2, combined with the insight from investigations on power counting in finite density systems, motivate both continued work on the DME and a renewal of efforts to apply EFT directly to nuclear DFT.

Finite density power counting. A major accomplishment of Dyhdalo's thesis work was to develop power counting estimates and test many-body perturbation theory (MBPT) for uniform matter using low-momentum interactions [14]. At densities near nuclear matter saturation, Pauli blocking dramatically changes the counting one expects in free-space (e.g., fine-tuning in the S waves goes away). Dyhdalo introduced diagnostic tools to analyze many-body contributions and showed

Table 1: Root mean square (r.m.s.) deviations between experimental and theoretical binding energies in MeV [16].

EDF	r.m.s. residual
UNEDF-2	1.98
LO	1.99
NLO	2.02
N2LO	1.57
N2LO+3N	1.58
NLOΔ	1.41
NLOΔ+ 3N	1.46
N2LOΔ	1.26
N2LOΔ + 3N	1.72

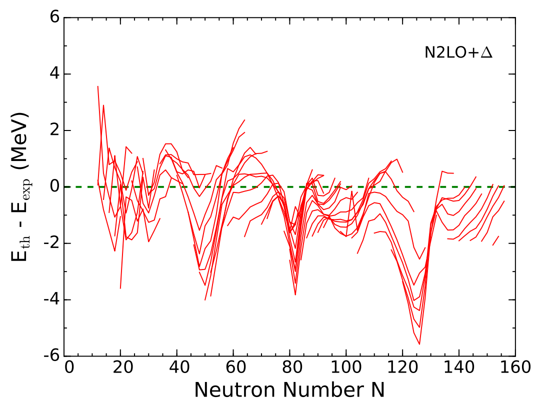

Figure 3: Residuals for N2LOΔ.

that quantitative estimates were feasible in the particle-particle channel [14]. With Drischler, we will extend these methods to the two-body particle-hole channels, where a power counting prescription is less clear. Drischler, Kai Hebeler, Phillips, and the PI will explore the role of three- and higher-body forces in χEFT calculations of nuclear matter. In carrying out these investigations, the dependence on EFT regulators (e.g., scale and scheme, local vs. nonlocal) will be a key issue.

Reference state EFT. An ongoing activity is to develop a many-body EFT formulation for which power counting is with respect to a reference state, such as the Hartree-Fock ground state. Expanding about such a reference state is key to ab initio basis methods such as coupled cluster and IM-SRG, but there is no established power counting. This is in contrast to finite-density EFTs that formalize Landau-Migdal theory, where the interacting Fermi surface is the reference, and one expands in small momentum deviations from the surface. We propose adapting the phase space methods and insights to formulate a metric for deviations from the reference state.

Further explorations of DME. Table 1 (from Ref. [16]) shows promising results from the application of the coordinate-space, regulated DME formulation by Dyhdalo, Bogner, and the PI [9]. In particular, with the same fitting protocol and the same free parameters, the r.m.s. residual for binding energies improved significantly compared to the UNEDF-2 reference when chiral NN contributions are added, particularly with an explicit Δ (e.g., to 1.41 MeV for NLOΔ and 1.26 MeV for N2LOΔ). But including three-body contributions does not improve the result or even makes it significantly worse (N2LOΔ+3N). Further explorations and testing of the DME approach and implementation will be carried out in collaboration with Bogner and the LLNL group, funded primarily through the NUCLEI-2 project. However, there will be complementary studies under this grant in collaboration with Bogner and colleagues at TU Darmstadt (this has just started with a visit to OSU in September, 2018). This includes extending the DME to the pairing channel, which requires renormalization even at the mean-field level. This is naturally formulated using an operator product expansion formalism [63, 64].

Merging with beyond-mean-field physics. The plot of binding energy residuals in Fig. 3 for the best case from Ref. [16] shows definite improvement when compared to the UNEDF-2 standard, but also manifests similar systematic deviations. The deviations are generally attributed to "beyond mean field" physics, meaning that one needs to go beyond the standard Hartree-Fock-Bogoliubov (HFB) energy density functional (EDF), such as doing symmetry restoration and incorporating coupling to vibrational modes. The LLNL team in the NUCLEI-2 project will be working on adding this physics to their codes and this will naturally be merged with the DME work. The PI will consult on this work but it will not be supported by this NSF grant. However, the need for this physics motivates a return to efforts for direct DFT from EFT by the PI and postdoc Zhang, as described in subsequent projects.

DFT from EFT with HS fields. A wide range of EFTs are useful in strong interaction physics, with applicability to different phenomena. One might observe that behind every successful emergent phenomenology there is an EFT (or EFTs) waiting to be uncovered. Past explorations of an EFT expansion for nuclear DFT by the PI and collaborators were based on a controlled low-density expansion, whereby the free-space momentum expansion translates into a $k_{\rm F}$ expansion [50, 65–72]. There are interesting recent developments by others building on this foundation, such as requiring renormalizability (see Ref. [73] for a review). Here we propose going in a different direction, building on the insights from the phase space approach and the successful phenomenology of nuclear EDFs. In particular, we want to build in that the pairing and particle-hole channels seem to have different associated scales and that vibrational modes are important beyond the mean fields. To accomplish both, we look to the textbook treatment for condensed matter systems, which introduces auxiliary bosonic fields for fermion bilinears via Hubbard-Stratonovich (HS) transformations [74, 75].

In an EFT approach, one would directly introduce a complete (but not redundant) set of bosonic operators coupled to quadratic fermion bilinears. The "trick" in this case is to introduce fields for all of the channels, not just one. If one summed to all orders, this would lead to double counting. But for small momenta near the Fermi surface, the different channels are effectively independent (these are different small momenta in the different channels), so one should include both [74, 75], which is consistent with nuclear EDF phenomenology. A saddlepoint expansion gives a mean-field approximation in leading order (with freedom to choose how this is organized, e.g., Hartree, HF, HFB [76]) and then the next order has vibrational contributions at the RPA level. This is naturally done within a path integral formulation of the effective action. In an earlier grant, Furnstahl and Hans-Werner Hammer extended an effective action pionless EFT approach for a dilute expansion for a uniform Fermi system to include pairing motivated by the DFT/EFT framework [71, 77, 78]. The first steps for the HS formulation is to apply it to the same uniform system and then to extend to a system in a trap.

Dealing with zero modes. In conventional discussions of EDFs the issue of symmetry breaking plays an important role. The dilemma with properly treating symmetries in the nuclear many-body problem is that one wants simple wave functions (e.g., Slater determinants) but this misses correlations from symmetries (e.g., plane waves won't describe clustering into nuclei) [79]. We hope to develop nuclear density functional theory (DFT), or some variation of it, within a field theory (effective action) formalism and as an effective field theory (EFT) expansion. A key technical problem to address is how to deal with zero modes that arise when one does a saddlepoint expansion of a path integral for the nuclear ground state, which leads one to pick out a mean-field reference state. The quantum corrections will naively be found to be infinite because there are fluctuations possible in flat (symmetry-wise) directions. Mathematically, one must calculate a determinant when evaluating quadratic fluctuations and there are zero eigenvalues ("zero modes") that cause divergences. We propose to use BRST methods as advocated by Bes and collaborators [80–82] but in a path integral rather than operator-based formulation. This has been a background project of the PI for many years, without significant progress; now it is time to make it a priority foreground project! The strategy will be to develop the method through application to basic demonstration problems, including the one-dimensional model studied by Engel for translational symmetry breaking [83] and a simple pairing model for fermion number symmetry.

Toy model for Becher/Leutwyler/Tang Covariant EFT/DFT Formalism. While the NUCLEI project has focused on generalizing nonrelativistic energy functionals, the covariant "mean-field" framework has continued to have phenomenological success. A covariant approach may offer a useful organization of the problem because the two underlying short-distance scales evident in EFT treatments of NN scattering [84, 85] correspond to the natural Lorentz scalar and vector short-distance scales. Past NSF research by Tang and the PI looked at making rigorous a covariant EFT with systematic power counting in loops. Tang's work at Minnesota [86, 87] was eventually systematized for πN by Becher and Leutwyler [88] under the name "infrared regularization" and several variations and extensions were subsequently developed [89–92]. A project to use this formalism to investigate a model covariant DFT for a dilute Fermi system with short-range interactions only (i.e., no pions) in an external trap, with the short distance scale Λ comparable to the fermion mass M (instead of $\Lambda \ll M$), was proposed in collaboration with the late Brian Serot, but was put on hold because of his illness. With postdoc Zhang (who was Serot's last PhD student) we propose to carry out the project, using the confined, finite system as a laboratory to explore the spin-orbit force, few-body forces, and other aspects of relativistic phenomenology in a systematic expansion.

5 Calculating and extracting process-independent quantities

Many nuclear quantities of interest, such as momentum distributions, are extracted from experiment via a factorization of nuclear structure from the description of the probe. However, this factorization is known in general to be scale and scheme dependent [41], and understanding this dependence and the limits of factorization may be critical for interpreting experiments and in particular for identifying and extracting *process-independent* quantities (which will inherit scale and scheme dependence) that can be compared to theory. In Refs. [15, 41], the SRG was used to investigate the simplest knockout reaction: deuteron electrodisintegration, where the factorization of the unitary transformation follows from a nonrelativistic operator product expansion [93]. We found that the scale dependence depends on kinematics in a systematic and understandable way. Here we propose a set of projects that explore or exploit factorization.

Extensions of deuteron electrodisintegration studies. Deuteron electrodistintegration is an excellent laboratory for exploring scale dependence in nuclear knock-out reactions. Figure 4 illustrates how the resolution scale can change the physics interpretation. The cartoons on the left show the dominant contributions to the longitudinal structure function in two kinematic regions. With quasifree kinematics, wave function components with low relative momentum between proton and neutron dominate, so the description is insensitive to the resolution. But with large momentum transfer q^2 and relatively small energy E', at high resolution one is sensitive to short-range correlation (SRC) configurations while at low resolution it is low relative momenta that are again probed, now with a simple two-body current. A consequence is seen on the right, where the percentage of D-state contribution to the cross section is extremely scale dependent (changes from dominant to zero). This example shows how the kinematics alone does not always uniquely determine what is probed in the reaction and is a cautionary lesson for those seeking to extract absolute nuclear

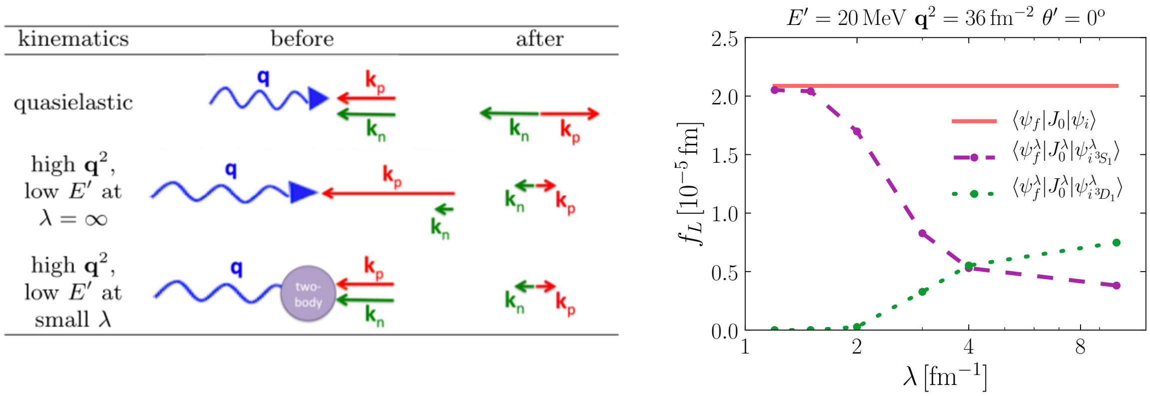

Figure 4: Left: schematic representation of dominant contributions to deuteron electrodisintegration on the quasielastic peak and near threshold [15] in the final state rest frame. Right: Contributions to the longitudinal structure function f_L from the deuteron S and D states as a function of the SRG λ, which controls the resolution scale for SRC kinematics [15].

structure information from knock-out reactions. This holds for other components as well, such as final-state interactions. One goal of further analysis is to help answer a key question: what is the best scale for analyses of experiment?

Planned extensions by Zhang, Bogner, and the PI include adding two-body currents, studying the transverse response, extending to few-body systems, and connecting to other knock-out processes. This includes studying the axial current response in neutrino-deuteron scattering. The latter could have its own significance in extracting the nucleon axial form factor, which plays a fundamental role in neutrino-nucleus calculations, from neutrino-deuteron scattering data [94]. A longer-term goal is to apply the soft-NN-interaction-based many-body methods to study GeV-neutrino–nucleus reactions, which are important to the long-baseline neutrino oscillation experiment.

Optical potentials. Optical potentials are a key ingredient in conventional reaction models. These are usually of phenomenological form and constrained by empirical data, although ab initio and EFT-based optical potentials are now being studied. The Feshbach projection formalism implies that an optical potential should be complex, energy dependent, and non-local [95–97]. We propose to gain insight into the scale and scheme dependence of optical potentials and the validity of common approximations by considering how transfer reactions behave under unitary transformations. To start we consider one-dimensional scattering in simple models as a theoretical laboratory; one-dimensional models have proven to be of great use in past SRG investigations of few-body forces [98]. NSF graduate fellow Ryan Caulfield has taken the first steps by solving a model of a nucleon scattering off a two-level "nucleus" with contact potentials [99] both directly and using an optical potential. One can then perform a unitary transformation on the interaction Hamiltonian to determine the consequences for the optical potential. Interesting results are already seen at this level. Extensions to the case of a three-body problem will allow study of the scale dependence of non-locality, the effectiveness of common approximations (impulse, Glauber, ADWA, CDCC), and the possibilities of decoupling. Caulfield has left nuclear physics (for Battelle) for family reasons, but this project is well suited for Tropiano.

Factorization for radiative capture. Halo-EFT has been applied successfully to study radiative capture reactions involving shallow bound states [100]. However there are many capture reactions with astrophysical importance whose final nuclear state is far below the incoming channel threshold, i.e., the Q value is much larger than the typical kinetic energy in the incoming channel [101]. In the extrapolation of their cross-section data down to astrophysical energies [101], the cluster-based potential models are plagued with uncontrolled theoretical uncertainties. One of these reactions, $^{12}\mathrm{C}\,(\alpha, \gamma)^{16}\,\mathrm{O}$, known as the "holy grail" in nuclear astrophysics [102], will be the focus of a study by Zhang. The previous Halo-EFT approach cannot be applied here because the reaction is dominated by the short-distance region. However, in this limit, factorization of the short- and long-distance physics can be used to parametrize the reaction amplitude's energy dependence in terms of local operators operating *only* on initial state at low energy with the coefficients dictated by the short-distance physics including the final bound state and EM transition multipoles. In the end, Bayesian inference will be applied to constrain the unknown parameters in the theory using available data, and provide error estimates of the low-energy cross sections that have not been measured directly.

Nuclear elastic scattering and the Busch formula. The Busch formula has been derived and generalized in Ref. [103–106] to connect the energy spectrum of a two cold atom system confined in a harmonic oscillator potential to their scattering phase shifts. The formula was applied in low-energy nuclear physics in Ref. [107, 108] to study two- and three-nucleon systems. Unfortunately, the formula is only exact when the trap becomes infinitely shallow [107]. In the framework of EFT, Zhang has found that in the low-energy region, the formula can be improved systematically by introducing two-body-current-like terms to the EFT lagrangian. He will work with Ragnar Stroberg and collaborators to extract *ab initio* α–neutron and ^{24}O–neutron scattering phase shifts from the energy spectrum of ^{5}He and ^{25}O confined in harmonic traps. Such systems pose significant challenges to conventional many-body methods, which cannot incorporate configurations with clusters having large separation. The strategy amounts to reducing the continuum physics for the many-body calculation by trapping the systems, while relying on cluster-based EFT to describe the large-separation physics. The EFT is fixed by matching the calculation of physical observables such as eigenenergies with the many-body method.

Nuclear contact. Recent theoretical work by Chen and collaborators has shown that the two-nucleon short-range correlation (SRC) scaling factor,

$$a_2(A, x) = \left.\frac{2\sigma_A}{A\sigma_2}\right|_{1.5<x<2}, \tag{1}$$

extracted from quasi-elastic scattering cross sections for nuclei, is approximately independent of renormalization scale and scheme [109, 110]. It has been repeatedly demonstrated that a_2 exhibits approximate x-independence in this region for a wide range of nuclei [111–114]. a_2 also shows only small Q^2 dependence. Thus it seems to be a process-independent quantity under the leading-order approximations considered. We propose to further examine these claims for a variety of light and medium mass closed-shell nuclei, using the IM-SRG. This is complementary to parallel efforts using quantum Monte Carlo methods by Lynn, Lonardoni, and collaborators. The IM-SRG is not restricted to local interactions, so we can explore the full range of state-of-the-art chiral potentials. Preliminary results by Parzuchowski show the feasibility of the project, but much is left to be done by the PI and Bogner. This includes extending past results on harmonic oscillator basis extrapolations for operators [59–62] to the relevant operators for contacts.