

NUCLEAR MATTER FROM IN-MEDIUM SIMILARITY RENORMALIZATION GROUP
AND EMULATOR-BASED UNCERTAINTY QUANTIFICATION

By

Kang Yu

A DISSERTATION

Submitted to
Michigan State University
in partial fulfillment of the requirements
for the degree of

Physics —Doctor of Philosophy
Computational Mathematics, Science and Engineering—Dual Major

2026

ABSTRACT

The nuclear matter equation of state (EOS) is essential for understanding a broad range of nuclear and astrophysical phenomena, including supernova explosions and neutron stars. In this thesis, we extend the in-medium similarity renormalization group (IMSRG) method to nuclear matter calculations and develop a many-body framework for constructing EOSs over a range of proton fractions and nuclear interactions. We compare IMSRG predictions for the EOS with results from other ab initio many-body methods, including many-body perturbation theory (MBPT) and coupled-cluster (CC) theory, using two classes of chiral effective field theory (EFT) interactions. We find generally good agreement for more perturbative systems, such as pure neutron matter, and for softer interactions in which the nucleon-nucleon interaction has been evolved to a lower resolution scale by the similarity renormalization group. Larger differences are observed for less perturbative systems, such as symmetric nuclear matter, and for harder interactions with unevolved nucleon-nucleon and three-nucleon forces. Beyond the EOS, we apply the same framework to nuclear matter observables and present proof-of-principle calculations of the single-nucleon momentum distribution and static structure factor. Comparisons between IMSRG(2) and free Fermi gas results exhibit systematics consistent with those observed in the EOS calculations.

To address the computational cost of the IMSRG framework, we subsequently introduce a hybrid emulator for IMSRG calculations of nuclear matter, based on chiral nucleon-nucleon and three-nucleon interactions and an implicit-reduced-basis method emulator constructed from parametric matrix models (PMMs) which is capable of rigorously estimating its uncertainties via conformal predictions. The resulting PMM–IMSRG emulator enables fast and accurate predictions with trustworthy confidence intervals of the nuclear EOS across a wide range of input parameters, including low-energy couplings, IMSRG flow parameters, densities, and basis sizes. This framework provides the foundation for principled uncertainty quantification of the nuclear EOS and enables computationally demanding applications such as Bayesian parameter estimation using our IMSRG calculations. As a first application, we present results for the coupling constants of the two quark-mass-dependent three-nucleon interactions, recently identified to contribute at next-to-next-

to-leading order in the chiral expansion based on a renormalization-group analysis, by fitting them to empirical saturation properties. We then propagate both parametric and emulator uncertainties to the EOS in the limits of pure neutron matter and symmetric nuclear matter.

Copyright by
KANG YU
2026

ACKNOWLEDGEMENTS

First, I would like to express my deep appreciation to my supervisor, Dr. Scott Bogner, who introduced me to the real world of physics research. Thanks to his lasting support and guidance, I have made it through a long journey filled with both wonder and unexpected challenges to reach this finish line.

I would like to thank my collaborators, Dr. Christian Drischler, Dr. Omokuyani Udiani, and Dr. Patrick Cook, for the rewarding work we have accomplished together. Dr. Christian Drischler has set an excellent academic example as an early-career researcher with high standards. He provided me with detailed guidance throughout the two projects we worked on together and, in many ways, has been like a second supervisor to me. Dr. Omokuyani Udiani, a senior student in Scott's group, has always been an icebreaker in group meetings with his characteristic sense of humor. He gave me tremendous help at the beginning of my research and helped me find my footing in the field. Dr. Patrick Cook is an inspiring colleague who is highly motivated and full of ideas, earning him the nickname "PatGPT". I learned a great deal from collaborating with him. I would also like to thank the junior members of the group, Brandon Lem and Aryan Vaidya, for many useful discussions.

I am grateful to my other committee members, Dr. Heiko Hergert, Dr. Morten Hjorth-Jensen, Dr. Sean Couch, and Dr. Brian O'Shea, for their guidance, support, and service throughout the years. I am also grateful to Elizabeth Deliyski for her warmth, kindness, and help with many different aspects of life and work at FRIB.

Thanks to all physicists who have been working tirelessly toward a deeper understanding of our world. Your efforts make the ultimate goal of understanding everything more than just a dream.

To my friends, both near and far, thank you for making my PhD years a more interesting and fulfilling experience and for exploring the world beyond academics with me. I hope our friendships will last for many years to come.

Finally, special thanks go to my partner, Dr. Nian Liu, for her companionship and unwavering support, and to my parents, Youwen Yu and Jilian Yuan, for always being there for me under any circumstances, from my decision to begin this journey to its unexpectedly long-awaited finish.

TABLE OF CONTENTS

LIST OF TABLES	viii
LIST OF FIGURES	ix
LIST OF ABBREVIATIONS	xii
CHAPTER 1 INTRODUCTION	1
1.1 Nuclear Matter Equation of State	1
1.2 Chiral Effective Field Theory	2
1.3 Ab Initio Nuclear Many-Body Theory	4
1.4 Emulators	5
1.5 Thesis Outline	6
CHAPTER 2 IMSRG FRAMEWORK FOR NUCLEAR MATTER CALCULATIONS	8
2.1 The Nuclear Many-Body Problem	9
2.2 Hartree–Fock Theory	10
2.3 Normal Ordering and NO2B Approximation	12
2.4 Many-Body Perturbation Theory	15
2.5 Coupled-Cluster Theory	17
2.6 Similarity Renormalization Group	19
2.7 In-Medium Similarity Renormalization Group	21
2.8 IMSRG for Nuclear Matter in a Finite Box	26
2.9 Benchmark	31
CHAPTER 3 IMSRG CALCULATIONS OF THE NUCLEAR MATTER EQUATION OF STATE AND OBSERVABLES	33
3.1 Convergence and Scaling	33
3.2 Finite Size Effects	40
3.3 Nuclear Matter Equation of State	42
3.4 Nuclear Matter Observables	50
3.5 Summary and Outlook	58
CHAPTER 4 PMM-IMSRG FRAMEWORK FOR NUCLEAR MATTER CALCULATIONS	59
4.1 Parametric Matrix Model	60
4.2 PMM for IMSRG Nuclear Matter Calculations	62
4.3 Conformal Prediction	67
4.4 Emulator Performance	68
CHAPTER 5 APPLICATIONS OF PMM-IMSRG FRAMEWORK WITH QUARK-MASS-DEPENDENT THREE-NUCLEON INTERACTIONS	70
5.1 Exploring Saturation Properties of 3N Forces	70
5.2 Variations of c_D and c_E about the Triton Binding Energy	72

5.3	Calibrating 3N Forces to Empirical Saturation Properties with Emulator Uncertainties	75
5.4	Propagating LEC Uncertainties to the EOS	83
5.5	Summary and Outlook	87
CHAPTER 6	CLOSING REMARKS	90
6.1	Summary	90
6.2	Outlook	92
BIBLIOGRAPHY		92

LIST OF TABLES

Table 2.1	Momentum shells and cumulative single-particle degeneracy.	28
Table 3.1	Convergence of the IMSRG calculation with respect to the flow parameter s	35

LIST OF FIGURES

Figure 2.1	A schematic view of IMSRG decoupling [25]. The many-body Hamiltonian is depicted in blocks, with the reference state $ \Phi\rangle$ and its particle-hole excitations (see the main text). During the IMSRG flow, the reference state is decoupled from its excitations.	22
Figure 2.2	Energy per particle of pure neutron matter computed in the IMSRG(2) approximation with the Minnesota interaction model for different single-particle basis sizes with $A = 114$	32
Figure 3.1	Convergence of the IMSRG(2) energy per particle for SNM with $N = Z = 66$ as a function of the flow parameter s at density $\rho = 0.07 \text{ fm}^{-3}$	34
Figure 3.2	Convergence of the IMSRG(2) energy per particle for SNM ($N = Z = 66$) versus the number of shells N_{shells} above the reference state (top panel) and versus the total number of single-particle states N_{sp} (bottom panel) at density $\rho = 0.16 \text{ fm}^{-3}$	37
Figure 3.3	Runtime (top panel) and memory usage (bottom panel) of the IMSRG(2) transformation for SNM with $N = Z = 66$ versus the number of states N_{sp} in the single-particle basis.	39
Figure 3.4	A -dependence of the energy per particle for PNM (top panel) and SNM (bottom panel) at the density $\rho = 0.16 \text{ fm}^{-3}$ using the $\text{N}^2\text{LO}_{\text{opt}}$ NN potential [96]. The blue curve denotes the IMSRG(2) energy per particle, which is decomposed into its Hartree–Fock (orange curve) and correlation energy (green curve) components.	41
Figure 3.5	Comparison of IMSRG(2) and MBPT calculations of the energy per particle (top panel) and correlation energy per particle (bottom panel) for PNM using the $\text{EM}(1.8/2.0)$ interaction treated in the NO2B approximation.	43
Figure 3.6	Comparison of IMSRG(2) and MBPT calculations of the energy per particle (top panel) and correlation energy per particle (bottom panel) for PNM using the $\text{EM}(2.8/2.0)$ interaction treated in the NO2B approximation.	44
Figure 3.7	Comparison of IMSRG(2) and MBPT calculations of the energy per particle (top panel) and correlation energy per particle (bottom panel) for PNM using the $\text{N}^2\text{LO EMN } 500 \text{ MeV NN} + 3\text{N}$ interactions treated in the NO2B approximation.	45
Figure 3.8	A subset of the MBPT(4) Hugenholtz diagrams corresponding to irreducible triples ($3p3h$) and quadruples ($4p4h$) excitations. The IMSRG(2) misses the triples diagrams T_1 – T_{16} completely, and undercounts the asymmetric quadruples diagrams Q_1 , Q_2 , Q_6 and Q_7 by a factor of $1/2$	47

Figure 3.9	Comparison of IMSRG(2) to MBPT and non-perturbative CC calculations of SNM for the EM(1.8/2.0) (top panel) and EM(2.8/2.0) (bottom panel) NN + 3N interactions treated in the NO2B approximation.	48
Figure 3.10	Comparison of IMSRG(2) to MBPT and non-perturbative CC calculations of SNM for the N^2 LO EMN 500 MeV NN + 3N interactions treated in the NO2B approximation.	49
Figure 3.11	Comparison of IMSRG(2) and MBPT calculations of asymmetric nuclear matter with proton fraction $Y_p = 0.05$ for the EM(2.8/2.0) NN+3N interaction, with the 3N interaction treated in the NO2B approximation.	50
Figure 3.12	Single neutron momentum distribution of PNM with $N = 66$ at $\rho = 0.05 \text{ fm}^{-3}$. The blue points show the IMSRG(2) results obtained with the N^2 LO EMN 500 MeV NN+3N interaction, with the 3N contribution treated in the NO2B approximation. The black dashed line shows the results for free Fermi gas at the same density. Here, k_F denotes the corresponding Fermi momentum in the box.	53
Figure 3.13	Static structure factor (top panel) and pair distribution function of PNM with $N = 66$ at $\rho = 0.05 \text{ fm}^{-3}$. The blue points and solid line show the IMSRG(2) results obtained with the N^2 LO EMN 500 MeV NN+3N interaction, with the 3N contribution treated in the NO2B approximation. The black dashed lines show the results for free Fermi gas at the same density. Here, k_F denotes the corresponding Fermi momentum in the box.	57
Figure 4.1	Comparison of PMM-predicted energies at the 95.45% confidence level and withheld test IMSRG results for both PNM (here, 66 neutrons) and SNM (here, 66 protons and 66 neutrons) as all degrees of freedom, including LECs and density, are varied for both N^2 LO (panel a) and N^3 LO (panel b). Insets show additional detail around the empirical saturation energy. All values are in units of MeV.	69
Figure 5.1	Saturation point distributions in SNM obtained from 10 000 uniform random samples in the range specified by the legends of c_D and c_E (panel a) and c_D , c_E , and F_2 (panel b) with $\{N_s, s\} = \{\infty, \infty\}$ at N^3 LO. The color of each point is determined by a color average of the corresponding colors given by the value of each LEC indicated in the legends. Each saturation point is shown with the associated confidence intervals at the 68.27% level. The empirical saturation point [115] is depicted by the star (mean value), and the associated 68.27% (inner ellipse) and 95.45% credible contours (outer ellipse) are shown in black.	71

Figure 5.2	Confidence regions of the EOS in the limit of SNM at N ³ LO when varying the widened c_D - c_E correlation that fits the triton binding energy as obtained in Ref. [98, see Fig. 1 in the Supplemental Material]. The error bands are obtained through ordinary Monte Carlo sampling from the probability distributions of the emulator and EFT truncation errors. See the main text for details.	73
Figure 5.3	Low-density EOS parameters associated with the sampled EOSs depicted in Fig. 5.2 (black). The units are MeV, except for n_{sat} , which is in fm ⁻³ . The blue lines and stars depict the empirical ranges defined in Eq. (5.3). The reported uncertainties in the titles correspond to 68% credible intervals centered on the median.	74
Figure 5.4	Corner plot showing the posterior distributions and pairwise correlations of the low-energy constants c_D , c_E , and F_2 obtained from the PMM-IMSRG Bayesian analysis. The LECs c_D and c_E are dimensionless, whereas F_2 is given in fm ⁴ . The reported uncertainties in the titles correspond to 68% credible intervals centered on the median. Note that the uniform prior enforces the constraint $ c_D \leq 5$	80
Figure 5.5	Corner plot showing the posterior distributions and pairwise correlations of the saturation properties n_{sat} , E_{sat} , S , L , and K obtained from the PMM-IMSRG Bayesian analysis. All observables are given in MeV, except for n_{sat} , which is given in fm ⁻³ . The diagonal panels display the marginal posterior distributions with median values and credible intervals, while the off-diagonal panels show the corresponding joint posterior contours. The blue curves indicate the prior distributions: a bivariate student- t distribution for $(n_{\text{sat}}, E_{\text{sat}})$ and independent Gaussian distributions for (S, L, K) , with the blue star marking the distributions' mean values. The 68% and 95% credible contours are shown, and the reported uncertainties (centered on the median) are at the 68% credibility level.	81
Figure 5.6	Same as Fig. 5.2 but for the LEC samples in Fig. 5.4.	84
Figure 5.7	Same as Fig. 5.6 but for PNM, where c_D and c_E do not contribute in contrast to F_2	85
Figure 5.8	Median expectation values of each term in the emulated Hamiltonian with 68% and 95% credible intervals from posterior LEC samples at N ² LO (panel a) and N ³ LO (panel b) at three different densities for SNM. The labels on the horizontal axis indicate the individual $c_i V_i$ term where “const.” denotes the fixed V_0 term in the emulator.	86

LIST OF ABBREVIATIONS

FRIB	Facility for Rare Isotope Beams
EOS	Equation of State
IMSRG	In-Medium Similarity Renormalization Group
MBPT	Many-Body Perturbation Theory
CC	Coupled-Cluster
EFT	Effective Field Theory
QCD	Quantum Chromodynamics
LEC	Low-Energy Constant
LO	Leading Order
NLO	Next-to-Leading Order
N²LO	Next-to-Next-to-Leading Order
N³LO	Next-to-Next-to-Next-to-Leading Order
SRG	Similarity Renormalization Group
SCGF	Self-Consistent Green's Function
QMC	Quantum Monte Carlo
EC	Eigenvector Continuation
RBM	Reduced-Basis Method
DMD	Dynamic Mode Decomposition
GP	Gaussian Process
ANN	Artificial Neural Network
PMM	Parametric Matrix Model
NN	Nucleon–Nucleon
3N	Three-Nucleon
3NF	Three-Nucleon Force

PNM	Pure Neutron Matter
SNM	Symmetric Nuclear Matter
ANM	Asymmetric Nuclear Matter
EDF	Energy Density Functional
HF	Hartree–Fock
NO2B	Normal-Ordered Two-Body
CCSD	Coupled-Cluster Singles and Doubles
CCSDT	Coupled-Cluster Singles, Doubles, and Triples
CCD	Coupled-Cluster Doubles
BCH	Baker–Campbell–Hausdorff
ODE	Ordinary Differential Equation
TABC	Twist-Averaged Boundary Conditions
EMN	Entem–Machleidt–Nosyk
SNMD	Single-Nucleon Momentum Distribution
SSF	Static Structure Factor
UQ	Uncertainty Quantification
AE-PMM	Affine Eigenvalue Parametric Matrix Model
AO-PMM	Affine Observable Parametric Matrix Model
RBF	Radial Basis Function
CDF	Cumulative Distribution Function

CHAPTER 1

INTRODUCTION

Neutron stars are among the densest objects in the universe. Formed in the aftermath of core-collapse supernovae, they typically contain about one to two solar masses within radii of only approximately 10 km. Their extreme densities and pressures make them unique astrophysical laboratories for studying strongly interacting matter under conditions that are difficult to create or directly probe on Earth. Neutron stars have a layered internal structure consisting of an outer crust, inner crust, outer core, and inner core, each with distinct compositions and physical properties, thereby encompassing rich physics that can be explored through astronomical observations.

Over the past decades, substantial observational progress has been made toward unraveling the properties of neutron stars through multiple astrophysical messengers, including pulsar timing, X-ray observations, and gravitational-wave measurements of binary neutron star mergers [1, 2, 3]. The key link between these macroscopic observations and the underlying microscopic nuclear physics is the neutron star equation of state (EOS). The EOS describes the thermodynamic relation among the energy density, pressure, density, temperature, and composition of matter inside neutron stars. It determines the neutron star mass-radius relation and therefore constrains the maximum mass a neutron star can support, as well as other observable properties such as the tidal deformability and response of neutron star matter. Astrophysical observations of neutron stars thus provide unique and essential constraints on the microscopic physics of strongly interacting matter at extreme densities. This connection motivates our investigation of the nuclear EOS in this work, where we develop new theoretical tools to compute the EOS starting from realistic inter-nucleon interactions with quantified uncertainties.

1.1 Nuclear Matter Equation of State

The core constitutes the largest region of a neutron star and contains most of its mass. The outer core consists of homogeneous matter composed primarily of neutrons, together with small fractions of protons, electrons and muons. Fermionic degeneracy pressure and repulsive nucleon–nucleon interactions support the neutron star against gravitational collapse. This phase of matter is of

particular interest to us because its properties are governed directly by the underlying interactions among nucleons. The inner core, on the other hand, may reach densities several times nuclear saturation density and remains the least well understood region of a neutron star because of the considerable uncertainty surrounding the possible emergence of additional degrees of freedom at such high densities. The matter in the inner core lies beyond the scope of this work.

Our work focuses on the outer core of a neutron star. We model neutron star matter in this regime, over densities ranging from approximately one half to twice nuclear saturation density, as nuclear matter — an idealized system of interacting nucleons in the thermodynamic limit. The properties of nuclear matter, such as its EOS, are closely connected to those of neutron stars but are very difficult to determine directly from data because nuclear matter itself is hard to realize in terrestrial experiments. Nevertheless, astronomical observations of neutron stars [4], together with terrestrial experiments on neutron-rich nuclei [5, 6] and heavy-ion collisions [7], can provide important constraints. Furthermore, these properties can be extracted from theoretical calculations [8]. The combination of experimental, observational and theoretical approaches makes nuclear matter both an interesting testing ground for quantum many-body theories and a subject of practical importance for understanding neutron stars. Its EOS plays a central role in determining its bulk properties and is therefore central to the present research.

A microscopic understanding of the nuclear matter EOS begins with the interactions among nucleons. In the next section, we introduce chiral effective field theory (EFT) as the framework used to describe these interactions.

1.2 Chiral Effective Field Theory

Many models based on meson exchange and varying degrees of phenomenology have been developed to describe the two-nucleon interactions by fitting to nucleon-nucleon scattering data and the properties of the deuteron [9, 10, 11, 12]. However, nuclear Hamiltonians containing only two-nucleon interactions fail to reproduce the binding energies of nuclei with $A \geq 3$ [13, 14] and the empirical saturation properties of nuclear matter [15]. These deficiencies, together with the composite nature of nucleons, motivate the inclusion of three-nucleon interactions, whose parameters

are commonly constrained using properties of light nuclei, such as the binding energies and radii of tritium or helium nuclei. The inclusion of three-nucleon forces provides essential contributions to nuclear binding and plays a crucial role in reproducing realistic saturation properties. Despite these successes [16, 17, 18], phenomenological models lack a systematic framework for treating two- and three-nucleon interactions consistently or for improving them in a controlled manner. Chiral effective field theory offers a modern approach that addresses these limitations.

Chiral EFT provides a systematic description of low-energy nuclear physics in terms of nucleons and pions, the relevant effective degrees of freedom for describing matter throughout the outer core of neutron stars. All other degrees of freedom are "integrated out", with their effects encoded in the effective couplings of the remaining degrees of freedom. It is rooted in, and therefore consistent with, the symmetries of quantum chromodynamics (QCD), the underlying theory of the strong interaction. Chiral EFT organizes nuclear interactions as an expansion in powers of the ratio $Q = \frac{\max(p, m_\pi)}{\Lambda_b}$, where p denotes the typical momentum scale of the nucleons, m_π is the pion mass, and Λ_b is the breakdown scale of the theory. This organization is known as power counting [19, 20]. In infinite nuclear matter, the typical nucleon momentum scale is generally taken to be of the order of the Fermi momentum k_F [8]. The breakdown scale is the scale beyond which the chiral EFT expansion is no longer expected to be valid and has been estimated to be of the order of 500-600 MeV. The strengths of the pion–nucleon couplings and the unresolved short-range physics, parametrized in terms of contact interactions, are encoded in low-energy constants (LECs), which are fitted to experimental data. A key advantage of chiral EFT over purely phenomenological models is its consistent and systematically improvable treatment of nuclear interactions, with the resulting order-by-order convergence pattern providing a natural basis for quantifying theoretical uncertainties [21, 22].

Even with nuclear Hamiltonians derived from chiral EFT, solving the many-body Schrödinger equation remains a non-trivial task. First, the many-body Hilbert space grows rapidly with particle number and is infinite dimensional in principle, requiring controlled truncations for practical calculations. Second, the couplings between low- and high-momentum states make nuclear interactions

hard and hinder the convergence of many-body methods. The development of the similarity renormalization group (SRG) and ab initio nuclear many-body methods has opened a practical pathway toward addressing these challenges [23, 24, 25].

1.3 Ab Initio Nuclear Many-Body Theory

The SRG has become a standard preprocessing tool for many-body Hamiltonians in low-energy nuclear physics [23, 24]. Through continuous unitary transformations, the SRG suppresses couplings between low- and high-momentum modes. The result is that low-energy nuclear wavefunctions have suppressed momentum components above this decoupling scale, which is often called the resolution scale or resolution. This decoupling softens nuclear interactions at low resolutions, and thereby substantially improves the convergence of many-body calculations, although at the cost of inducing higher-body operators [23, 24, 25].

A variety of many-body methods have been developed to solve the nuclear Schrödinger equation. Configuration space methods include many-body perturbation theory (MBPT) [26], coupled-cluster (CC) [27], the in-medium similarity renormalization group (IMSRG) [25, 28], and self-consistent Green’s function (SCGF) [29, 30]. In these approaches, a chosen single-particle basis is used to construct a many-body basis of Slater determinants, and correlations are incorporated through particle–hole excitations relative to a reference state. To make the problem computationally tractable, these methods employ controlled truncations of the many-body expansion. The resulting approximations can be systematically improved by retaining higher-order many-body contributions. At a fixed truncation level, the configuration-space methods achieve polynomial scaling with the size of the single-particle basis, allowing calculations in otherwise prohibitively large many-body Hilbert spaces. As in chiral EFT, controlled truncation schemes and systematic convergence patterns provide a natural foundation for quantifying theoretical uncertainties. QMC methods, by contrast, commonly employ coordinate-space representations of the many-body wavefunction. Starting from a trial wavefunction, they use imaginary-time evolution to project out the ground state in a nearly exact manner [31], although the fermion sign problem generally restricts their use to Hamiltonians that are local or whose nonlocality is at most quadratic in the momenta [32, 33].

Advances in EFT, SRG, and *ab initio* nuclear many-body methods have substantially enhanced the predictive power of nuclear theory and broadened its reach across the nuclear chart [28, 34, 35]. Most applications of these approaches have focused on finite nuclei, while MBPT, CC, SCGF, and QMC have also been recently used to study infinite nuclear matter. At the outset of this project, however, the IMSRG had not yet been applied to realistic calculations of infinite nuclear matter. We therefore sought to extend the IMSRG framework to this regime.

1.4 Emulators

Predicting the nuclear EOS from chiral EFT interactions using the IMSRG is only the first step. Although the IMSRG has polynomial computational scaling at a fixed truncation level, realistic calculations remain expensive because ultraviolet convergence requires a sufficiently large single-particle basis. Moreover, a small set of EOS predictions obtained from selected chiral interactions is not sufficient for many applications. Reliable predictions require the relevant theoretical uncertainties to be quantified and propagated to the EOS.

Within chiral EFT, important sources of uncertainty include truncation of the EFT expansion [21, 22] and uncertainties in the calibration of the LECs [36]. Propagating these uncertainties generally requires evaluating the EOS across a broad region of the parameter space of the input interactions, often requiring millions of calculations. A direct IMSRG calculation for each sample would therefore be computationally prohibitive. This challenge motivates the use of emulators, which approximate the outputs of the original model — in our case, computationally expensive many-body methods — at a much lower computational cost. The construction of emulators relies on the fact that much of the information contained in high-fidelity models is superfluous for tracing parametric dependencies and can therefore be represented in a lower-dimensional space [37, 38]. For this reason, emulators are also referred to as reduced-order models.

Emulators can generally be classified into three categories. The first consists of model-driven emulators, which derive and solve reduced-order equations from the governing equations of the high-fidelity model. Because they preserve the underlying structure of the original model, these approaches are often described as physics-based. Examples include eigenvector continuation

(EC) [39] and the broad class of reduced-basis methods (RBMs) [38, 40]. The second category consists of data-driven emulators, which do not require explicit knowledge of the governing physics. Instead, they learn the parametric dependence of model outputs directly from training data. This category includes dynamic mode decomposition (DMD) [37, 41], as well as machine-learning techniques such as Gaussian processes (GPs) [42] and artificial neural networks (ANNs) [43]. The third category comprises hybrid emulators, which combine model-driven and data-driven elements. These approaches incorporate known physical structure while using data to learn components that are unknown or computationally expensive to evaluate. A recently developed machine-learning approach known as the parametric matrix model (PMM) belongs to this category [44]. In this work, we use the PMM to emulate IMSRG calculations of the nuclear EOS.

By dramatically accelerating model evaluations, emulators enable large-scale computations that would be impractical using high-fidelity calculations alone, thereby supporting subsequent Bayesian inference and uncertainty quantification analyses.

1.5 Thesis Outline

The background introduced above motivates our extension of the IMSRG to nuclear matter and the further development of the PMM-IMSRG emulator for large-scale nuclear EOS calculations required for uncertainty quantification.

The remainder of this thesis is organized as follows. Chapter 2 describes our IMSRG framework for nuclear matter calculations with nucleon–nucleon (NN) and three-nucleon (3N) interactions treated at the normal-ordered two-body level. Chapter 3 presents IMSRG results for the nuclear matter equation of state obtained from a range of chiral interactions and compares the predictions of several many-body methods. Chapter 4 introduces the PMM emulation framework for IMSRG calculations of the nuclear EOS, including its general formalism, strategies for emulation across chiral EFT LECs, IMSRG flow parameters, densities, and basis sizes, as well as the associated uncertainty quantification. Chapter 5 presents proof-of-principle applications of the PMM-IMSRG framework. In particular, we assess the emulator’s performance, constrain higher-order quark-mass-dependent chiral three-nucleon forces that have been argued [45] should be promoted to

N2LO in the chiral expansion, and propagate parametric uncertainties to the nuclear EOS. Finally, Chapter 6 summarizes the main findings and discusses directions for future work.

CHAPTER 2

IMSRG FRAMEWORK FOR NUCLEAR MATTER CALCULATIONS

Microscopic studies of the nuclear matter EOS are important for various reasons [46]. For example, the EOS in the limit of pure neutron matter (PNM) is crucial in understanding supernova explosions and the properties of neutron stars, including their internal composition and structure, thermal evolution, mass-radius relationships, and the maximum mass before collapsing into a black hole [47, 48, 49]. Moreover, the symmetry energy, which quantifies the energy penalty for having an imbalance of protons and neutrons, determines the neutron skin thickness in neutron-rich nuclei [50, 51, 52], while the incompressibility, which gives a measure of the stiffness of matter, is probed in the study of giant resonances [53, 54]. Finally, empirical saturation properties of symmetric nuclear matter (SNM) such as the density and energy per nucleon control the bulk features of nuclei across the mass table [55, 56], and provide important constraints for nuclear energy density functionals (EDFs) and mass models [57, 58], and may be helpful to constrain microscopic nucleon-nucleon (NN) and 3N interactions to improve their performance beyond light nuclei [59, 56, 60].

In recent years, significant progress has been made in constraining nuclear matter as a function of the baryon density, isospin asymmetry, and temperature [46]. This progress has been driven by advances in chiral effective field theory for nuclear forces [61, 62, 63, 64, 60] and in microscopic many-body frameworks, including many-body perturbation theory [65, 66, 67, 68, 69], coupled cluster theory [70, 71, 59, 72], quantum Monte Carlo (QMC) methods [73, 74, 75, 76, 77], and the self-consistent Green's function method [78, 29, 79]. Here, we develop, implement, and test the IMSRG, which has been a powerful nonperturbative many-body framework for nuclear structure calculations of atomic nuclei, for nuclear matter calculations in a finite volume [80, 81]. Specifically, we focus here on the IMSRG at the normal-ordered two-body (NO2B) level, or IMSRG(2), and benchmark it to CC and MBPT calculations, all of which have different, but well-understood, diagrammatic content.

This chapter discusses the formalism and implementation of the IMSRG for nuclear matter calculations. It begins by formulating the nuclear many-body problem and introducing Hartree–

Fock (HF) theory and normal ordering, which together establish the reference-state representation used in subsequent many-body methods. Many-body perturbation theory and coupled-cluster theory are then reviewed to connect the IMSRG with other widely used many-body approaches. The similarity renormalization group is introduced next as the foundation for continuous unitary transformations, followed by the IMSRG formalism, including the IMSRG(2) truncation, the choice of generator, and the Magnus formulation. Finally, the framework is specialized to nuclear matter in a finite periodic box, with discussions of the single- and many-particle basis, and the computational workflow used to calculate the equation of state and other observables.

2.1 The Nuclear Many-Body Problem

The properties of an A -nucleon system are determined by solving the time-independent Schrödinger equation,

$$\hat{H}|\Psi_k^A\rangle = E_k|\Psi_k^A\rangle, \quad (2.1)$$

where $\hat{H}$ is the nuclear many-body Hamiltonian operator and $|\Psi_k^A\rangle$ is an A -body eigenstate with energy E_k . In this work, we are primarily interested in the ground state, corresponding to the lowest eigenvalue of H .

In second quantization, the Hamiltonian can take the following general form in a given single-particle basis, retaining interactions up to the three-body level:

$$\hat{H} = \sum_{pq} T_{pq} a_p^\dagger a_q + \frac{1}{4} \sum_{pqrs} V_{pqrs}^{(2)} a_p^\dagger a_q^\dagger a_s a_r + \frac{1}{36} \sum_{pqrst} V_{pqrst}^{(3)} a_p^\dagger a_q^\dagger a_r^\dagger a_u a_t a_s, \quad (2.2)$$

where $a_p^\dagger$ and a_p are the creation and annihilation operators for the single-particle state p . T_{pq} denotes the one-body kinetic-energy matrix elements; $V_{pqrs}^{(2)}$ and $V_{pqrst}^{(3)}$ denote the antisymmetrized matrix elements of the bare two-nucleon and three-nucleon interactions.

A general A -body state can be expanded in a basis of Slater determinants constructed from the

chosen single-particle states:

$$\begin{aligned}
|\Psi_k^A\rangle &= \sum_{p_1 < \dots < p_A} C_{p_1 \dots p_A}^{(k)} a_{p_1}^\dagger \dots a_{p_A}^\dagger |0\rangle \\
&= \sum_{p_1 < \dots < p_A} C_{p_1 \dots p_A}^{(k)} |p_1 p_2 \dots p_A\rangle,
\end{aligned} \tag{2.3}$$

where $|0\rangle$ is the particle vacuum, $C_{p_1 \dots p_A}^{(k)}$ are expansion coefficients, and $|p_1 p_2 \dots p_A\rangle = a_{p_1}^\dagger \dots a_{p_A}^\dagger |0\rangle$ denotes the Slater determinant constructed from the occupied single-particle states $p_1, \dots, p_A$. The restriction $p_1 < \dots < p_A$ ensures that each Slater determinant is counted only once and enforces the Pauli exclusion principle.

Suppose that the single-particle basis contains N states. Before imposing additional symmetry constraints, the number of distinct A -particle Slater determinants is

$$\dim \mathcal{H}_A = \binom{N}{A}. \tag{2.4}$$

The dimension of the many-body Hilbert space therefore grows combinatorially with both the size of the single-particle basis and the number of nucleons. Direct construction and diagonalization of the full Hamiltonian matrix therefore become computationally prohibitive for large systems with many particles and realistic model spaces.

This rapid growth motivates the development of approximate many-body methods that avoid diagonalization in the full configuration space while retaining the relevant correlations. In the following sections, we introduce the theoretical ingredients and many-body methods relevant to this work: Hartree–Fock theory for constructing the reference state, normal ordering for reorganizing the Hamiltonian with respect to that reference, many-body perturbation theory and coupled-cluster theory, which will later provide benchmarks at different truncation levels for comparison with the IMSRG results, the similarity renormalization group as the conceptual foundation of the IMSRG, and finally the IMSRG formalism used in our nuclear matter calculations [25, 82, 28, 83].

2.2 Hartree–Fock Theory

Many-body methods such as MBPT, CC, and the IMSRG are formulated relative to a reference state that incorporates essential physical information about the system. The reference state provides

a zeroth-order approximation to the many-body ground state, defines the occupied and unoccupied single-particle orbitals, and allows correlations to be organized in terms of particle-hole excitations. It also serves as the state with respect to which the Hamiltonian is normal ordered in the subsequent formulation.

In the single-reference framework considered in this work, the reference state $|\Phi\rangle$ is chosen to be a single Slater determinant. Hartree–Fock theory determines the energetically optimal Slater determinant by variationally minimizing the expectation value of the Hamiltonian,

$$E_{\text{HF}} = \min_{|\Phi\rangle} \langle \Phi | \hat{H} | \Phi \rangle, \quad (2.5)$$

where the minimization is carried out over all Slater determinants. The Slater determinant that attains this minimum is the Hartree–Fock state, denoted by $|\Phi^{\text{HF}}\rangle$. Applying the variational principle leads to the Hartree–Fock equations,

$$\sum_q F_{pq} C_{qi} = \varepsilon_i C_{pi}, \quad (2.6)$$

where C_{pi} is the expansion coefficient of the HF orbital i in the original single-particle basis, ε_i is the corresponding HF single-particle energy, and F_{pq} denotes matrix elements of the Fock operator. For a Hamiltonian containing up to three-nucleon interactions, the Fock operator is given by

$$F_{pq} = T_{pq} + \sum_{i \in \text{occ}} \langle pi | \hat{V}^{(2)} | qi \rangle + \frac{1}{2} \sum_{ij \in \text{occ}} \langle pij | \hat{V}^{(3)} | qij \rangle, \quad (2.7)$$

where the sums run over the occupied orbitals of the HF reference and the interaction matrix elements are antisymmetrized.

Because the Fock operator depends on the occupied orbitals, the HF equations must be solved self-consistently. Starting from an initial set of single-particle orbitals, one constructs and diagonalizes the Fock matrix to obtain an updated set of single-particle orbitals and their energies. The lowest-energy orbitals are then selected as occupied and used to construct a new Fock matrix. This procedure is repeated until the energies, density matrix, or orbitals change by less than a prescribed numerical tolerance. The resulting HF state is the lowest-energy state within the space of single Slater determinants. The Fock operator provides a one-body mean-field description of the system:

the contributions of the two- and three-nucleon interactions are incorporated by summing over the occupied orbitals. Although HF does not capture correlations beyond a single Slater determinant, it provides a physically motivated reference state for many reference-based many-body methods, including MBPT, CC, and the IMSRG.

2.3 Normal Ordering and NO2B Approximation

Having introduced Hartree–Fock theory as a method for constructing a physically motivated reference state, we now reorganize the Hamiltonian by normal ordering it with respect to the HF reference $|\Phi^{\text{HF}}\rangle$. For notational simplicity, we denote this reference state by $|\Phi\rangle$ throughout the remainder of this section. Normal ordering reorganizes an operator into contributions already contained in the reference state and normal-ordered terms that describe excitations relative to it.

We begin by illustrating normal ordering with respect to the reference state using the simplest one-body example:

$$a_p^\dagger a_q =: a_p^\dagger a_q : + \overline{a_p^\dagger a_q}, \quad (2.8)$$

where the colons denote normal ordering with respect to the reference state. The contraction is defined as the expectation value of the contracted operators in the reference state,

$$\overline{a_p^\dagger a_q} \equiv \langle \Phi | a_p^\dagger a_q | \Phi \rangle = \rho_{pq}, \quad (2.9)$$

where ρ_{pq} is the one-body density matrix element. From the definition in Eq. (2.8), the expectation value of the normal-ordered one-body operator must vanish in the reference state:

$$\langle \Phi | : a_p^\dagger a_q : | \Phi \rangle = 0. \quad (2.10)$$

The one-body definition can be generalized recursively to an arbitrary A -body operator,

$$\begin{aligned} & a_{p_1}^\dagger \cdots a_{p_A}^\dagger a_{q_A} \cdots a_{q_1} \\ & =: a_{p_1}^\dagger \cdots a_{p_A}^\dagger a_{q_A} \cdots a_{q_1} : \\ & + \overline{a_{p_1}^\dagger a_{q_1}} : a_{p_2}^\dagger \cdots a_{p_A}^\dagger a_{q_A} \cdots a_{q_2} : - \overline{a_{p_1}^\dagger a_{q_2}} : a_{p_2}^\dagger \cdots a_{p_A}^\dagger a_{q_A} \cdots a_{q_3} a_{q_1} : + \text{singles} \\ & + \left(\overline{a_{p_1}^\dagger a_{q_1}} \overline{a_{p_2}^\dagger a_{q_2}} - \overline{a_{p_1}^\dagger a_{q_2}} \overline{a_{p_2}^\dagger a_{q_1}} \right) : a_{p_3}^\dagger \cdots a_{p_A}^\dagger a_{q_A} \cdots a_{q_3} : + \text{doubles} \\ & + \cdots + \text{full contractions.} \end{aligned} \quad (2.11)$$

Here, singles and doubles denote the remaining terms containing one and two contractions, respectively. The relative signs arise from the fermionic anti-commutation relations when the operators are permuted to form the contractions. The result $\langle \Phi | : a_p^\dagger a_q : | \Phi \rangle = 0$ for the one-body case can also be readily generalized to an arbitrary A -body operator:

$$\langle \Phi | : a_{p_1}^\dagger \cdots a_{p_A}^\dagger a_{q_A} \cdots a_{q_1} : | \Phi \rangle = 0. \quad (2.12)$$

This is an important property of normal-ordered operators.

With these definitions in place, we can now write the Hamiltonian containing up to three-nucleon interactions in normal-ordered form as

$$\begin{aligned} \hat{H} = E &+ \sum_{pq} f_{pq} : a_p^\dagger a_q : \\ &+ \frac{1}{4} \sum_{pqrs} \Gamma_{pqrs} : a_p^\dagger a_q^\dagger a_s a_r : \\ &+ \frac{1}{36} \sum_{pqrst} W_{pqrst} : a_p^\dagger a_q^\dagger a_r^\dagger a_u a_t a_s : . \end{aligned} \quad (2.13)$$

Here, E , $\hat{f}$, $\hat{\Gamma}$, and $\hat{W}$ are the normal-ordered zero-, one-, two-, and three-body components of the Hamiltonian, respectively. Unlike the corresponding free-space operators, the lower-rank normal-ordered terms contain contributions from higher-rank interactions through contractions with occupied states in the reference.

We choose the HF state as the reference state and work in the corresponding canonical HF single-particle basis. In this basis, the one-body density matrix is diagonal:

$$\rho_{pq} = \delta_{pq} n_p, \quad (2.14)$$

where n_p is the occupation number of the single-particle state p . Because the HF reference is a single Slater determinant, n_p is either zero or one. Occupied states with $n_i = 1$ are referred to as hole states and are denoted by $i, j, k, \dots$, whereas unoccupied states with $n_a = 0$ are referred to as particle states and are denoted by $a, b, c, \dots$. Indices $p, q, r, \dots$ denote general single-particle states. In this basis, the normal-ordered components of the Hamiltonian can be expressed in terms

of the kinetic-energy matrix elements and the antisymmetrized two- and three-nucleon interaction matrix elements as

$$E = \sum_i \langle i | \hat{T} | i \rangle + \frac{1}{2} \sum_{ij} \langle ij | \hat{V}^{(2)} | ij \rangle + \frac{1}{6} \sum_{ijk} \langle ijk | \hat{V}^{(3)} | ijk \rangle, \quad (2.15)$$

$$f_{pq} = \langle p | \hat{T} | q \rangle + \sum_i \langle pi | \hat{V}^{(2)} | qi \rangle + \frac{1}{2} \sum_{ij} \langle pij | \hat{V}^{(3)} | qij \rangle, \quad (2.16)$$

$$\Gamma_{pqrs} = \langle pq | \hat{V}^{(2)} | rs \rangle + \sum_i \langle pqi | \hat{V}^{(3)} | rsi \rangle, \quad (2.17)$$

$$W_{pqrstu} = \langle pqr | \hat{V}^{(3)} | stu \rangle. \quad (2.18)$$

These expressions show that contractions of the three-nucleon interaction with occupied states generate contributions to the normal-ordered zero-, one-, and two-body terms. Thus, part of the physics associated with the bare three-nucleon interaction is incorporated into the lower-rank operators. In particular, the normal-ordered one-body component f has the same form as the Fock operator introduced in the previous section. In the canonical HF basis, its matrix representation is diagonal.

If we neglect the residual normal-ordered three-nucleon interaction and retain the remaining terms in Eq. (2.13), the Hamiltonian becomes

$$H = E + \sum_{pq} f_{pq} : a_p^\dagger a_q : + \frac{1}{4} \sum_{pqrs} \Gamma_{pqrs} : a_p^\dagger a_q^\dagger a_s a_r : . \quad (2.19)$$

This truncation is known as the NO2B approximation. Although the residual normal-ordered three-body term is omitted, the effects of the bare three-nucleon interaction are still retained through its contributions to the normal-ordered zero-, one-, and two-body terms. The resulting Hamiltonian therefore incorporates a substantial portion of the three-body physics while preserving the computational scaling of a two-body Hamiltonian. For low-momentum interactions, the NO2B approximation has been shown to be accurate, with the omission of the residual three-body term producing differences of only about 1–2% in the ground-state energies of light- and medium-mass nuclei [84, 14, 85]. We therefore employ the NO2B approximation throughout this work.

2.4 Many-Body Perturbation Theory

Many-body perturbation theory extends the basic ideas of Rayleigh–Schrödinger perturbation theory to interacting many-body systems. It has long been used in condensed-matter physics and quantum chemistry, where the Coulomb interaction can often be treated perturbatively around an appropriate mean-field solution. In nuclear physics, the development of low-resolution interactions through the SRG has substantially improved the perturbative behavior of nuclear Hamiltonians and has therefore enabled broader applications of MBPT [86, 87].

The starting point of MBPT is to partition the Hamiltonian into an unperturbed part $\hat{H}_0$, whose eigenvalue problem can be solved directly, and a residual interaction $\hat{H}_I$:

$$\hat{H} = \hat{H}_0 + \hat{H}_I. \quad (2.20)$$

The exact ground state $|\Psi_0\rangle$ then satisfies

$$\hat{H}|\Psi_0\rangle = (\hat{H}_0 + \hat{H}_I)|\Psi_0\rangle = E|\Psi_0\rangle, \quad (2.21)$$

where E is the exact ground-state energy. In the canonical HF basis, the normal-ordered one-body operator is diagonal,

$$f_{pq} = \varepsilon_p \delta_{pq}, \quad (2.22)$$

where ε_p denotes the HF single-particle energy. A natural choice for the unperturbed Hamiltonian is therefore

$$\hat{H}_0 = E_0 + \sum_p \varepsilon_p : a_p^\dagger a_p :, \quad (2.23)$$

where $E_0 = E_{\text{HF}}$ is the HF reference energy. Within the NO2B approximation, the residual interaction is

$$\hat{H}_I = \frac{1}{4} \sum_{pqrs} \Gamma_{pqrs} : a_p^\dagger a_q^\dagger a_s a_r :. \quad (2.24)$$

This choice of $\hat{H}_0$ and $\hat{H}_I$, known as the Møller–Plesset partition, makes the HF reference $|\Phi\rangle$ an eigenstate of $\hat{H}_0$:

$$\hat{H}_0|\Phi\rangle = E_0|\Phi\rangle. \quad (2.25)$$

Multiplying Eq. (2.21) from the left by $\langle\Phi|$ and inserting Eq. (2.25) gives

$$(E - E_0) \langle\Phi|\Psi_0\rangle = \langle\Phi|\hat{H}_I|\Psi_0\rangle. \quad (2.26)$$

We impose the intermediate-normalization condition $\langle\Phi|\Psi_0\rangle = 1$, so that the correlation energy $\Delta E \equiv E - E_0$ can be written as

$$\Delta E = \langle\Phi|\hat{H}_I|\Psi_0\rangle. \quad (2.27)$$

To construct the perturbative expansion, we introduce the projection operator

$$\hat{Q} = 1 - |\Phi\rangle\langle\Phi|, \quad (2.28)$$

which projects onto the subspace orthogonal to the reference state, and the corresponding reduced resolvent,

$$\hat{R}_0 = \frac{\hat{Q}}{E_0 - \hat{H}_0}. \quad (2.29)$$

Here, the inverse of $E_0 - \hat{H}_0$ is defined only within the subspace orthogonal to $|\Phi\rangle$. Projecting the Schrödinger equation onto this complementary subspace gives

$$\hat{Q}|\Psi_0\rangle = \hat{R}_0 (\hat{H}_I - \Delta E) |\Psi_0\rangle. \quad (2.30)$$

Under the intermediate-normalization condition $\langle\Phi|\Psi_0\rangle = 1$, the exact ground state can be written as

$$|\Psi_0\rangle = |\Phi\rangle + \hat{R}_0 (\hat{H}_I - \Delta E) |\Psi_0\rangle. \quad (2.31)$$

Repeated substitution of Eq. (2.31) into its right-hand side yields the formal expansions

$$|\Psi_0\rangle = |\Phi\rangle + \sum_{m=1}^{\infty} [\hat{R}_0 (\hat{H}_I - \Delta E)]^m |\Phi\rangle, \quad (2.32)$$

$$E = E_0 + \sum_{m=0}^{\infty} \langle\Phi|\hat{H}_I [\hat{R}_0 (\hat{H}_I - \Delta E)]^m |\Phi\rangle. \quad (2.33)$$

Equations (2.32) and (2.33) provide compact, implicit expressions for the exact ground-state wavefunction and energy. They show how successive applications of the perturbation and the reduced resolvent generate corrections to the reference state and its energy.

To derive the energy correction at each perturbative order, we assume that the exact ground state and correlation energy can be expanded in powers of $\hat{H}_I$:

$$|\Psi_0\rangle = |\Phi\rangle + \sum_{i=1}^{\infty} |\Psi^{(i)}\rangle, \quad (2.34)$$

$$\Delta E = \sum_{i=1}^{\infty} \Delta E^{(i)}, \quad (2.35)$$

where $|\Psi^{(i)}\rangle$ and $\Delta E^{(i)}$ denote the i th-order corrections in $\hat{H}_I$. Substituting these expansions into Eq. (2.31) and equating terms of the same perturbative order yields the individual energy corrections. The first three are

$$\Delta E^{(1)} = \langle \Phi | \hat{H}_I | \Phi \rangle, \quad (2.36)$$

$$\Delta E^{(2)} = \langle \Phi | \hat{H}_I \hat{R}_0 \hat{H}_I | \Phi \rangle, \quad (2.37)$$

$$\begin{aligned} \Delta E^{(3)} = & \langle \Phi | \hat{H}_I \hat{R}_0 \hat{H}_I \hat{R}_0 \hat{H}_I | \Phi \rangle \\ & - \langle \Phi | \hat{H}_I | \Phi \rangle \langle \Phi | \hat{H}_I \hat{R}_0^2 \hat{H}_I | \Phi \rangle. \end{aligned} \quad (2.38)$$

In the Møller–Plesset partition, the residual interaction $\hat{H}_I$ is normal ordered with respect to the HF reference. Its expectation value in the reference state therefore vanishes:

$$\langle \Phi | \hat{H}_I | \Phi \rangle = 0. \quad (2.39)$$

Consequently, the first three corrections to the correlation energy simplify to

$$\Delta E^{(1)} = 0, \quad (2.40)$$

$$\Delta E^{(2)} = \langle \Phi | \hat{H}_I \hat{R}_0 \hat{H}_I | \Phi \rangle, \quad (2.41)$$

$$\Delta E^{(3)} = \langle \Phi | \hat{H}_I \hat{R}_0 \hat{H}_I \hat{R}_0 \hat{H}_I | \Phi \rangle. \quad (2.42)$$

2.5 Coupled-Cluster Theory

Coupled-cluster theory is closely related to the IMSRG framework introduced below [28, 27]. It parametrizes the correlated many-body wavefunction through an exponential ansatz acting on a

reference state $|\Phi\rangle$:

$$|\Psi_{\text{CC}}\rangle = e^{\hat{T}}|\Phi\rangle, \quad (2.43)$$

where $\hat{T}$ is the cluster operator. It is written as a sum of particle-hole excitation operators of increasing rank,

$$\hat{T} = \hat{T}_1 + \hat{T}_2 + \cdots, \quad (2.44)$$

with

$$\hat{T}_1 = \sum_{ai} t_i^a : a_a^\dagger a_i :, \quad (2.45)$$

$$\hat{T}_2 = \frac{1}{4} \sum_{abij} t_{ij}^{ab} : a_a^\dagger a_b^\dagger a_j a_i :, \quad (2.46)$$

where $t_i^a, t_{ij}^{ab}, \dots$ are the cluster amplitudes. The operators $\hat{T}_1$ and $\hat{T}_2$ generate one-particle–one-hole (1p1h) and two-particle–two-hole (2p2h) excitations, respectively.

If excitation operators of all ranks are retained, the CC ansatz is formally exact. In practical calculations, however, the cluster operator must be truncated. Retaining only single and double excitations,

$$\hat{T} = \hat{T}_1 + \hat{T}_2, \quad (2.47)$$

defines the coupled-cluster singles and doubles (CCSD) approximation. Including triple excitations as well gives CCSDT, while several intermediate schemes incorporate triples approximately, such as perturbative corrections built on a CCSD solution.

Substituting the CC ansatz into the Schrödinger equation and multiplying from the left by $e^{-\hat{T}}$ gives

$$\overline{H}|\Phi\rangle = E_{\text{CC}}|\Phi\rangle, \quad (2.48)$$

where $\overline{H} = e^{-\hat{T}}\hat{H}e^{\hat{T}}$ is the similarity-transformed Hamiltonian. The cluster amplitudes are determined by requiring the reference state to be decoupled from the particle-hole excitations in $\overline{H}$. For

CCSD, the projected equations enforcing the decoupling are

$$\langle \Phi | \bar{H} | \Phi \rangle = E_{\text{CC}}, \quad (2.49)$$

$$\langle \Phi_i^a | \bar{H} | \Phi \rangle = 0, \quad (2.50)$$

$$\langle \Phi_{ij}^{ab} | \bar{H} | \Phi \rangle = 0, \quad (2.51)$$

where $|\Phi_i^a\rangle = a_a^\dagger a_i |\Phi\rangle$ and $|\Phi_{ij}^{ab}\rangle = a_a^\dagger a_b^\dagger a_j a_i |\Phi\rangle$ are 1p1h and 2p2h excitations of the reference state. The singles and doubles projection equations form a coupled nonlinear system that determines the cluster amplitudes, while the reference-state projection yields the CC ground-state energy. These equations together constitute the CC equations.

Unlike the SRG and IMSRG transformations introduced in the following sections, the CC similarity transformation is not unitary. Consequently, the similarity-transformed Hamiltonian $\bar{H}$ is generally non-Hermitian.

2.6 Similarity Renormalization Group

The basic idea of the similarity renormalization group is to simplify the nuclear many-body Hamiltonian through a continuous sequence of unitary transformations. These transformations are parametrized by a scalar flow parameter s , giving the flow-dependent Hamiltonian

$$\hat{H}(s) = \hat{U}^\dagger(s) \hat{H}(0) \hat{U}(s), \quad (2.52)$$

where $\hat{H}(0)$ denotes the initial Hamiltonian and $\hat{U}(s)$ is the unitary transformation at flow parameter s . Because the transformation is unitary, the eigenvalues of the Hamiltonian are preserved throughout the flow.

The SRG is commonly used to soften free-space nuclear interactions by decoupling low- and high-momentum states. This is achieved by driving the Hamiltonian toward a more diagonal or block-diagonal form and suppressing matrix elements that connect states with widely separated momenta. As a result, low-energy observables become less sensitive to the short-range, high-momentum details of the interaction. In this sense, the SRG lowers the resolution scale of the nuclear interactions and improves the convergence of subsequent many-body calculations. To

describe this decoupling, the flowing Hamiltonian is partitioned as

$$\hat{H}(s) = \hat{H}_d(s) + \hat{H}_{od}(s), \quad (2.53)$$

where $\hat{H}_d(s)$ and $\hat{H}_{od}(s)$ denote the parts designated as diagonal and off-diagonal, respectively.

The flow is constructed to suppress $\hat{H}_{od}(s)$, ideally such that

$$\lim_{s \rightarrow \infty} \hat{H}_{od}(s) = 0. \quad (2.54)$$

Differentiating Eq. (2.52) with respect to s and defining the anti-Hermitian generator

$$\hat{\eta}(s) \equiv \frac{d\hat{U}^\dagger(s)}{ds} \hat{U}(s), \quad (2.55)$$

gives the SRG flow equation

$$\frac{d\hat{H}(s)}{ds} = [\hat{\eta}(s), \hat{H}(s)]. \quad (2.56)$$

The choice of generator determines how the Hamiltonian evolves during the flow. A commonly used choice is the Wegner generator [88],

$$\hat{\eta}(s) = [\hat{H}_d(s), \hat{H}_{od}(s)]. \quad (2.57)$$

As the off-diagonal part is suppressed, the generator approaches zero, and the flow reaches a fixed point.

The labels “diagonal” and “off-diagonal” do not necessarily refer to the literal diagonal and off-diagonal matrix elements of the Hamiltonian. Instead, $\hat{H}_d$ and $\hat{H}_{od}$ are defined according to the desired decoupling pattern: $\hat{H}_d$ contains the structure to be retained, while $\hat{H}_{od}$ contains the couplings to be suppressed.

An important complication arises from the operator structure of the flow equation. Commutators of many-body operators generally generate terms of higher particle rank. Thus, even if the initial Hamiltonian contains only two-body interactions, the SRG evolution induces three-body and higher-body operators. For an A -body system, an exact evolution can therefore generate operators of rank up to A , and retaining all of these induced operators becomes computationally prohibitive as the particle number increases.

Truncating the induced operators breaks the exact unitarity of the SRG evolution in systems whose particle number exceeds the highest retained operator rank. For example, if the flow equations are truncated at the two-body level, observables in the two-nucleon system remain invariant, including nucleon–nucleon scattering phase shifts and the deuteron binding energy. For systems with $A > 2$, however, omitting induced three-body and higher-body interactions introduces a residual dependence of calculated observables on the SRG flow parameter. Similarly, retaining operators through the three-body level preserves observables for systems with $A \leq 3$, such as the ground-state energies of ^3H and ^3He , while calculations for heavier systems remain affected by omitted four-body and higher-body terms.

Because an exact SRG evolution of the full A -body Hamiltonian in free space is computationally prohibitive, SRG is most commonly used as a preprocessor to dial the resolution scale of nuclear interactions and thereby soften them [25, 23, 24, 89, 90], improving the convergence of subsequent many-body methods such as MBPT and CC. There is also a many-body method based on the same continuous unitary-transformation idea as the SRG: the in-medium similarity renormalization group (IMSRG), which is the topic of the next section.

2.7 In-Medium Similarity Renormalization Group

Having introduced the basic idea of the SRG, we now take a step further and apply the same continuous unitary-transformation framework directly to the many-body problem. The goal of the in-medium similarity renormalization group (IMSRG) is to solve the many-body Schrödinger equation by decoupling a chosen reference state from its particle-hole excitations. By formulating the problem relative to a reference state that captures important features of the many-body system, parts of the higher-rank contributions are incorporated into lower-rank operators, making subsequent truncations less detrimental to calculated observables. The key step is to normal order the Hamiltonian with respect to this reference state.

Once we have normal ordered the Hamiltonian with respect to the reference state, we can use the idea of SRG to choose a generator to evolve the Hamiltonian operator, to decouple our reference state from the excited states (including 1p1h, 2p2h, $\dots$ and so on) via the continuous

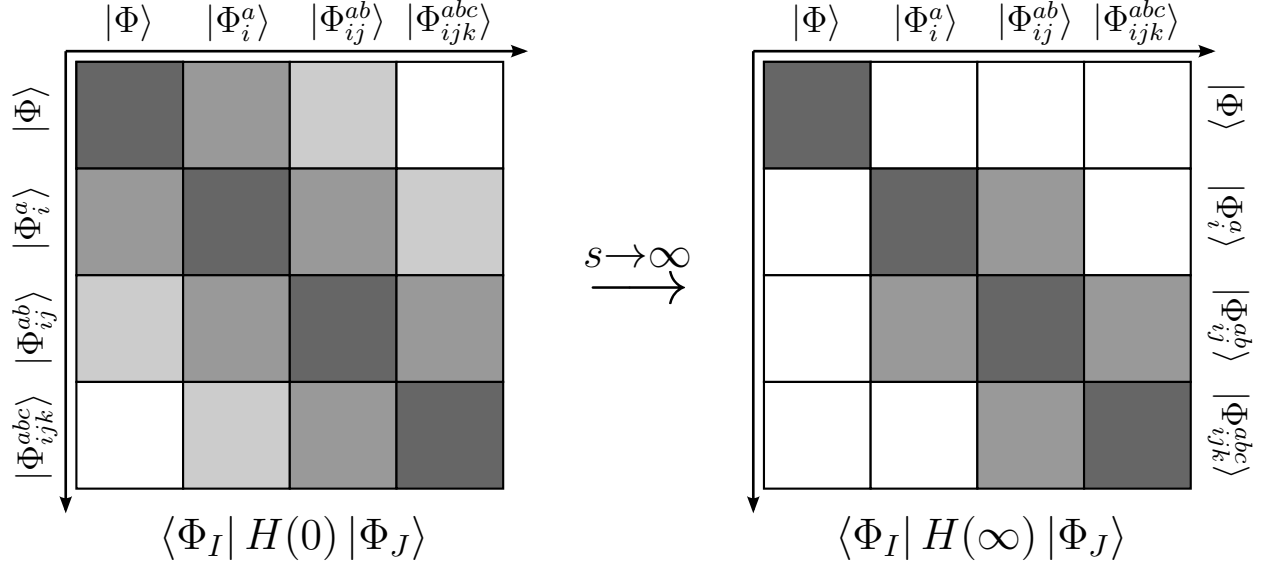


Figure 2.1 A schematic view of IMSRG decoupling [25]. The many-body Hamiltonian is depicted in blocks, with the reference state $|\Phi\rangle$ and its particle-hole excitations (see the main text). During the IMSRG flow, the reference state is decoupled from its excitations.

unitary transformation. At the end of the flow, when the reference state is completely decoupled, it becomes the true ground state of our evolved Hamiltonian and the evolved zero-body part becomes our ground state energy.

For a single-reference ground-state calculation, the off-diagonal Hamiltonian $\hat{H}_{\text{od}}$ is defined to contain the terms that couple the reference state $|\Phi\rangle$ to its particle-hole excitations. In the normal-ordered two-body approximation, these couplings are represented by the 1p1h and 2p2h matrix elements

$$\langle\Phi|\hat{H} : a_a^\dagger a_i : |\Phi\rangle = f_{ai}, \quad (2.58)$$

and

$$\langle\Phi|\hat{H} : a_a^\dagger a_b^\dagger a_j a_i : |\Phi\rangle = \Gamma_{abij}, \quad (2.59)$$

together with their Hermitian conjugates. The IMSRG flow is constructed to suppress these matrix elements, so that

$$\lim_{s \rightarrow \infty} f_{ai}(s) = 0, \quad \lim_{s \rightarrow \infty} \Gamma_{abij}(s) = 0. \quad (2.60)$$

The reference state is then decoupled from the corresponding particle-hole excitations, as shown schematically in Fig. 2.1.

2.7.1 IMSRG(2) Scheme

As discussed in the context of the SRG, the problem of induced higher-body operators also arises in the IMSRG. Although the Hamiltonian is normal ordered with respect to a reference state, commutators of normal-ordered operators generally generate higher-rank terms. For example, the commutator of two normal-ordered two-body operators has the schematic structure

$$[\hat{\eta}^{(2)}, \hat{H}^{(2)}] = \hat{C}^{(0)} + \hat{C}^{(1)} + \hat{C}^{(2)} + \hat{C}^{(3)}, \quad (2.61)$$

where $\hat{C}^{(n)}$ denotes the normal-ordered n -body part of the commutator. The four-body contribution cancels in the commutator, but a normal-ordered three-body operator is induced. Retaining this term in subsequent commutators would generate operators of still higher particle rank, eventually producing operators up to rank A in an A -body system.

To keep the computational cost manageable, we apply the NO2B approximation consistently to all operators and commutators throughout the flow. Thus, each operator is truncated at the normal-ordered two-body level, retaining only its zero-, one-, and two-body components while discarding the residual normal-ordered three-body terms. This truncation scheme is known as IMSRG(2) and is analogous in spirit to CCSD.

This truncation breaks the exact unitarity of the IMSRG evolution, so the resulting ground-state energy is approximate. Nevertheless, by normal ordering all operators with respect to a reference state that provides a good approximation to the ground state, important many-body contributions are incorporated into the retained lower-rank operators, so the effects of induced three-body operators are preserved in part. The empirical success of the NO2B approximation for low-momentum NN+3N Hamiltonians provides support for the IMSRG(2) truncation scheme: omitting the residual normal-ordered three-body term in exact calculations produces deviations of only $\sim 1\%$ for oxygen, calcium, and nickel isotopes [14, 13, 91].

Under the IMSRG(2) scheme, we decompose all many-body operators into normal-ordered

zero-, one-, and two-body parts:

$$\hat{\eta}(s) \approx \hat{\eta}^{(1)}(s) + \hat{\eta}^{(2)}(s), \quad (2.62)$$

$$\hat{H}(s) \approx E(s) + \hat{f}(s) + \hat{\Gamma}(s), \quad (2.63)$$

$$\frac{d\hat{H}(s)}{ds} \approx \frac{dE(s)}{ds} + \frac{d\hat{f}(s)}{ds} + \frac{d\hat{\Gamma}(s)}{ds}. \quad (2.64)$$

Substituting these expressions into the flow equation, Eq. (2.56), gives the IMSRG(2) flow equations

$$\frac{dE}{ds} = \sum_{ab} (n_a - n_b) \eta_{ab} f_{ba} + \frac{1}{2} \sum_{abcd} \eta_{abcd} \Gamma_{cdab} n_a n_b \bar{n}_c \bar{n}_d, \quad (2.65)$$

$$\begin{aligned} \frac{df_{ij}}{ds} = & \sum_a (1 + P_{ij}) \eta_{ia} f_{aj} + \sum_{ab} (n_a - n_b) (\eta_{ab} \Gamma_{biaj} - f_{ab} \eta_{biaj}) \\ & + \frac{1}{2} \sum_{abc} (n_a n_b \bar{n}_c + \bar{n}_a \bar{n}_b n_c) (1 + P_{ij}) \eta_{ciab} \Gamma_{abcj}, \end{aligned} \quad (2.66)$$

$$\begin{aligned} \frac{d\Gamma_{ijkl}}{ds} = & \sum_a \left\{ (1 - P_{ij}) (\eta_{ia} \Gamma_{ajkl} - f_{ia} \eta_{ajkl}) \right. \\ & \left. - (1 - P_{kl}) (\eta_{ak} \Gamma_{ijal} - f_{ak} \eta_{ijal}) \right\} \\ & + \frac{1}{2} \sum_{ab} (1 - n_a - n_b) (\eta_{ijab} \Gamma_{abkl} - \Gamma_{ijab} \eta_{abkl}) \\ & + \sum_{ab} (n_a - n_b) (1 - P_{ij}) (1 - P_{kl}) \eta_{aibk} \Gamma_{bjal}. \end{aligned} \quad (2.67)$$

Here, $\bar{n}_i = 1 - n_i$, P_{ij} denotes the permutation operator that interchanges the indices i and j , and the explicit s dependence has been omitted for simplicity.

In this work, we adopt the White generator with Møller–Plesset (MP) denominator, which in the NO2B approximation is given by

$$\begin{aligned} \hat{\eta} = & \sum_{ai} \frac{f_{ai}}{\Delta_{ai}} : a_a^\dagger a_i : + \frac{1}{4} \sum_{abij} \frac{\Gamma_{abij}}{\Delta_{abij}} : a_a^\dagger a_b^\dagger a_j a_i : \\ & - \text{H.c.}, \end{aligned} \quad (2.68)$$

where

$$\Delta_{ai} = f_{aa} - f_{ii}, \quad (2.69)$$

is the unperturbed energy difference between the reference state and its 1p1h excitation in the Møller–Plesset partition, and

$$\Delta_{abij} = f_{aa} + f_{bb} - f_{ii} - f_{jj}, \quad (2.70)$$

is the corresponding unperturbed energy difference for a 2p2h excitation.

2.7.2 Magnus Formulation

In this work, we use the Magnus expansion formulation of the IMSRG [89, 92], which offers a number of practical advantages over the direct integration of Eq. (2.56). The idea is to express the IMSRG unitary transformation as a true exponential,

$$\hat{U}^\dagger(s) = e^{\hat{\Omega}(s)}, \quad (2.71)$$

where the anti-Hermitian Magnus operator $\hat{\Omega}(s)$ obeys the flow equation, with the explicit s dependence suppressed for brevity,

$$\frac{d\hat{\Omega}}{ds} = \sum_{k=0}^{\infty} \frac{B_k}{k!} \text{ad}_{\hat{\Omega}}^{(k)}(\hat{\eta}), \quad (2.72)$$

where B_k are the Bernoulli numbers, and the adjoint $\text{ad}_{\hat{\Omega}}^{(k)}(\hat{\eta})$ signifies a recursively defined nested commutator:

$$\text{ad}_{\hat{\Omega}}^{(k)}(\hat{\eta}) = \left[\hat{\Omega}, \text{ad}_{\hat{\Omega}}^{(k-1)}(\hat{\eta}) \right], \quad \text{ad}_{\hat{\Omega}}^{(0)}(\hat{\eta}) = \hat{\eta}. \quad (2.73)$$

The evolved Hamiltonian, or any other operator of interest, can then be expressed via the Baker–Campbell–Hausdorff (BCH) formula,

$$\begin{aligned} \hat{H}(s) &= e^{\hat{\Omega}(s)} \hat{H}(0) e^{-\hat{\Omega}(s)} \\ &= \hat{H}(0) + [\hat{\Omega}(s), \hat{H}(0)] + \frac{1}{2} [\hat{\Omega}(s), [\hat{\Omega}(s), \hat{H}(0)]] + \cdots \end{aligned} \quad (2.74)$$

Fortunately, in most practical applications, only the first few terms of the infinite series in Eqs. (2.74) and (2.72) are important, and so the commutator may be evaluated iteratively until the size of a given term is below some numerical threshold.

The Magnus expansion formulation allows one to use a simple forward first-order Euler method to solve Eq. (2.72) without accumulating time-step errors in the computed ground-state energy [89]. In contrast, the direct integration of Eq. (2.56) requires a high-order adaptive ODE solver, since time-step errors are accumulated directly in the evolved Hamiltonian. Consequently, the memory savings from the Magnus expansion formulation can be significant.

Another major advantage of the Magnus method is that, by solving for $\hat{\Omega}(s)$, we can compute arbitrary effective operators besides the Hamiltonian in a consistent and efficient way [92, 93]. In the next chapter, we will illustrate this by carrying out proof-of-principle computations of single-nucleon momentum distributions and static structure factors for nuclear matter.

2.8 IMSRG for Nuclear Matter in a Finite Box

In this section, we describe how the IMSRG, which has been widely applied to finite nuclei, is extended to nuclear matter to calculate the EOS and other observables of interest. Nuclear matter is an idealized infinite system defined in the thermodynamic limit. In practical calculations, it is therefore natural to represent the system in a finite volume with periodic boundary conditions. Following previous work [70, 72, 81], we model infinite nuclear matter as a system of A nucleons confined to a cubic box of length L with periodic boundary conditions. In the next chapter, we will discuss how we correct the finite-size effects introduced by this modeling scheme.

2.8.1 Single-Particle Basis

In this scenario, the single-particle basis states are momentum eigenstates,

$$|p\rangle \equiv |\mathbf{k}_p \sigma_p \tau_p\rangle, \quad (2.75)$$

where p labels a single-particle state, and σ_p and τ_p denote the spin and isospin projections, respectively. Its coordinate-space representation is given by the plane wave

$$\psi_{\mathbf{k}_p, \sigma_p, \tau_p}(\mathbf{r}) = \frac{e^{i\mathbf{k}_p \cdot \mathbf{r}}}{\sqrt{\mathcal{V}}} |\sigma_p \tau_p\rangle, \quad (2.76)$$

where $\mathcal{V} = L^3$ is the volume of the cubic box, and the momentum components are quantized as

$$k_i = \frac{2\pi}{L}n_i, \quad \text{for } i = x, y, z, \quad (2.77)$$

with $n_i = 0, \pm 1, \pm 2, \dots$. The spin-isospin degeneracies for each momentum state are $g_s = 2$ (PNM) and $g_s = 4$ (SNM), respectively. Therefore, filling up the discrete lattice of momentum points in accordance with the Pauli principle leads to Fermi spheres (closed-shell configurations) with $A = g_s \mathcal{N}$ nucleons, where $\mathcal{N} = 1, 7, 19, 27, 33, 57, \dots$

All of our calculations are performed in a truncated single-particle model space defined by

$$n_x^2 + n_y^2 + n_z^2 \leq n_{\max}^2. \quad (2.78)$$

The size of the model space is then increased until the computed energy per nucleon is practically independent of $n_{\max}$. This occurs once the basis is large enough to resolve the high-momentum (i.e., short-distance) structure of the nucleon-nucleon and three-nucleon interactions. The approach used to control the systematic error arising from working in a truncated single-particle basis will also be discussed in Chapter 3.

To clarify the relation between $n_{\max}^2$ and the number of allowed single-particle states, Table 2.1 lists the cumulative number $N_{\uparrow\downarrow}$ of states for each value of $n_x^2 + n_y^2 + n_z^2$ up to 4 for a single spin- $\frac{1}{2}$ species [82]. For matter containing both protons and neutrons, the total degeneracy should be multiplied by a factor of two. The table also illustrates how the degeneracies of successive momentum shells give rise to the closed-shell particle numbers.

In this work, we also use N_{shells} to characterize the truncation of the single-particle basis. Specifically, N_{shells} denotes the number of unoccupied momentum shells retained above the Fermi surface. The number of occupied momentum shells is fixed by the chosen closed-shell particle number A . For example, for a closed-shell system with $A = 66$, the reference state occupies the first five momentum shells. Thus, $N_{\text{shells}} = 1$ indicates that one additional momentum shell above the highest occupied shell is included in the single-particle basis.

Table 2.1 Momentum shells and cumulative single-particle degeneracy.

$n_x^2 + n_y^2 + n_z^2$	n_x	n_y	n_z	$N_{\uparrow\downarrow}$
0	0	0	0	2
1	-1	0	0	
1	1	0	0	
1	0	-1	0	
1	0	1	0	
1	0	0	-1	
1	0	0	1	14
2	-1	-1	0	
2	-1	1	0	
2	1	-1	0	
2	1	1	0	
2	-1	0	-1	
2	-1	0	1	
2	1	0	-1	
2	1	0	1	
2	0	-1	-1	
2	0	-1	1	
2	0	1	-1	
2	0	1	1	38
3	-1	-1	-1	
3	-1	-1	1	
3	-1	1	-1	
3	-1	1	1	
3	1	-1	-1	
3	1	-1	1	
3	1	1	-1	
3	1	1	1	54
4	-2	0	0	
4	2	0	0	
4	0	-2	0	
4	0	2	0	
4	0	0	-2	
4	0	0	2	66

2.8.2 Many-Particle Basis

Starting from the single-particle basis, we construct the corresponding many-particle basis subject to the Pauli exclusion principle, which requires that no identical fermions occupy the same single-particle state.

Working in the discrete momentum basis, translational invariance is automatically enforced, with NN and 3N interaction matrix elements vanishing unless the total momentum is conserved. In addition, the nuclear interaction conserves the total isospin projection, which further eliminates many possible combinations when evaluating the interaction matrix elements.

For two-particle states (p, q) and (r, s) , these conservation laws are expressed as

$$\mathbf{k}_p + \mathbf{k}_q = \mathbf{k}_r + \mathbf{k}_s, \quad (2.79)$$

$$(\tau_z)_p + (\tau_z)_q = (\tau_z)_r + (\tau_z)_s, \quad (2.80)$$

with $p \neq q$ and $r \neq s$.

For three-particle states (p, q, r) and (s, t, u) , the corresponding constraints are

$$\mathbf{k}_p + \mathbf{k}_q + \mathbf{k}_r = \mathbf{k}_s + \mathbf{k}_t + \mathbf{k}_u, \quad (2.81)$$

$$(\tau_z)_p + (\tau_z)_q + (\tau_z)_r = (\tau_z)_s + (\tau_z)_t + (\tau_z)_u, \quad (2.82)$$

where p, q , and r are all distinct, and likewise s, t , and u are all distinct.

2.8.3 Computational Workflow

Based on the preceding discussion, we now summarize our IMSRG(2) computational workflow for calculating the nuclear matter equation of state and other observables. The main steps are:

1. Construct the single-particle basis from the plane-wave states in the finite periodic box.
2. Construct the corresponding two-particle and three-particle basis, subject to the Pauli exclusion principle and the conservation of total momentum and isospin projection.
3. Compute the kinetic-energy and NN interaction matrix elements and use them to construct the initial one- and two-body parts of the Hamiltonian.

4. Determine the Hartree–Fock reference state. For homogeneous nuclear matter, translational invariance ensures that the Fock operator is diagonal in momentum space, so the Hartree–Fock orbitals are the plane-wave basis states. The Hartree–Fock reference is then obtained by occupying the lowest-energy single-particle states up to the chosen particle number. For the closed-shell particle numbers considered here, this corresponds to a filled Fermi-sea configuration.
5. Normal order the Hamiltonian with respect to the Hartree–Fock reference. During this step, the normal-ordered zero-, one-, and two-body contributions from the initial 3N interaction are computed on the fly, avoiding the need to store the complete set of 3N matrix elements.
6. Construct the White generator from the resulting NO2B Hamiltonian.

7. Integrate the flow equation for the Magnus operator,

$$\frac{d\hat{\Omega}}{ds} = \sum_{k=0}^{\infty} \frac{B_k}{k!} \text{ad}_{\hat{\Omega}}^{(k)}(\hat{\eta}),$$

using the first-order forward Euler method.

8. At each step of the flow, apply the BCH expansion to transform the initial Hamiltonian,

$$\hat{H}(s) = e^{\hat{\Omega}(s)} \hat{H}(0) e^{-\hat{\Omega}(s)},$$

and extract its evolved zero-body component $E(s)$.

9. Continue the evolution until the chosen convergence criterion is satisfied. The final zero-body component,

$$E_{\text{IMSRG}} = E(s_{\text{final}}),$$

is then taken as the IMSRG(2) result of the ground-state energy of the nuclear matter system.

10. Repeat the IMSRG(2) calculation over a chosen grid of densities. The resulting ground-state energy per particle,

$$\frac{E_{\text{IMSRG}}(n)}{A},$$

as a function of the baryon density n defines the nuclear matter EOS.

11. To calculate an additional observable $\hat{O}$, store the final Magnus operator and apply the same BCH transformation to the normal-ordered target operator,

$$\hat{O}(s_{\text{final}}) = e^{\hat{\Omega}(s_{\text{final}})} \hat{O}(0) e^{-\hat{\Omega}(s_{\text{final}})}. \quad (2.83)$$

Its ground-state expectation value is obtained from the zero-body component of the evolved operator.

These steps constitute the main structure of the computational framework. In addition, second- and third-order many-body perturbation theory calculations are performed for the Hamiltonian at each stage of the flow to monitor the suppression of perturbative corrections. After the initial normal ordering, all operators and subsequent calculations are represented in the normal-ordered operator basis.

2.9 Benchmark

To benchmark our IMSRG(2) framework, we compute the EOS of pure neutron matter (PNM) with $A = 114$ for several single-particle basis sizes and compare the results with those obtained using coupled-cluster doubles (CCD). CCD, rather than CCSD, is sufficient for this application because the singles amplitudes vanish for the Hartree–Fock reference in homogeneous nuclear matter as a consequence of translational invariance. CCD and IMSRG(2) are distinct many-body methods, but they employ comparable truncation schemes. Although the two calculations use slightly different model spaces, the resulting EOS predictions are in close agreement, as shown by comparing our IMSRG(2) results in Fig. 2.2 with the CCD results presented in Fig. 8.8 of Ref. [94]. Such agreement is expected because the Minnesota potential is relatively perturbative.

The framework developed in this chapter provides the foundation for the nuclear matter calculations presented in Chapter 3, where we assess the main sources of uncertainty and apply it to the nuclear matter EOS and ground-state observables. In addition, the framework could be extended to other translationally invariant many-body systems with different underlying interactions, such as the electron gas.

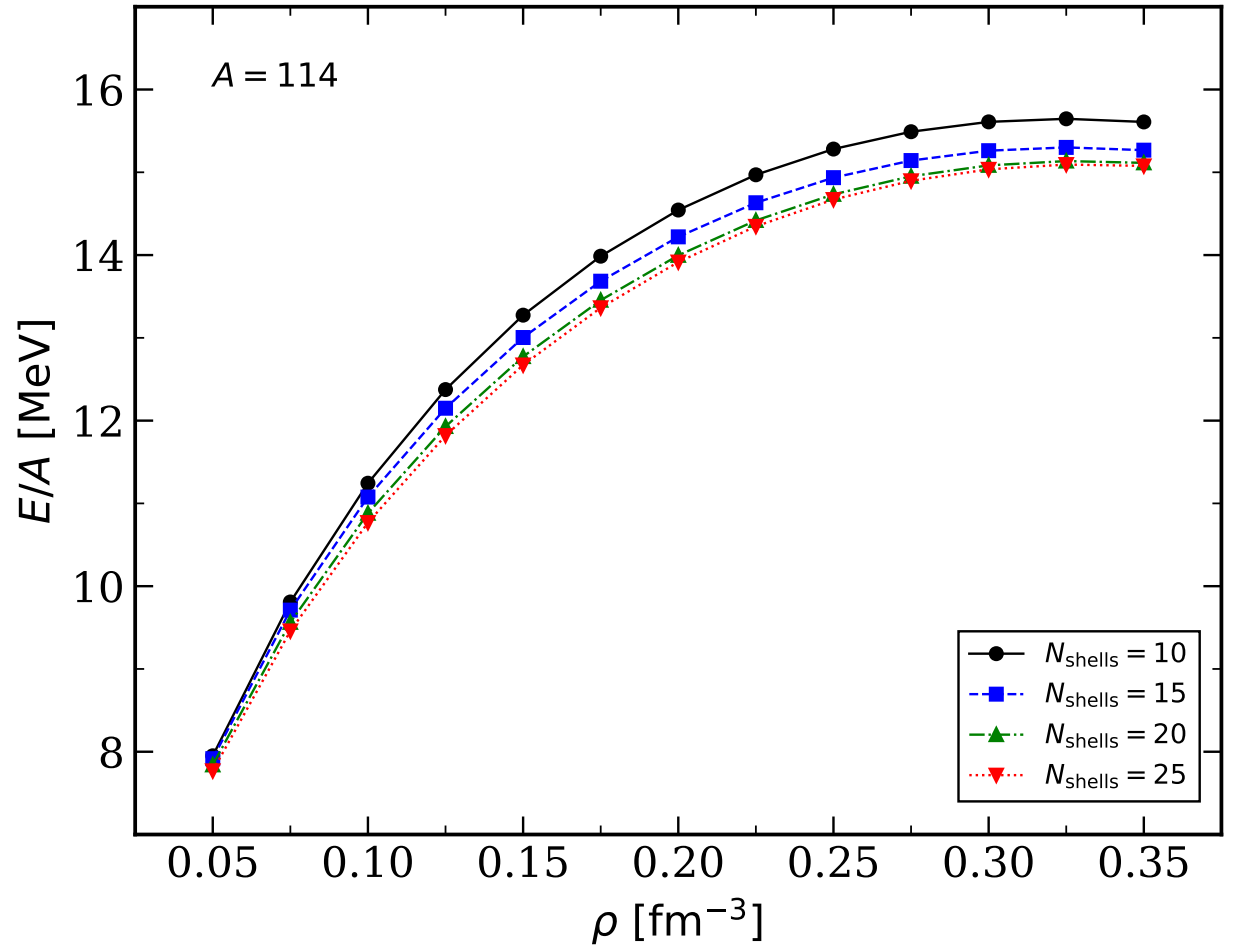


Figure 2.2 Energy per particle of pure neutron matter computed in the IMSRG(2) approximation with the Minnesota interaction model for different single-particle basis sizes with $A = 114$.

CHAPTER 3

IMSRG CALCULATIONS OF THE NUCLEAR MATTER EQUATION OF STATE AND OBSERVABLES

Chapter 2 introduces the formalism and implementation of our IMSRG framework for nuclear matter calculations [80]. In this chapter, we present the results obtained with this framework, including its convergence behavior and computational scaling, an analysis of finite-size effects and how they can be accounted for, and our main results for the energy per particle in pure neutron matter and symmetric nuclear matter, together with an additional example for asymmetric nuclear matter at proton fraction $Y_p = 0.05$. Detailed comparisons with other many-body methods are also presented and discussed. Finally, we demonstrate the framework’s capability to compute ground-state observables beyond the energy enabled by the Magnus formulation, with proof-of-principle calculations of the single-nucleon momentum distribution and static structure factor.

3.1 Convergence and Scaling

Let us start by examining the convergence of the IMSRG calculations with respect to both the flow parameter and the size of the single-particle basis. In particular, we demonstrate that one of the two major sources of systematic errors in our periodic-box calculations—the truncation of the single-particle basis—is small and under control. We then analyze the computational scaling of the framework.

3.1.1 Flow Convergence

We first discuss the convergence with respect to the flow parameter s . Because we employ the Magnus formulation of the IMSRG, we can use a relatively large step size of $\Delta s = 1$ in our calculations. As discussed in the previous chapter, the IMSRG flow is considered converged when the chosen off-diagonal part of the Hamiltonian has been sufficiently suppressed. The degree of suppression can be quantified using many-body perturbation theory (MBPT) corrections evaluated with the IMSRG-evolved Hamiltonian. As the off-diagonal part is suppressed, the evolved Hamiltonian becomes increasingly perturbative, resulting in smaller MBPT corrections.

We denote the second- and third-order MBPT energy corrections to the IMSRG-evolved Hamil-

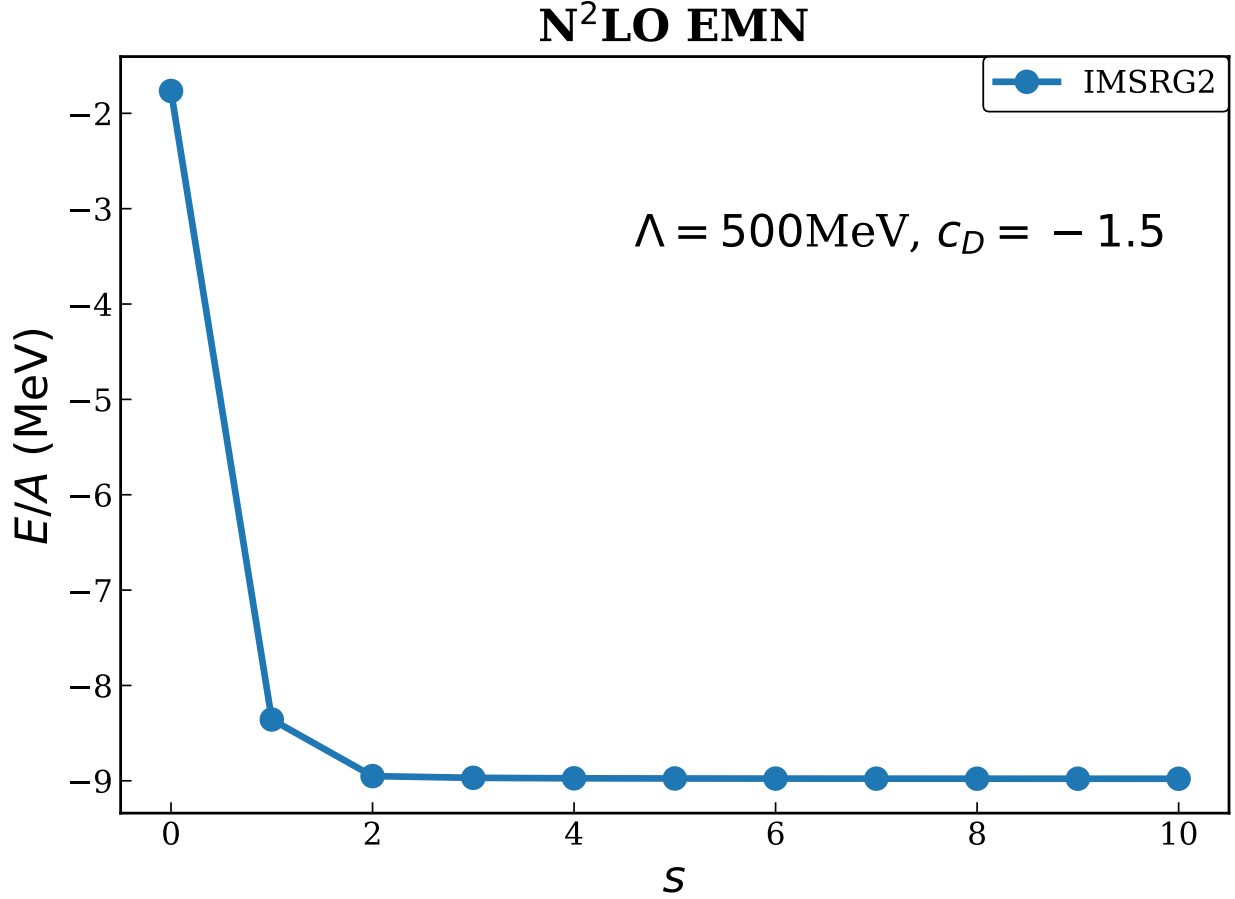


Figure 3.1 Convergence of the IMSRG(2) energy per particle for SNM with $N = Z = 66$ as a function of the flow parameter s at density $\rho = 0.07 \text{ fm}^{-3}$.

tonian by ΔE_2 and ΔE_3 , respectively. The magnitude of the total MBPT energy corrections through third order, $|\Delta E_2 + \Delta E_3|$, therefore serves as a diagnostic of flow convergence, with smaller values indicating better convergence. The convergence criterion implemented in our code is

$$\frac{|\Delta E_2 + \Delta E_3|}{A} < \epsilon, \quad (3.1)$$

where ϵ is set to 10^{-6} MeV in the calculations presented here. The resulting convergence pattern is shown in Fig. 3.1.

As shown in the figure, the energy converges rapidly during the first few flow steps. The convergence exhibits an approximately exponential decay pattern, consistent with the perturbative arguments discussed in Ref. [25]. The numerical values corresponding to Fig. 3.1 are listed in Table 3.1.

Table 3.1 Convergence of the IMSRG calculation with respect to the flow parameter s .

s	E/A	$(E + \Delta E_2)/A$	$(E + \Delta E_2 + \Delta E_3)/A$	$\ \eta^{(2)}\ $	$\ \Gamma_{\text{od}}\ $
0	-1.76560417	-9.70149552	-9.50129238	9.43046754	1056.87066128
1	-8.35711814	-9.03147960	-8.93208229	2.80840851	283.75908138
2	-8.95069265	-8.97480352	-8.97296399	0.45017137	63.77034791
3	-8.96865390	-8.97095071	-8.97130061	0.16114162	16.85533181
4	-8.97380056	-8.97433119	-8.97454238	0.08357917	7.54766045
5	-8.97550718	-8.97570403	-8.97579976	0.05306634	4.34369148
6	-8.97663651	-8.97672476	-8.97676998	0.03635445	2.83999642
7	-8.97730747	-8.97734948	-8.97737132	0.02530700	1.94225962
8	-8.97775016	-8.97777068	-8.97778139	0.01781887	1.34745937
9	-8.97804308	-8.97805321	-8.97805850	0.01256433	0.94362475
10	-8.97824219	-8.97824722	-8.97824984	0.00887725	0.66285005

At the end of the flow, the change in E/A relative to the preceding step has decreased to approximately 2×10^{-4} MeV, indicating that the residual dependence on the flow parameter is at the sub-keV level per particle. The Frobenius norm $\|\Gamma_{\text{od}}\|$, which measures overall magnitude of the off-diagonal two-body matrix elements targeted by the transformation, decreases steadily throughout the flow and approaches zero, as expected.

3.1.2 Basis Convergence

We then discuss the convergence with respect to the size of the single-particle basis. As has been introduced in the previous chapter, all calculations are performed in a truncated single-particle model space defined by

$$n_x^2 + n_y^2 + n_z^2 \leq n_{\text{max}}^2.$$

The model space is then increased until results are nearly independent of n_{max} . The top panel of Fig. 3.2 shows the convergence of the ground-state energy for SNM as a function of the number of shells¹ kept above the filled reference state. For $A = 132$ ($N = Z = 66$), the reference state corresponds to the first five shells being fully occupied, so $N_{\text{shells}} = 1$ corresponds to $n_{\text{max}}^2 = 5$, etc. Note that in the bottom panel of Fig. 3.2, a much smoother convergence pattern is obtained when the energy is plotted as a function of the number of single-particle states, N_{sp} . Empirically, we find

¹A shell is comprised of all single-particle states with a given value of $n^2 \equiv n_x^2 + n_y^2 + n_z^2$.

that the IMSRG(2) energies can be extrapolated reasonably well using an exponential of the form

$$E(N_{\text{sp}}) = E(\infty) + ae^{-bN_{\text{sp}}}, \quad (3.2)$$

although we have not explored this systematically since we find that convergence sets in rapidly once the maximum single-particle momentum $k_{\text{max}} = \frac{2\pi}{L}n_{\text{max}} \gtrsim \Lambda$, where Λ is the momentum cutoff in the chiral EFT regulators, typically in the range of 400 – 600 MeV. For $n_{\text{max}}^2 = 34$ ($N_{\text{shells}} = 25$), which corresponds to k_{max} ranging from 585 – 850 MeV for the densities considered, our results are converged at the 10 keV level (few keV level) for SNM (PNM). Unless otherwise specified, the results in the following are calculated at $n_{\text{max}}^2 = 34$.

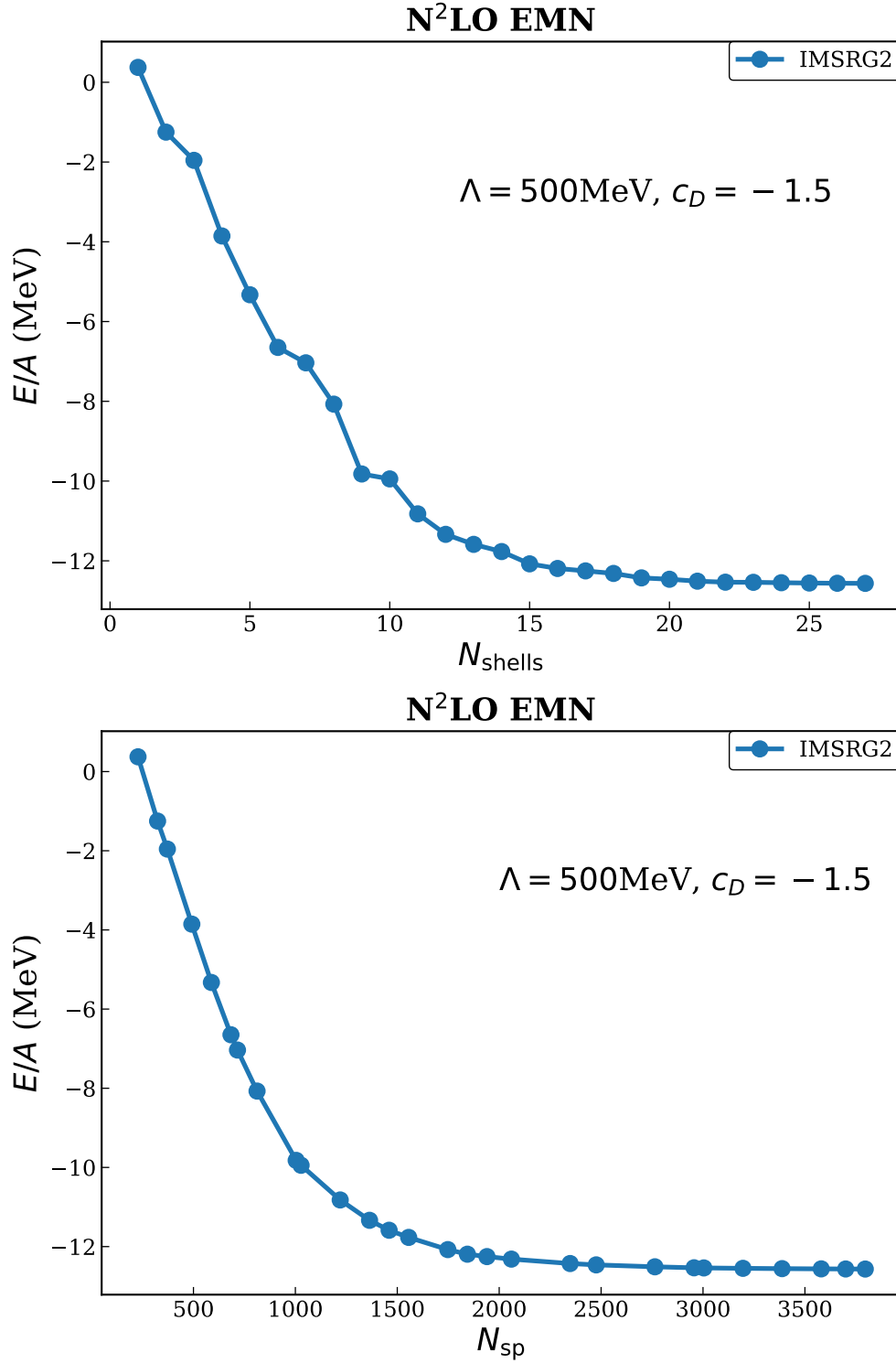


Figure 3.2 Convergence of the IMSRG(2) energy per particle for SNM ($N = Z = 66$) versus the number of shells N_{shells} above the reference state (top panel) and versus the total number of single-particle states N_{sp} (bottom panel) at density $\rho = 0.16 \text{ fm}^{-3}$.

3.1.3 Computational Scaling

The computational cost of IMSRG(2) is dominated by the two-body flow equation (2.67), which naively scales as $O(N_{\text{sp}}^6)$, where N_{sp} denotes the number of states in the single-particle basis. In our implementation, we employ the White generator. For homogeneous nuclear matter, its one-body part vanishes, while its two-body part contains only pphh contributions. The computational scaling is therefore reduced to $O(N_h^2 N_p^4)$, where N_h and N_p denote the numbers of hole and particle states in the single-particle basis, respectively. In the model spaces considered here, N_p is generally much larger than N_h , so that $N_p \sim N_{\text{sp}}$. IMSRG(2) therefore has the same leading-order computational scaling as CCSD.

The memory requirement naively scales as $O(N_{\text{sp}}^4)$ because the largest objects stored in our implementation are two-body operators. Fig. 3.3 shows the runtime and memory usage of the IMSRG(2) calculations with respect to N_{sp} . The approximately linear trends on the log–log scale are consistent with the scaling estimates discussed above.

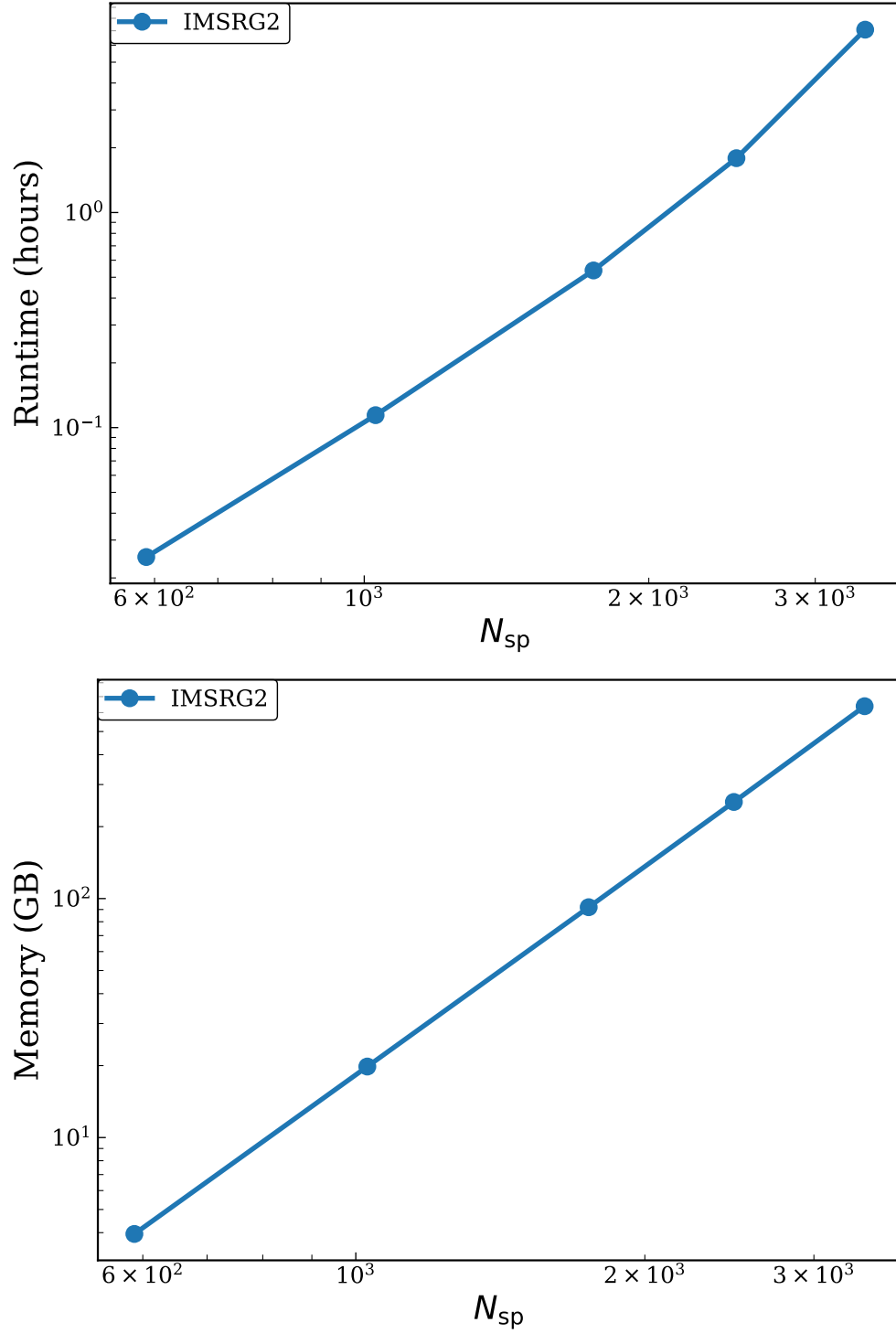


Figure 3.3 Runtime (top panel) and memory usage (bottom panel) of the IMSRG(2) transformation for SNM with $N = Z = 66$ versus the number of states N_{sp} in the single-particle basis.

3.2 Finite Size Effects

The other source of systematic error, finite-size effects, arises from the fact that we are simulating our system away from the thermodynamic limit. This is illustrated in Fig. 3.4, where we see that the computed E/A (blue curve) at a fixed density fluctuates with particle number due to shell effects. To correct for this, twist-averaged boundary conditions (TABCs) can be used to dampen these fluctuations, allowing for a smooth extrapolation to the $A \rightarrow \infty$ limit. However, this comes at a steep cost for non-stochastic methods like the IMSRG, as one must perform multiple calculations at the different twist angles used to carry out the averaging.

We do not use TABCs in the present work. Instead, we work at particular particle numbers, namely $A = 66$ for PNM and $A = 132$ for SNM, that are known to minimize finite size effects [95, 70]. We note that a computationally cheap but phenomenological correction for finite-size effects can be made based on the following observation. Decomposing E/A into its Hartree–Fock (orange curve) and correlation energy (green curve) components in Fig. 3.4, we see that the A -dependent fluctuations of the correlation energy are significantly less pronounced than those of the Hartree–Fock energy. For both PNM and SNM, the standard deviation of the correlation energies is reduced by about a factor of 10 compared to that of the Hartree–Fock energies. This suggests that the thermodynamic limit of the periodic box calculations can be estimated as

$$\left(\frac{E}{A}\right)_{\text{TD}} \approx \left(\frac{E}{A}\right)_{\text{Box}} + \left(\frac{E^{\text{HF}}}{A}\right)_{\text{TD}} - \left(\frac{E^{\text{HF}}}{A}\right)_{\text{Box}}. \quad (3.3)$$

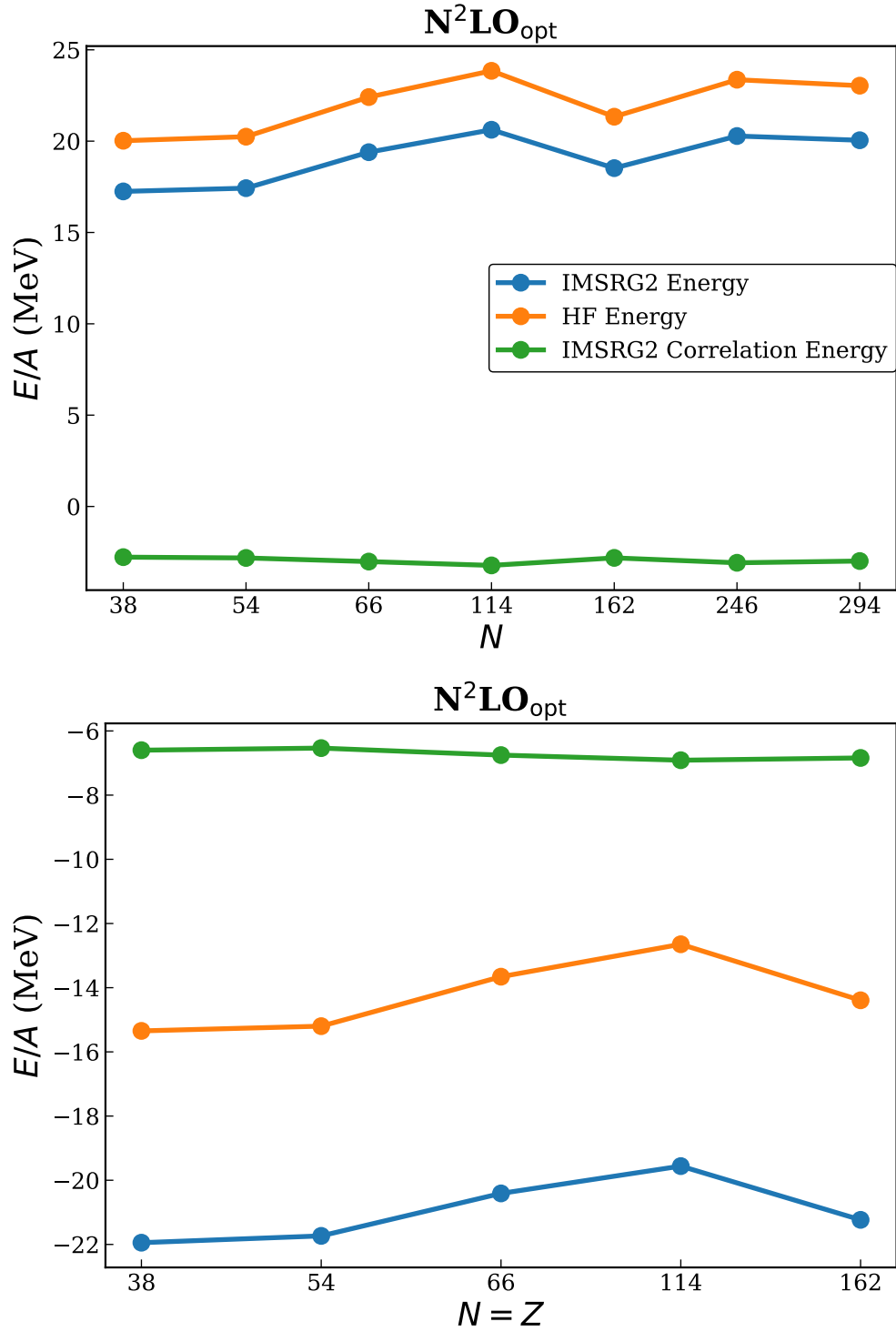


Figure 3.4 A -dependence of the energy per particle for PNM (top panel) and SNM (bottom panel) at the density $\rho = 0.16 \text{ fm}^{-3}$ using the $N^2\text{LO}_{\text{opt}}$ NN potential [96]. The blue curve denotes the IMSRG(2) energy per particle, which is decomposed into its Hartree-Fock (orange curve) and correlation energy (green curve) components.

3.3 Nuclear Matter Equation of State

3.3.1 Chiral Interactions

Before presenting our results for the nuclear EOS, we briefly introduce the two classes of chiral interactions employed in this work. The first consists of the Hebeler interactions [86]. These interactions are based on the $N^3\text{LO}$ nucleon–nucleon (NN) potential of Entem and Machleidt [97] with a cutoff of 500 MeV. The NN interaction is evolved to lower resolution using the SRG, with the evolution characterized by the resolution scale $\lambda = s^{-1/4}$, which has dimensions of momentum in natural units. For each 3N cutoff Λ , the two low-energy constants (LECs) that govern the shorter-range components of the $N^2\text{LO}$ three-nucleon force (3NF), c_D and c_E , are fitted to the ^3H binding energy and the ^4He matter radius. Each Hebeler interaction is labeled by the combination λ/Λ , which specifies the NN resolution scale and the 3N cutoff.

The second class consists of the $N^2\text{LO}$ Entem–Machleidt–Nosyk (EMN) NN interaction with a cutoff of 500 MeV [61], combined with a 3NF at the same chiral order [98]. In this case, the NN interaction is not SRG evolved and is therefore used consistently with the unevolved 3N interaction. The two 3N couplings, c_D and c_E , are fitted to the ^3H binding energy and empirical nuclear-matter saturation properties. Because the EMN 500 MeV NN+3N interaction is not softened through an SRG evolution, it is generally expected to be harder than the Hebeler interactions.

3.3.2 Pure Neutron Matter

We start by presenting our results for pure neutron matter, which provides a check on the validity of our IMSRG(2) implementation through comparisons to MBPT3 and MBPT4 calculations. As is well known from previous studies [98, 46], correlation effects in PNM are rather weak and are well described at low orders of MBPT when working with relatively soft chiral EFT interactions². Therefore, when working with relatively soft chiral EFT interactions such as those used here, we expect to find good agreement between our IMSRG(2) results and low-order MBPT. We consider three different chiral Hamiltonians at different resolution scales, each treated in the NO2B approximation. Fig. 3.5 and Fig. 3.6 show the PNM results for the softer EM(1.8/2.0)

²One expects to see larger discrepancies between low-order MBPT and non-perturbative methods like IMSRG(2) even in PNM for chiral interactions at higher resolution scales, see, e.g., the recent results in Ref. [81].

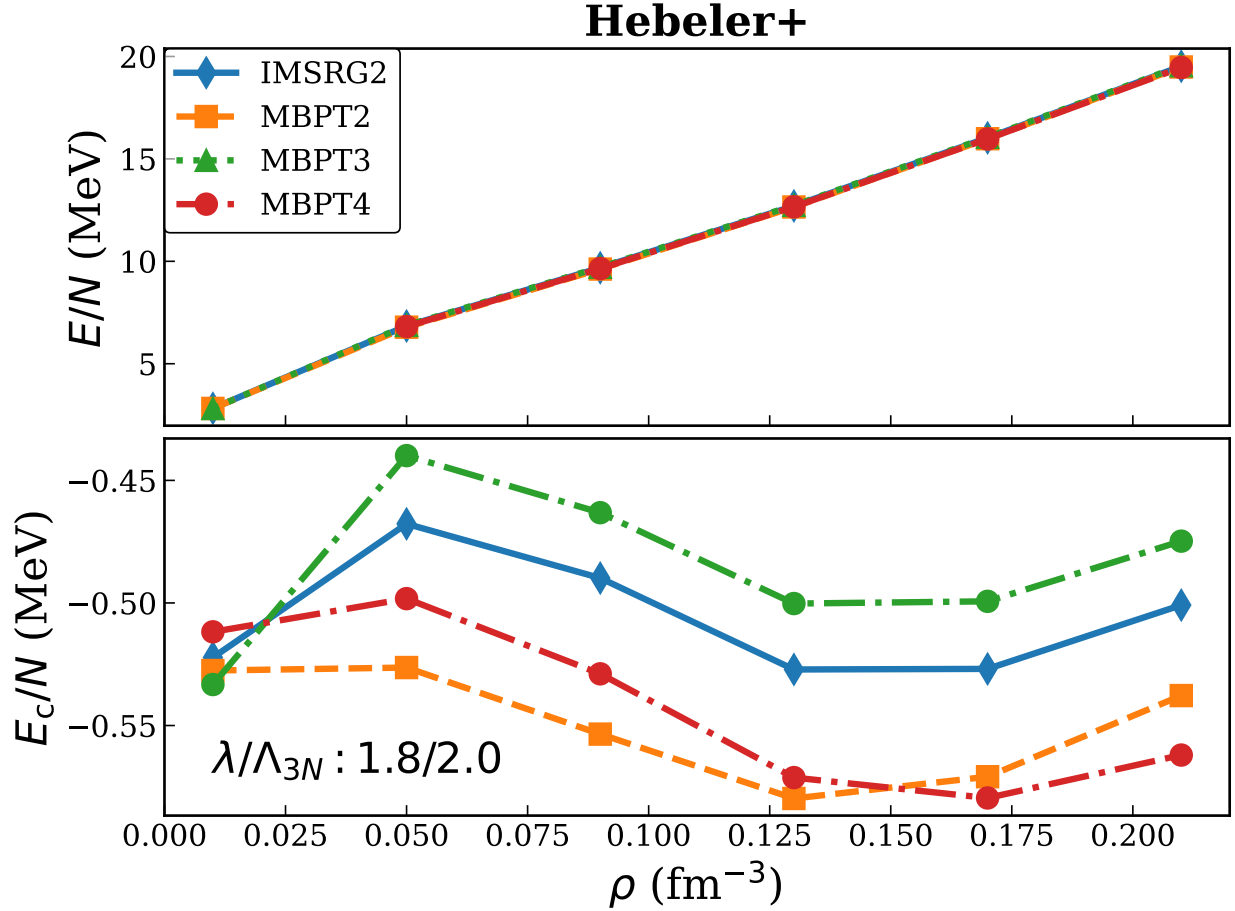


Figure 3.5 Comparison of IMSRG(2) and MBPT calculations of the energy per particle (top panel) and correlation energy per particle (bottom panel) for PNM using the EM(1.8/2.0) interaction treated in the NO2B approximation.

and EM(2.8/2.0) Hamiltonians, respectively, while Fig. 3.7 shows results for the N2LO(500) Hamiltonian, which is the hardest interaction we considered. In all three instances, we see that the IMSRG(2) and MBPT results are in close agreement with each other, with the IMSRG(2) results typically falling between the MBPT3 and MBPT4 curves.

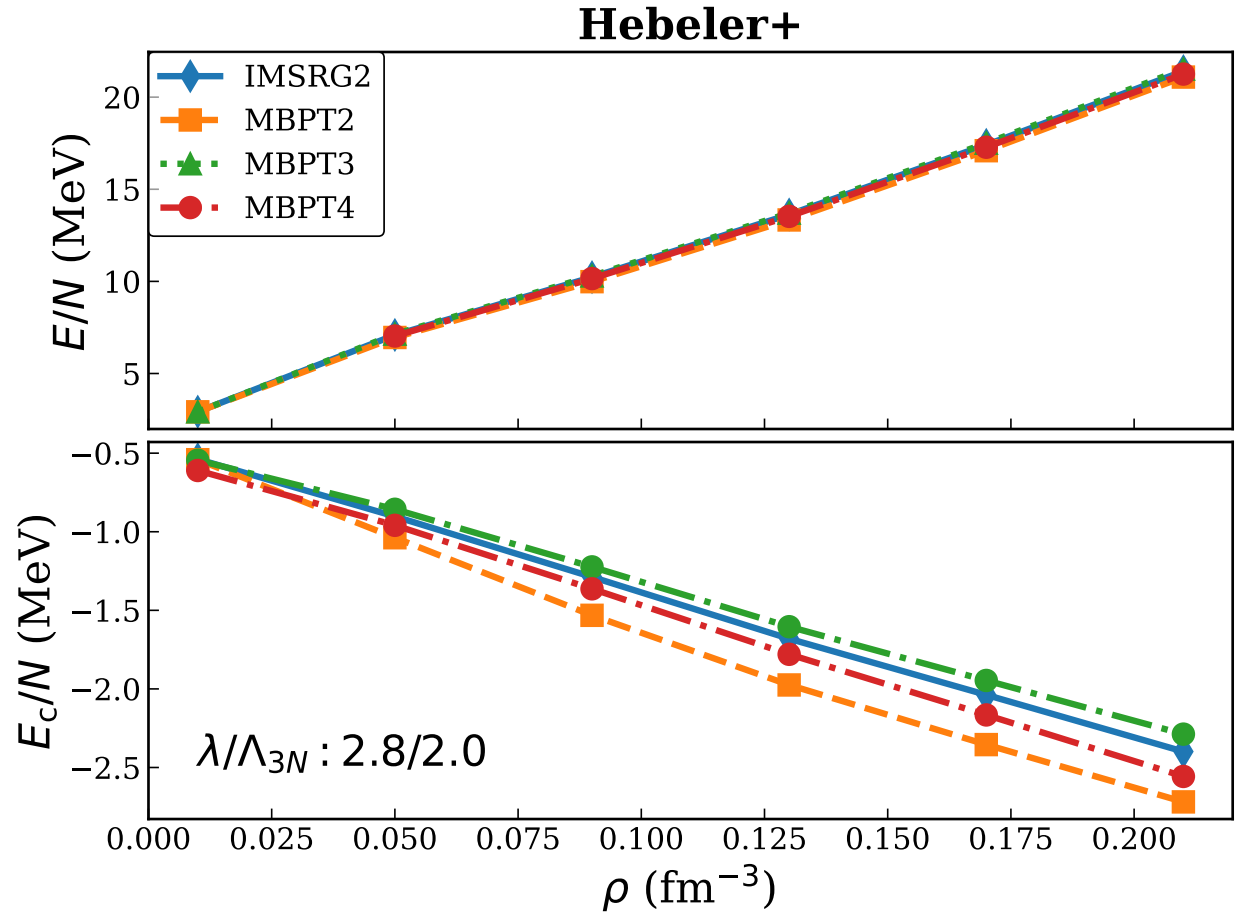


Figure 3.6 Comparison of IMSRG(2) and MBPT calculations of the energy per particle (top panel) and correlation energy per particle (bottom panel) for PNM using the EM(2.8/2.0) interaction treated in the NO2B approximation.

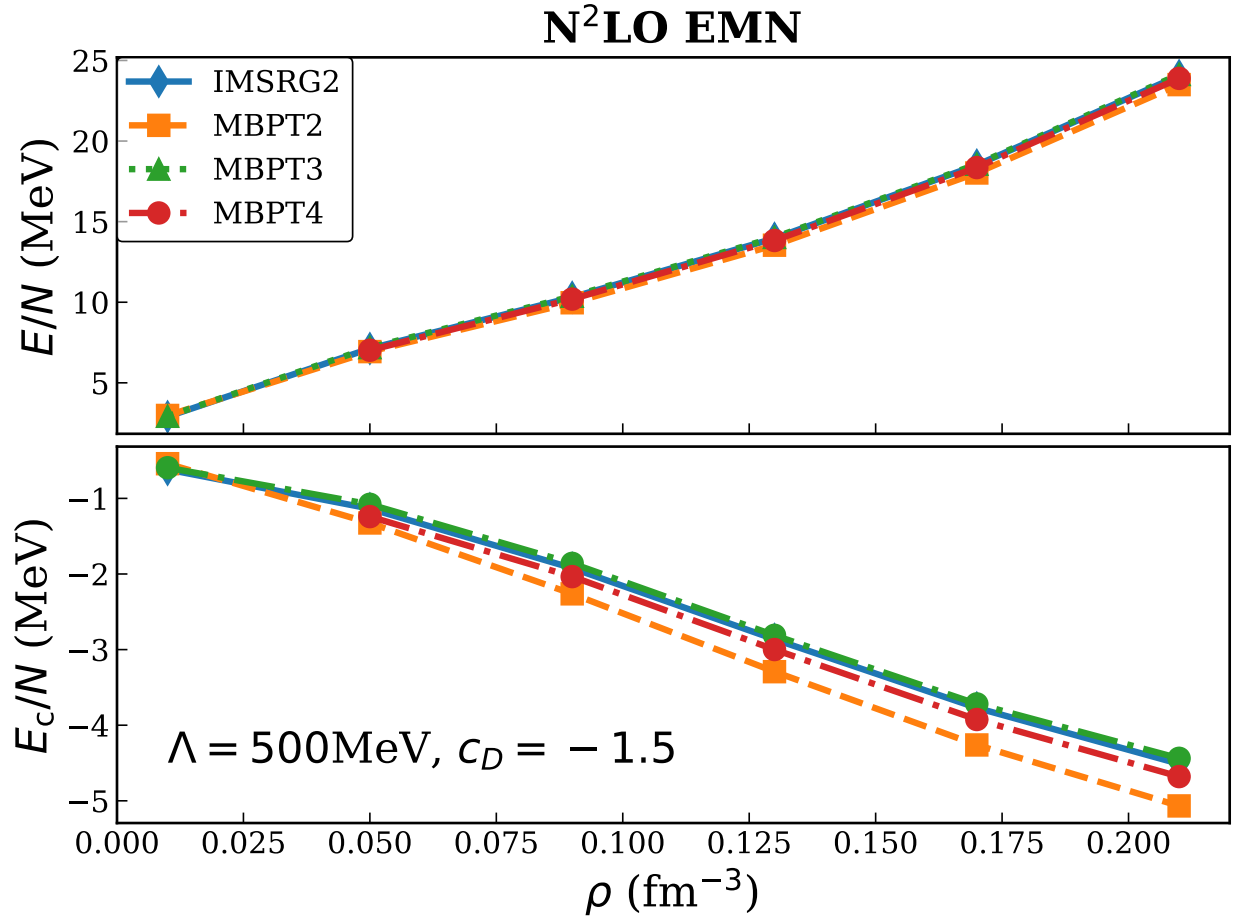


Figure 3.7 Comparison of IMSRG(2) and MBPT calculations of the energy per particle (top panel) and correlation energy per particle (bottom panel) for PNM using the N²LO EMN 500 MeV NN + 3N interactions treated in the NO2B approximation.

3.3.3 Symmetric Nuclear Matter

Turning now to SNM, we see a rather different picture due to the increased role played by correlations. This is primarily because the iterated tensor force in the $^3S_1 - ^3D_1$ channel, which is active in SNM but inactive in PNM, is known to produce significant correlations. Additionally, when using non-local 3N regulators as in the Hamiltonians used here, the two short-range c_E and c_D terms in the 3N interaction vanish in PNM due to the Pauli principle, but are non-vanishing in SNM. Referring to Figures 3.9 and 3.10, we compare our IMSRG(2) results to non-perturbative CC calculations containing doubles excitations (CCD) and approximate triples excitations (CCD(T)), as well as MBPT3 and MBPT4 calculations.

In marked contrast to PNM, we see discrepancies between the different many-body methods that increase as we progress from the softest EM(1.8/2.0) Hamiltonian to the hardest N2LO(500) Hamiltonian. Similar results were found in Ref. [72], where low-order MBPT and different non-perturbative many-body techniques can differ at the several MeV/particle level at the empirical saturation density. We note that the IMSRG(2) results tend to track between the CCD and CCD(T) results for all cases considered. Similar trends have been observed in IMSRG(2) calculations of ground-state energies for closed-shell nuclei, where it can be qualitatively understood from a diagrammatic analysis of the perturbative content of the IMSRG [25].

The IMSRG(2) can be shown to be third-order-exact, which means that it exactly contains all MBPT contributions through third order. At fourth order, the IMSRG(2) starts to miss some contributions, omitting the net-attractive triples excitation contributions completely, see diagrams T_1 through T_{16} in Fig. 3.8, and undercounting the net-repulsive asymmetric quadruples excitation contributions by a factor of 1/2, see diagrams Q_1 , Q_2 , Q_6 and Q_7 . Similarly, CCD is third-order-exact, omitting the fourth-order triples excitation diagrams, but it includes the fourth-order asymmetric quadruples diagrams with their full weight. This explains why our IMSRG(2) ground-state energies are more bound than those from CCD³. CCD(T) can be shown to be fourth-order-exact,

³Note this contradicts the recent SNM results reported in Ref. [81], where their IMSRG(2) results appear to be *less* bound than CCD. While the argument that $E_{\text{IMSRG}(2)} < E_{\text{CCD}}$ is perturbative in nature, we expect this bound to be robust for the relatively soft chiral Hamiltonians studied here and in Ref. [81].

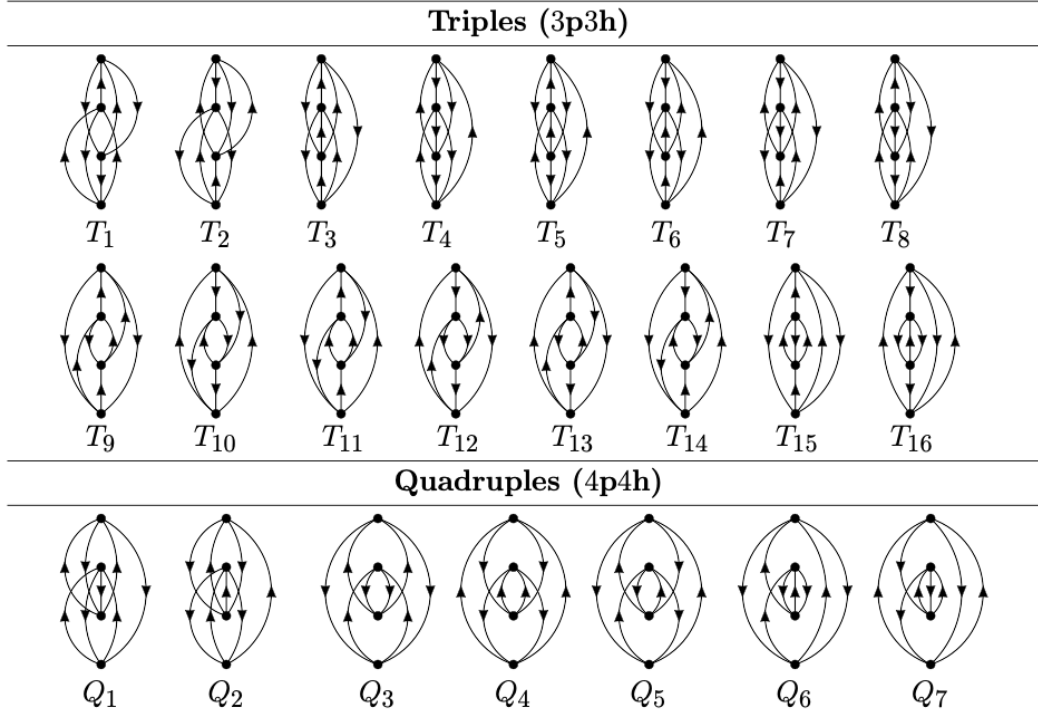


Figure 3.8 A subset of the MBPT(4) Hugenholtz diagrams corresponding to irreducible triples ($3p3h$) and quadruples ($4p4h$) excitations. The IMSRG(2) misses the triples diagrams T_1 - T_{16} completely, and undercounts the asymmetric quadruples diagrams Q_1 , Q_2 , Q_6 and Q_7 by a factor of $1/2$.

as it includes the fourth-order triples-excitation diagrams that are omitted in CCD.

The undercounting of the fourth-order asymmetric quadruple-excitation diagrams is consistent with the empirical observation seen in finite nuclei that IMSRG(2) results tend to fall between CCD and CCD(T), at least when using relatively soft chiral Hamiltonians. Diagrams Q_1 , Q_2 , Q_6 and Q_7 are positive-definite, while the dominant 4th-order triples diagrams, T_{15} and T_{16} , can be shown to be negative-definite⁴. The IMSRG(2)'s undercounting of diagrams Q_1 , Q_2 , Q_6 and Q_7 therefore roughly mimics some of the attraction that would be gained if the triple-excitation contributions were included. We stress that this argument is perturbative in nature and can break down. Indeed, as shown in Ref. [99], the undercounting of the asymmetric quadruples in IMSRG(2) can lead to a diverging flow for the ground state energy under certain circumstances when the interactions become strong.

⁴For the interactions studied here, these two diagrams accounted for more than 95% of the total triples-excitation energy contribution.

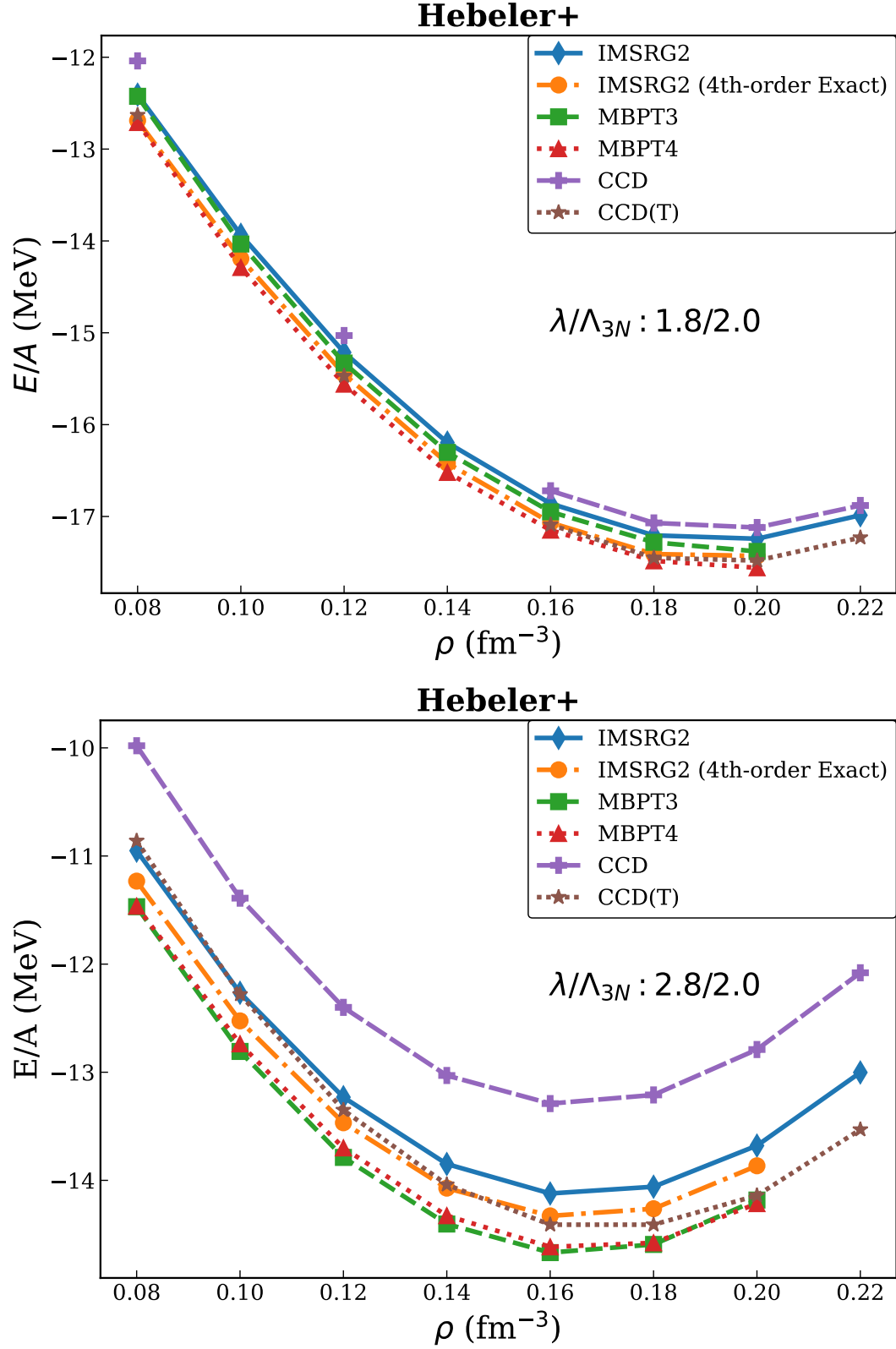


Figure 3.9 Comparison of IMSRG(2) to MBPT and non-perturbative CC calculations of SNM for the EM(1.8/2.0) (top panel) and EM(2.8/2.0) (bottom panel) NN + 3N interactions treated in the NO2B approximation.

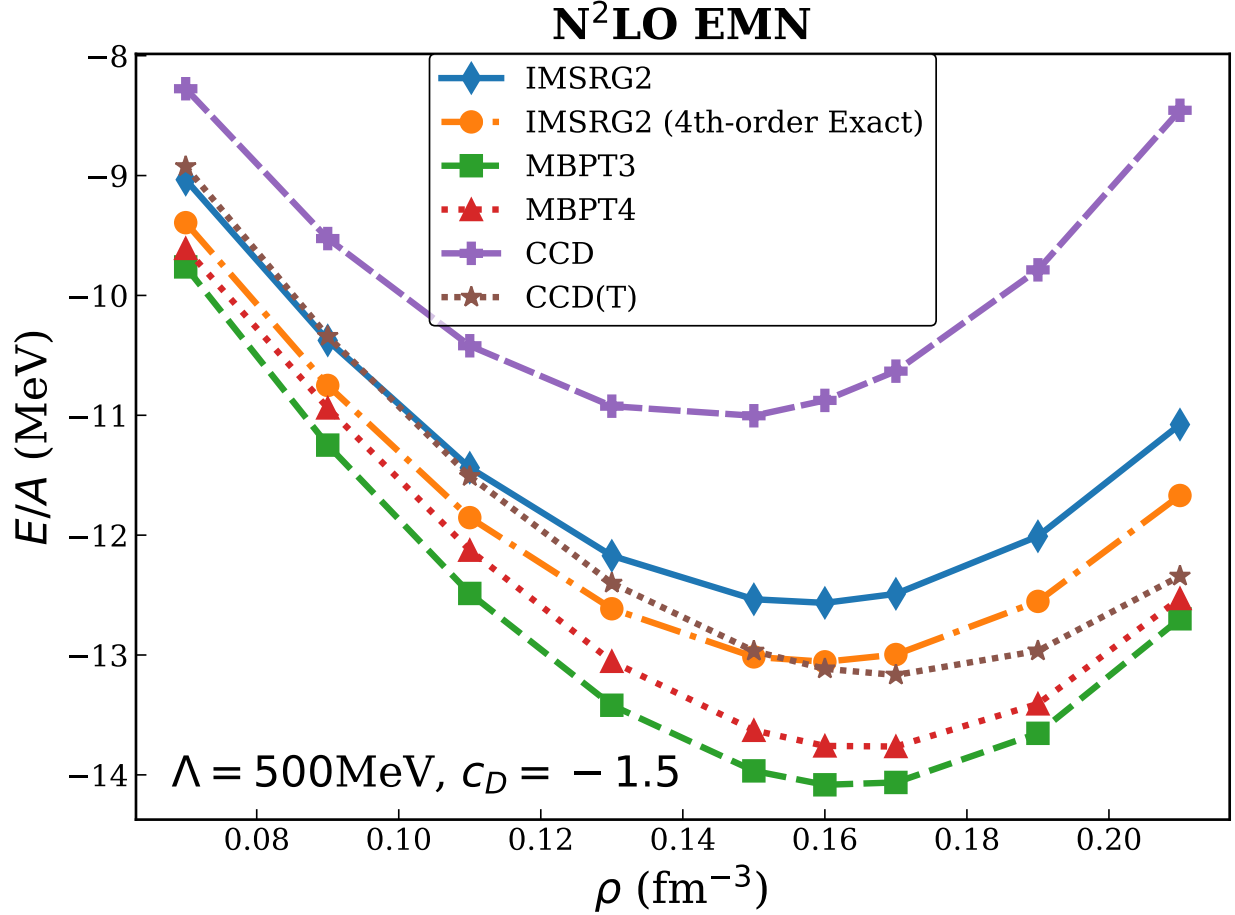


Figure 3.10 Comparison of IMSRG(2) to MBPT and non-perturbative CC calculations of SNM for the $N^2\text{LO EMN}$ 500 MeV NN + 3N interactions treated in the NO2B approximation.

3.3.4 Asymmetric Nuclear Matter

Beyond PNM and SNM, our framework can also compute the EOS of asymmetric nuclear matter (ANM) at selected proton fractions Y_p by choosing different closed-shell particle numbers for neutrons and protons. In this case, the single-particle basis truncation, specified by n_{max} or N_{shells} , is defined relative to the species with the larger particle number.

As an example, Fig. 3.11 shows the EOS of asymmetric nuclear matter with a proton fraction of $Y_p = 0.05$, obtained using $N = 38$ and $Z = 2$. This capability is particularly relevant to neutron-star applications because neutron-star matter is not pure neutron matter, but rather highly neutron-rich matter in beta equilibrium, with a typical proton fraction of $\sim 5\%$ around nuclear saturation density. Although the closed-shell constraint prevents us from performing calculations at arbitrary proton

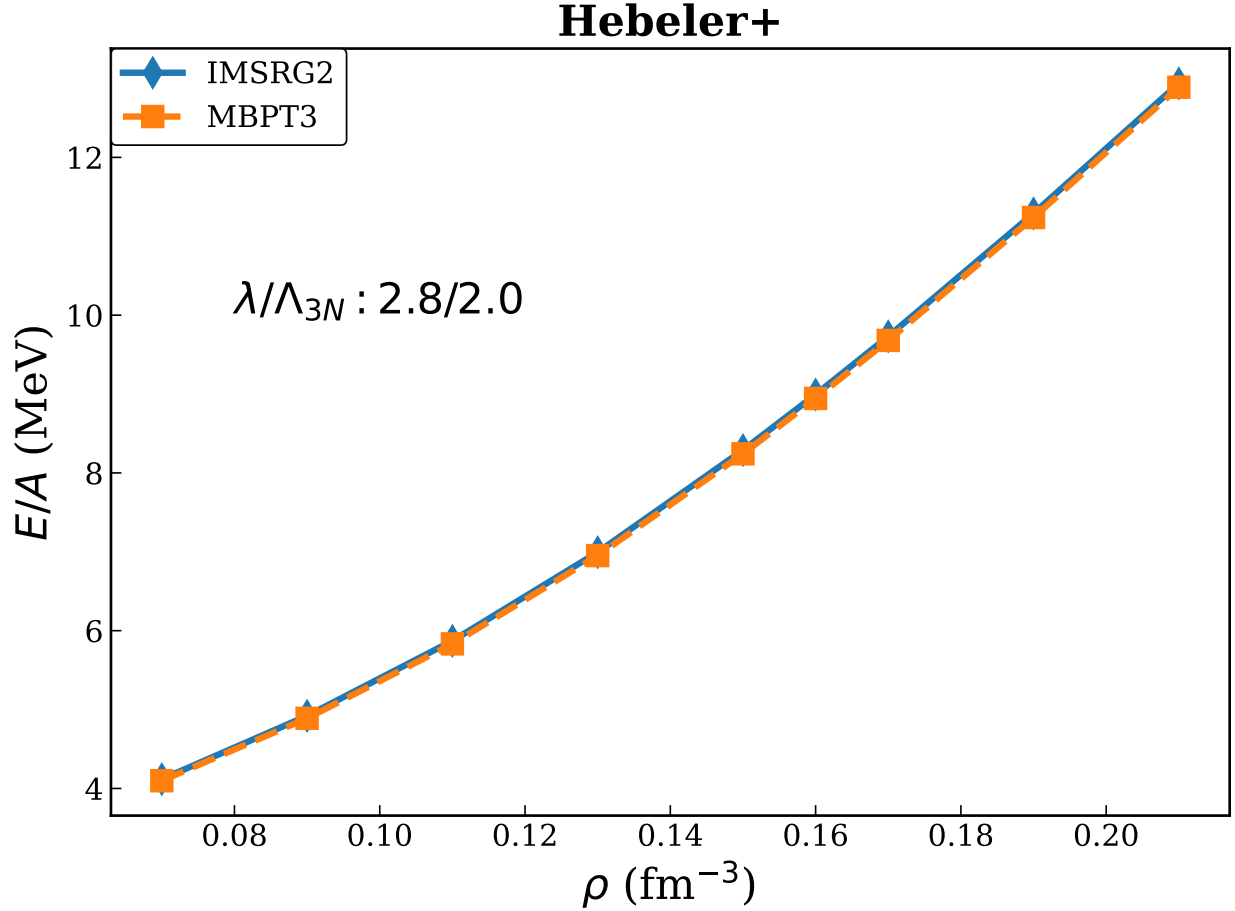


Figure 3.11 Comparison of IMSRG(2) and MBPT calculations of asymmetric nuclear matter with proton fraction $Y_p = 0.05$ for the EM(2.8/2.0) NN+3N interaction, with the 3N interaction treated in the NO2B approximation.

fractions, interpolation methods can be used to construct the EOS over the full range $Y_p \in [0, 0.5]$.

As shown in Fig. 3.11, the IMSRG(2) results are in close agreement with the third-order MBPT results. This behavior is similar to that observed for PNM and indicates that asymmetric nuclear matter with a small proton fraction also remains relatively perturbative, as expected.

3.4 Nuclear Matter Observables

In addition to the EOS, our framework can be used to compute other nuclear matter observables of interest. A key advantage of the Magnus formulation is that the observable operator does not need to be evolved simultaneously with the Hamiltonian throughout the flow. As discussed in Sec. 2.8.3, once the final Magnus operator has been obtained and stored, an observable $\hat{O}$ can be

evolved by applying the same BCH transformation to the corresponding normal-ordered operator,

$$\hat{O}(s_{\text{final}}) = e^{\hat{\Omega}(s_{\text{final}})} \hat{O}(0) e^{-\hat{\Omega}(s_{\text{final}})}.$$

The ground-state expectation value is then given by the zero-body component of the evolved operator.

In this section, we present proof-of-principle calculations of two observables—the single-nucleon momentum distribution and the static structure factor—to demonstrate the capabilities of the framework. These observables provide additional probes of the correlated many-body wavefunction and facilitate comparisons with other many-body approaches, while also laying the groundwork for future microscopic calculations of response functions and transport properties of dense matter.

3.4.1 Single Nucleon Momentum Distribution

We first apply our framework to the single-nucleon momentum distribution (SNMD), which characterizes the occupation of single-particle states with different momenta [100]. In the plane-wave basis, a single-particle state p is specified by the quantum numbers $p \equiv (\mathbf{k}, \sigma, \tau)$. The corresponding occupation-number operator is

$$\hat{n}_p = a_{\mathbf{k}\sigma\tau}^\dagger a_{\mathbf{k}\sigma\tau}. \quad (3.4)$$

For a fixed momentum vector $\mathbf{k}$ and nucleon species with isospin projection τ , the occupation operator summed over the spin projections is

$$\hat{N}_\tau(\mathbf{k}) = \sum_{\sigma} a_{\mathbf{k}\sigma\tau}^\dagger a_{\mathbf{k}\sigma\tau}. \quad (3.5)$$

Because homogeneous nuclear matter is isotropic, no particular momentum direction is preferred. We therefore define the SNMD as the average occupation of all single-particle states belonging to a momentum shell with magnitude k ,

$$\hat{n}_\tau(k) = \frac{1}{g_k} \sum_{\substack{\mathbf{k}' \\ |\mathbf{k}'|=k}} \sum_{\sigma} a_{\mathbf{k}'\sigma\tau}^\dagger a_{\mathbf{k}'\sigma\tau}, \quad (3.6)$$

where g_k is the total number of single-particle states in the shell, including both the momentum-direction and spin degeneracies. With this definition, the expectation value satisfies

$$0 \leq n_\tau(k) \leq 1, \quad (3.7)$$

and particle-number conservation requires

$$\sum_k g_k n_\tau(k) = N_\tau. \quad (3.8)$$

The one-body matrix elements of the operator in Eq. (3.6) are

$$\langle p | \hat{n}_\tau(k) | q \rangle = \frac{1}{g_k} \delta_{pq} \delta_{\tau_p \tau} \delta_{|k_p|, k}, \quad (3.9)$$

where $p \equiv (\mathbf{k}_p, \sigma_p, \tau_p)$ and $q \equiv (\mathbf{k}_q, \sigma_q, \tau_q)$. Normal ordering with respect to the Hartree–Fock reference gives

$$\hat{n}_\tau(k) = n_\tau^{\text{HF}}(k) + \frac{1}{g_k} \sum_{\substack{\mathbf{k}' \\ |\mathbf{k}'|=k}} \sum_{\sigma} \left\{ a_{\mathbf{k}'\sigma\tau}^\dagger a_{\mathbf{k}'\sigma\tau} \right\}, \quad (3.10)$$

where $n_\tau^{\text{HF}}(k)$ is the average shell occupation in the Hartree–Fock reference. For a closed-shell Fermi-sea reference, $n_\tau^{\text{HF}}(k) = 1$ below the Fermi surface and vanishes above it.

We construct the operator using Eq. (3.9), normal order it with respect to the Hartree–Fock reference, and then evolve it using the Magnus operator obtained from the Hamiltonian flow. The zero-body component of the evolved operator yields the correlated ground-state momentum distribution. Fig. 3.12 shows the single neutron momentum distribution obtained from an IMSRG(2) calculation of PNM with $N = 66$. The computed momentum distribution satisfies the normalization condition in Eq. (3.8). Relative to the step-function distribution of the HF reference, which has the same form as that of a free Fermi gas in homogeneous nuclear matter, correlations slightly deplete the occupations below the Fermi momentum k_F and generate small but nonzero occupations above it. This qualitative behavior is generally expected for an interacting Fermi system. The modest size of the redistribution is consistent with the relatively perturbative character of PNM for the interaction considered here.

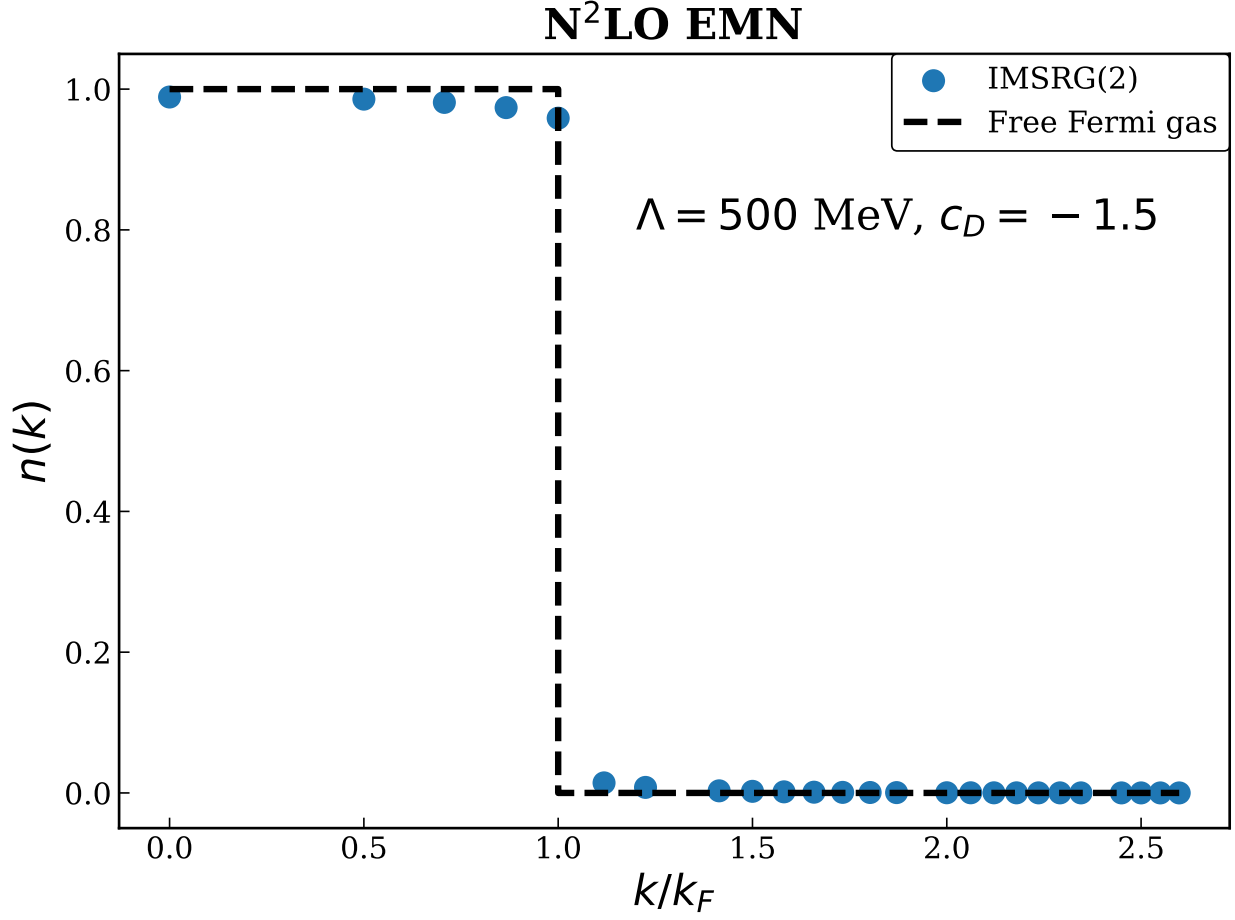


Figure 3.12 Single neutron momentum distribution of PNM with $N = 66$ at $\rho = 0.05 \text{ fm}^{-3}$. The blue points show the IMSRG(2) results obtained with the N²LO EMN 500 MeV NN+3N interaction, with the 3N contribution treated in the NO2B approximation. The black dashed line shows the results for free Fermi gas at the same density. Here, k_F denotes the corresponding Fermi momentum in the box.

3.4.2 Static Structure Factor

We next apply our framework to the static structure factor (SSF), which characterizes density correlations in the ground state. We first introduce the Fourier component of the density operator,

$$\hat{\rho}(\mathbf{Q}) = \sum_{\mathbf{k}, \sigma \tau} a_{\mathbf{k}+\mathbf{Q}, \sigma \tau}^\dagger a_{\mathbf{k}, \sigma \tau}, \quad (3.11)$$

where $\mathbf{Q}$ denotes the momentum transfer. The corresponding density-fluctuation operator is defined as

$$\Delta \hat{\rho}(\mathbf{Q}) = \hat{\rho}(\mathbf{Q}) - \langle \Psi_0 | \hat{\rho}(\mathbf{Q}) | \Psi_0 \rangle, \quad (3.12)$$

and, for a system of A particles, the SSF is given by the equal-time density-fluctuation correlation function [100],

$$S(\mathbf{Q}) = \frac{1}{A} \langle \Psi_0 | \Delta \hat{\rho}^\dagger(\mathbf{Q}) \Delta \hat{\rho}(\mathbf{Q}) | \Psi_0 \rangle. \quad (3.13)$$

Equivalently,

$$S(\mathbf{Q}) = \frac{1}{A} \left[\langle \Psi_0 | \hat{\rho}^\dagger(\mathbf{Q}) \hat{\rho}(\mathbf{Q}) | \Psi_0 \rangle - |\langle \Psi_0 | \hat{\rho}(\mathbf{Q}) | \Psi_0 \rangle|^2 \right]. \quad (3.14)$$

Because the ground-state density of homogeneous nuclear matter is spatially uniform, its Fourier components vanish for all nonzero momentum transfers. Hence,

$$\langle \Psi_0 | \hat{\rho}(\mathbf{Q}) | \Psi_0 \rangle = A \delta_{\mathbf{Q}, \mathbf{0}}. \quad (3.15)$$

The density-fluctuation operator therefore takes the form

$$\Delta \hat{\rho}(\mathbf{Q}) = \begin{cases} \hat{\rho}(\mathbf{0}) - A, & \mathbf{Q} = \mathbf{0}, \\ \hat{\rho}(\mathbf{Q}), & \mathbf{Q} \neq \mathbf{0}. \end{cases} \quad (3.16)$$

Since $\hat{\rho}(\mathbf{0})$ is the particle-number operator and the ground state has a fixed particle number A ,

$$\Delta \hat{\rho}(\mathbf{0}) | \Psi_0 \rangle = [\hat{\rho}(\mathbf{0}) - A] | \Psi_0 \rangle = 0. \quad (3.17)$$

Consequently, the SSF can be written as

$$S(\mathbf{Q}) = \begin{cases} 0, & \mathbf{Q} = \mathbf{0}, \\ \frac{1}{A} \langle \Psi_0 | \hat{\rho}^\dagger(\mathbf{Q}) \hat{\rho}(\mathbf{Q}) | \Psi_0 \rangle, & \mathbf{Q} \neq \mathbf{0}. \end{cases} \quad (3.18)$$

We therefore consider only nonzero momentum transfers when constructing the SSF operator below.

For $\mathbf{Q} \neq \mathbf{0}$, the corresponding SSF operator is

$$\begin{aligned} \hat{S}(\mathbf{Q}) &= \frac{1}{A} \hat{\rho}^\dagger(\mathbf{Q}) \hat{\rho}(\mathbf{Q}) \\ &= \frac{1}{A} \sum_{\mathbf{k}, \sigma \tau} \sum_{\mathbf{k}', \sigma' \tau'} a_{\mathbf{k}, \sigma \tau}^\dagger a_{\mathbf{k}+\mathbf{Q}, \sigma \tau} a_{\mathbf{k}'+\mathbf{Q}, \sigma' \tau'}^\dagger a_{\mathbf{k}', \sigma' \tau'}. \end{aligned} \quad (3.19)$$

Applying the fermionic anticommutation relations separates this expression into one- and two-body parts,

$$\begin{aligned}\hat{S}(\mathbf{Q}) &= \frac{1}{A} \sum_{\mathbf{k}, \sigma\tau} a_{\mathbf{k}, \sigma\tau}^\dagger a_{\mathbf{k}, \sigma\tau} \\ &+ \frac{1}{A} \sum_{\mathbf{k}, \sigma\tau} \sum_{\mathbf{k}', \sigma'\tau'} a_{\mathbf{k}, \sigma\tau}^\dagger a_{\mathbf{k}'+\mathbf{Q}, \sigma'\tau'}^\dagger a_{\mathbf{k}', \sigma'\tau'} a_{\mathbf{k}+\mathbf{Q}, \sigma\tau}.\end{aligned}\quad (3.20)$$

The one-body term is the particle-number operator and represents the self-correlation contribution, whereas the two-body term describes correlations between distinct nucleons.

Let p denote the index of the single-particle state associated with the quantum numbers $(\mathbf{k}_p, \sigma_p, \tau_p)$, and similarly for q , r , and s . We first evaluate the two-body matrix elements for $p < q$ and $r < s$:

$$\begin{aligned}S_{pqrs}^{(2)}(\mathbf{Q}) &= \frac{1}{A} \sum_{\eta=\pm 1} \left[\delta_{\sigma_p \sigma_r} \delta_{\sigma_q \sigma_s} \delta_{\tau_p \tau_r} \delta_{\tau_q \tau_s} \delta_{\mathbf{k}_r - \mathbf{k}_p, \eta \mathbf{Q}} \delta_{\mathbf{k}_q - \mathbf{k}_s, \eta \mathbf{Q}} \right. \\ &\quad \left. - \delta_{\sigma_p \sigma_s} \delta_{\sigma_q \sigma_r} \delta_{\tau_p \tau_s} \delta_{\tau_q \tau_r} \delta_{\mathbf{k}_s - \mathbf{k}_p, \eta \mathbf{Q}} \delta_{\mathbf{k}_q - \mathbf{k}_r, \eta \mathbf{Q}} \right].\end{aligned}\quad (3.21)$$

The first term is the direct contribution, while the second is the exchange contribution. The sum over $\eta = \pm 1$ includes both orientations of the momentum transfer and ensures that the constructed matrix elements satisfy the Hermiticity condition

$$S_{pqrs}^{(2)}(\mathbf{Q}) = S_{rs pq}^{(2)*}(\mathbf{Q}). \quad (3.22)$$

For $\mathbf{Q} \neq 0$, the $\eta = +1$ and $\eta = -1$ terms populate Hermitian-conjugate matrix elements rather than duplicating the same contribution. Therefore, no additional factor of $1/2$ is required.

After the matrix elements for $p < q$ and $r < s$ have been evaluated, the remaining entries are populated using antisymmetry:

$$S_{qprs}^{(2)}(\mathbf{Q}) = -S_{pqrs}^{(2)}(\mathbf{Q}), \quad S_{pqsr}^{(2)}(\mathbf{Q}) = -S_{pqrs}^{(2)}(\mathbf{Q}), \quad S_{qp sr}^{(2)}(\mathbf{Q}) = S_{pqrs}^{(2)}(\mathbf{Q}). \quad (3.23)$$

Following the same procedure used for the SNMD, we construct the SSF operator, normal order it with respect to the Hartree–Fock reference, and evolve it using the Magnus operator obtained from the Hamiltonian flow. The zero-body component of the evolved operator then gives the IMSRG(2)

ground-state expectation value. Again, owing to the isotropy of homogeneous nuclear matter, the SSF depends only on the magnitude of the momentum transfer, $Q = |\mathbf{Q}|$, and is therefore denoted by $S(Q)$.

For comparison, the static structure factor of a free Fermi gas is

$$S_{\text{FG}}(Q) = \begin{cases} \frac{3}{4} \frac{Q}{k_F} - \frac{1}{16} \left(\frac{Q}{k_F} \right)^3, & Q \leq 2k_F, \\ 1, & Q > 2k_F, \end{cases} \quad (3.24)$$

where k_F is the Fermi momentum at the corresponding density.

The SSF is closely related to the pair distribution function. For the homogeneous nuclear matter considered here, the SSF $S(Q)$ and the pair distribution function $g(r)$ are related by

$$S(Q) = 1 + 4\pi\rho \int_0^\infty dr [g(r) - 1] r^2 \frac{\sin(Qr)}{Qr}, \quad Q \neq 0, \quad (3.25)$$

where $\rho = A/V$ is the particle-number density. Thus, the pair distribution function can be obtained directly from the SSF through the inverse Fourier transform. Fig. 3.13 compares the IMSRG(2) SSF and the corresponding pair distribution function of PNM with $N = 66$ to the free-Fermi-gas results. The IMSRG(2) results exhibit the expected asymptotic behavior, with both $S(Q)$ and $g(r)$ approaching 1 at large Q and large r , respectively. The relatively small deviations from the free-Fermi-gas results indicate that correlations beyond the Hartree–Fock reference produce only moderate modifications to these observables, consistent with the pattern found for the SNMD.

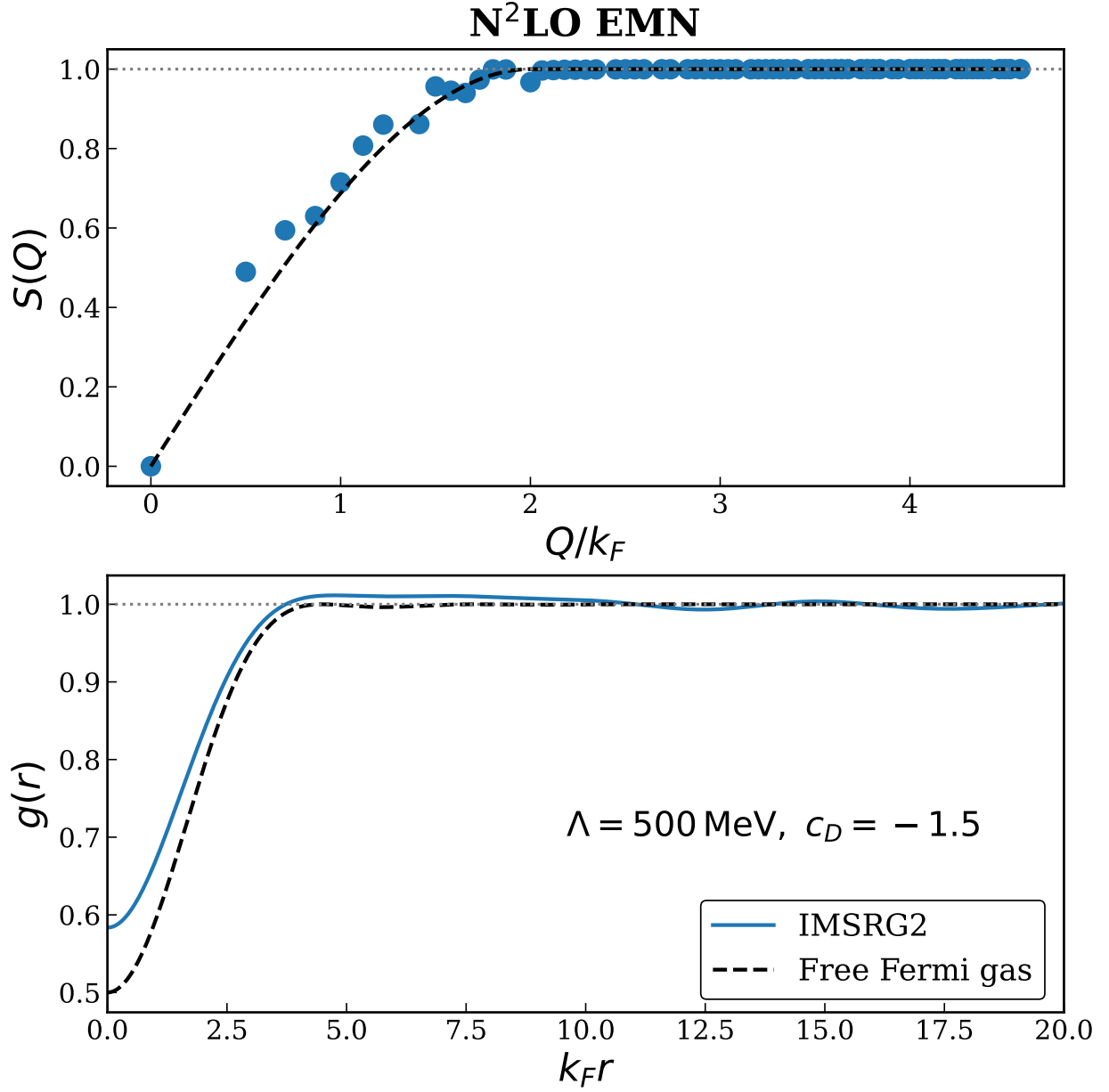


Figure 3.13 Static structure factor (top panel) and pair distribution function of PNM with $N = 66$ at $\rho = 0.05 \text{ fm}^{-3}$. The blue points and solid line show the IMSRG(2) results obtained with the N²LO EMN 500 MeV NN+3N interaction, with the 3N contribution treated in the NO2B approximation. The black dashed lines show the results for free Fermi gas at the same density. Here, k_F denotes the corresponding Fermi momentum in the box.

3.5 Summary and Outlook

We have extended the IMSRG to carry out calculations of infinite nuclear matter in a finite periodic box and presented benchmark results at the IMSRG(2) level using chiral two- and three-nucleon interactions. We demonstrated that the method exhibits rapid convergence with respect to single-particle basis size and that residual finite-size effects can be controlled using a simple Hartree–Fock-based correction scheme. For pure neutron matter, where correlations are comparatively weak for the interactions considered, the IMSRG(2) results are in close agreement with low-order many-body perturbation theory. For symmetric nuclear matter, where tensor and three-body correlations are more pronounced, larger method-dependent differences emerge, though the IMSRG(2) energies are found to lie systematically between CCD and CCD(T) calculations, consistent with the known perturbative content of the truncation and consistent with analogous trends in calculations of finite nuclei. We have also shown that the Magnus formulation naturally enables calculations of ground-state observables beyond the energy, illustrating this capability with proof-of-principle calculations of the SNMD and SSF, with the latter further used to obtain the pair distribution function. These results establish the IMSRG as a promising nonperturbative framework for nuclear matter studies and provide a foundation for future developments including approximate IMSRG(3) truncations, finite-temperature and uncertainty-quantified equation-of-state predictions relevant to nuclei and astrophysics.

Despite this progress, our capability to efficiently perform the large number of EOS calculations required for uncertainty-quantification studies remains limited by the computational cost. This motivates the application of reduced-order modeling techniques to construct fast and accurate IMSRG EOS emulators. The development of such an emulator is presented in Chapter 4, enabling large-scale uncertainty-quantification studies of IMSRG EOS calculations, with proof-of-principle applications presented in Chapter 5.

CHAPTER 4

PMM-IMSRG FRAMEWORK FOR NUCLEAR MATTER CALCULATIONS

The nuclear EOS plays a central role in connecting microscopic nuclear physics to the properties of dense astrophysical objects such as neutron stars [8, 7, 101, 4, 102]. In the previous chapter, we developed an IMSRG framework for computing the nuclear EOS from chiral effective field theory interactions [80, 103] (see also Ref. [81]). However, repeated predictions of the nuclear EOS pose significant computational challenges, e.g., when sampling the parameter spaces of the underlying interactions for principled uncertainty quantification (UQ), because these *ab initio* many-body calculations are often prohibitively expensive. Emulators provide an efficient means to overcome these computational challenges by constructing fast and accurate surrogate models for high-fidelity *ab initio* calculations. See Refs. [104, 40] for recent review articles and Refs. [105, 106, 107, 108] for recent applications of nuclear matter emulators.

In this work, we develop a hybrid emulator using a PMM approach [44] for IMSRG nuclear matter calculations, designed to embed as much relevant physics as possible while learning the remaining unknown or inaccessible structure from data. Unlike purely data-driven approaches, PMMs preserve the operator structure of the many-body problem by learning low-dimensional representations of the Hamiltonian itself. This feature enables the PMM to retain important physical properties dictated by the structure of the underlying Hamiltonian, while providing a natural route to emulate across model parameters. Compared to eigenvector continuation [39] and other intrusive reduced-basis emulators [38, 40], which rely on explicitly constructed subspaces from high-fidelity training states, PMMs implicitly parameterize the relevant low-dimensional subspaces through learned operators. Using this approach avoids, e.g., the need to store or manipulate large many-body wavefunctions, while still capturing the dominant parametric dependence of the ground-state energy. These features make PMMs particularly well-suited for IMSRG calculations, in which the underlying physics is governed by smoothly varying operators, yet direct evaluation remains computationally expensive.

The remainder of this chapter is organized as follows. Section 4.1 provides a brief introduction

to the general PMM framework. Section 4.2 describes its application to IMSRG nuclear-matter calculations, including the relevant parameter dependencies and the construction of the PMM-IMSRG emulator across chiral EFT LECs, IMSRG flow parameters, densities, and basis sizes. Section 4.3 briefly introduces the uncertainty quantification of the PMM-IMSRG emulator, and Section 4.4 demonstrates its accuracy in predicting the nuclear EOS.

4.1 Parametric Matrix Model

The parametric matrix model is a recently developed class of machine-learning methods in which the dependence of model outputs on input parameters is represented through trainable parametric matrices. In applications to physical systems, PMMs can be used as emulators by learning low-dimensional matrix representations that reproduce the outputs of computationally expensive high-fidelity calculations. A natural way to understand the basic idea of the PMM is through its connection to explicit reduced-basis methods, such as EC [39, 104].

Consider a Hamiltonian that depends affinely on a set of parameters $\mathbf{c} = \{c_i\}$, with “affine” meaning that the dependence of the matrix elements on the input parameters is at most linear,

$$H(\mathbf{c}) = H_0 + \sum_{i=1}^p c_i H_i, \quad (4.1)$$

where $H(\mathbf{c})$ is an $n \times n$ matrix acting in a high-dimensional Hilbert space. Suppose our goal is to determine the ground-state energy for arbitrary values of $\mathbf{c}$ within a prescribed parameter domain. In EC, one first performs high-fidelity calculations at a selected set of training points $\{\mathbf{c}^{(k)}\}$ and obtains the corresponding ground-state eigenvectors,

$$|\Psi_0(\mathbf{c}^{(1)})\rangle, |\Psi_0(\mathbf{c}^{(2)})\rangle, \dots, |\Psi_0(\mathbf{c}^{(r)})\rangle. \quad (4.2)$$

These eigenvectors span a reduced subspace intended to approximate the ground-state manifold over this domain. After orthonormalization, the reduced basis vectors can be collected into an $n \times r$ matrix P , whose columns form an orthonormal basis of the reduced space, such that

$$P^\dagger P = I_r, \quad (4.3)$$

where $r \ll n$. If the reduced basis provides a good representation of the ground state, the projection onto the reduced space should satisfy

$$PP^\dagger |\Psi_0(c)\rangle \approx |\Psi_0(c)\rangle \quad (4.4)$$

throughout the domain.

The full Hamiltonian can then be projected into the reduced space,

$$h(c) = P^\dagger H(c) P = h_0 + \sum_{i=1}^p c_i h_i, \quad (4.5)$$

where

$$h_0 = P^\dagger H_0 P, \quad h_i = P^\dagger H_i P. \quad (4.6)$$

The reduced Hamiltonian therefore retains the same affine dependence on the input parameters as the full Hamiltonian, while its dimension is reduced from $n \times n$ to $r \times r$, with $r \ll n$. If the reduced basis is sufficiently accurate, the lowest eigenvalue of $h(c)$ provides a good approximation to the ground-state energy of the original Hamiltonian. Once the reduced matrices h_i have been constructed, predictions at new parameter values require only the diagonalization of a small $r \times r$ matrix and are therefore computationally efficient.

Although explicit reduced-basis methods such as EC can be highly effective, they are intrusive in the sense that they require access to the high-dimensional many-body states and operators. In particular, one must explicitly construct the reduced basis and the associated projection operator P from the high-dimensional many-body states. For many-body problems in large model spaces, storing and manipulating the full eigenvectors and operators can itself be computationally demanding or impractical.

The affine eigenvalue PMM (AE-PMM) can be viewed as a data-driven, non-intrusive alternative to this physics-based construction. Rather than explicitly constructing the reduced basis and projection operators, the AE-PMM assumes that an accurate low-dimensional matrix representation with the same affine parameter dependence exists and writes it directly as

$$M(c) = M_0 + \sum_{i=1}^p c_i M_i. \quad (4.7)$$

Here, M_0 and M_i are independent Hermitian matrices of the same dimension $m \times m$. In contrast to the reduced matrices h_i obtained through explicit projection, the independent matrix elements of M_0 and M_i are treated as trainable parameters and learned directly from high-fidelity data. The output of the AE-PMM is the lowest eigenvalue of $M(c)$, which serves as an approximation to the ground-state energy of $H(c)$. The matrix elements are therefore optimized by minimizing a loss function, such as the mean squared error, between the lowest eigenvalues of PMM and the corresponding high-fidelity ground-state energies over the training set. The matrix dimension m is treated as a model hyperparameter that can be selected during the training process. In this way, the AE-PMM retains the affine matrix structure motivated by projection-based model reduction while bypassing the explicit construction of the reduced basis and projection operators.

Despite its simple form, the AE-PMM has been proven to be a universal function approximator. The same basic PMM framework can therefore be extended beyond eigenvalue prediction to more general regression problems. This generalized form is referred to as the affine observable PMM (AO-PMM), in which the model output is constructed from the parametric matrices and their eigenvectors rather than being restricted to the eigenvalues themselves. This allows the PMM framework to represent more general observables and functions of the input parameters. In this work, we employ both the AE-PMM and AO-PMM. We do not discuss the technical details of the AO-PMM construction; instead, we use it as a general function approximator, similar in spirit to other machine-learning models such as neural networks.

4.2 PMM for IMSRG Nuclear Matter Calculations

We next discuss how this reduced-order model is applied to the IMSRG framework for nuclear matter calculations. The nuclear Hamiltonians depend affinely on the LECs, making them naturally suited to the AE-PMM framework. The IMSRG results, however, also depend on several other quantities, including the chiral order, density, single-particle basis size, and IMSRG flow parameter. We will first analyze how the Hamiltonian and the IMSRG ground-state energy depend on these different parameters. Based on these observations and our physical understanding of the system, we will then introduce the PMM-IMSRG framework used to emulate these dependencies through

projection onto a reduced basis.

4.2.1 Chiral Order and LEC Dependence

We first consider the dependence of the underlying free-space Hamiltonian on the chiral order and LECs. At a fixed momentum cutoff, the Hamiltonian is constructed up to $N^3\text{LO}$ and depends on the chosen chiral order, indicated by $\nu = 0, 2, 3, 4$, and the associated LECs $\mathbf{c}$,¹ with the affine parameter dependence [40]:

$$H_{\text{free}}(\mathbf{c}, \nu) = \sum_{j=0}^{\nu} \sum_{k=1}^{N_k} h_{jk}(\mathbf{c}) V_k^{(j)}. \quad (4.8)$$

That is, H_{free} can be written as a sum of N_k products of parameter-dependent functions $h_{jk}(\mathbf{c})$ and parameter-independent operators $V_k^{(j)}$, with $V_k^{(1)} \equiv 0$ in Weinberg power counting.

In this proof-of-principle work, we consider only the $N^2\text{LO}$ 3N LECs $\mathbf{c} \equiv [c_D, c_E, D_2, F_2]$ and hold all other LECs fixed at their best-fit values, corresponding to $N_k = 4$ in Eq. (4.8). Consequently, the dependence represented by the functions h_{jk} is linear, with $h_{jk}(c_i) = c_k$. This affine dependence on the LECs naturally matches the structure of the AE-PMM introduced in Sec. 4.1.

Following Ref. [98], we use the order-by-order NN potentials developed by Entem, Machleidt, and Nosyk [61] with the momentum cutoff $\Lambda = 450$ MeV and combine them with 3N forces, when present, at the same chiral order. Additionally, PNM does not depend on c_D and c_E for the nonlocal regulator functions considered here [109].

4.2.2 Density and Basis Size Dependence

We next consider the dependence introduced when the free-space Hamiltonian is represented in the finite single-particle basis used for the nuclear matter calculation. The dependence on the number of allowed single-particle states N_s , the proton fraction Y_p , and the nuclear density n enters through the transformation from the free-space Hamiltonian to the in-medium Hamiltonian. Denoting the Hamiltonian parameters by $X_H \equiv [\mathbf{c}, \nu, N_s, Y_p, n]$, we have

$$H_{\text{IM}}(X_H) = U^\dagger(N_s, Y_p, n) H_{\text{free}}(\mathbf{c}, \nu) U(N_s, Y_p, n), \quad (4.9)$$

¹The c_i 's are considered here generic LECs and are not to be confused with the πN LECs.

where $U(N_s, Y_p, n)$ is a partial isometry—the operator which induces the projection $U^\dagger U$ —parameterized by the aforementioned values.

Equation (4.9) separates the dependence associated with the underlying interaction, contained in $H_{\text{free}}(\mathbf{c}, \nu)$, from the dependence on density, proton fraction, and basis size, which enters through $U(N_s, Y_p, n)$. In this work, however, we consider only PNM and SNM, corresponding to $Y_p = 0$ and $Y_p = 0.5$, respectively. No interpolation or emulation in proton fraction is therefore performed.

4.2.3 IMSRG Flow Parameter Dependence

Finally, we consider the dependence on the IMSRG flow parameter s . In principle, the IMSRG result can be viewed as the ground-state energy of Eq. (4.9) together with corrections parameterized by the Hamiltonian parameters that decay exponentially with the flow parameter,

$$E_0^{\text{IMSRG}}(X_H; s) = E_0(X_H) + \sum_{i=1}^r \alpha_i(X_H) \exp[-\beta_i(X_H)s], \quad (4.10)$$

where $\alpha(X_H), \beta(X_H) \geq 0$ are smooth, non-negative functions parameterized by the Hamiltonian parameters, and $E_0(X_H)$ satisfies

$$H_{\text{IM}}(X_H) |\Psi_0\rangle = E_0(X_H) |\Psi_0\rangle. \quad (4.11)$$

The asymptotic quantity of interest is therefore $E_0(X_H)$, while the finite- s dependence is described by exponentially decaying correction terms motivated by perturbative analyses of the IMSRG flow [25]. Eqs. (4.8)–(4.10) establish the parameter dependencies that will be incorporated into the PMM-IMSRG framework.

4.2.4 PMM-IMSRG Emulation Framework

With the relevant parameter dependencies of the Hamiltonian and IMSRG ground-state energy established, we now construct the PMM-IMSRG framework that incorporates these dependencies into a reduced-order model.

Consider now the subspace of a chosen dimension $k_1 \leq \dim(H_{\text{IM}})$ that best² preserves Eq. (4.11). Let P_1 be the partial isometry whose columns span this space. We can then compress Eq. (4.11)

²Here, “best” refers to optimality for the entire emulator’s predictions. In this work, this refers only to the ground state energy.

into this space,

$$h_{\text{IM}}(X_H) |\psi_0\rangle \approx E_0(X_H) |\psi_0\rangle, \quad (4.12)$$

where $h_{\text{IM}}(X_H) \equiv P_1^\dagger H_{\text{IM}}(X_H) P_1$ and $|\psi_0\rangle \equiv P_1^\dagger |\Psi_0\rangle$. The reduced space is chosen such that the ground-state energy $E_0(X_H)$ is preserved as accurately as possible under this compression.

We next consider another subspace of a given dimension k_2 with $k_1 < k_2 \leq \dim(H_{\text{free}})$ that best^2 preserves Eq. (4.9). As before, let P_2 be the partial isometry whose columns span this space. Compressing the $H_{\text{free}}(\mathbf{c}, \nu)$ present in the expression for $h_{\text{IM}}(X_H)$ using P_2 yields

$$h_{\text{IM}}(X_H) \approx u^\dagger(N_s, Y_p, n) h_{\text{free}}(\mathbf{c}, \nu) u(N_s, Y_p, n), \quad (4.13)$$

where $u(N_s, Y_p, n) \equiv P_2^\dagger U(N_s, Y_p, n) P_1$ and $h_{\text{free}}(\mathbf{c}, \nu) \equiv P_2^\dagger H_{\text{free}}(\mathbf{c}, \nu) P_2$.

It is straightforward to show that the functional form of $h_{\text{free}}(\mathbf{c}, \nu)$, the compressed $H_{\text{free}}(\mathbf{c}, \nu)$, is identical to that of the full-dimensional Hamiltonian in Eq. (4.8), leading us to define $v_i^{(j)}$ of dimension k_2 just as before. The affine dependence on the chiral order and LECs can therefore be retained explicitly in the reduced Hamiltonian.

The reduced spaces themselves, however, do not need to be known explicitly. Instead of constructing the particular partial isometries P_1 and P_2 , we can absorb them into the definitions of the reduced operators and treat the corresponding reduced basis as an implicit learned basis. The reduced operators can then be learned directly from data for $\{X_H, E_0(X_H)\}$ without explicitly performing the full-dimensional compressions. This is the central idea behind the PMM construction used here: the known functional structure of the underlying physics is retained while the reduced representation required to reproduce the target observable is learned directly from data.

The remaining dependence on N_s , Y_p , and n enters through the reduced transformation $u(N_s, Y_p, n)$. Since the functional dependence of $U(N_s, Y_p, n)$, and therefore $u(N_s, Y_p, n)$, is not known, we instead substitute a universal form capable of approximating all possible forms given a sufficiently large “hidden model” size. For such an operator which compresses from a space of dimension N to one of dimension $k \leq N$,

$$U_{\text{univ}}(x_i) \equiv \exp \left[i \sum_{j=1}^l f_j(x_i) M_j \right] (:, 1 : k), \quad (4.14)$$

where M_j are Hermitian operators of dimension N , $f_j(x_i)$ are universal functions (e.g., the output of a neural network), and $A(:, 1 : k)$ denotes taking the first k columns of A . For sufficiently large l and expressive f_j , this can represent any parameterized partial isometry to arbitrary accuracy.

Finally, we model the flow dependence of the IMSRG predictions through the exponentially decaying corrections introduced in Eq. (4.10). The magnitudes and decay rates of these corrections are learned in a purely data-driven way by fitting universal data-driven PMM forms, namely the AO-PMM [44]. Since the deployed emulator needs only to produce accurate predictions at $s \rightarrow \infty$, reproducing the exact finite- s physics of these corrections is less important than accurately capturing the asymptotic ground-state energy $E_0(X_H)$.

The explicit process of using the PMM to make an emulated prediction is as follows. Given input parameters $c_D, c_E, D_2, F_2, \nu, N_s, Y_p, n$, and s , trained operators $v_i^{(j)}, m_1, m_2, \dots, m_l \in \mathbb{H}(k_2)$, and trained scalar functions $f_1, f_2, \dots, f_l, \alpha_1, \dots, \alpha_r, \beta_1, \dots, \beta_r$, we first form $h_{\text{free}}(\mathbf{c}, \nu) \in \mathbb{H}(k_2)$ using the form of Eq. (4.8). We then compute

$$u(N_s, Y_p, n) = \exp \left[i \sum_{j=1}^l f_j(N_s, Y_p, n) m_j \right] (:, 1 : k_1) \quad (4.15)$$

and transform $h_{\text{free}}(\mathbf{c}, \nu)$ as in Eq. (4.13) to form $h_{\text{IM}}(X_H)$. An exact diagonalization of $h_{\text{IM}}(X_H)$ then yields the emulated $E_0(X_H)$. The entire process can be carried out in $\mathcal{O}(k_2^3)$ time. If the emulated flow dependence is desired, one can evaluate all α_i and β_i and then compute $E(X_H; s)$ as in Eq. (4.10).

4.2.5 From EOS to Saturation Properties

The procedure described above provides predictions of the EOS for a given input Hamiltonian. These predictions can in turn be used to determine several derived nuclear-matter saturation properties, including the saturation density n_{sat} , saturation energy E_{sat} , symmetry energy S , slope parameter L , and incompressibility K .

Denote $X_{\text{SNM or PNM}} \equiv [\mathbf{c}, \nu, N_s, Y_p = 0.5 \text{ or } 0.0, n]$. The saturation density is obtained by

minimizing the emulated SNM energy with respect to n ,

$$n_{\text{sat}} = \arg \inf_{n \in \left(\min_{n' \in \mathcal{T}} n', \max_{n' \in \mathcal{T}} n' \right)} E(X_{\text{SNM}}; s), \quad (4.16)$$

where the minimization is restricted to the open density interval spanned by the training dataset $\mathcal{T}$.

Denote $X_{\text{SNM or PNM}}^{\text{sat}} \equiv [\mathbf{c}, \nu, N_s, 0.5 \text{ or } 0.0, n_{\text{sat}}]$. The emulator predictions for the saturation energy, symmetry energy and its slope parameter within the standard quadratic approximation, and the incompressibility of SNM are then given by

$$\begin{aligned} E_{\text{sat}} &= E(X_{\text{SNM}}^{\text{sat}}; s), \\ S &= E(X_{\text{PNM}}^{\text{sat}}; s) - E(X_{\text{SNM}}^{\text{sat}}; s), \\ L &= 3n_{\text{sat}} \frac{\partial}{\partial n} \left[E(X_{\text{PNM}}; s) - E(X_{\text{SNM}}; s) \right] \Big|_{n_{\text{sat}}}, \\ K &= 9n_{\text{sat}}^2 \frac{\partial^2 E(X_{\text{SNM}}; s)}{\partial n^2} \Big|_{n_{\text{sat}}}. \end{aligned} \quad (4.17)$$

An important advantage of the PMM is that its prediction is differentiable with respect to the continuous input parameters. The density derivatives entering L and K can therefore be evaluated directly from the emulator.

4.3 Conformal Prediction

Reliable uncertainty quantification is essential for assessing the trustworthiness of emulator predictions. We use split conformal prediction to quantify the statistical uncertainty associated with the PMM-IMSRG emulator. Split conformal prediction provides distribution-free finite-sample confidence guarantees that rely only on the exchangeability of data. The method uses an uncertainty heuristic and a calibration dataset that is disjoint from the training, validation, and test sets to calibrate the emulator uncertainty. For comprehensive introductions to this technique, see Refs. [110, 111]; recent applications in nuclear physics can be found in Refs. [112, 113].

For a prescribed miscoverage level α , split conformal prediction returns the lower and upper bounds of a prediction interval, which we refer to as the conformal interval, for each test point, with target coverage $1 - \alpha$. Under the assumption that the calibration and test data are exchangeable,

the corresponding true value for a new test point is contained within the conformal interval with probability at least $1 - \alpha$, up to the finite-sample discreteness determined by the size of the calibration set.

In this work, the uncertainty heuristic incorporates the sensitivity of the PMM prediction to its trainable parameters and continuous inputs, together with the distance of the test point from the training set. The calibration set is then used to calibrate this heuristic and construct the final conformal prediction intervals for the PMM-IMSRG emulator.

4.4 Emulator Performance

At the end of this chapter, we demonstrate the accuracy of the emulator on withheld test data for both SNM and PNM at $N^2\text{LO}$ and $N^3\text{LO}$ in Fig. 4.1. The test set spans both matter types, varies all LECs considered in this work (c_D, c_E, D_2, F_2) as well as the nuclear density, and includes the most converged IMSRG results obtained with the largest number of shells. Neither the largest basis size nor these test samples are represented in the training or validation data. We compare the predicted energies with the corresponding IMSRG results and show the associated 95% confidence intervals, demonstrating both strong agreement and tight predictive uncertainties.

The PMM-IMSRG framework developed here provides the basis for the uncertainty-quantification applications presented in Chapter 5. More generally, the framework can in principle be extended to emulate the dependence on the full set of relevant chiral EFT LECs, including those in the NN interaction and the πN 3N couplings c_1, c_3 , and c_4 . This would enable applications such as global sensitivity analyses and more comprehensive uncertainty-quantification studies of the nuclear EOS.

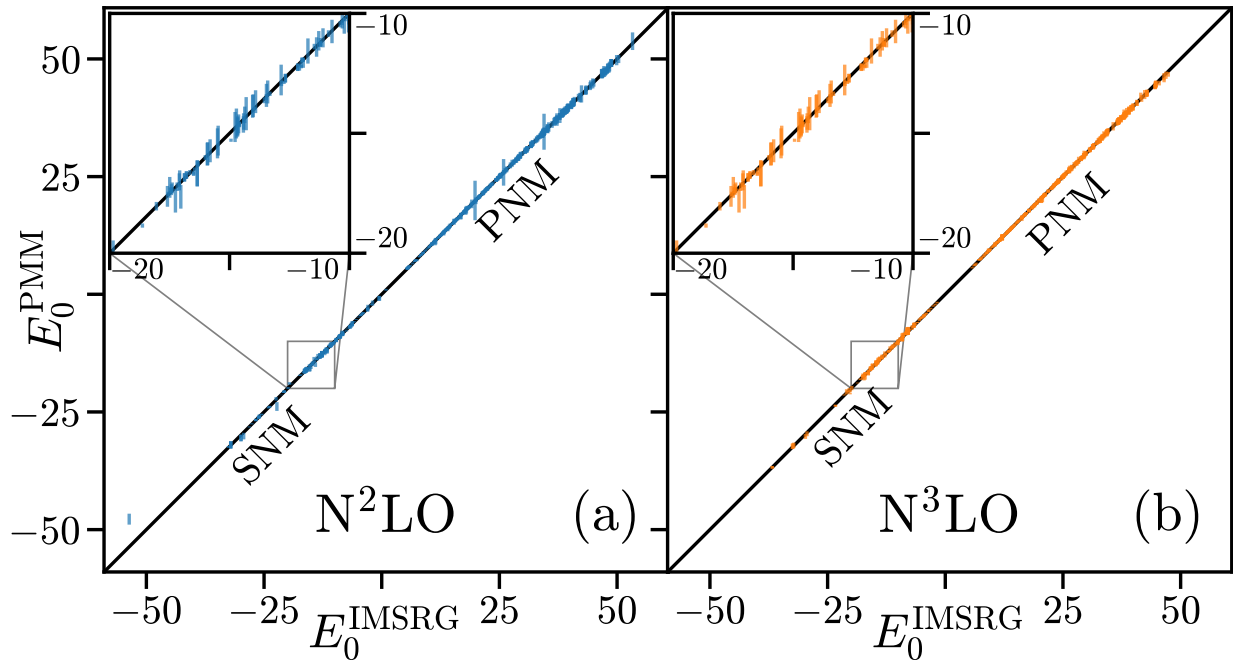


Figure 4.1 Comparison of PMM-predicted energies at the 95.45% confidence level and withheld test IMSRG results for both PNM (here, 66 neutrons) and SNM (here, 66 protons and 66 neutrons) as all degrees of freedom, including LECs and density, are varied for both $N^2\text{LO}$ (panel a) and $N^3\text{LO}$ (panel b). Insets show additional detail around the empirical saturation energy. All values are in units of MeV.

CHAPTER 5

APPLICATIONS OF PMM-IMSRG FRAMEWORK WITH QUARK-MASS-DEPENDENT THREE-NUCLEON INTERACTIONS

In Chapter 4, we developed the PMM–IMSRG emulator framework, which enables fast and accurate predictions of the EOS across a wide range of physical and computational inputs, including chiral EFT low-energy constants, IMSRG flow parameters, densities, and basis sizes. This capability establishes the foundation for principled UQ of the nuclear EOS and opens the door to a variety of computationally demanding applications. To demonstrate the efficacy of this framework, we present exploratory results for the coupling constants of the two quark-mass-dependent three-nucleon interactions (D_2 , F_2) [114] at next-to-next-to-leading order (N^2 LO) in the chiral expansion based on a renormalization-group analysis [45], by fitting them to empirical saturation properties. We then propagate both parametric and emulator uncertainties to the EOS in the limits of PNM and SNM.

In this chapter, we discuss our main results. Following the methodology outlined in Chapter 4, we construct a PMM–IMSRG emulator that is trained on IMSRG-generated PNM and SNM calculations encompassing a range of densities, basis sizes, and four chiral orders (i.e., up to N^3 LO). Specifically, we perform IMSRG training calculations across $n = [0.08, 0.24] \text{ fm}^{-3}$ and broad ranges $[-5, 5]$ for c_D and c_E , $[-4.2, 4.2] \text{ fm}^4$ for D_2 and F_2 ¹, based on the N^3 LO EMN NN interaction with a cutoff of 450 MeV, combined with 3N forces at the same chiral order. We then present proof-of-principle applications of the PMM–IMSRG emulator, assess its efficacy, constrain quark-mass-dependent chiral 3N forces at N^2 LO in the chiral expansion, and propagate parametric uncertainties to the nuclear EOSs. Finally, we provide a summary and outlook.

5.1 Exploring Saturation Properties of 3N Forces

Fig. 5.1 shows the distributions of emulated saturation points (n_{sat} , E_{sat}) resulting from randomly sampling 10 000 3N LECs $\mathbf{c} = [c_D, c_E]$ in panel (a) and $[c_D, c_E, F_2]$ in panel (b). For simplicity, we sample all 3N LECs *uniformly* in the broad range $[-5, +5]$, where we use fm^4 as the units for F_2

¹These ranges are chosen to match the prior ranges adopted in the Bayesian parameter-estimation framework discussed in Section 5.3.1

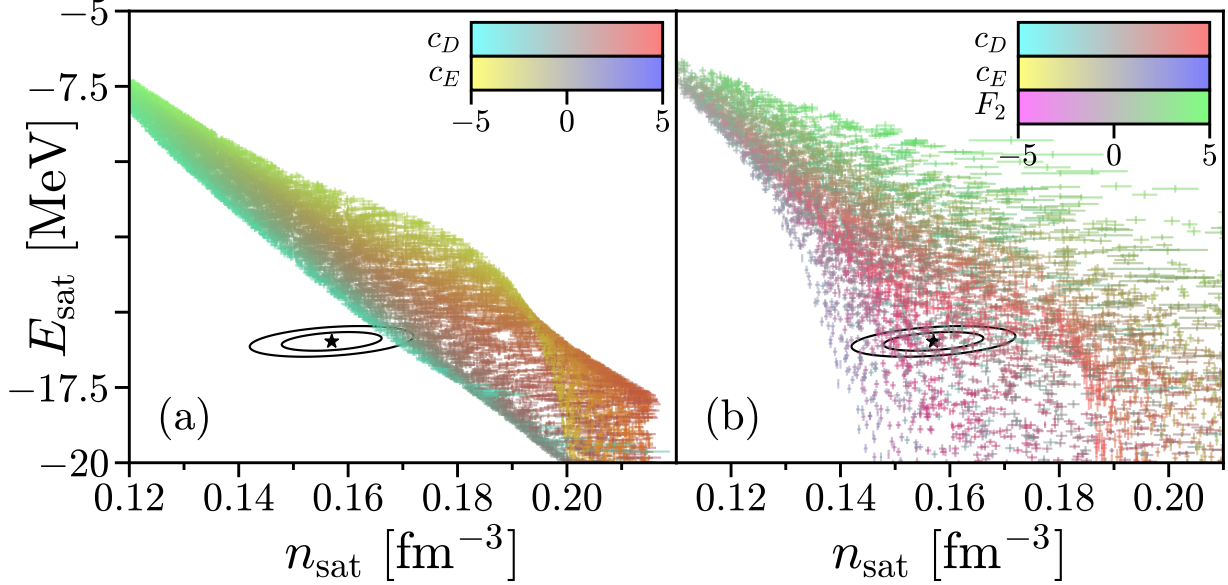


Figure 5.1 Saturation point distributions in SNM obtained from 10 000 uniform random samples in the range specified by the legends of c_D and c_E (panel a) and c_D , c_E , and F_2 (panel b) with $\{N_s, s\} = \{\infty, \infty\}$ at $N^3\text{LO}$. The color of each point is determined by a color average of the corresponding colors given by the value of each LEC indicated in the legends. Each saturation point is shown with the associated confidence intervals at the 68.27% level. The empirical saturation point [115] is depicted by the star (mean value), and the associated 68.27% (inner ellipse) and 95.45% credible contours (outer ellipse) are shown in black.

(see the legends), while keeping the $N^3\text{LO}$ EMN 450 MeV NN potential and the $N^3\text{LO}$ 3N forces constant. The color of the samples shown in Fig. 5.1 is determined by the average color of the colors associated with the individual LECs given in the legends. The empirical saturation point, which is given by a bivariate student- t distribution and depicted by the star (i.e., mean value) and two credible ellipses at 68% and 95% credibility, respectively, was obtained in Ref. [115] by Bayesian model mixing of the empirical constraints of the saturation points obtained from various Skyrme and relativistic mean field functionals. As shown in panel (a) of Fig. 5.1, this sampling strategy results in a Coester-like anti-correlation band [15]. However, with only c_D and c_E as degrees of freedom, this Coester band is markedly shifted to higher energies per particle and densities relative to the empirical points, consistent with the findings in the literature (e.g., see Ref. [8]).

Motivated by this well-known shortcoming, we add a quark-mass-dependent 3N force, which was recently shown to contribute at $N^2\text{LO}$, F_2 . Previous studies [45, 114] indicate that the

contribution from F_2 is more significant than that from D_2 , a trend that we have verified with our IMSRG calculations. Accordingly, we follow Ref. [114] and focus on F_2 throughout the remainder of this work; i.e., $D_2 = 0$. As shown in panel (b) of Fig. 5.1, we find that including F_2 enables, while significantly widening the Coester band, these forces to saturate closer to the empirical point. This improved agreement motivates us to employ the PMM–IMSRG emulator to investigate more systematically the LEC dependence of the EOS on F_2 and to further constrain its value in Sec. 5.3.

5.2 Variations of c_D and c_E about the Triton Binding Energy

Next, we explore parametric uncertainties in the NN and 3N interactions constructed in Ref. [98] by fitting c_D and c_E to the triton binding energy and the empirical saturation point using MBPT calculations. To this end, we consider the $c_E(c_D)$ correlation constrained by the triton binding energy, as shown in Figure 1 in the supplemental material of Ref. [98], and assume a somewhat arbitrary symmetric uncertainty about the blue-dashed line in that Figure 1, as described below. In future work, this additional uncertainty could be due to EFT truncation errors in the triton binding energy predictions, which were not considered in Ref. [98]. We construct a GP [42] with a fixed mean function and covariance function (or kernel) to represent this uncertainty band. Specifically, we use a cubic spline interpolating the discrete $c_D(c_E)$ data obtained in Ref. [98] as the mean function and choose constant values for the hyperparameters of the radial basis function (RBF) kernel:

$$\kappa_{\text{RBF}}(c_D, c'_D) = \sigma_f^2 \exp \left[-\frac{(c_D - c'_D)^2}{\ell^2} \right], \quad (5.1)$$

with variance $\sigma_f^2 = 0.1^2$ and correlation length $\ell = 10$.

We evaluate the GP at 100 equally spaced c_D values over the interval $[-5, 5]$ and generate 100 $c_E(c_D)$ sample curves. This procedure yields a total of 10 000 (c_D, c_E) pairs. Figures 5.2 and 5.3 show the resulting SNM and associated low-density EOS parameters.²

In Fig. 5.2, we use the PMM–IMSRG emulator to predict the EOS at all four chiral orders for each of the 10 000 sampled (c_D, c_E) pairs. We construct an approximate quantile function for

²We do not show the PNM EOS because its energy per particle is independent of the 3N LECs considered [109], so varying these LECs would yield a single line rather than an uncertainty band.

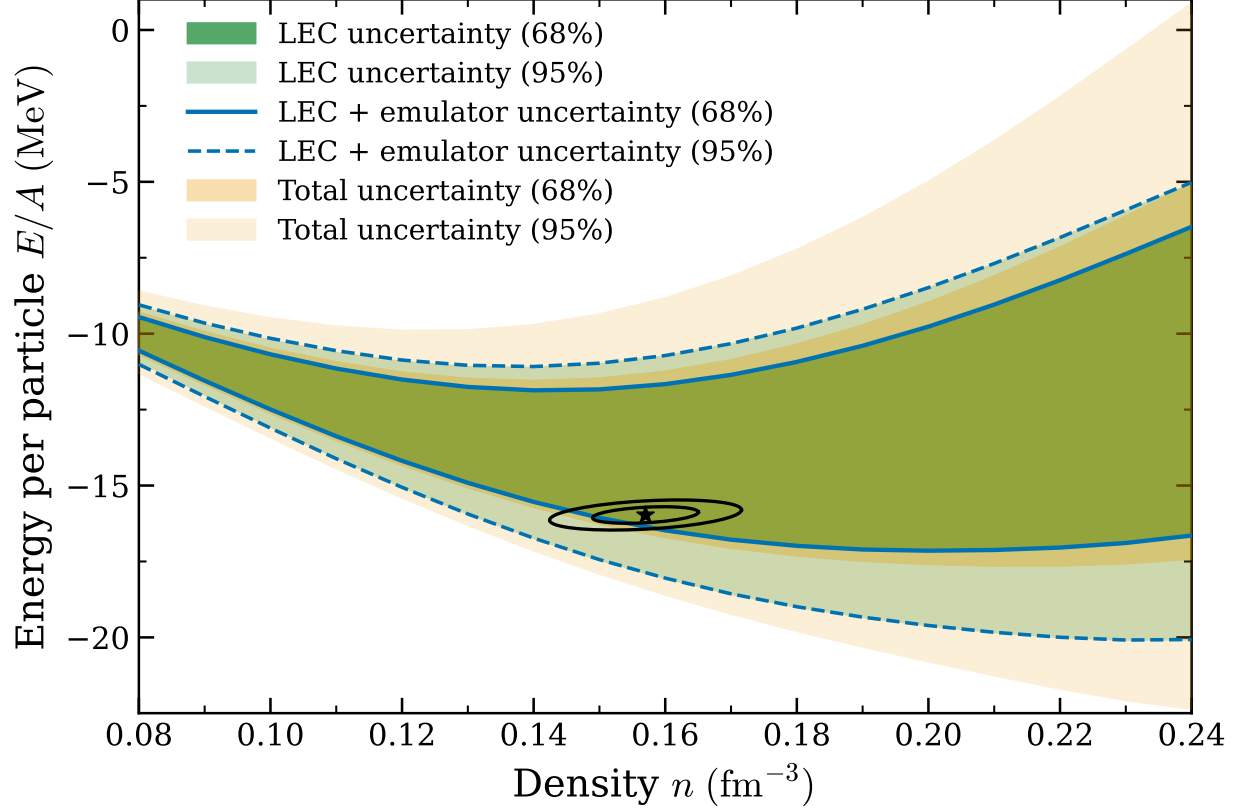


Figure 5.2 Confidence regions of the EOS in the limit of SNM at N³LO when varying the widened c_D - c_E correlation that fits the triton binding energy as obtained in Ref. [98, see Fig. 1 in the Supplemental Material]. The error bands are obtained through ordinary Monte Carlo sampling from the probability distributions of the emulator and EFT truncation errors. See the main text for details.

the emulator error at each chiral order, using the conformal intervals over a range of miscoverage levels. Assuming the emulator errors are independent across chiral orders, we draw samples from the emulator error distributions using inverse-transform sampling. For each (c_D, c_E) pair, we draw 100 emulator error samples at each chiral order and add them to the corresponding emulator predictions. For each resulting set of emulator-error-adjusted EOS predictions, we use the BUQEYE pipeline [21, 22], described in more detail in section 5.4, to determine the N³LO EFT truncation error distribution at each density point and draw an additional 100 EFT truncation error samples. This ordinary Monte Carlo procedure therefore produces $10^4 \times 10^2 \times 10^2 = 10^8$ EOS samples, incorporating uncertainties from the LECs, emulator errors, and EFT truncation errors. The LEC uncertainty bands (depicted in green) are obtained by taking pointwise quantiles over

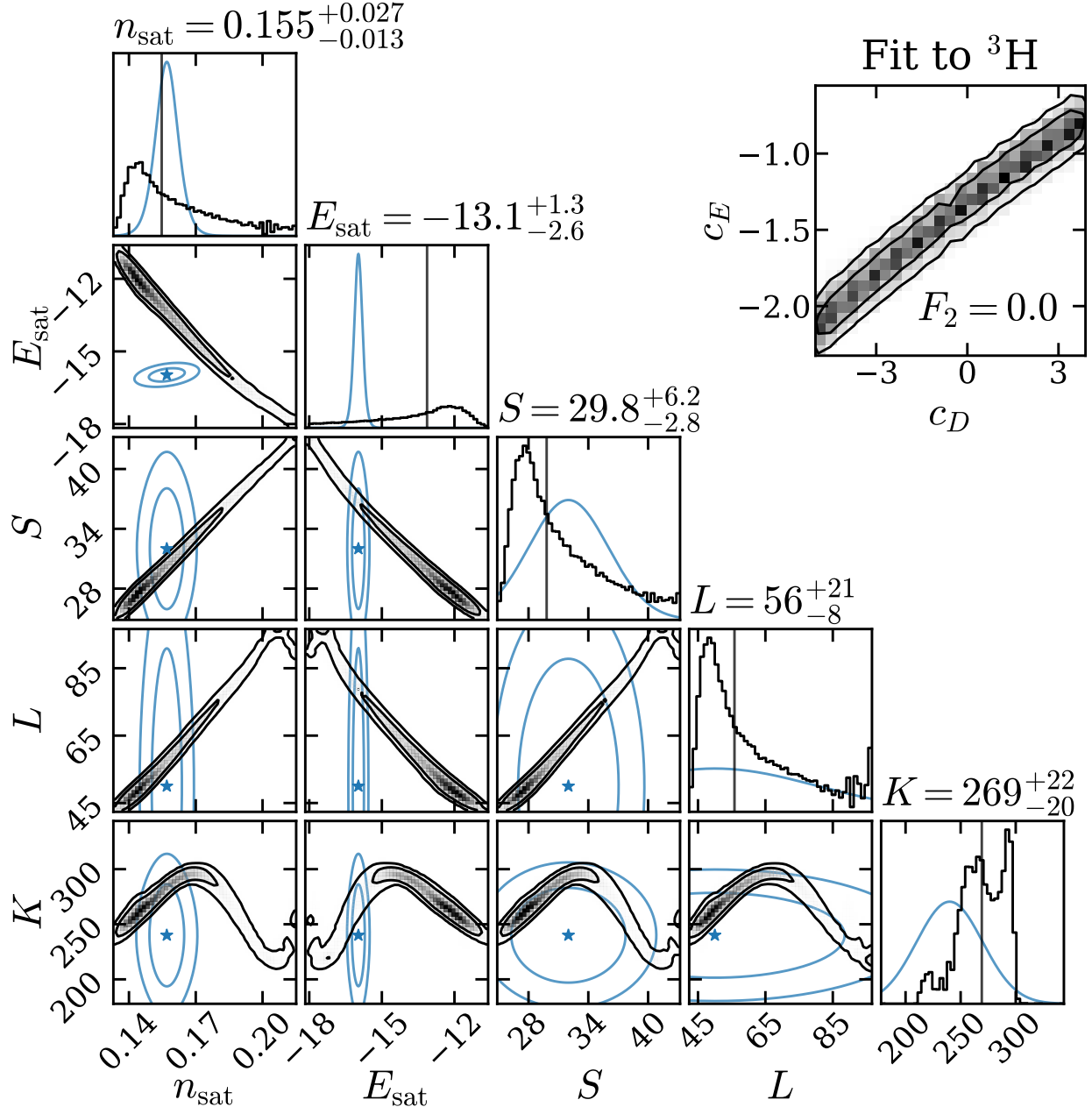


Figure 5.3 Low-density EOS parameters associated with the sampled EOSs depicted in Fig. 5.2 (black). The units are MeV, except for n_{sat} , which is in fm^{-3} . The blue lines and stars depict the empirical ranges defined in Eq. (5.3). The reported uncertainties in the titles correspond to 68% credible intervals centered on the median.

the EOS distribution associated with the sampled LECs after marginalizing over the emulator and EFT truncation errors. The combined LEC and emulator uncertainty bands (depicted in blue) are obtained by taking pointwise quantiles after marginalizing over the EFT truncation error. Finally, the total uncertainty bands (depicted in orange) in Fig. 5.2 are obtained from the pointwise quantiles of the full EOS sample, including the LEC, emulator, and EFT truncation uncertainties.

We find that, even when relaxing the requirement to exactly reproduce the triton binding as discussed, these chiral NN and 3N forces still cannot reproduce the empirical saturation point at the 68%-level or better. However, as shown in the correlation plot in Fig. 5.3, the predicted Coester band is slightly shifted toward the empirical saturation point, while the other low-density EOS parameters explore a wide range of values. For example, the symmetry energy $S = 29.8^{+6.2}_{-2.8}$ MeV and its slope parameter $L = 56^{+21}_{-8}$ MeV at n_{sat} . In the following, we study the consequence of adding the F_2 term to the N²LO 3N forces. To this end, we choose to constrain its coupling constant to empirical saturation properties.

5.3 Calibrating 3N Forces to Empirical Saturation Properties with Emulator Uncertainties

We devise a Bayesian parameter-estimation framework based on the PMM–IMSRG emulator, with emulator uncertainties quantified using conformal prediction. In this exploratory study, we account only for emulator uncertainty and defer the inclusion of EFT truncation errors to future work.³ For a given set of 3N LECs $\mathbf{c} = [c_D, c_E, F_2]$, the emulator efficiently generates the EOS in the limits of PNM and SNM. The saturation properties are obtained by locating the minimum of the SNM EOS and evaluating the relevant derivatives at that point (see Eqs. (4.17) for the expressions), with associated emulator uncertainties propagated accordingly.

5.3.1 Bayesian Fit Protocol

The empirical observables used to constrain these LECs include the saturation density (n_{sat}), saturation energy (E_{sat}), symmetry energy (S), slope of the symmetry energy (L), and incompressibility of SNM (K). For the first two parameters, we adopt the joint bivariate student- t distribution,

³LEC uncertainties and the EFT truncation errors are correlated. While neglecting these correlations may lead to misestimation of EFT predictions, rigorously quantifying and incorporating these uncertainties remains a work in progress [116].

$t_9(\boldsymbol{\mu}, \boldsymbol{\Psi})$, obtained in Ref. [115], with 9 degrees of freedom and mean value and scale matrix, respectively, given by (in units of fm^{-3} and MeV)⁴

$$\boldsymbol{\mu} \approx \begin{bmatrix} 0.157 \\ -15.97 \end{bmatrix}, \quad \boldsymbol{\Psi} \approx \begin{bmatrix} 0.005^2 & 0.017^2 \\ 0.017^2 & 0.17^2 \end{bmatrix}. \quad (5.2)$$

At the prior level, we assume that S , L , and K have the independent normal distributions:

$$\begin{aligned} S &\sim \mathcal{N}(32, 3^2), \\ L &\sim \mathcal{N}(60, 25^2), \\ K &\sim \mathcal{N}(240, 20^2), \end{aligned} \quad (5.3)$$

where the mean values and standard deviations are given in MeV . The priors for S and L are chosen to encompass, at the prior's $\approx 2\sigma$ level [65], the relatively large mean values from the recent PREX-II-informed extraction [5], while the prior for K is chosen to be consistent to (but slightly less informed than) the one obtained in Ref. [6] based on several analyses of isoscalar giant monopole resonances. We adopt uniform priors for the dimensionless c_D and c_E over the range $[-5, 5]$ to impose naturalness, and for F_2 over the range $[-(5f_\pi^4)^{-1}, (5f_\pi^4)^{-1}]$,⁵ with the pion decay constant f_π , as determined by renormalization-group analysis [45].

We consider the statistical discrepancy model of the emulator error:

$$y_{\text{IMSRG}} = y_{\text{emu}} + \delta y_{\text{emu}}, \quad (5.4)$$

where y_{emu} denotes the emulator's approximation to the high-fidelity prediction y_{IMSRG} . The difference between the two is given by the emulator error δy_{emu} . We emphasize that y_{IMSRG} is not the “true” value of the observable in nature, but rather the high-fidelity IMSRG prediction that we seek to emulate; it therefore carries additional theoretical uncertainties, e.g., from many-body approximations and EFT truncations, which we omit in the following. Since δy_{emu} is not directly observed in practice, we model it as a random variable.

⁴This distribution function for the empirical saturation point is depicted throughout this article in figures showing the SNM EOS.

⁵This range corresponds to $|F_2| \lesssim 4.2 \text{ fm}^4$, so slightly smaller than the range used to generate the results for panel (b) in Fig. 5.1.

With the discrepancy model (5.4), the likelihood of observing saturation properties y_{IMSRG} for a given set of LECs $\mathbf{c}$ is obtained by marginalizing the emulator error via the convolution integral [117]

$$p(y_{\text{IMSRG}} | \mathbf{c}) = \int p(y_{\text{IMSRG}} - \delta y_{\text{emu}}) \times p(\delta y_{\text{emu}}) d(\delta y_{\text{emu}}), \quad (5.5)$$

where $p(\cdot)$ indicates probability density distributions. The likelihood (5.5) can be rewritten in terms of the quantile function of the emulator error, $q(u)$ with $u \in [0, 1]$,⁶ using the probability integral transform [118]⁷

$$p(y_{\text{IMSRG}} | \mathbf{c}) = \int_0^1 p(y_{\text{IMSRG}} - q(u)) du. \quad (5.6)$$

Here, we use a set of conformal intervals over a range of α values to approximate the quantile function $q(u)$ in Eq. (5.6), as follows. For a given miscoverage level $\alpha \in (0, 1)$, conformal prediction yields an interval (a_α, b_α) that satisfies

$$p(a_\alpha \leq y_{\text{IMSRG}} \leq b_\alpha) \approx 1 - \alpha. \quad (5.7)$$

The confidence intervals are central by construction, implying that the cumulative distribution function (CDF) F_y satisfies

$$F_y(a_\alpha) \approx \frac{\alpha}{2}, \quad F_y(b_\alpha) \approx 1 - \frac{\alpha}{2}, \quad (5.8)$$

which, together with Eq. (5.4), results in the shifted CDF for δy_{emu} evaluated at the end points:

$$F_\delta(a_\alpha - y_{\text{emu}}) \approx \frac{\alpha}{2}, \quad F_\delta(b_\alpha - y_{\text{emu}}) \approx 1 - \frac{\alpha}{2}. \quad (5.9)$$

The corresponding quantile function is then given by $q(u) = F_\delta^{-1}(u)$, with $u \in (0, 1)$, and thus

$$q\left(\frac{\alpha}{2}\right) \approx a_\alpha - y_{\text{emu}}, \quad q\left(1 - \frac{\alpha}{2}\right) \approx b_\alpha - y_{\text{emu}}. \quad (5.10)$$

Computing the conformal intervals $[a_\alpha, b_\alpha]$ over a range of α values allows us to estimate the corresponding values of $q(u)$ on a grid of u and then numerically interpolate them to obtain $q(u)$

⁶The quantile function $q(u)$ depends on the input LECs $\mathbf{c}$. For notational simplicity, we write $q(u)$ in place of $q_{\mathbf{c}}(u)$ throughout this paper.

⁷See Theorem 2.1.10 in Ref. [118] for more details.

over the interval $(0, 1)$ for each given set of LECs $\mathbf{c}$. Specifically, we use an equidistant grid of $N_\alpha = 500$ values of $\alpha \in (0, 1)$, resulting in N_α central confidence intervals, from which we obtain the quantile function evaluated at $\alpha/2$ and $1 - \alpha/2$ simultaneously. Hence, we obtain $q(u)$ sampled at $2N_\alpha = 1000$ grid points. We then use linear interpolation between these points to approximate the full quantile function while preserving its monotone non-decreasing structure.

Let $X(\mathbf{c})$ denote the central emulator prediction of the saturation property X for a given set of LECs $\mathbf{c}$, and let $q_X(u)$ denote the corresponding quantile function of the emulator error, where

$$X \in \{n_{\text{sat}}, E_{\text{sat}}, S, L, K\}.$$

We collect the empirical saturation point into the vector

$$\mathbf{y}_{nE}^{\text{emp}} \equiv \begin{pmatrix} n_{\text{sat}}^{\text{emp}} \\ E_{\text{sat}}^{\text{emp}} \end{pmatrix}, \quad (5.11)$$

the central emulator predictions of n_{sat} and E_{sat} into

$$\boldsymbol{\mu}_{nE}(\mathbf{c}) \equiv \begin{pmatrix} n_{\text{sat}}(\mathbf{c}) \\ E_{\text{sat}}(\mathbf{c}) \end{pmatrix}, \quad (5.12)$$

and their emulator-error quantile functions into

$$\mathbf{q}_{nE}(u) \equiv \begin{pmatrix} q_n(u) \\ q_E(u) \end{pmatrix}. \quad (5.13)$$

For a given $u \in (0, 1)$, we define the emulator-error-adjusted empirical saturation point by

$$\Delta \mathbf{y}_{nE}(u) \equiv \mathbf{y}_{nE}^{\text{emp}} - \mathbf{q}_{nE}(u). \quad (5.14)$$

For the remaining saturation properties, we define

$$\Delta X(u) \equiv X^{\text{inf}} - q_X(u), \quad X \in \{S, L, K\}. \quad (5.15)$$

Here, X^{inf} denotes the adopted prior-level calibration mean for the saturation property X . The complete calibration-data vector is

$$\mathbf{y}_{\text{cal}} \equiv \left(n_{\text{sat}}^{\text{emp}}, E_{\text{sat}}^{\text{emp}}, S^{\text{inf}}, L^{\text{inf}}, K^{\text{inf}} \right)^{\top}. \quad (5.16)$$

Assuming that, conditional on $\mathbf{c}$ and u , $(n_{\text{sat}}, E_{\text{sat}})$ is independent of (S, L, K) , and that S , L , and K are mutually independent, the likelihood of the calibration data, marginalized over the emulator uncertainty, is

$$p(\mathbf{y}_{\text{cal}} \mid \mathbf{c}) = \int_0^1 t_9(\Delta \mathbf{y}_{nE}(u) \mid \boldsymbol{\mu}_{nE}(\mathbf{c}), \Psi) \times \mathcal{N}^{(S,L,K)}(u) \, du, \quad (5.17)$$

where

$$\mathcal{N}^{(S,L,K)}(u) \equiv \prod_{X \in \{S,L,K\}} \mathcal{N}(\Delta X(u) \mid X(\mathbf{c}), \sigma_X^2). \quad (5.18)$$

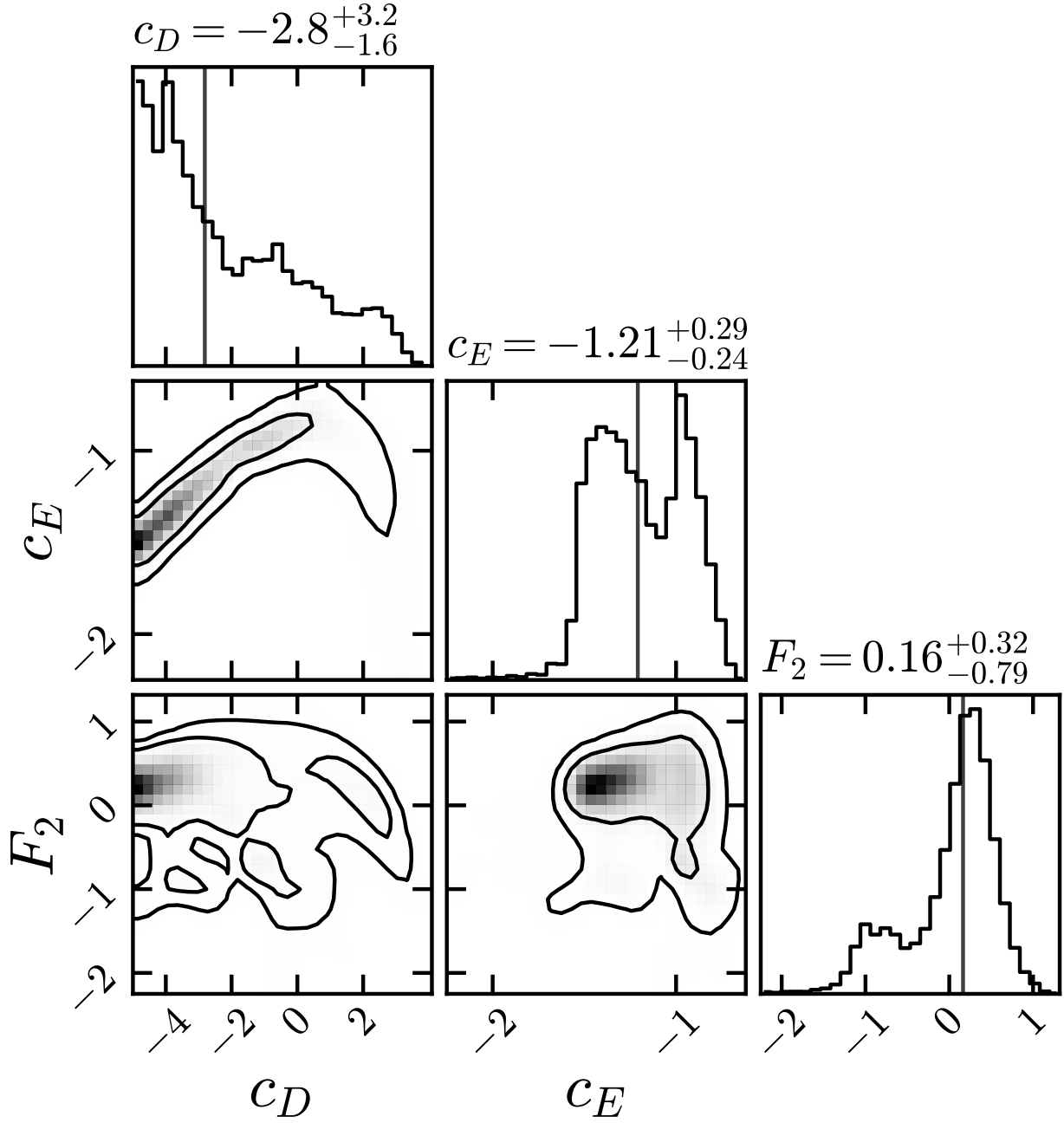


Figure 5.4 Corner plot showing the posterior distributions and pairwise correlations of the low-energy constants c_D , c_E , and F_2 obtained from the PMM-IMSRG Bayesian analysis. The LECs c_D and c_E are dimensionless, whereas F_2 is given in fm^4 . The reported uncertainties in the titles correspond to 68% credible intervals centered on the median. Note that the uniform prior enforces the constraint $|c_D| \leq 5$.

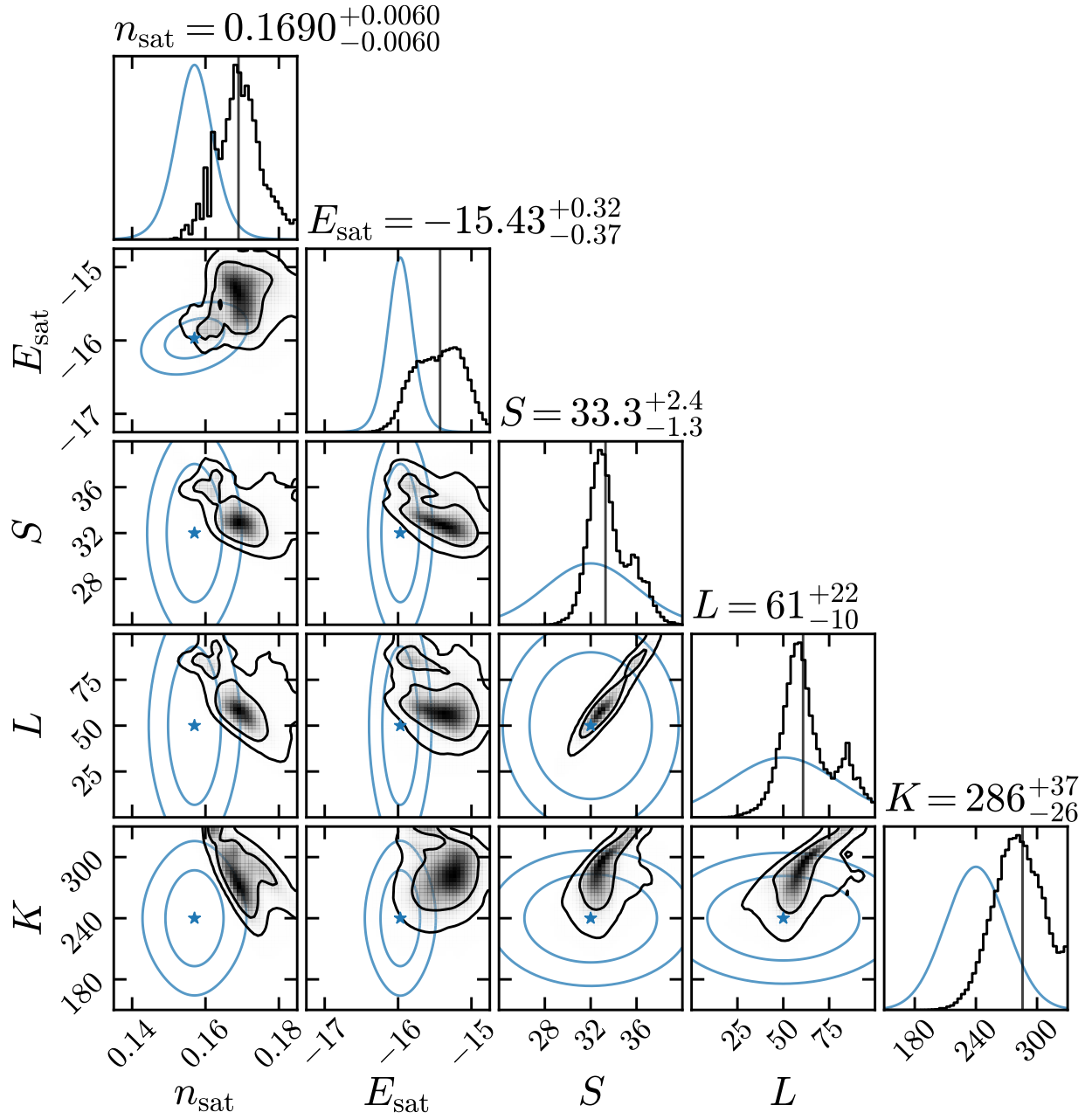


Figure 5.5 Corner plot showing the posterior distributions and pairwise correlations of the saturation properties n_{sat} , E_{sat} , S , L , and K obtained from the PMM-IMSRG Bayesian analysis. All observables are given in MeV, except for n_{sat} , which is given in fm^{-3} . The diagonal panels display the marginal posterior distributions with median values and credible intervals, while the off-diagonal panels show the corresponding joint posterior contours. The blue curves indicate the prior distributions: a bivariate student- t distribution for $(n_{\text{sat}}, E_{\text{sat}})$ and independent Gaussian distributions for (S, L, K) , with the blue star marking the distributions' mean values. The 68% and 95% credible contours are shown, and the reported uncertainties (centered on the median) are at the 68% credibility level.

5.3.2 LEC Constraints and Predictions for the Low-Density EOS

With the standard Monte Carlo sampler implemented in the Python package `emcee` [119], we sample the posterior distribution of the LECs. We use 32 random walkers, initialized at the maximum a posteriori (MAP) estimate plus random perturbations, discard 4000 burn-in steps, and generate 20 000 production steps. The production chain was thinned by retaining every fifth sample. Fig. 5.4 shows the resulting posterior samples of the LEC posterior distribution, which were subsequently propagated through the PMM–IMSRG emulator to evaluate the posterior distributions of the saturation properties shown in Fig. 5.5. The titles report the 68% confidence regions centered on the median value.

Fig. 5.4 shows that, particularly, $c_D = -2.8^{+3.2}_{-1.6}$ is not well constrained by this fit protocol, exhibiting long tails, and its distribution is cut off at the lower edge of the prior, $|c_D| \leq 5$. While positive values of F_2 are slightly favored, our constraints are statistically consistent with $F_2 = 0$ at the 68% level. We emphasize again that these NN and 3N interactions are constructed only for exploratory purposes, serving to investigate how PMM–IMSRG can constrain nuclear forces to reproduce empirical saturation properties.

In Fig. 5.5, the associated posterior for the saturation properties (black contours) remains consistent with empirical expectations (blue contours representing the prior), although the posterior consistently suggests higher values for those low-density EOS parameters, especially for $K \approx 286^{+37}_{-26}$ MeV. In addition, we no longer observe a Coester-like anticorrelation of n_{sat} and E_{sat} , as reflected by the Pearson correlation coefficient $\rho = 0.21$ [115]. This is likely a consequence of the relatively tight constraints imposed on n_{sat} and E_{sat} , which restrict the posterior LECs to a narrow region of parameter space. When these constraints are relaxed, the Coester-like anticorrelation reemerges. However, the mode of the predicted saturation point distribution, $p(n_{\text{sat}}, E_{\text{sat}})$, is close to the 68% contour of the empirical point, so closer than with $F_2 = 0$ alone, as was expected. These features reflect the fact that, in the present analysis, the LECs are constrained only by empirical saturation properties. Consequently, the calibration does not yet incorporate important information from few-body observables, which is essential for further constraining the magnitudes of the LECs.

In future work, it will be interesting to incorporate constraints from finite nuclei, including the ^3H binding energy and ^4He charge radius, but also heavier nuclei, as was done in Ref. [114]. Our PMM–IMSRG emulator with conformal prediction can be applied straightforwardly to these nuclear structure calculations, providing a unified IMSRG framework for both finite nuclei and infinite matter.

Finally, we stress that this type of Bayesian calibration, based on our IMSRG calculations without PMM–IMSRG, would have been computationally challenging, if not impossible, given the computational resources available to us. Our emulator accelerates IMSRG calculations of the nuclear EOS by roughly five orders of magnitude, enabling efficient propagation of LEC uncertainties to the EOS and derived quantities, thereby enabling Bayesian workflows such as parameter estimation.

5.4 Propagating LEC Uncertainties to the EOS

Next, we propagate 10 000 posterior LEC samples (c_D, c_E, F_2) , as depicted in Fig. 5.4, to the nuclear EOS to quantify its parametric uncertainties. Specifically, using the PMM–IMSRG emulator, we evaluate the energies of particles in PNM and SNM for $n = [0.08, 0.24] \text{ fm}^{-3}$ with a constant spacing of 0.01 fm^{-3} .

In addition to these parametric uncertainties, for each LEC sample, we employ the pointwise Bayesian truncation error model developed by the BUQEYE collaboration [21, 22] to estimate EFT truncation error in the energy per particle. This truncation error arises from performing EFT calculations in practice at a finite chiral order. Given a set of order-by-order many-body calculations in the chiral EFT expansion and physics-informed priors, the BUQEYE model learns the convergence pattern of these successive calculations and sums the contributions from omitted orders to all orders. The pointwise model neglects important correlations in the density, which is an approximation that should be revisited.

We adopt $Q(k_F) = k_F/\Lambda_b$ as the EFT expansion parameter in medium, where $k_F(n) = 4\pi\sqrt[3]{n/N}$ denotes the Fermi momentum in the finite box and N the particle number (i.e., $N = 66$ for PNM and $N = 132$ for SNM), and take the breakdown scale to be $\Lambda_b = 600 \text{ MeV}$. The model’s

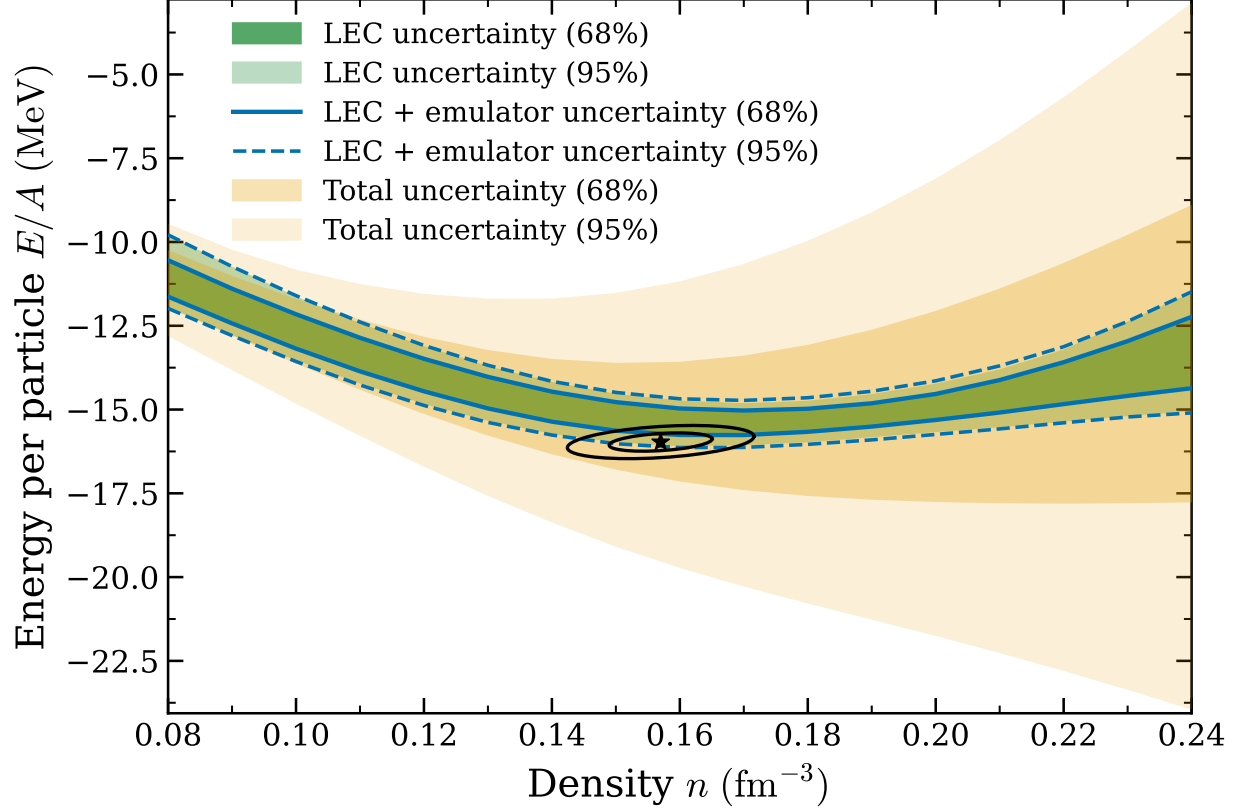


Figure 5.6 Same as Fig. 5.2 but for the LEC samples in Fig. 5.4.

hyperparameters are set to $\mu_0 = \tau_0 = 1$, and the reference scale is chosen to be $y_{\text{ref}} = 16$ MeV for both PNM and SNM calculations.

With these prerequisites in place, we construct credible intervals for our IMSRG calculations. Figures 5.6 and 5.7 show the corresponding uncertainty bands in the SNM and PNM EOSs, respectively, obtained using the PMM–IMSRG emulator. The green bands correspond to the LEC uncertainty; the blue solid and dashed curves delimit the combined LEC and emulator uncertainties at the 68% and 95% credibility levels, respectively; the orange bands represent the total uncertainty, including the EFT truncation error, at the corresponding credibility levels. In SNM, as one might have expected, we observe a clear hierarchy of uncertainties, with the EFT truncation error as the dominant source and the emulator uncertainties the smallest, indicating that omitting EFT truncation errors from the likelihood is an important limitation of the present Bayesian calibration and should be revisited in the future. In PNM, we find that the propagated LEC uncertainty band is

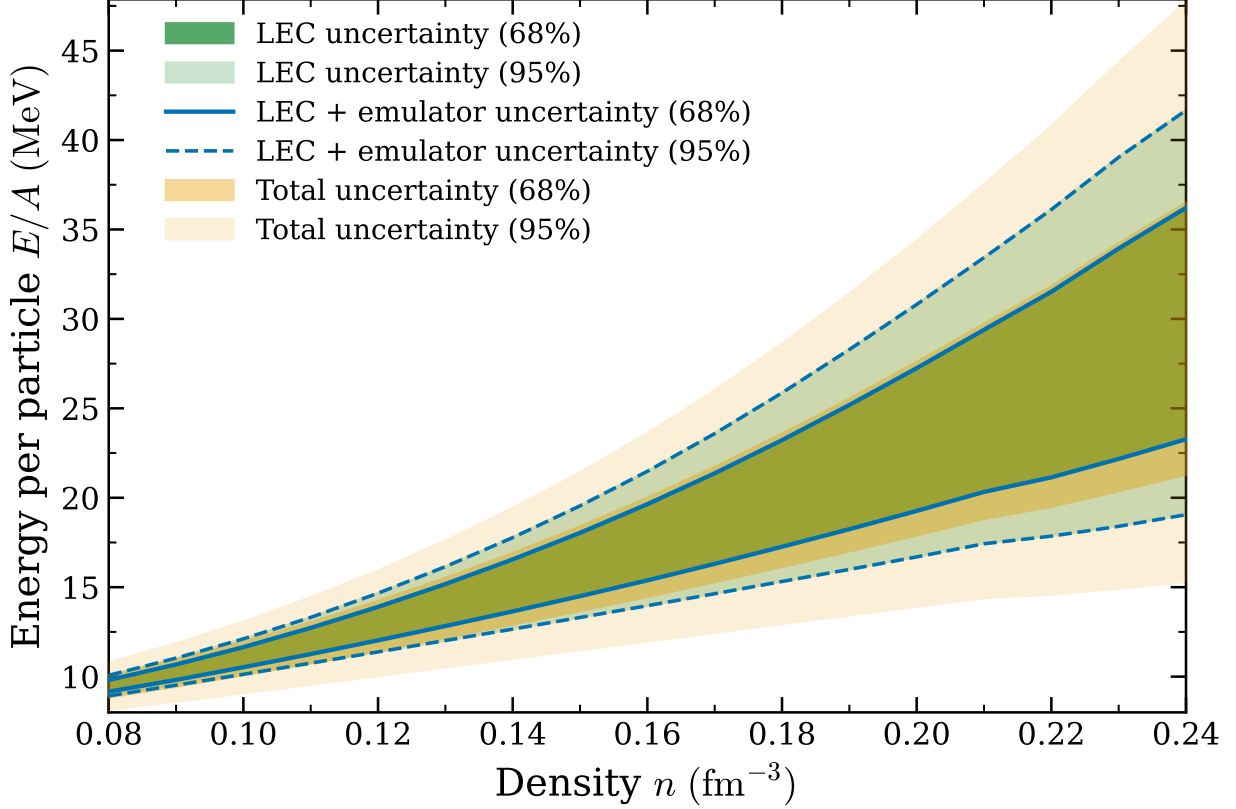


Figure 5.7 Same as Fig. 5.6 but for PNM, where c_D and c_E do not contribute in contrast to F_2 .

wider than in SNM at densities above 0.09 fm^{-3} , and the hierarchy of uncertainties found in SNM is no longer observed. Although this may appear counterintuitive at first, it is a direct consequence of the applied fit protocol. The PNM EOS is mainly constrained by the weakly informed prior on the symmetry energy and its slope parameter evaluated at the saturation density. The latter is proportional to the pressure in PNM at that density. Since the saturation point in SNM is more tightly constrained and F_2 contributes to the PNM EOS, whereas c_D and c_E do not, we obtain only weakly constrained results for the PNM EOS. It would be interesting to incorporate additional PNM constraints, e.g., from nuclear experiments and neutron star observations, into this fit protocol.

In Ref. [114], the impact of including F_2 was analyzed for light- and medium-mass nuclei. They found that while its inclusion can have a significant impact on the ground state energies and charge radii, this is mainly due to changes in the other short-range 3N couplings, c_D and c_E . In particular, they found that the expectation value of the F_2 term was much smaller than the c_D and c_E terms.

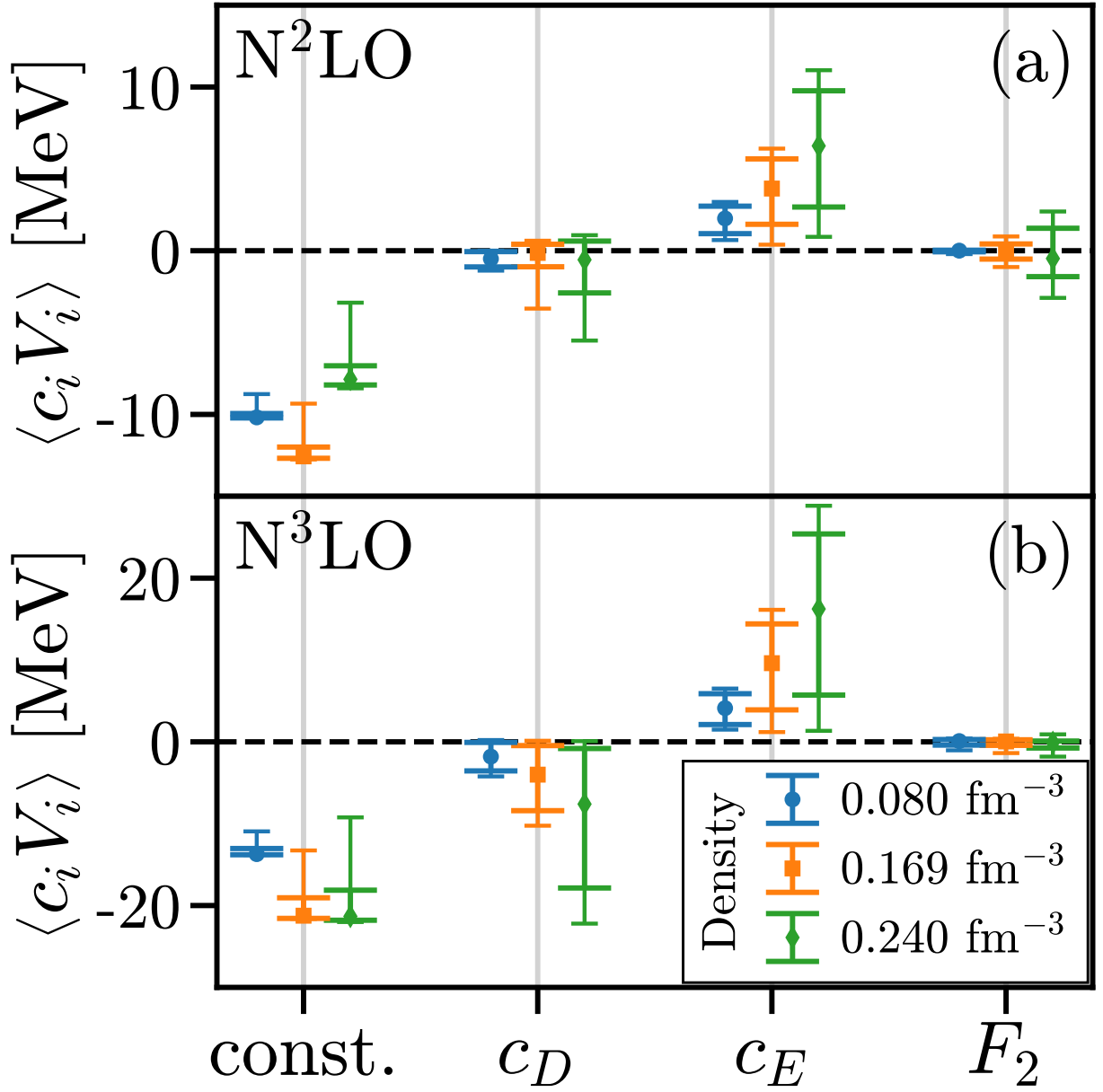


Figure 5.8 Median expectation values of each term in the emulated Hamiltonian with 68% and 95% credible intervals from posterior LEC samples at N²LO (panel a) and N³LO (panel b) at three different densities for SNM. The labels on the horizontal axis indicate the individual $c_i V_i$ term where “const.” denotes the fixed V_0 term in the emulator.

Since our emulator internally mimics the form of the Hamiltonian for the EMN interaction via Eq. (4.8), this allows us to extract the individual operators from the PMM, along with the emulated ground state wavevector, to compute the expectation values of the F_2 , c_D , and c_E terms, as well as the remaining part of the Hamiltonian, denoted by V_0 , that does not depend on these 3N LECs in the ground state. Fig. 5.8 shows these expectation values and the associated 68% and 95% credible intervals obtained from posterior LEC samples at N²LO (panel a) and N³LO (panel b), at the posterior median saturation density $n_{\text{sat}} = 0.169 \text{ fm}^{-3}$, and the minimum and maximum densities considered in the training data, $n_{\text{min}} = 0.08 \text{ fm}^{-3}$ and $n_{\text{max}} = 0.240 \text{ fm}^{-3}$. Consistent with the findings of Ref. [114], the expectation value of the F_2 term in all cases is significantly smaller in magnitude than the c_D , c_E , and V_0 terms at all three densities.

Taken together, the results of our exploratory studies of F_2 contributions demonstrate the viability of the present emulator-driven Bayesian framework and highlight an important limitation. Additional constraints from light (and even medium-mass) nuclei would help improve the predictive power of these chiral NN and 3N forces for nuclear structure and nuclear matter calculations. Adding these complementary constraints to the Bayesian fit protocol will be an important direction for future work [114].

5.5 Summary and Outlook

We have developed a fast, accurate, and physically-consistent PMM emulator for (nonperturbative) IMSRG calculations of the nuclear EOS [80, 103] in PNM and SNM across the space of LECs, density, flow parameter, and basis size. This emulator enables principled UQ of the nuclear EOS, including emulator error estimation and LEC variations, a task that was previously computationally prohibitive. The emulator uncertainty estimation via conformal predictions developed in this work is generally applicable and not limited to EOS or IMSRG calculations. It also enables controlled extrapolation of slowly converging (or even diverging) IMSRG calculations to much lower resolution scales. The resulting low-resolution potentials could be used to accelerate the convergence of many-body approaches based on diagrammatic expansions of the many-body Schrödinger equation, such as MBPT, thereby facilitating *ab initio* studies of low-density nuclear matter across a wide

range of many-body frameworks.

To demonstrate the efficacy of this framework, we propagated parametric uncertainties of order-by-order chiral NN and 3N interactions up to $N^3\text{LO}$ developed in Ref. [98] to the EOS in the limits of PNM and SNM. Leveraging our PMM–IMSRG emulator, we achieved computational speedups of five orders of magnitude, emphasizing that these calculations would not have been feasible (given our computational resources) without emulation. Together with quantified emulator and EFT truncation errors, this enabled principled UQ that captured the dominant sources of theoretical uncertainty in the nuclear EOS.

We then constructed exploratory chiral NN and 3N interactions that incorporate the promoted quark-mass-dependent 3N interaction governed by F_2 (with the other proportional to D_2 omitted, following Ref. [114]), and calibrated the leading 3N LECs c_D , c_E , and F_2 to empirical saturation properties of nuclear matter using Bayesian parameter estimation. These interactions are not intended to be state-of-the-art, but rather to serve as explorations of constraining nuclear forces using the IMSRG to reproduce empirical saturation properties. Taken together, our results demonstrate the viability and efficacy of the PMM–IMSRG framework for Bayesian calibration and uncertainty quantification, while highlighting the need for complementary constraints from few-body systems and finite nuclei to pin down the allowed values and the impact of these LECs.

Looking ahead, we plan to extend this framework to emulate the EOS across a range of proton fractions and temperatures, enabling the construction of uncertainty-quantified nuclear EOSs derived from microscopic Hamiltonians and directly applicable to astrophysical simulations of supernovae and binary mergers. Furthermore, it will be of interest to perform a joint analysis of light- to medium-mass nuclei and nuclear matter within our PMM–IMSRG emulator framework, and to systematically combine EFT truncation and emulator uncertainties in the Bayesian calibration, which can be straightforwardly extended to these nuclear-structure calculations. This effort can be complemented by recent Bayesian analysis of two- and three-body scattering observables facilitated by fast and accurate scattering emulators [120, 121, 122, 117, 123]. Such a combined analysis has the potential to shed light on the importance of nuclear saturation properties in infinite matter for

reproducing binding energies and charge radii of medium-mass to heavy nuclei [55, 56]. Altogether, these advances in emulator-driven *ab initio* calculations, with theoretical uncertainties rigorously quantified, are highly exciting, as they pave the way for new insights into strongly interacting, strongly correlated systems that appeared computationally infeasible until recently.

CHAPTER 6

CLOSING REMARKS

6.1 Summary

Nuclear matter is a system of both theoretical and practical importance, and its EOS provides a key connection between microscopic nuclear physics and the properties of dense astrophysical objects such as neutron stars. In this thesis, we have developed an IMSRG framework for nonperturbative calculations of the zero-temperature nuclear matter EOS for PNM, SNM, and generic ANM at selected proton fractions, based on a finite-volume modeling of the many-body system. We analyzed the convergence behavior and computational scaling of our implementation and showed that two important sources of systematic uncertainty—the convergence with respect to the single-particle basis size and finite-size effects—are small and can be controlled.

We then applied this framework to two classes of chiral EFT interactions, including the Hebeler interactions and the EMN interactions at a momentum cutoff of 500MeV, with the 3N contributions treated in the NO2B approximation, and compared the resulting IMSRG EOSs with calculations from other many-body methods, including MBPT and CC. For the more perturbative PNM system, the agreement among the different many-body methods is generally very good. For SNM, where correlations are stronger, good agreement is still found for the softer Hebeler interactions, whereas more noticeable differences emerge for the harder EMN interactions. A detailed analysis of these discrepancies shows that the observed systematics are consistent with those found in IMSRG studies of finite nuclei. Beyond PNM and SNM, the framework can also be applied to generic ANM at selected proton fractions, which is of particular interest for connection to neutron-star matter in beta equilibrium.

Our implementation is based on the Magnus formulation of the IMSRG, which naturally enables the consistent evolution of operators and therefore calculations of ground-state observables beyond the energy. We demonstrated this capability through proof-of-principle calculations of the single-nucleon momentum distribution and static structure factor, with the latter also used to obtain the pair distribution function. As expected, comparisons with the corresponding free-Fermi-gas results

reveal systematics similar to those found for the EOS.

Having established the IMSRG–EOS framework, however, our plan to carry out large-scale uncertainty-quantification studies of the nuclear EOS was delayed by the computational cost of performing the large number of IMSRG calculations required. To address this limitation, we constructed a fast and accurate emulator for the IMSRG–EOS framework based on the recently developed PMM. The PMM can be viewed as a non-intrusive reduced-order modeling approach that retains the low-dimensional matrix structure and parameter dependence motivated by explicit projection-based reduced-basis methods while learning the reduced representation directly from data. By incorporating our knowledge of both the underlying physical system and the IMSRG calculation, we constructed an emulator capable of capturing the dependence of the IMSRG EOS on the chiral EFT LECs, density, single-particle basis size, and IMSRG flow parameter. Derived quantities, including nuclear matter saturation properties, can then be computed directly through the PMM from the emulated EOS. We also incorporated conformal prediction to quantify the emulator uncertainty and found that the resulting emulator achieves high accuracy on withheld test data while providing speedups of approximately five orders of magnitude over the corresponding high-fidelity IMSRG calculations.

We subsequently applied the emulator to investigate the effects of quark-mass-dependent 3N interactions, recently shown to contribute at $N^3\text{LO}$, on the saturation properties of nuclear matter. Using a Bayesian parameter-estimation framework, we constrained the coupling D_2 associated with the interaction that produces the significantly larger contribution at the Hartree–Fock level, using empirical information on the nuclear saturation point together with inferred ranges for S , L , and K from nuclear experiments. We then propagated the resulting posterior uncertainties in the LECs to the PNM and SNM equations of state. This proof-of-principle application demonstrates how the combination of IMSRG calculations, reduced-order emulation, and statistical inference can enable uncertainty-quantified predictions that would otherwise be prohibitively expensive to obtain.

6.2 Outlook

Beyond the results presented in this thesis, the two frameworks developed here provide a foundation for a wide range of extensions and future applications.

The IMSRG–EOS framework can be extended in several directions. One natural development is to improve the many-body truncation, for example through the implementation of approximate IMSRG(3) schemes [124, 99]. The framework could also be extended to finite-temperature nuclear matter EOS by building on existing finite-temperature IMSRG formulations for finite nuclei [125]. In addition, the capability to calculate physical quantities beyond the energy can be further extended to calculating more general observables, including response functions of nuclear matter [126, 127]. Such calculations would provide a more direct connection to experimentally accessible quantities and could be explored through equation-of-motion techniques [128, 93] and other approaches.

The PMM–IMSRG framework also offers several possibilities for further development. Beyond the four LECs considered in this work, the emulator can also be generalized to include LECs entering the NN interaction and the πN sector of the 3N interaction. Such an extension would make it possible to perform more complete uncertainty and sensitivity studies of the nuclear EOS. The emulator could also be extended to include emulation in the proton fraction by incorporating training data for a broader set of proton fractions.

More generally, the methodology is not restricted to IMSRG calculations or to infinite nuclear matter. The same framework could be adapted to other many-body methods, such as MBPT, and to other nuclear systems, including finite nuclei, without requiring a fundamental restructuring of the framework. Extending the framework to finite nuclei would be particularly interesting for studying the quark-mass-dependent 3N interactions considered in this work. Combining constraints from nuclear matter saturation properties with information from few-body scattering and finite-nuclei observables could provide a more comprehensive picture of their impact and lead to stronger and more consistent constraints on their couplings.

BIBLIOGRAPHY

- [1] F. Özel and P. Freire, “Masses, radii, and the equation of state of neutron stars,” *Annual Review of Astronomy and Astrophysics*, vol. 54, no. Volume 54, 2016, pp. 401–440, 2016.
- [2] L. Baiotti, “Gravitational waves from neutron star mergers and their relation to the nuclear equation of state,” *Progress in Particle and Nuclear Physics*, vol. 109, p. 103714, 2019.
- [3] A. L. Watts, N. Andersson, D. Chakrabarty, M. Feroci, K. Hebeler, G. Israel, F. K. Lamb, M. C. Miller, S. Morsink, F. Özel, A. Patruno, J. Poutanen, D. Psaltis, A. Schwenk, A. W. Steiner, L. Stella, L. Tolos, and M. van der Klis, “Colloquium: Measuring the neutron star equation of state using x-ray timing,” *Rev. Mod. Phys.*, vol. 88, p. 021001, Apr 2016.
- [4] K. Chatziioannou, H. T. Cromartie, S. Gandolfi, I. Tews, D. Radice, A. W. Steiner, and A. L. Watts, “Neutron stars and the dense matter equation of state,” *Rev. Mod. Phys.*, vol. 97, no. 4, p. 045007, 2025.
- [5] B. T. Reed, F. J. Fattoyev, C. J. Horowitz, and J. Piekarewicz, “Implications of PREX-II on the equation of state of neutron-rich matter,” *Phys. Rev. Lett.*, vol. 126, no. 17, p. 172503, 2021.
- [6] X. Roca-Maza and N. Paar, “Nuclear equation of state from ground and collective excited state properties of nuclei,” *Prog. Part. Nucl. Phys.*, vol. 101, pp. 96–176, 2018.
- [7] A. Sorensen *et al.*, “Dense nuclear matter equation of state from heavy-ion collisions,” *Prog. Part. Nucl. Phys.*, vol. 134, p. 104080, 2024.
- [8] C. Drischler, J. W. Holt, and C. Wellenhofer, “Chiral Effective Field Theory and the High-Density Nuclear Equation of State,” *Annu. Rev. Nucl. Part. Sci.*, vol. 71, no. 1, pp. 403–432, 2021.
- [9] R. Machleidt, “The Meson theory of nuclear forces and nuclear structure,” *Adv. Nucl. Phys.*, vol. 19, pp. 189–376, 1989.
- [10] R. Machleidt, “The high-precision, charge-dependent Bonn nucleon-nucleon potential (CD-Bonn),” *Phys. Rev. C*, vol. 63, p. 024001, 2001.
- [11] R. B. Wiringa, V. G. J. Stoks, and R. Schiavilla, “An Accurate nucleon-nucleon potential with charge independence breaking,” *Phys. Rev. C*, vol. 51, pp. 38–51, 1995.
- [12] V. G. J. Stoks, R. A. M. Klomp, C. P. F. Terheggen, and J. J. de Swart, “Construction of high-quality NN potential models,” *Phys. Rev. C*, vol. 49, pp. 2950–2962, 6 1994.
- [13] R. Roth, J. Langhammer, A. Calci, S. Binder, and P. Navratil, “Similarity-Transformed Chiral $NN+3N$ Interactions for the Ab Initio Description of ^{12}C and ^{16}O ,” *Phys. Rev. Lett.*, vol. 107, p. 072501, 2011.
- [14] R. Roth, S. Binder, K. Vobig, A. Calci, J. Langhammer, and P. Navratil, “Ab Initio Calculations of Medium-Mass Nuclei with Normal-Ordered Chiral $NN+3N$ Interactions,” 2011.

- [15] F. Coester, S. Cohen, B. Day, and C. M. Vincent, “Variation in Nuclear-Matter Binding Energies with Phase- Shift-Equivalent Two-Body Potentials,” *Phys. Rev. C*, vol. 1, pp. 769–776, 1970.
- [16] S. C. Pieper, V. R. Pandharipande, R. B. Wiringa, and J. Carlson, “Realistic models of pion-exchange three-nucleon interactions,” *Phys. Rev. C*, vol. 64, p. 014001, 2001.
- [17] S. C. Pieper and R. B. Wiringa, “Quantum Monte Carlo Calculations of Light Nuclei,” *Ann. Rev. Nucl. Part. Sci.*, vol. 51, pp. 53–90, 2001.
- [18] A. Akmal, V. R. Pandharipande, and D. G. Ravenhall, “The equation of state for nucleon matter and neutron star structure,” *Phys. Rev. C*, vol. 58, pp. 1804–1828, 1998.
- [19] E. Epelbaum, H.-W. Hammer, and U.-G. Meißner, “Modern Theory of Nuclear Forces,” *Rev. Mod. Phys.*, vol. 81, pp. 1773–1825, 2009.
- [20] R. Machleidt and D. R. Entem, “Chiral effective field theory and nuclear forces,” *Phys. Rept.*, vol. 503, pp. 1–75, 2011.
- [21] J. A. Melendez, S. Wesolowski, and R. J. Furnstahl, “Bayesian truncation errors in chiral effective field theory: nucleon-nucleon observables,” *Phys. Rev. C*, vol. 96, no. 2, p. 024003, 2017.
- [22] J. A. Melendez, R. J. Furnstahl, D. R. Phillips, M. T. Pratola, and S. Wesolowski, “Quantifying Correlated Truncation Errors in Effective Field Theory,” *Phys. Rev. C*, vol. 100, no. 4, p. 044001, 2019.
- [23] S. K. Bogner, R. J. Furnstahl, and R. J. Perry, “Similarity renormalization group for nucleon-nucleon interactions,” *Phys. Rev. C*, vol. 75, p. 061001, 2007.
- [24] S. K. Bogner, R. J. Furnstahl, and A. Schwenk, “From low-momentum interactions to nuclear structure,” *Prog. Part. Nucl. Phys.*, vol. 65, pp. 94–147, 2010.
- [25] H. Hergert, S. K. Bogner, T. D. Morris, A. Schwenk, and K. Tsukiyama, “The in-medium similarity renormalization group: A novel ab initio method for nuclei,” *Physics Reports*, vol. 621, pp. 165–222, 3 2016.
- [26] A. Tichai, R. Roth, and T. Duguet, “Many-body perturbation theories for finite nuclei,” *Front. in Phys.*, vol. 8, p. 164, 2020.
- [27] G. Hagen, T. Papenbrock, M. Hjorth-Jensen, and D. J. Dean, “Coupled-cluster computations of atomic nuclei,” *Rept. Prog. Phys.*, vol. 77, no. 9, p. 096302, 2014.
- [28] H. Hergert, “A guided tour of ab initio nuclear many-body theory,” *Frontiers in Physics*, vol. 8, p. 379, 2020.
- [29] W. H. Dickhoff and C. Barbieri, “Self-consistent Green’s function method for nuclei and nuclear matter,” *Prog. Part. Nucl. Phys.*, vol. 52, pp. 377–496, 2004.

- [30] V. Somà, “Self-consistent green’s function theory for atomic nuclei,” *Frontiers in Physics*, vol. 8, p. 340, 2020.
- [31] J. Carlson, S. Gandolfi, F. Pederiva, S. C. Pieper, R. Schiavilla, K. E. Schmidt, and R. B. Wiringa, “Quantum Monte Carlo methods for nuclear physics,” *Rev. Mod. Phys.*, vol. 87, p. 1067, 2015.
- [32] A. Gezerlis, I. Tews, E. Epelbaum, M. Freunek, S. Gandolfi, K. Hebeler, A. Nogga, and A. Schwenk, “Local chiral effective field theory interactions and quantum Monte Carlo applications,” *Phys. Rev. C*, vol. 90, no. 5, p. 054323, 2014.
- [33] S. Gandolfi, D. Lonardoni, A. Lovato, and M. Piarulli, “Atomic nuclei from quantum monte carlo calculations with chiral eft interactions,” *Frontiers in Physics*, vol. 8, p. 117, 2020.
- [34] T. Miyagi, S. R. Stroberg, P. Navrátil, K. Hebeler, and J. D. Holt, “Converged ab initio calculations of heavy nuclei,” *Phys. Rev. C*, vol. 105, no. 1, p. 014302, 2022.
- [35] B. Hu, W. Jiang, T. Miyagi, Z. Sun, A. Ekström, C. Forssén, G. Hagen, J. D. Holt, T. Papenbrock, S. R. Stroberg, and I. Vernon, “Ab initio predictions link the neutron skin of 208pb to nuclear forces,” *Nature Physics*, vol. 18, pp. 1196–1200, 2022.
- [36] I. Svensson, A. Ekström, and C. Forssén, “Bayesian estimation of the low-energy constants up to fourth order in the nucleon-nucleon sector of chiral effective field theory,” *Phys. Rev. C*, vol. 107, no. 1, p. 014001, 2023.
- [37] J. N. Kutz, S. L. Brunton, B. W. Brunton, and J. L. Proctor, *Dynamic Mode Decomposition*. Other Titles in Applied Mathematics, SIAM-Society for Industrial and Applied Mathematics, 2016.
- [38] J. A. Melendez, C. Drischler, R. J. Furnstahl, A. J. Garcia, and X. Zhang, “Model reduction methods for nuclear emulators,” *J. Phys. G*, vol. 49, no. 10, p. 102001, 2022.
- [39] D. Frame, R. He, I. Ipsen, D. Lee, D. Lee, and E. Rrapaj, “Eigenvector continuation with subspace learning,” *Phys. Rev. Lett.*, vol. 121, no. 3, p. 032501, 2018.
- [40] C. Drischler, J. A. Melendez, R. J. Furnstahl, A. J. Garcia, and X. Zhang, “BUQEYE Guide to Projection-Based Emulators in Nuclear Physics,” *Front. Phys.*, vol. 10, p. 92931, 12 2023. supplemental, interactive Python code can be found on the companion website <https://github.com/buqeye/frontiers-emulator-review>.
- [41] J. A. Davison, *Theoretical and Computational Improvements to the In-Medium Similarity Renormalization Group*. Ph. d. thesis, Michigan State University, United States – Michigan, 2023.
- [42] C. E. Rasmussen and C. K. I. Williams, *Gaussian Processes for Machine Learning*. Adaptive computation and machine learning series, Cambridge, MA: University Press Group Limited, 2006.
- [43] G. Cybenko, “Approximation by superpositions of a sigmoidal function,” *Math. Control Signal Systems*, vol. 2, pp. 303–314, 1989.

- [44] P. Cook, D. Jammooa, M. Hjorth-Jensen, D. D. Lee, and D. Lee, “Parametric matrix models,” *Nature Communications*, vol. 16, p. 5929, Jul 2025.
- [45] V. Cirigliano, M. Dawid, W. Dekens, and S. Reddy, “New class of three-nucleon forces and their implications,” *Phys. Rev. Lett.*, vol. 135, p. 022501, Jul 2025.
- [46] C. Drischler, J. Holt, and C. Wellenhofer, “Chiral effective field theory and the high-density nuclear equation of state,” *Annual Review of Nuclear and Particle Science*, vol. 71, no. Volume 71, 2021, pp. 403–432, 2021.
- [47] J. M. Lattimer and M. Prakash, “Neutron Star Observations: Prognosis for Equation of State Constraints,” *Phys. Rept.*, vol. 442, pp. 109–165, 2007.
- [48] J. M. Lattimer, “Neutron Stars and the Nuclear Matter Equation of State,” *Ann. Rev. Nucl. Part. Sci.*, vol. 71, pp. 433–464, 2021.
- [49] J. M. Lattimer, “The nuclear equation of state and neutron star masses,” *Ann. Rev. Nucl. Part. Sci.*, vol. 62, pp. 485–515, 2012.
- [50] B. A. Brown, “Neutron radii in nuclei and the neutron equation of state,” *Phys. Rev. Lett.*, vol. 85, pp. 5296–5299, 2000.
- [51] R. J. Furnstahl, “Neutron radii in mean field models,” *Nucl. Phys. A*, vol. 706, pp. 85–110, 2002.
- [52] J. M. Lattimer, “Constraints on the Nuclear Symmetry Energy from Experiments, Theory and Observations,” *J. Phys. Conf. Ser.*, vol. 2536, no. 1, p. 012009, 2023.
- [53] S. Shlomo and D. H. Youngblood, “Nuclear matter compressibility from isoscalar giant monopole resonance,” *Phys. Rev. C*, vol. 47, pp. 529–536, 1993.
- [54] U. Garg and G. Colò, “The compression-mode giant resonances and nuclear incompressibility,” *Prog. Part. Nucl. Phys.*, vol. 101, pp. 55–95, 2018.
- [55] J. Hoppe, C. Drischler, K. Hebeler, A. Schwenk, and J. Simonis, “Probing chiral interactions up to next-to-next-to-next-to-leading order in medium-mass nuclei,” *Phys. Rev. C*, vol. 100, no. 2, p. 024318, 2019.
- [56] B. S. Hu, A. Ekström, C. Forssén, G. Hagen, W. G. Jiang, T. Miyagi, and T. Papenbrock, “The neutron dripline in calcium isotopes from a chiral interaction,” 12 2025.
- [57] M. Bender, P.-H. Heenen, and P.-G. Reinhard, “Self-consistent mean-field models for nuclear structure,” *Rev. Mod. Phys.*, vol. 75, pp. 121–180, 2003.
- [58] M. Kortelainen, T. Lesinski, J. More, W. Nazarewicz, J. Sarich, N. Schunck, M. V. Stoitsov, and S. Wild, “Nuclear Energy Density Optimization,” *Phys. Rev. C*, vol. 82, p. 024313, 2010.
- [59] W. G. Jiang, C. Forssén, T. Djärv, and G. Hagen, “Nuclear-matter saturation and symmetry energy within Δ -full chiral effective field theory,” *Phys. Rev. C*, vol. 109, no. 6, p. L061302, 2024.

- [60] A. Ekström, G. R. Jansen, K. A. Wendt, G. Hagen, T. Papenbrock, B. D. Carlsson, C. Forssén, M. Hjorth-Jensen, P. Navrátil, and W. Nazarewicz, “Accurate nuclear radii and binding energies from a chiral interaction,” *Phys. Rev. C*, vol. 91, no. 5, p. 051301, 2015. [Erratum: *Phys.Rev.C* 109, 059901 (2024)].
- [61] D. R. Entem, R. Machleidt, and Y. Nosyk, “High-quality two-nucleon potentials up to fifth order of the chiral expansion,” *Phys. Rev. C*, vol. 96, no. 2, p. 024004, 2017.
- [62] E. Epelbaum, H. Krebs, and U. G. Meißner, “Precision nucleon-nucleon potential at fifth order in the chiral expansion,” *Phys. Rev. Lett.*, vol. 115, no. 12, p. 122301, 2015.
- [63] P. Reinert, H. Krebs, and E. Epelbaum, “Semilocal momentum-space regularized chiral two-nucleon potentials up to fifth order,” *Eur. Phys. J. A*, vol. 54, no. 5, p. 86, 2018.
- [64] W. G. Jiang, A. Ekström, C. Forssén, G. Hagen, G. R. Jansen, and T. Papenbrock, “Accurate bulk properties of nuclei from $A = 2$ to ∞ from potentials with Δ isobars,” *Phys. Rev. C*, vol. 102, no. 5, p. 054301, 2020.
- [65] C. Drischler, K. S. McElvain, and P. Arthuis, “Many-body perturbation theory for the nuclear equation of state up to fifth order,” 3 2026.
- [66] J. Keller, C. Wellenhofer, K. Hebeler, and A. Schwenk, “Neutron matter at finite temperature based on chiral effective field theory interactions,” *Phys. Rev. C*, vol. 103, no. 5, p. 055806, 2021.
- [67] J. Keller, K. Hebeler, and A. Schwenk, “Nuclear Equation of State for Arbitrary Proton Fraction and Temperature Based on Chiral Effective Field Theory and a Gaussian Process Emulator,” *Phys. Rev. Lett.*, vol. 130, no. 7, p. 072701, 2023.
- [68] J. W. Holt and N. Kaiser, “Equation of state of nuclear and neutron matter at third-order in perturbation theory from chiral effective field theory,” *Phys. Rev. C*, vol. 95, no. 3, p. 034326, 2017.
- [69] P. Wen, J. W. Holt, and A. Blackburn, “Application of normalizing flows to nuclear many-body perturbation theory,” 12 2024.
- [70] G. Hagen, T. Papenbrock, A. Ekström, K. A. Wendt, G. Baardsen, S. Gandolfi, M. Hjorth-Jensen, and C. J. Horowitz, “Coupled-cluster calculations of nucleonic matter,” *Phys. Rev. C*, vol. 89, no. 1, p. 014319, 2014.
- [71] G. Baardsen, A. Ekström, G. Hagen, and M. Hjorth-Jensen, “Coupled-cluster studies of infinite nuclear matter,” *Phys. Rev. C*, vol. 88, p. 054312, 2013.
- [72] F. Marino, W. Jiang, and S. J. Novario, “Diagrammatic ab initio methods for infinite nuclear matter with modern chiral interactions,” *Phys. Rev. C*, vol. 110, no. 5, p. 054322, 2024.
- [73] D. Lonardoni, I. Tews, S. Gandolfi, and J. Carlson, “Nuclear and neutron-star matter from local chiral interactions,” *Phys. Rev. Res.*, vol. 2, no. 2, p. 022033(R), 2020.

- [74] P. Arthuis, C. Barbieri, F. Pederiva, and A. Roggero, “Quantum Monte Carlo calculations in configuration space with three-nucleon forces,” *Phys. Rev. C*, vol. 107, no. 4, p. 044303, 2023.
- [75] B. Fore, J. Kim, M. Hjorth-Jensen, and A. Lovato, “Investigating the crust of neutron stars with neural-network quantum states,” *Commun. Phys.*, vol. 8, no. 1, p. 108, 2025.
- [76] A. Lovato, G. Carleo, B. Fore, M. Hjorth-Jensen, J. Kim, A. Rios, and N. Rocco, “Neural-network quantum states for the nuclear many-body problem,” 2 2026.
- [77] R. Hu, S. Jin, X. Zhen, H. Shang, J. Pei, F. Xu, and F. Marino, “*Ab Initio* Exact Calculation of Strongly-Correlated Nucleonic Matter,” 8 2025.
- [78] F. Marino, C. Barbieri, and G. Colò, “Gorkov algebraic diagrammatic construction for infinite nuclear matter,” *Phys. Rev. C*, vol. 113, no. 6, p. 064301, 2026.
- [79] A. Rios, “Green’s Function Techniques for Infinite Nuclear Systems,” *Front. in Phys.*, vol. 8, p. 387, 2020.
- [80] O. C. Udiani, *Extending the In-Medium Similarity Renormalization Group to Nuclear Matter with Novel Insights on Unitary Coupled-Cluster Theory*. PhD thesis, Michigan State University, East Lansing, MI, 2025.
- [81] X. Zhen, R. Hu, H. Shang, J. Chen, J. Pei, and F. Xu, “Non-perturbative calculations of nuclear matter using in-medium similarity renormalization group,” *Phys. Lett. B*, vol. 862, p. 139350, 2025.
- [82] H. Hergert, S. K. Bogner, J. G. Lietz, T. D. Morris, S. J. Novario, N. M. Parzuchowski, and F. Yuan, *In-Medium Similarity Renormalization Group Approach to the Nuclear Many-Body Problem*, pp. 477–570. Cham: Springer International Publishing, 2017.
- [83] S. R. Stroberg, H. Hergert, S. K. Bogner, and J. D. Holt, “Nonempirical interactions for the nuclear shell model: An update,” *Annu. Rev. Nucl. Part. Sci.*, vol. 69, pp. 307–362, 2019/10/22 2019.
- [84] S. Binder, J. Langhammer, A. Calci, P. Navratil, and R. Roth, “*AbInitio* calculations of medium-mass nuclei with explicit chiral $3N$ interactions,” *Phys. Rev. C*, vol. 87, no. 2, p. 021303, 2013.
- [85] T. Djärv, A. Ekström, C. Forssén, and G. R. Jansen, “Normal-ordering approximations and translational (non)invariance,” *Phys. Rev. C*, vol. 104, no. 2, p. 024324, 2021.
- [86] K. Hebeler, S. K. Bogner, R. J. Furnstahl, A. Nogga, and A. Schwenk, “Improved nuclear matter calculations from chiral low-momentum interactions,” *Phys. Rev. C*, vol. 83, p. 031301(R), 2011.
- [87] L. Coraggio, J. W. Holt, N. Itaco, R. Machleidt, L. E. Marcucci, and F. Sammarruca, “Nuclear-matter equation of state with consistent two- and three-body perturbative chiral interactions,” *Phys. Rev. C*, vol. 89, no. 4, p. 044321, 2014.

- [88] F. Wegner *Ann. Phys.*, vol. 506, p. 77, 1994.
- [89] T. D. Morris, N. M. Parzuchowski, and S. K. Bogner, “Magnus expansion and in-medium similarity renormalization group,” *Phys. Rev. C*, vol. 92, p. 034331, Sep 2015.
- [90] H. Hergert, “In-medium similarity renormalization group for closed and open-shell nuclei,” *Phys. Scripta*, vol. 92, no. 2, p. 023002, 2017.
- [91] G. Hagen *et al.*, “Coupled-cluster theory for three-body hamiltonians,” *Phys. Rev. C*, vol. 76, p. 034302, 2007.
- [92] T. D. Morris, *Systematic improvements of ab-initio in-medium similarity renormalization group calculations*. PhD thesis, Michigan State University, East Lansing, MI, 2016.
- [93] N. M. Parzuchowski, S. R. Stroberg, P. Navrátil, H. Hergert, and S. K. Bogner, “Ab initio electromagnetic observables with the in-medium similarity renormalization group,” *Phys. Rev. C*, vol. 96, no. 3, p. 034324, 2017.
- [94] J. G. Lietz, S. Novario, G. R. Jansen, G. Hagen, and M. Hjorth-Jensen, *Computational Nuclear Physics and Post Hartree-Fock Methods*, pp. 293–399. Cham: Springer International Publishing, 2017.
- [95] C. Lin, F. H. Zong, and D. M. Ceperley, “Twist-averaged boundary conditions in continuum quantum Monte Carlo,” *Phys. Rev. E*, vol. 64, p. 016702, 2001.
- [96] A. Ekström, G. Baardsen, C. Forssén, G. Hagen, M. Hjorth-Jensen, *et al.*, “An optimized chiral nucleon-nucleon interaction at next-to-next-to-leading order,” *Phys. Rev. Lett.*, vol. 110, p. 192502, 2013.
- [97] D. R. Entem and R. Machleidt, “Accurate charge-dependent nucleon-nucleon potential at fourth order of chiral perturbation theory,” *Phys. Rev. C*, vol. 68, p. 041001, 2003.
- [98] C. Drischler, K. Hebeler, and A. Schwenk, “Chiral interactions up to next-to-next-to-next-to-leading order and nuclear saturation,” *Phys. Rev. Lett.*, vol. 122, no. 4, p. 042501, 2019.
- [99] S. R. Stroberg, T. D. Morris, and B. C. He, “IMSRG with flowing 3 body operators, and approximations thereof,” *preprint*, 6 2024.
- [100] A. Fetter and J. Walecka, *Quantum Theory of Many-particle Systems*. Dover Books on Physics, Dover Publications, 2003.
- [101] R. Kumar *et al.*, “Theoretical and experimental constraints for the equation of state of dense and hot matter,” *Living Rev. Rel.*, vol. 27, no. 1, p. 3, 2024.
- [102] K. Agarwal, J. Jahan, B. Kardan, P. T. H. Pang, T. Reichert, and A. C. Semposki, “Toward a Unified Understanding of the Dense Matter Equation of State,” 11 2025.
- [103] O. Udiani, K. Yu, C. Drischler, S. J. Novario, and S. K. Bogner, “In-medium similarity renormalization group calculations of nuclear matter.” in *prep.*, 2026.

- [104] T. Duguet, A. Ekström, R. J. Furnstahl, S. König, and D. Lee, “Colloquium: Eigenvector continuation and projection-based emulators,” *Rev. Mod. Phys.*, vol. 96, no. 3, p. 031002, 2024.
- [105] C. L. Armstrong, B. T. Reed, T. Plohr, H. Rose, S. De, R. Somasundaram, and I. Tews, “Constraining Hamiltonians from chiral effective field theory with neutron-star data,” 1 2026.
- [106] C. L. Armstrong, P. Giuliani, K. Godbey, R. Somasundaram, and I. Tews, “Emulators for Scarce and Noisy Data: Application to Auxiliary-Field Diffusion Monte Carlo for Neutron Matter,” *Phys. Rev. Lett.*, vol. 135, no. 14, p. 142501, 2025.
- [107] R. Somasundaram, C. L. Armstrong, P. Giuliani, K. Godbey, S. Gandolfi, and I. Tews, “Emulators for scarce and noisy data: Application to auxiliary field diffusion Monte Carlo for the deuteron,” *Phys. Lett. B*, vol. 866, p. 139558, 2025.
- [108] W. G. Jiang, C. Forssén, T. Djärv, and G. Hagen, “Emulating ab initio computations of infinite nucleonic matter,” *Phys. Rev. C*, vol. 109, no. 6, p. 064314, 2024.
- [109] K. Hebeler and A. Schwenk, “Chiral three-nucleon forces and neutron matter,” *Phys. Rev. C*, vol. 82, p. 014314, 2010.
- [110] A. N. Angelopoulos and S. Bates, “Conformal prediction: A gentle introduction,” *Foundations and Trends in Machine Learning*, vol. 16, pp. 494–591, 03 2023.
- [111] R. Hulsman, “Distribution-free finite-sample guarantees and split conformal prediction,” 2022.
- [112] H. Y. Dezdaran, R. Curry, and A. Gezerlis, “Conformal prediction for uncertainties in nucleon-nucleon scattering,” *Phys. Rev. C*, vol. 113, no. 1, p. 014004, 2026.
- [113] H. Y. Dezdaran, R. Curry, C. L. Armstrong, and A. Gezerlis, “Conformal prediction for uncertainties in the neutron star equation of state,” 4 2026.
- [114] U. Vernik, K. Hebeler, and A. Schwenk, “Exploring quark mass dependent three-nucleon forces in medium-mass nuclei,” 12 2025.
- [115] C. Drischler, P. G. Giuliani, S. Bezoui, J. Piekarewicz, and F. Viens, “Bayesian mixture model approach to quantifying the empirical nuclear saturation point,” *Phys. Rev. C*, vol. 110, no. 4, p. 044320, 2024.
- [116] N. L. Carter, R. J. Furnstahl, J. A. Melendez, and D. R. Phillips, “Neglecting correlations leads to misestimated model errors in EFT predictions,” 2 2026.
- [117] A. Giri, J. Kim, C. Drischler, C. Elster, and R. J. Furnstahl, “Active learning emulators for nuclear two-body scattering in momentum space,” *Phys. Rev. C*, vol. 113, no. 4, p. 044001, 2026.
- [118] G. Casella and R. L. Berger, *Statistical Inference*. Chapman & Hall/CRC Texts in Statistical Science, Pacific Grove, CA: Duxbury Press, 2 ed., 2002.

- [119] D. Foreman-Mackey, D. W. Hogg, D. Lang, and J. Goodman, “emcee: The MCMC Hammer,” , vol. 125, p. 306, Mar. 2013.
- [120] A. Gnech, X. Zhang, C. Drischler, R. J. Furnstahl, A. Grassi, A. Kievsky, L. E. Marcucci, and M. Viviani, “Accurate and Efficient Emulation of Proton-Deuteron Scattering via the Reduced Basis Method and Active Learning,” 11 2025.
- [121] A. Gnech, X. Zhang, C. Drischler, R. J. Furnstahl, A. Grassi, A. Kievsky, L. E. Marcucci, and M. Viviani, “Emulation of Proton-Deuteron Scattering via the Reduced Basis Method and Active Learning: Detailed Description,” 11 2025.
- [122] J. M. Maldonado, C. Drischler, R. J. Furnstahl, and P. Mlinarić, “Greedy emulators for nuclear two-body scattering,” *Phys. Rev. C*, vol. 112, no. 2, p. 024002, 2025.
- [123] S. Heihoff, A. A. Filin, and E. Epelbaum, “Exact emulation of few-body systems at low cost,” 4 2026.
- [124] B. C. He and S. R. Stroberg, “Factorized Approximation to the IMSRG(3),” *preprint*, 5 2024.
- [125] I. G. Smith, H. Hergert, and S. K. Bogner, “In-medium similarity renormalization group at finite temperature,” *Phys. Rev. C*, vol. 111, no. 4, p. 044318, 2025.
- [126] G. I. Lykasov, C. J. Pethick, and A. Schwenk, “A unified approach to structure factors and neutrino processes in nucleon matter,” *Phys. Rev. C*, vol. 78, p. 045803, 2008.
- [127] S. Bacca, K. Hally, C. J. Pethick, and A. Schwenk, “Chiral effective field theory calculations of neutrino processes in dense matter,” *Phys. Rev. C*, vol. 80, p. 032802, 2009.
- [128] N. M. Parzuchowski, T. D. Morris, and S. K. Bogner, “Ab initio excited states from the in-medium similarity renormalization group,” *Phys. Rev. C*, vol. 95, p. 044304, Apr 2017.