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Ab initio nuclear structure theory

Gianina Alina Negoita

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Ab initio nuclear structure theory

by

Gianina Alina Negoita

A dissertation submitted to the graduate faculty
in partial fulfillment of the requirements for the degree of

DOCTOR OF PHILOSOPHY

Major: Nuclear Physics

Program of Study Committee:
James Vary, Major Professor
James Evans
Marzia Rosati
Kirill Tuchin
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Iowa State University
Ames, Iowa
2010

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DEDICATION

This thesis is dedicated to my wonderful grandparents, Gheorghe and Maria Croitoru, who passed away while I was writing it. They have raised me to be the person I am today and they always loved me, supported me, and appreciated me...

I love you and I will never forget you!
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Thank you for everything!
Ab initio no core methods have become major tools for understanding the properties of light nuclei based on realistic nucleon-nucleon ($NN$) and three-nucleon ($NNN$) interactions. A brief description is provided for the inter-nucleon interactions that fit two-body scattering and bound state data, as well as $NNN$ interactions. Major new progress, including the goal of applying these interactions to solve for properties of nuclei, is limited by convergence issues. That is, with the goal of obtaining high precision solutions of the nuclear many-body Hamiltonian with no core methods (all nucleons treated on the same footing), one needs to proceed to very large basis spaces to achieve a convergence pattern suitable for extrapolation to the exact result. This thesis investigates (1) the similarity renormalization group (SRG) approach to soften the interaction, while preserving its phase shift properties, and (2) adoption of a realistic basis space using Woods-Saxon (WS) single-particle wavefunctions. Both have their advantages and limitations, discussed here. For (1), SRG was demonstrated by applying it to a realistic $NN$ interaction, JISP16, in a harmonic oscillator (HO) representation. The degree of interaction softening achieved through a regulator parameter is examined. For (2), new results are obtained with the realistic JISP16 $NN$ interaction in ab initio calculations of light nuclei $^4$He, $^6$He and $^{12}$C, using a WS basis optimized to minimize the ground-state energy within the truncated no core shell model. These are numerically-intensive many-body calculations.

Finally, to gain insight into the potential for no core investigations of heavier nuclei, an initial investigation was obtained for the odd mass $A = 47 - 49$ region nuclei straddling $^{48}$Ca. The motivation for selecting these nuclei stems from the aim of preparing for nuclear double beta-decay studies of $^{48}$Ca. In these heavier systems, phenomenological additions to
the realistic $NN$ interaction determined by previous fits to $A = 48$ nuclei are needed to fit the data. The modified Hamiltonian produces reasonable spectra for these odd mass nuclei. A look at future pathways opened up with the results presented here concludes this investigation.
CHAPTER 1. INTRODUCTION

The formulation of a many-body problem, based on the two-body interaction, is an old idea first used for the gravitational force by Newton. Newton’s theory of gravitation explains many phenomena successfully. For instance, the trajectories of celestial bodies can be predicted almost precisely by this theory. A two-body interaction can be used easily for a many-body system by imposing the force acting between each of the two bodies in the system, sometimes called the additivity principle.

The additivity principle works for Coulomb’s electrical potential as well as the Newtonian gravitational potential. The electromagnetic theory and Newton’s theory of mechanics worked successfully until the late 19th century, when it appeared the Galilean transformation, under which Newton’s laws are invariant, cannot be used for Maxwell’s equations. During that time, it was not known which of the theories needed correction. Moreover, there were a few new phenomena, such as black body radiation, that could not be explained by these theories. During the early 20th century, two new theories were introduced that could explain all known phenomena: relativity and quantum mechanics. Relativity solved the inconsistency between Newtonian theory and Maxwell’s theory of electromagnetism. It improved Newtonian theory and kept Maxwell’s equations as derived by Maxwell. It was shown the relativistic formulation of mechanics becomes Newtonian mechanics for a low velocity. Quantum mechanics could also explain other new phenomena, such as the photo-electric phenomenon. As far as Newtonian gravitation and electromagnetic interactions are concerned, the two-body potential is adequate to explain the natural phenomena of many-body systems, if the sizes of the bodies are small in comparison with the distance between them (the bodies are essentially point-like objects). However, massive gravitational objects are composites and, sometimes, they cannot
be considered as point-like bodies.

During the 20th century, the discovery of weak and strong interactions opened a new world for physics and raised new questions. The weak interaction is responsible for $\beta$-decay and the strong interaction keeps the nucleons together in nuclei. In contrast to Newton’s gravitation theory, it was not easy to establish a potential function for the new forces, due to the lack of experimental evidence and knowledge about these forces in the early 20th century. However, some of the physical aspects of the forces were understood phenomenologically. For example, the strong interaction must be much stronger than the electromagnetic interaction, since the protons are held together within nuclei by the attractive strong force, which more than compensates for the repulsive Coulomb force. Also, the strong force must be a short-range force. If it were a long-range potential, as the electromagnetic potential, the whole universe would collapse or the universe would not have evolved from the Big Bang. The weak interaction is weaker than the electromagnetic interaction, as its name suggests. Discussion about the weak interaction is outside the scope of this thesis and, therefore, it is not further mentioned. Below is a discussion of how the concepts of the strong force in the nuclear system have developed over the past few decades.

The ultimate goal of nuclear physics would be to describe all nuclear interactions beginning with the basic interactions between nucleons. This is the goal of the microscopic or ab initio approach of nuclear physics. There are two major obstacles to overcome before this dream can become a reality:

1. Calculations in many-body systems are difficult and require advanced computation techniques

2. There is evidence that three-nucleon forces (and possibly higher multi-particle interactions) play a significant role.

This means that three-nucleon potentials must be included in the approach. This active area of research includes recent advances in computational techniques leading to better first-principles calculations of the nuclear shell structure. Two- and three-nucleon (NN and NNN) potentials have been implemented for nuclear masses up to $A = 17$. 
The first step in understanding the strong force is to establish the $NN$ potential. If this force is under control, one might then employ the additivity principle to solve problems involving three or more bodies. This picture looks very classical. Nevertheless, it can answer questions about many-body systems to a certain degree of accuracy. To achieve a realistic $NN$ potential, there are many unanswered questions, such as:

- What is the functional form of the potential?
- What is the range of the potential?
- What is the mechanism for exchanging the force?
- What are the spin and isospin characteristics of the interaction?

As two nucleons approach, the attractive force increases, but this attraction stops at some point and turns to repulsion. This is empirically established through the property of the $S$-wave phase shifts that turn negative at higher momentum transfers. Therefore, the potential seems to be highly repulsive at distances of less than 1 $fm$. The behavior of the $NN$ potential is explained by the exchange of mesons [1]. It turned out that only the long-range of the potential is governed by the $\pi$-meson exchange and the middle-range attraction is modelled by scalar mesons, such as the $\sigma$-meson. The heavier vector mesons, such as the $\omega$-meson, contribute to the repulsive short-range part of the $NN$ potential.

In the 1960s and early 70s, the theory of Quantum Chromo-Dynamics (QCD) is developed to explain the strong force. In this theory, the hadrons are not elementary, but are made up of quarks. Quarks have color charge and interact by exchanging gluons. Hadrons are colorless compositions of quarks. Unfortunately, at low energies the interaction is so strong one cannot apply perturbative methods. Therefore, it is difficult to use QCD at low energies. One way to resolve this problem is to model the $NN$ potential semi-phenomenologically.

At the present time, there are several recent high-quality $NN$ models [2–4], which will be discussed in Sec. 1.1. There are many parameters in each model determined by fits to the world data set on $NN$ scattering and the deuteron bound state.
There is also a systematic attempt to explain the $NN$ potential fully based on effective field theory. In particular, chiral symmetry breaking can be analysed in terms of an effective field theory (called chiral perturbation theory), which allows perturbative calculations of the interactions between nucleons with pions as exchange particles. This work started with Weinberg’s idea about the low-energy expansion of the Lagrangian of QCD \[4\]. This will be discussed in Sec. 1.1.3.

1.1 A Brief History of the Intra-nucleon Interactions

The $NN$ potentials that describe the available two-nucleon data have a long and multifaceted history. High precision fits have improved with time, even as more precise experimental data have become available. $NNN$ potentials have a shorter history, but are intensively investigated at the present time.

Disparate foundations for these potentials, both $NN$ and $NNN$, have emerged. On the one hand, one sees the predominant meson-exchange potentials sometimes supplemented with phenomenological terms to achieve a high accuracy in fitting $NN$ data (Yukawa, CD-Bonn, Nijmegen I and II, Argonne v18, Idaho) and $NNN$ data (Urbana, Illinois, Tucson-Melbourne). On the other hand, one sees the emergence of potentials with ties to QCD, either meson-free or intertwined with meson-exchange theory (Chiral N3LO).

All these potentials are used with unprecedented success to explain a vast amount of data on light nuclei in various microscopic approaches, such as the no core shell model (NCSM) addressed in this present work. The overwhelming success of these efforts have led some to characterize these approaches as leading to a ‘Standard Model’ of non-relativistic nuclear physics.

Chief among the outstanding challenges is the computational intensity of using these $NN$ + $NNN$ potentials within the presently available many-body methods. For this reason, most ab initio investigations have been limited to $A \leq 12$. The situation would be dramatically simpler, if either the $NN$ potential alone would be sufficient or the potentials would couple less strongly between the low-momentum and the high-momentum degrees of freedom. If both
simplifications are obtained, the future for applications would be greatly simplified.

1.1.1 JISP16 interactions

JISP16 [2] stands for J-matrix Inverse Scattering Potential tuned up to $^{16}$O. In this approach, the $NN$ interaction is constructed by means of the J-matrix version of inverse scattering theory. The matrix of the $NN$ potential in the oscillator basis is obtained for each partial wave independently and is determined by the $NN$ scattering phase shifts. The experimental $NN$ scattering data and deuteron properties have been reproduced with low-dimensional matrices. This $NN$ interaction is sufficiently “soft” that it can be directly used in no core calculations of light nuclei without additional truncation. Since it has been adjusted off-shell to reproduce selected properties of light nuclei, it is not surprising this $NN$ interaction reproduces energy spectra and other observables in a range of light nuclei [5], as well as deuteron properties and $NN$ scattering data. From this point of view, this $NN$ interaction can be treated as a realistic interaction which has been tuned to simulate the role of $NNN$ interactions that appear in other formalisms. This interaction is not related to meson exchange theory. However, one can obtain the deuteron and scattering wavefunctions very close to the ones obtained with realistic meson exchange potentials.

The potential derived by the J-matrix inverse scattering approach has ambiguities that are eliminated by a phenomenological ansatz that the potential matrix in the uncoupled partial waves is tridiagonal in the harmonic oscillator basis states of relative motion. Therefore, these potentials are referred to as Inverse Scattering Tridiagonal Potentials (ISTP).

The non-central nature of the $NN$ interaction was manifested in the coupling of some partial waves, and the tridiagonal potential ansatz was conventionally extended to allow for the coupling of these partial waves. Shirokov et al. [2] postulated phenomenologically the simplest generalization of the tridiagonal form of the potential matrix in this case. They found a simple tridiagonal ansatz produced scattering wavefunctions very close to the ones provided by the Nijmegen [6] meson exchange realistic $NN$ potentials. However, in the case of the coupled $SD$-waves, these same authors found it necessary to perform a phase equivalent
potential transformation to improve the description of the deuteron properties. The resulting ISTP potentials were used in the NCSM calculations for $^3H$ and $^4He$. The predicted $^3H$ and $^4He$ binding energies were determined very close to the experimental values. Note, $NNN$ interactions were not used here, but the predictions of the $^3H$ and $^4He$ bindings were found close to the experimental results as the theoretical predictions based on the best realistic meson exchange $NN + NNN$ forces.

The J-matrix formalism has been developed as an approach, based on the analytic properties of the harmonic oscillator (HO) representation of scattering theory. Some important relations needed to understand the inverse scattering J-matrix approach are provided below with some of the key notations adopted for this work.

The Schrödinger equation in the partial wave with orbital angular momentum, $l$, reads as

$$H^l \Psi_{lm}(E, \vec{r}) = E \Psi_{lm}(E, \vec{r}) , \quad (1.1)$$

$H^l$ indicates the potential is channel dependent. Spin is neglected in this simplified introduction, but is included in the full scattering treatment. The wavefunction is given by

$$\Psi_{lm}(E, \vec{r}) = \frac{1}{r} u_l(E, r) Y_{lm}(\hat{r}) , \quad (1.2)$$

where $Y_{lm}(\hat{r})$ is the spherical harmonic and $u_l$ is the radial wavefunction. Within the J-matrix formalism, the radial wavefunction $u_l(E, r)$ is expanded in the basis of the radial solutions of the 3-dimensional HO, $R_{nl}$ as follows

$$u_l(E, r) = \sum_{n=0}^{\infty} a_{nl}(E) R_{nl}(r) , \quad (1.3)$$

where

$$R_{nl}(r) = (-1)^n \sqrt{\frac{2n!}{r_0 \Gamma(n + l + 3/2)}} \left( \frac{r}{r_0} \right)^{l+1} \exp \left( -\frac{r^2}{2r_0^2} \right) L_{\frac{n-1}{2}} \left( \frac{r^2}{r_0^2} \right) , \quad (1.4)$$

with $L_{\alpha}(x)$ the associated Laguerre polynomial, the oscillator radius $r_0 = \sqrt{\hbar/\mu \Omega}$, and $\mu$ is the reduced mass. All energies are given in the units of the oscillator basis parameter, $\hbar \Omega$. The wavefunction expressed in the oscillator representation, $a_{nl}(E)$, is a solution of the infinite set of algebraic equations,

$$\sum_{n'=0}^{\infty} (H^l_{nn'} - \delta_{nn'}E) a_{n'l}(E) = 0 , \quad (1.5)$$
where the Hamiltonian matrix elements, \( H_{nn'}^l = T_{nn'}^l + V_{nn'}^l \), the kinetic energy matrix elements

\[
T_{n,n-1}^l = -\frac{1}{2}\sqrt{n(n+l+1/2)} ,
\]

\[
T_{n,n}^l = \frac{1}{2}(2n+l+3/2) ,
\]

\[
T_{n,n+1}^l = -\frac{1}{2}\sqrt{(n+1)(n+l+3/2)} ,
\]

and the potential energy \( V^l \) within the J-matrix formalism is approximated by the truncated matrix with elements

\[
\tilde{V}_{nn'}^l = \begin{cases} 
V_{nn'}^l & \text{if } n \text{ and } n' \leq N \\
0 & \text{if } n \text{ or } n' > N .
\end{cases}
\]

In the inverse scattering J-matrix approach, the potential energy is constructed in the form of the finite matrix of the type in Eq. (1.7). Therefore, the J-matrix solutions of the phase shifts for all energies with such an interaction are exact when the potential can be exactly truncated, according to Eq. (1.7). In the external part of the model space spanned by the functions given in Eq. (1.4) with \( n \geq N \), Eq. (1.5) takes the form of a three-term recurrence relation,

\[
T_{n,n-1}^l a_{n-1,l}(E) + (T_{nn}^l - E)a_{nl}(E) + T_{n,n+1}^l a_{n+1,l}(E) = 0 .
\]

Any solution of Eq. (1.8) is a superposition of the fundamental regular \( S_{nl}(E) \) and irregular \( C_{nl}(E) \) of the Schrödinger equation in the scattering domain:

\[
a_{nl}(E) = \cos(\delta(E))S_{nl}(E) + \sin(\delta(E))C_{nl}(E) ,
\]

where

\[
S_{nl}(E) = \sqrt{\frac{\pi r_0 n!}{\Gamma(n+l+3/2)}} q^{l+1} \exp \left( -\frac{q^2}{2} \right) \frac{1}{2^{l+1/2}} I_{n+1/2}(q^2) ,
\]

\[
C_{nl}(E) = (-1)^l \sqrt{\frac{\pi r_0 n!}{\Gamma(n+l+3/2)}} q^{-l} \exp \left( -\frac{q^2}{2} \right) \Phi(-n-l-1/2, -l+1/2; q^2) ,
\]

\( \Phi(a, b; z) \) is a confluent hypergeometric function, \( q = \sqrt{2E} \), and \( \delta(E) \) is the scattering phase shift. The wavefunction expansion coefficients in the oscillator representation \( a_{nl}(E) \) in the internal part of the model space spanned by the functions given in Eq. (1.4) with \( n \leq N \), can
be expressed through the external solution \( a_{N+1,l}(E) \):

\[
a_{nl}(E) = \zeta_{nN} T_{N,N+1}^l a_{N+1,l}(E) .
\]  

(1.12)

The matrix elements,

\[
\zeta_{nn'} = - \sum_{\lambda'=0}^{N} \frac{\langle n|\lambda'\rangle\langle \lambda'|n'\rangle}{E_{n'} - E} ,
\]  

(1.13)

are expressed through the eigenvalues, \( E_\lambda \), and eigenvectors, \( \langle n|\lambda\rangle \), of the truncated Hamiltonian matrix, i.e., \( E_\lambda \) and \( \langle n|\lambda\rangle \) are obtained by solving the algebraic problem,

\[
\sum_{n'=0}^{N} H_{nn'}^l \langle n'|\lambda\rangle = E_\lambda \langle n|\lambda\rangle , \quad n \leq N ,
\]  

(1.14)

where \( \lambda \) is just a label, such as a sequence number for the eigenvalues. The matrix element \( \zeta_{NN} \), is of primary importance in the calculation of the phase shift \( \delta(E) \), containing the information about the potential:

\[
\tan \delta(E) = - \frac{S_{Ni}(E) - \zeta_{NN} T_{N,N+1}^l S_{N+1,i}(E)}{C_{Ni}(E) - \zeta_{NN} T_{N,N+1}^l C_{N+1,i}(E)} .
\]  

(1.15)

In the direct J-matrix approach, Eq. (1.14) is solved to provide inputs for calculating the phase shift, \( \delta(E) \), by means of Eq. (1.15). In the inverse scattering J-matrix approach, the phase shift, \( \delta(E) \), is taken to be known at any energy, \( E \), and, instead of solving Eq. (1.14), one extracts the eigenvalues, \( E_\lambda \), and the eigenvectors, \( \langle n|\lambda\rangle \), from the phase shifts. First, some value is assigned to \( N \), the rank of the desired potential matrix [see Eq. (1.7)]. Generally, with a finite rank potential matrix, it is possible to reproduce the phase shift, \( \delta(E) \), only in a finite energy interval; larger \( N \) supports a larger energy interval. However, from the point of view of achieving convergence in many-body applications, it is desirable to have \( N \) as small as possible. The components, \( a_{nl}(E) \), of the wavefunction in the oscillator representation should be finite at arbitrary energy, \( E \). This is seen from Eqs. (1.12) and (1.13) to be possible at energies \( E = E_\lambda , \lambda = 0, 1, ..., N \) only if

\[
a_{N+1,l}(E_\lambda) = 0 .
\]  

(1.16)

Due to Eq. (1.16), one obtains

\[
a_{N+1,l}(E) \xrightarrow{E \to E_\lambda} a_\lambda^l(E - E_\lambda) ,
\]  

(1.17)
where

\[ \alpha^\lambda_l = \frac{d a_{N+1,l}(E)}{dE} \bigg|_{E=E^\lambda}. \]  

(1.18)

Now, it is easy to derive from Eqs. (1.12) and (1.13) the following equation:

\[ a_{Nl}(E^\lambda) = |\langle n|\lambda \rangle|^2 \alpha^\lambda_l T^l_{N,N+1}, \]  

(1.19)

or, equivalently,

\[ |\langle n|\lambda \rangle|^2 = \frac{a_{Nl}(E^\lambda)}{\alpha^\lambda_l T^l_{N,N+1}}. \]  

(1.20)

Within the J-matrix formalism, both \( a_{Nl}(E) \) and \( a_{N+1,l}(E) \) fit Eq. (1.9) and can be calculated using this equation at any energy, \( E \). Hence, one can also calculate \( \alpha^\lambda_l \) by means of Eq. (1.18).

Therefore, the components \( \langle N|\lambda \rangle \) can be obtained from Eq. (1.20) (the sign of the components \( \langle N|\lambda \rangle \) is of no importance). Equations (1.16) and (1.20) provide the general solution of the J-matrix inverse scattering problem. Solving these equations, one can obtain the sets of \( E^\lambda \) and \( \langle N|\lambda \rangle \), and these quantities completely determine the phase shifts, \( \delta(E) \). However, \( \langle N|\lambda \rangle \) are supposed to be the components of the eigenvectors, \( \langle n|\lambda \rangle \), of the truncated Hamiltonian matrix [see Eq. (1.14)] that should fit the completeness relation

\[ \sum_{\lambda=0}^{N} \langle n|\lambda \rangle \langle \lambda|n' \rangle = \delta_{nn'}. \]  

(1.21)

Hence, one should have

\[ \sum_{\lambda=0}^{N} \langle N|\lambda \rangle \langle \lambda|N \rangle = 1. \]  

(1.22)

Generally the set of \( \langle N|\lambda \rangle \) obtained by means of Eq. (1.20) violates the completeness relation for Eq. (1.22). Therefore, this set of \( \langle N|\lambda \rangle \) ideally describing the phase shifts cannot be treated as the set of last components of the normalized eigenvectors \( \langle n|\lambda \rangle \) of any truncated Hermitian-Hamiltonian matrix. In other words, the set of \( \langle N|\lambda \rangle \) violating Eq. (1.22) cannot be used to construct a Hermitian-Hamiltonian matrix. To overcome this difficulty, Eq. (1.22) can be fitted by changing the value of the component, \( \langle N|\lambda = N \rangle \), corresponding to the highest eigenvalue, \( E^\lambda=N \). This modification spoils the description of the phase shifts, \( \delta(E) \), at energies, \( E \), different from \( E^\lambda, \lambda = 0,1,...,N \). The phase shift description in the energy interval \([0,E^\lambda=N-1]\) can be restored by variation of \( E^\lambda=N \). From the above consideration, it is
clear that larger $N$ values make it possible to reproduce phase shifts in larger energy intervals $[0, E_{\lambda=N-1}]$.

There is an ambiguity in determining the potential matrix describing the given phase shifts, $\delta(E)$. Any of the phase equivalent transformations discussed in Ref. [7] that do not change the truncated Hamiltonian eigenvalues, $E_\lambda$, and respective eigenvector components, $\langle N|\lambda \rangle$, results in a potential matrix that brings the same phase shifts, $\delta(E)$, at any energy, $E$. Additional model assumptions are needed to resolve this ambiguity. A tridiagonal form of the potential matrix in the harmonic oscillator basis is assumed for simplicity. The construction of the tridiagonal potential matrix discussed by Shirokov et al. [2], assumes $N$, the sets of $E_\lambda$ and $\langle N|\lambda \rangle$ are known. If the potential matrix is tridiagonal, Eq. (1.14) can be rewritten. The authors, [2] demonstrated it was possible to calculate all unknown quantities. After calculating the Hamiltonian matrix elements, $H^l_{nn'}$, they derived the ISTP matrix elements by the obvious equations:

$$V^l_{n,n} = H^l_{n,n} - T^l_{n,n}$$ \hspace{1cm} (1.23a)


and

$$V^l_{n,n\pm 1} = H^l_{n,n\pm 1} - T^l_{n,n\pm 1}.$$ \hspace{1cm} (1.23b)

Their earlier theory was used to construct the $NN$ ISTP matrix elements in uncoupled partial waves.

JISP16 has the same symmetries as other conventional $NN$ potentials, but is not constrained by meson exchange theory, QCD or locality. It is constructed as matrices using input from the $np$ scattering phase shifts reconstructed from the experimental data by the Nijmegen group [6]. The oscillator basis parameter $\hbar\Omega = 40 \ MeV$. The dimension of the potential matrix is specified by the maximum value of $N = 2n + l$ and is referred to as the $N\hbar\Omega$ potential. To be applicable to all $p$-shell nuclei in accessible model spaces, $8\hbar\Omega$ and $7\hbar\Omega$ was suggested, i.e., the rank of the ISTP matrix $N$ is chosen such that $2N + l = 8$ in the partial waves with even orbital angular momentum, $l$, and $2N + l = 7$ in the partial waves with odd orbital angular momentum, $l$. 
The JISP16 potential in Sec. 2.2.2 is transformed with the Similarity Renormalization Group method and examine the degree of interaction softening achieved through a regulator parameter. Also, new results are obtained with the realistic bare JISP16 interaction in \textit{ab initio} calculations of light nuclei \(^4\)He, \(^6\)He and \(^{12}\)C, using a Woods-Saxon basis in Chapter 6.

To improve the description of phase shifts, Shirokov et al. [2] developed \(9\hbar\Omega\)-ISTP in odd waves, instead of the \(7\hbar\Omega\)-ISTP, retaining \(8\hbar\Omega\)-ISTP in even partial waves. To generate a high quality description of two-body data, these low values of “N” required \(\hbar\Omega = 40\ MeV\). They used unitary transformations to tune the off-shell interaction to binding energy of \(^3\)He, the low-lying spectrum of \(^6\)Li, and the binding energy of \(^{16}\)O. The \(NN\) off-shell freedom was sufficient to describe these limited data without the need of \(NNN\) potentials. The phase shifts were seen as well reproduced by ISTP up to the laboratory energy, \(E_{lab} = 350\ MeV\), as one of the best realistic meson exchange potentials Nijmegen II [2].

1.1.2 CD-Bonn

This section presents a charge-dependent \(NN\) potential developed by Machleidt [3] fitted to the world proton-proton data below 350 \(MeV\) available in the year of 2000 with a \(\chi^2\) per datum of 1.01 for 2932 data and the corresponding neutron-proton data with \(\chi^2/\text{datum}\) of 1.02 for 3058 data. This reproduction of the \(NN\) data was more accurate than any other \(NN\) potential at that time.

During the 1970s and 80s, a comprehensive field-theoretic meson-exchange model for the \(NN\) interaction was developed at the University of Bonn. The final version, published in 1987, has become known as the Bonn Full Model [9]. For a pedagogical review see Ref. [10].

The charge-dependence of the potential, named “CD-Bonn”, is based upon predictions by the Bonn Full Model for charge-symmetry and charge-independence breaking in all partial waves with \(J \leq 4\). The potential was represented in terms of the covariant Feynman amplitudes for one-boson exchange, which are non-local. Therefore, the off-shell behavior of the CD-Bonn potential differs from commonly used local potentials and leads to larger binding energies in nuclear few- and many-body systems, where underbinding is a persistent problem.
In the language of field-theoretic perturbation theory, the lowest order contributions to the $NN$ interaction generated by mesons are the one-boson exchange diagrams. Furthermore, there are many irreducible multi-meson exchanges. The diagrams of two-pion ($2\pi$) exchange are most prominent, since they provide the intermediate-range attraction of the nuclear force. However, once explicit diagrams of $2\pi$ exchange (with intermediate $\Delta$ isobars) are used in a model, then it is vital to also include the corresponding diagrams of $\pi\rho$ exchange. There are characteristic (partial) cancellations between the two groups of diagrams, crucial for a quantitative reproduction of the $NN$ data. Moreover, the Bonn model contains additional classes of irreducible three-pion ($3\pi$) and four-pion ($4\pi$) exchanges, important conceptually rather than quantitatively, since they appear to indicate convergence of the diagrammatic expansion chosen by the Bonn group [9].

The development of the Bonn Full Model was necessary to test reliably the meson-exchange concept for nuclear forces and to assess systematically the range of its validity. Thus, the model represents a benchmark for any alternative attempt (based, e.g., on quark models, chiral perturbation theory, or other ideas) to explain the nuclear force. The Bonn model addressed many important issues. One was the charge dependence of nuclear forces. The charge-symmetry-breaking (CSB) of the $NN$ interaction due to nucleon mass splitting has been investigated in Ref. [11]. It turns out that considerable CSB is generated by the $2\pi$ exchange contribution to the $NN$ interaction and the $\pi\rho$ diagrams, such that the CSB difference in the singlet scattering lengths can be fully explained from nucleon mass splitting. Also, noticeable CSB effects occur in $P$ and $D$ waves.

The charge-independence breaking (CIB) of the $NN$ interaction has also been investigated earlier in Ref. [12]. Pion mass splitting was the major cause. It was known the one-pion-exchange (OPE) explains about 50% of the CIB difference in the singlet scattering lengths. However, the $2\pi$ exchange model and the diagrams of the irreducible $3\pi$ and $4\pi$ exchanges contributed additionally to CIB, which could sum up to 50% of the OPE CIB contribution in $S$, $P$, and $D$ waves. This effect was not negligible.

Other important issues related to the nuclear force are relativistic effects, medium effects,
and many-body forces. The medium effects on the nuclear force, when inserted into nuclear matter, have been calculated thoroughly. A large repulsive contribution to these medium effects came from intermediate $\Delta$ isobar states, which also give rise to energy-dependence. On the other hand, isobars create attractive many-body forces. Thus, large cancellations between these two classes of many-body forces/effects occurred. It has been shown the net contribution was very small [13]. Relativistic effects, however, may play an important role in the nuclear many-body problem [10].

For these reasons, already early in the history of the meson theory of nuclear forces, the so-called one-boson-exchange (OBE) model was designed which, by definition, includes only single-meson exchanges (which could be represented in an energy-independent way). The model includes all mesons with masses below the nucleon mass, i.e., $\pi$, $\eta$, $\rho(770)$, and $\omega(782)$ [14]. In addition, the OBE model typically introduces a scalar, isoscalar boson, commonly denoted by $\sigma$.

Based upon the philosophy just outlined, Machleidt has constructed a $NN$ potential that is energy-independent and defined in the framework of the usual (nonrelativistic) Lippmann-Schwinger equation [3]. Thus, it can be applied in the same way as any other conventional $NN$ potential. The charge-dependence (CD) predicted by the Bonn Full Model was reproduced accurately by this potential, the reason it was named CD-Bonn potential. The off-shell behavior of CD-Bonn was based upon the relativistic Feynman amplitudes for meson-exchange. Therefore, the CD-Bonn potential differs off-shell from conventional $NN$ potentials—a fact that has attractive consequences in nuclear structure applications. However, an earlier version of the CD-Bonn potential did not contain all the charge-dependence and was published in Ref. [15], where the off-shell aspects were discussed in great detail.

By definition, charge independence is invariance under any rotation in isospin space. A violation of this symmetry is referred to as charge dependence or charge independence breaking (CIB). Charge symmetry is invariance under a rotation by 180° about the $y$-axis in isospin space, if the positive $z$-direction is associated with the positive charge. The violation of this symmetry is known as charge symmetry breaking (CSB). Obviously, CSB is a special case
of charge dependence. CIB of the strong $NN$ interaction means that, in the isospin $T = 1$ state, the proton-proton ($T_z = +1$), neutron-proton ($T_z = 0$), or neutron-neutron ($T_z = -1$) interactions are (slightly) different, after electromagnetic effects have been removed. CSB of the $NN$ interaction refers to a difference between proton-proton ($pp$) and neutron-neutron ($nn$) interactions, only. For recent reviews on these, see Ref. [16].

The major cause of CIB in the $NN$ interaction is pion mass splitting. Based upon the Bonn Full Model for the $NN$ interaction mentioned above, the CIB due to pion mass splitting has been calculated carefully and systematically in Ref. [12]. If the pion masses were all the same, neutron-proton ($np$) and proton-proton ($pp$) potentials would be identical. However, due to the mass splitting, the $T = 1$ $np$ potential is weaker as compared to the $pp$ potential. This causes a difference between $T = 1$ $pp$ and $np$ known as CIB.

Machleidt constructed three $NN$ interactions—$pp$, $nn$, and $np$ potential. These three potentials were not independent. They were all based upon the model described previously and the differences between them were determined by CSB and CIB. Thus, when one of the three potentials was fixed, then the $T = 1$ parts of the other two potentials were also fixed, due to CSB and CIB.

The CD-Bonn potential had been fitted to the empirical value for the deuteron binding energy $B_d = 2.224575$ $MeV$ [17] using relativistic kinematics. Once this adjustment had been made, the other deuteron properties, like deuteron matter radius, deuteron quadrupole moment, deuteron $D$-state probability $P_D$, etc, were predictions. The deuteron $D$-state probability $P_D$ is not an observable, but it is of great theoretical interest. CD-Bonn predicted $P_D = 4.85\%$, while local potentials typically predict $P_D \approx 5.7\%$, clearly reflected in the deuteron $D$-waves [3]. The smaller $P_D$ value of CD-Bonn could be traced to the non-localities contained in the tensor force as discussed and demonstrated in Ref. [3]. The CD-Bonn and the Nijmegen I [6] potentials have non-local central forces, which explain the smooth behavior of their deuteron $S$-waves at short distances.

The trend of the non-local Bonn potential to increase binding energies had a very favorable impact on predictions for nuclear matter [13] and the structure of finite nuclei [18].
Due to the very accurate fit of even the latest high-precision \(NN\) data, sophisticated charge-dependence incorporated in the model and well-founded off-shell behavior, the CD-Bonn potential \([3]\) represents a promising starting point for exact few-body calculations and microscopic nuclear many-body theory. To gain insight into this potential for no core investigations of heavier nuclei, an initial investigation is made of the odd mass, \(A = 47 - 49\) region nuclei straddling \(^{48}\text{Ca}\) \([19]\). These results are based on phenomenological additions to the realistic \(NN\) interaction determined by previous fits to \(A = 48\) nuclei explained in Ref. \([20]\), needed to fit the data. The results for the odd mass \(A = 47 - 49\) region nuclei using CD-Bonn interaction plus these phenomenological additions are presented in Chapter 4.

1.1.3 Chiral \(NN + NNN\)

One of the most fundamental problems of nuclear physics is to derive the force between two nucleons from first principles. A great obstacle for the solution of this problem has been the fact that the fundamental theory of strong interactions, QCD, is nonperturbative in the low energy regime characteristic for nuclear physics. The way out of this dilemma is the Effective Field Theory concept outlined by Weinberg \([21]\), which recognizes different energy scales in nature. Below the chiral symmetry breaking scale, \(\Lambda_{QCD} \approx 1\ GeV\), the appropriate degrees of freedom are pions and nucleons interacting via a force governed by the symmetries of QCD, particularly (broken) chiral symmetry.

The derivation of the nuclear force from chiral effective field theory was initiated by Weinberg \([21]\), and subsequently many groups became involved in the subject. The starting point for the derivation of the \(NN\) interaction is an effective chiral \(\pi N\) Lagrangian given by a series of terms of increasing chiral dimension,

\[
\mathcal{L}_{\pi N} = \mathcal{L}_{\pi N}^{(1)} + \mathcal{L}_{\pi N}^{(2)} + \mathcal{L}_{\pi N}^{(3)} + \ldots ,
\]

where the superscript refers to the number of derivatives or pion mass insertions (chiral dimension) and the ellipsis denotes terms of chiral order four or higher.

The heavy baryon (HB) formulation of chiral perturbation theory has been applied \([22]\), in which the relativistic Lagrangian is subject to an expansion in terms of powers of \((\frac{1}{M_N})\)
(reminiscent of a nonrelativistic expansion). The lowest order is

\[ \hat{\mathcal{L}}_{\pi N}^{(1)} = \bar{N}(iD_0 - \frac{g_A}{2}\vec{\sigma} \cdot \vec{u})N \approx \bar{N}[i\delta_0 - \frac{1}{4f_\pi^2} \tau \cdot (\pi \times \delta_0 \pi) - \frac{g_A}{2f_\pi} \tau \cdot (\vec{\sigma} \cdot \vec{V})]N + ... , \]  

where \( \pi \) is the pion field, \( \vec{u} \) is the vector field, and \( g_A \) is the nucleon axial decay constant, which satisfies the Goldberger-Treiman relation, \( g_A = \frac{g_{\pi NN}}{M_N} f_\pi \). \( M_N \) is the nucleon mass. The pion decay constant, \( f_\pi = 92.4 \text{ MeV} \), and \( N \) and \( \bar{N} \) are the upper components of the baryon wavefunctions, and \( D_0 \) and \( \delta_0 \) are first order derivatives.

The HB projected Lagrangian at order two is most conveniently broken into two components:

\[ \hat{\mathcal{L}}_{\pi N}^2 = \hat{\mathcal{L}}_{\pi N,fix}^2 + \hat{\mathcal{L}}_{\pi N,ct}^2 , \]  

with

\[ \hat{\mathcal{L}}_{\pi N,fix}^2 = \bar{N}[\frac{1}{2M_N} \vec{D} \cdot \vec{D} + i \frac{g_A}{4M_N} \{ \vec{\sigma} \cdot \vec{D}, u_0 \}]N \]  

and

\[ \hat{\mathcal{L}}_{\pi N,ct}^2 = \bar{N}[2c_1 m_\pi^2 (U + U^\dagger) + (c_2 - \frac{g_A^2}{8M_N})u_0^2 + c_3 u_\mu u^\mu + \frac{i}{2} (c_4 + \frac{1}{4M_N})\vec{\sigma} \cdot (\vec{u} \times \vec{u})]N . \]  

In Eqs. (1.27) and (1.28), \( \vec{D} \) is a derivative, \( U = u^2 \) is the coupling to the pions, and \( \vec{u} \) is the vector field. Note, \( \hat{\mathcal{L}}_{\pi N,fix}^2 \) is created entirely from HB expansion of the relativistic \( \hat{\mathcal{L}}_{\pi N}^{(1)} \). Thus, no free parameters (i.e., “fixed”), while \( \hat{\mathcal{L}}_{\pi N,ct}^2 \) is dominated by \( \pi N \) contact terms with proportionality parameters \( c_i \), besides some small \( \frac{1}{M_N} \) corrections. The parameters, \( c_i \), are known as low-energy constants (LECs) and must be determined empirically from fits to \( \pi N \) data. For example, \( c_1 = -0.81, \ c_3 = -4.70, \ c_4 = 3.40 \ (\text{GeV}^{-1}) \) (\( c_2 \) was not needed) for N2LO (cf. Ref. [23]). But, for the N3LO case in the fitting process, Entem and Machleidt varied three of the LECs, namely, \( c_2, \ c_3 \) and \( c_4 \), and they used \( g_A = 1.29 \).

The \( \pi N \) Lagrangian is the crucial ingredient for the evaluation of the pion-exchange contributions to the \( NN \) interaction. Since this is a low-energy effective theory, it is appropriate to analyze the contributions in terms of powers of small momenta: \( (\frac{Q}{\Lambda_{QCD}})^\nu \), where \( Q \) is a generic momentum or a pion mass, and \( \Lambda_{QCD} \approx 1 \text{ GeV} \) is the chiral symmetry breaking scale. This
procedure has become known as power counting. For the pion-exchange diagrams relevant to this problem, the power \( \nu \) of a diagram is determined by the simple formula

\[
\nu = 2l + \sum_j (d_j - 1),
\]

where \( l \) denotes the number of loops in the diagram, \( d_j \) is the number of derivatives involved in vertex \( j \), and the sum runs over all the vertices of the diagram. The Chiral Perturbation Theory (\( \chi PT \)) describes pion-pion (\( \pi\pi \)), pion-nucleon (\( \pi N \)), and inter-nucleon interactions at low energies. The \( NN \) sector has been proposed by S. Weinberg (1991) [21] and has been worked out by Van Kolck [24], Kaiser [25], Meissner [26], Epelbaum [27], and Machleidt [4, 23]. Hence, the chiral effective Lagrangian is given by an infinite series of terms with an increasing number of derivatives and/or nucleon fields, with the dependence of each term on the pion field prescribed by the rules of broken chiral symmetry of QCD. For a given order, \( \nu \), the number of contributions is finite and calculable.

One important advantage of \( \chi PT \) is that it makes specific predictions for many-body forces. For a given order of \( \chi PT \), both two-nucleon (2\( N \)) and three-nucleon (3\( N \)) forces are generated on the same footing. At NLO (next-leading-order), all 3\( N \) forces cancel; however, at NNLO (next-next-leading-order) and higher orders, well-defined, non-vanishing 3\( N \) forces occur.

Since 3\( N \) forces appear for the first time at NNLO, they are generally small compared to the 2\( N \) forces. Therefore, it is only possible to demonstrate their relevance when the 2\( N \) force is highly constrained.

In \( \chi PT \) the \( NN \) amplitude is determined by two classes of contributions: 1) contact terms and 2) pion-exchange diagrams. At N3LO there are two contact terms of \( O(Q^0) \), seven of \( O(Q^2) \) and fifteen of \( O(Q^4) \), making a total of 24 contact terms. Hence, 24 parameters are needed for the fit of the partial waves with orbital angular momentum \( l \leq 2 \). The peripheral partial waves of \( NN \) scattering with \( L \geq 3 \) are exclusively determined by one-pion exchange (OPE) and two-pion exchange (TPE) because the N3LO contact terms contribute to \( l \leq 2 \) only. In addition, there are two charge-dependent contact terms and, because three LEC are treated as semifree, the total number of parameters for N3LO potential is 29.

The 24 contact terms for N3LO were included for the first time in an earlier chiral \( NN \) potential constructed by Entem and Machleidt [23], where the importance of the \( O(Q^4) \) contact
terms for a quantitative reproduction of the $NN$ $D$-waves was demonstrated. However, this earlier potential included a two-pion exchange (TPE) only up to NNLO.

Now, turning to the pion contributions, at leading order [$LO \mathcal{O}(Q^0)$, $\nu = 0$], there is only the well known static OPE. TPE starts at NLO ($\nu = 2$) and there are further TPE’s in any higher order. Three-pion ($3\pi$) exchange shows up for the first time at N3LO (2 loops). It was shown that the $3\pi$ contributions at this order are negligible, which is why they have been left out [28]. For an accurate fit to the low energy $pp$ and $nn$ data, charge dependence is also important [29].

It was shown that $\chi PT$ at NNLO was poor in quantitative terms Ref. [23]; it reproduced $NN$ data below 290 $MeV$ lab energy with $\chi^2$/datum more than 20. This implies one must proceed to a higher order to obtain interactions competitive with those of meson exchange theory, where the $\chi^2$/datum is often around unity. At the fourth order of $\chi PT$ (N3LO), the accuracy was comparable to some of the high-precision phenomenological potentials like, for example, Argonne v18 [30].

In conclusion, the $NN$ potential at N3LO is the lowest order where a high-precision fit to $NN$ data can be made. This is the minimum order to meet the requirements for a reliable input potential for high-precision studies of nuclear structure and nuclear reactions.
CHAPTER 2. RENORMALIZATION TO A FINITE BASIS SPACE

2.1 Operators in Momentum Space

It is challenging to gain physical intuition for non-local operators, such as realistic \( NN \) interactions introduced in Chapter 1. In addition, whenever one truncates a local operator, such as approximating it in a finite matrix representation, one introduces non-locality.

This chapter presents contour plots in momentum space for the projector operator, kinetic energy operator as well as for the realistic \( NN \) interaction JISP16 truncated to a finite harmonic oscillator (HO) basis. Each is, in principle, an infinite dimensional matrix in the HO basis. The first two are local operators in the full basis, while the \( NN \) interaction is defined to be non-local even in the infinite representation.

This discussion begins with the harmonic oscillator radial wavefunctions, \( R_{nl}(r) \), Eq. (1.4) in the convention employed here and shows how they are normalized. In coordinate space, one needs to define a parameter, \( r_0 \), called the oscillator radius, as \( r_0 = \frac{\hbar}{\sqrt{m\Omega}} = \frac{\hbar c}{\sqrt{mc^2\Omega}} \), which has units of \([fm]\) (Sec. 1.1.1). In the notation used in the present chapter, \( m \) is the average mass of the nucleon, \( m = \frac{m_n + m_p}{2} \), and \( \mu \) is the reduced mass. Therefore, \( \mu = \frac{m}{2} \).

The total harmonic oscillator (HO) wavefunction is \( \Psi_{nlm}(\vec{r}) = R_{nl}(r)Y_{lm}(\hat{\vec{r}}) \), similar to Eq. (1.2). Using the notation, \( \overline{R_{nl}}(r) = \frac{R_{nl}(r)}{r} \), the radial part of the total wave function is related to the regular oscillator solutions \( S_{nl}(q) \) Eq. (1.10) as described below

\[
\overline{R_{nl}}(r) = \frac{\sqrt{2}}{r_0\sqrt{\pi}} \frac{r}{r} S_{nl}(q) .
\] (2.1)

The non-local Schrödinger equation to solve is

\[
-\frac{\hbar^2}{2\mu} \nabla^2 \Psi(\vec{r}) + \int d^3r' V(r, r') \Psi(\vec{r}') = E \Psi(\vec{r}) .
\] (2.2)
From here, the corresponding non-local NN interaction in coordinate space is

\[
V_{\text{JISP16}}^{lS_1J}(r, r') = \sum_{nn'} \sum_{nl}^{n_{\text{max}}} A_{nn'l}^{lS_1J} < r | nl > < n'l | r' > = \sum_{nn'}^{n_{\text{max}}} A_{nn'l}^{lS_1J} \bar{R}_{nl}(r) \bar{R}_{n'l}(r') .
\] (2.3)

Hence, the normalization condition for the radial part of the wavefunction can be written as

\[
\int \bar{R}_{nl}(r) \bar{R}_{n'l}(r) r^2 dr = \delta_{nn'} ,
\]

or as

\[
\int R_{nl}(r) R_{n'l}(r) r^2 dr = \delta_{nn'} .
\] (2.5)

In momentum-space, it is convenient to define the dimensionless parameter, \( \rho = kr_0 \), \( k \) being the relative momentum transfer with units of \([fm^{-1}]\). Define the momentum variables in the following way. If \( \vec{k}_1 \) and \( \vec{k}_2 \) are the momentum of the two particles before the scattering process and if \( \vec{k}'_1 \) and \( \vec{k}'_2 \) are the momentum of the same particles after the scattering, then one can define the total momentum before and after the scattering by \( |\vec{K}| = |\vec{k}_1 + \vec{k}_2| \) and \( |\vec{K}'| = |\vec{k}'_1 + \vec{k}'_2| \), respectively. The corresponding relative momenta for the same two particles before and after the scattering are \( |\vec{k}| = |\vec{k}_1 - \vec{k}_2| \) and \( |\vec{k}'| = |\vec{k}'_1 - \vec{k}'_2| \); thus, the momentum transfer is \( \vec{q} = \vec{k}' - \vec{k} \).

The JISP16 interaction in momentum-space is

\[
V_{\text{JISP16}}^{ll'S_1J}(k, k') = < k | V_{\text{JISP16}}^{ll'S_1J} | k' > \approx < k | \sum_{nn'}^{n_{\text{max}}} (-1)^{n+n'} < nl | \sum_{nn'}^{n_{\text{max}}} A_{nn'l'}^{S_1J} < n'l' | k' > \]

\[
= \sum_{nn'}^{n_{\text{max}}} (-1)^{n+n'} A_{nn'l'}^{S_1J} < k | nl > < n'l' | k' > \] (2.4)

\[
= \sum_{nn'}^{n_{\text{max}}} (-1)^{n+n'} A_{nn'l'}^{S_1J} \frac{R_{nl}(k) R_{n'l'}(k')}{k} ,
\]

where \( n_{\text{max}} \) is the maximum number of principle quantum number \( n \).

The normalization condition in momentum-space is also satisfied

\[
\int \frac{R_{nl}(k) R_{n'l'}(k)}{k} k^2 dk = \delta_{nn'} .
\] (2.5)

2.1.1 Projector matrix elements

The projector operator is a truncated version of the completeness relation, \( 1 = \sum_{nl} |nl\rangle\langle nl| \), where “1” on the right-hand side is the identity operator and “\( |nl\rangle \)” signify orthonormal eigenkets. The above sum is a useful mathematical tool, as it can be inserted wherever the identity operator can appropriately be inserted.
Similarly to the JISP16 interaction, Eq. (2.5), the projector operator in momentum-space can also be defined

\[
P_{ll'}(k,k') = \sum_{nn'} \delta_{nn'} \frac{\hbar \Omega}{k} R_n(k) R_{n'}(k')
\]

\[
P_{ll'}(k,k') = \sum_{n} \hbar \Omega \frac{R_n(k) R_{n'}(k')}{k}.
\] (2.6)

For consistency, the factor, \( \hbar \Omega [MeV] \), which has units of energy is inserted, giving the projector operator defined in Eq. (2.6) in units of \([MeV - fm^3]\). For a more convenient color gradient scale, one chooses to convert the matrix elements of the projector operator into units of \([fm]\), dividing the projector matrix elements in units of \([MeV - fm^3]\) by the factor,

\[
\frac{\hbar^2}{m} = 41.471 \ [MeV - fm^2],
\] (2.7)

where \( m \) is the nucleon mass. To obtain finite matrix representation, truncate the HO basis space and view the resulting quantities in momentum space. One selects a set of summation cutoffs, \( n_{max} = 7, 15, 31, 63, 127, 255 \), which relate to different HO basis space truncations defined by \( N_{max} = 2n_{max} \) and, conventionally, with a mention of the HO energy, \( \hbar \Omega \). Thus, \( n_{max} = 7, 15, 31, 63, 127, 255 \) correspond to \( 14\hbar \Omega, 30\hbar \Omega, 62\hbar \Omega, 126\hbar \Omega, 254\hbar \Omega, 510\hbar \Omega \), respectively.

Choose the results for the projector operator as a function of the cutoff scale, \( N_{max} \). The contour plots represent the projector operator \( P_{l=l'=0}(k,k') \) in units of \([fm]\) versus relative momentum square \( k^2 [fm^{-2}] \) and \( k'^2 [fm^{-2}] \), with \( l = l' = 0 \) referring to the \( S \)-waves representation, see Fig. 2.1. The color scale from the right side of each figure associates with the strength of the projector matrix elements, red is strongly repulsive and blue is strongly attractive. One can also notice in Fig. 2.1 the resolution of the representation is governed by the cutoff. The higher the cutoff, the higher the resolution and sharper details come into focus. The projector operator, as well as the kinetic energy operator, are local operators, meaning they converge into a very simple diagonal matrix in an infinite matrix limit. Figure 2.1 shows the evolution with increasing basis space truncation cutoffs, \( N_{max} \hbar \Omega \). The projector operator approaches the diagonal representation expected in an infinite matrix limit (see Fig. 2.1(f)).
The cutoff induces non-locality that disappears when going towards an infinite limit in the cutoff.

For a better visualization of the matrix elements situated at the same distance from the origin in momentum space, selected arc circles are presented separately. One presents plots for $S$-waves projector matrix elements, $P_{nn'}^l(\mathbf{k},\mathbf{k}')$ versus $k^2 [fm^{-2}]$, for all points situated on the arc circles, $k^2 + k'^2 = 4 [fm^{-2}]$ and $k^2 + k'^2 = 8 [fm^{-2}]$, respectively, for selected basis space cutoffs in Figs. 2.2 and 2.3. It is interesting to see how the matrix elements on the chosen arc circles shows the correct behavior of a $\delta$-function. The set of figures from Figs. 2.2 and 2.3 shows clearly a $\delta$-function behavior when going toward an infinite limit in the cutoff. One can see the reduction in the off-diagonal matrix elements and an increase in the diagonal matrix elements, when increasing the basis space cutoff. Comparing Figs. 2.2 and 2.3, two extra nodes in the set of figures are seen in Fig. 2.3.
Fig. 2.1  Momentum-space contour plots for S-waves projector matrix elements at different HO basis space cutoff scales—14ℏΩ, 30ℏΩ, 62ℏΩ, 126ℏΩ, 254ℏΩ, and 510ℏΩ. The color gradient scale represents the strength of the projector operator, red is strongly repulsive and blue is strongly attractive. The contour plots are presented versus momentum transfer square $k^2 \ [fm^{-2}]$ and $k'^2 \ [fm^{-2}]$ as $P(k,k') \ [fm]$ strength.
Fig. 2.2  $S$-waves projector matrix elements on the arc circle $k^2 + k'^2 = 4 \text{ [fm}^{-2}]$ plotted versus $k^2 \text{ [fm}^{-2}]$. 
Fig. 2.3 S-waves projector matrix elements on the arc circle $k^2 + k'^2 = 8 \ [fm^{-2}]$ plotted versus $k^2 \ [fm^{-2}]$. 
2.1.2 Kinetic energy matrix elements

Kinetic energy is also an infinite dimensional matrix in the HO basis and a local operator. The matrix elements of the kinetic energy in the HO basis are defined as

\[ T_{nn'} = 0 \text{ if } |n - n'| > 1, \quad (2.8a) \]
\[ T_{nn}^l = \frac{\hbar \Omega}{2} (2n + l + \frac{3}{2}), \quad (2.8b) \]
\[ T_{n+1,n}^l = T_{n,n+1}^l = \frac{\hbar \Omega}{2} \sqrt{(n + 1)(n + l + \frac{3}{2})}, \quad (2.8c) \]

with non-zero matrix elements \( T_{nn}^l \) and \( T_{n,n+1}^l \) increasing linearly with the principle quantum number \( n \) (see also Eq. (1.6)).

Keeping the anterior notations, the kinetic energy operator in momentum-space can be defined similarly to the JISP16 interaction Eq. (2.5) and projector operator Eq. (2.6)

\[ KE_{nn'}^l(k, k') = \sum_{nn'} (-1)^{n+n'} T_{nn'}^l \frac{R_{nl}(k)}{k} \frac{R_{n'l'}(k')}{k'}. \quad (2.9) \]

The same set of plots are produced for the kinetic energy operator in Fig. 2.4, similar to the projector operator case shown in Fig. 2.1. Increasing the basis space cutoff scale, \( N_{max} \) up to \( 510 \hbar \Omega \), one can see again the tendency toward a \( \delta \)-function in the infinite limit, the matrix becoming almost diagonal. The kinetic energy operator is a stronger operator and the off-diagonal matrix elements are more evident than in the projector operator case (Fig. 2.1), being proportional to \( k^2 \ [fm^{-2}] \). In this case, a stronger colored texture comes into focus and disappears when increasing the cutoff scale towards an infinite limit.
Fig. 2.4  Momentum-space contour plots for $S$-waves kinetic energy operator. See caption for Fig. 2.1.
2.1.3 JISP16 matrix elements

The JISP16 interaction comes in the form of truncated matrices, \( n \) and \( n' \), being the principal quantum numbers and can be any integer between 0 and 4. Potential matrix elements are obtained in a harmonic oscillator (HO) basis using \( \hbar \Omega = 40 \text{ MeV} \) as presented in Sec. 1.1.1. One represents the JISP16 interaction in momentum-space, see Eq. (2.5).

The coefficients, \( A_{nlnt'}^{SJ} \), represent the JISP16 matrix elements in the HO basis and \( R_{nl}(k) \) are the HO wavefunctions in momentum space. The JISP16 matrix elements in momentum space, initially in units of \([\text{MeV} - \text{fm}^3]\), are divided by the factor given by Eq. (2.7), converting the interaction matrix elements in units of \([\text{fm}]\). This would facilitate a direct comparison of the JISP16 bare [8] interaction results with SRG and \( V_{\text{lowk}} \) versions of N3LO (see Sec. 2.2.2). To obtain the same color gradient scale as Furnstahl et al. for N3LO Ref. [31], one imposes the boundary conditions that \( V_{JISP16}^{nlnt'}(k,k') = 0.5 \text{ fm} \) for all values of the potential matrix elements bigger than 0.5 \text{ fm} and \( V_{JISP16}^{nlnt'}(k,k') = -0.5 \text{ fm} \) for all values of the potential smaller than −0.5 \text{ fm}.

Contour plots for the JISP16 interaction in momentum-space are presented with respect to \( k^2 \) and \( k'^2 \) \([\text{fm}^{-2}]\) for selected partial waves in Fig. 2.5. The notation for the partial waves that labels this set of figures is \( {}^{(2S+1)L_J} \), where \( S \) is the spin quantum number, \( L \) stands for the orbitals \( S, P, D, ... \) corresponding to the orbital angular momentum quantum number \( l = 0, 1, 2, ..., \) respectively, and \( J \) is the total angular momentum quantum number.

For example, \( {}^1S_0 \) partial waves refer to the following set of quantum numbers (Spin \( S = 0 \), Orbital Angular Momentum \( l = 0 \), Total Angular Momentum \( J = 0 \)), where \( {}^3P_2 \) partial waves stands for (Spin \( S = 2 \), Angular Momentum \( L = 1 \), Total Angular Momentum \( J = 1 \)). Figures 2.5(a) - 2.5(g) clearly show the JISP16 interaction is soft over the full range in \( k^2 \), except in a region around the origin, which is strongly attractive for \( {}^1S_0 \) partial waves, Fig. 2.5(a), and \( {}^3S_1 \) channel, Fig. 2.5(b). For \( {}^3P_2 \) partial waves, notice the interaction is smooth over the entire range in \( k^2 \), Fig. 2.5(c). For the other \( P \)-waves, the interaction is also smooth except in a momentum square area of about 6.25 \text{ fm}^{-2}, where nice repulsive wings come into focus, Figs. 2.5(e), 2.5(f), and 2.5(g). For the \( {}^3D_2 \) partial waves, the situation is quite interesting as
the interaction is strongly repulsive near the origin and has nice attractive wings in a region of momentum square area of about 6.25 $fm^{-2}$, Fig. 2.5(d).

Figure 2.6 presents $^1S_0$ partial waves for two basis space cutoff scales, 6$h\Omega$ and 8$h\Omega$. Due to the fact the JISP16 interaction comes as truncated matrices at 8$h\Omega$, then, the interaction would look the same at any higher truncation in the basis space presented in this work. Looking at Figs. 2.6(a) and 2.6(b), one can see the JISP16 interaction is soft over the full range in $k^2$,.
except in a region around the origin where it is strongly attractive. Figure 2.7 presents other selection of momentum-space $S$-waves kinetic energy matrix elements for different HO cutoff scales—$6\hbar\Omega$, $8\hbar\Omega$, $20\hbar\Omega$, $500\hbar\Omega$.

If one adds the $S$-waves kinetic energy matrix elements with the $^1S_0$ partial waves part of the JISP16 matrix elements in momentum space at the same cutoff scale, one obtains the $^1S_0$ part of the total Hamiltonian matrix elements. Figure 2.8 shows the momentum-space contour plots for the total Hamiltonian matrix elements at chosen cutoff scales. Comparing Figs. 2.7 and 2.8, one cannot detect any visual difference. This is due to the fact the kinetic energy operator dominates, JISP16 interaction being attractive in a small area around the origin. To better visualize what happens around the origin, produce a different set of plots for the kinetic energy and the total Hamiltonian matrix elements on a finer resolution scale, see Figs. 2.9 and 2.10. Now, one can more easily visualize the differences in their features.

To conclude, it is worth obtaining a physical intuition in the momentum space for the projector operator and kinetic energy operator that are local operators, as well as, for the JISP16 interaction, which is non-local. One can see the evolution towards a diagonal matrix in an infinite limit for the first two cases and one can also visualize how “soft” is the JISP16 interaction, making it difficult to see the differences between the kinetic energy and the total Hamiltonian operators.

![Fig. 2.6 Momentum-space JISP16 matrix elements for $^1S_0$ partial waves and two different cutoff scales—$6\hbar\Omega$ and $8\hbar\Omega$. See caption for Fig. 2.1.](image-url)
Fig. 2.7 Other selection of momentum-space $S$-waves kinetic energy matrix elements for different HO cutoff scales—$6\hbar\Omega$, $8\hbar\Omega$, $20\hbar\Omega$, $500\hbar\Omega$. See caption for Fig. 2.1.
Fig. 2.8  Momentum-space total Hamiltonian matrix elements for $^1S_0$ partial waves and for different HO cutoff scales—$6\hbar\Omega$, $8\hbar\Omega$, $20\hbar\Omega$, $500\hbar\Omega$. See caption for Fig. 2.1.

Fig. 2.9  Momentum-space total Hamiltonian matrix elements for $^1S_0$ partial waves and for different HO cutoff scales—$6\hbar\Omega$, $8\hbar\Omega$, $20\hbar\Omega$—at a smaller momentum transfer square region. See caption for Fig. 2.1.
Fig. 2.10  Momentum-space $S$-waves kinetic energy matrix elements for different HO cutoff scales—$6\hbar\Omega$, $8\hbar\Omega$, $20\hbar\Omega$—at a smaller momentum transfer square region. See caption for Fig. 2.1.
2.2 Introduction to Renormalization Methods

The concept of an effective interaction has been widely used in nuclear, atomic, and molecular physics. An effective interaction may be viewed as a model-space-dependent or basis-space-dependent interaction that simulates the features of the original (or “bare” \cite{8}) interaction in the infinite basis space. The main purpose of this subsection is to provide a deeper insight into nuclear structure calculations by introducing an effective interaction as a basic ingredient and a fundamentally derivable quantity of the nuclear many-body theory.

The NCSM \cite{32–37} is based on an effective Hamiltonian derived from realistic “bare” \cite{8} interactions and acting within a finite Hilbert space. All $A$-nucleons are treated on an equal footing. The approach is both computationally tractable and demonstrably convergent to the exact result of the full (infinite) Hilbert space.

Initial investigations used two-body interactions \cite{32}, based on a G-matrix approach. Later, a similarity transformation procedure, based on Okubo’s pioneering work \cite{38}, was implemented to derive two-body and three-body effective interactions from realistic $NN$ and $NNN$ interactions. Diagonalization and evaluation of observables from effective operators created with the same transformations are carried out on high-performance parallel computers.

Progress on the nuclear many-body problem has been hindered for decades because nucleon-nucleon ($NN$) potentials that reproduce elastic scattering phase shifts typically exhibit strong short-range repulsion, as well as a strong tensor force. This leads to strongly correlated many-body wavefunctions and highly non-perturbative few- and many-body systems. The more perturbative potentials at lower renormalization scale, defined by a variable characteristic of the maximum momentum scale $\lambda$, induce weaker short-range correlations in few- and many-body wavefunctions, which, in turn, lead to greatly improved convergence in variational calculations. This was illustrated via calculations of the binding energy of the deuteron and triton by diagonalization in a HO basis. For a fixed basis size, a more accurate estimate was obtained with smaller $\lambda$, or conversely, at fixed $\lambda$ the convergence with basis size became more rapid \cite{39}.

One path to decouple high-momentum from low-momentum physics is the Similarity Renor-
malization Group (SRG), based on unitary transformations that suppress off-diagonal matrix elements, driving the Hamiltonian towards a band-diagonal form. The transformation leads to $NN$ potentials, for which, calculations of few-nucleon binding energies and other observables converge rapidly. Hence, a simple SRG transformation applied to $NN$ interactions leads to greatly improved convergence properties, while preserving observables, and provides a method to consistently evolve many-body potentials and other operators.

2.2.1 Lee-Suzuki-Okamoto method for deriving the effective Hamiltonian

The $NN$ interaction has a strong repulsive core whose effects cannot be efficiently described using a finite HO basis. Therefore, from here, to achieve improved convergence of many-body applications, one is motivated to derive effective interactions from the underlying realistic $NN$ interaction.

To clarify the distinctions from the conventional shell model with a core, we briefly outline here the $ab$ initio NCSM approach with $NN$ interactions alone and point the reader to the literature for the extensions to include $NNN$ interactions. Begin with the purely intrinsic Hamiltonian for the $A$-nucleon system, i.e.,

$$H_A = T_{\text{rel}} + V = \frac{1}{4} \sum_{i<j}^A \frac{(\vec{p}_i - \vec{p}_j)^2}{2m} + \sum_{i<j=1}^A V_N(\vec{r}_i - \vec{r}_j),$$  \hspace{1cm} (2.10)

where $m$ is the nucleon mass and $V_N(\vec{r}_i - \vec{r}_j)$, the $NN$ interaction, with both strong and electromagnetic components. Note the absence of a phenomenological single-particle potential. One may use either coordinate-space $NN$ potentials, such as the Argonne potentials [30] or momentum-space dependent $NN$ potentials, such as the CD-Bonn [3]. Local and non-local interactions are treated on an equal footing.

Next, one adds to Eq. (2.10) the center-of-mass harmonic oscillator (HO) Hamiltonian $H_{\text{CM}} = T_{\text{CM}} + U_{\text{CM}}$, where $U_{\text{CM}} = \frac{1}{2} Am\Omega^2 \vec{R}^2$, $\vec{R} = \frac{1}{A} \sum_{i=1}^A \vec{r}_i$. At convergence, the added $H_{\text{CM}}$ term has no influence on the intrinsic properties. However, when introducing the cluster approximation below, the added $H_{\text{CM}}$ term facilitates convergence to exact results with increasing basis size. The modified Hamiltonian, with pseudo-dependence on the HO frequency,
\( \Omega \), can be given as

\[
H_A^\Omega = H_A + H_{CM} = \sum_{i=1}^{A} \left[ \frac{p_i^2}{2m} + \frac{1}{2} m \Omega^2 \tilde{r}_i^2 \right] + \sum_{i<j=1}^{A} \left[ V_N(ij) - \frac{m \Omega^2}{2A} (\tilde{r}_i - \tilde{r}_j)^2 \right].
\] (2.11)

Next step is to introduce a unitary transformation, designed to accommodate the short-range two-body correlations in a nucleus, by choosing an anti-hermitian operator \( S \), acting only on intrinsic coordinates, such that \( \mathcal{H} = e^{-S} H_A^\Omega e^S \). In this approach, \( S \) is determined by the requirements that \( \mathcal{H} \) and \( H_A^\Omega \) have the same symmetries and eigenspectra over the subspace \( \mathcal{K} \) of the full Hilbert space. In general, both \( S \) and the transformed Hamiltonian are \( A \)-body operators. The simplest, non-trivial approximation to \( \mathcal{H} \) is to develop a two-body (\( a = 2 \)) effective Hamiltonian, where the upper bound of the summations “\( A \)” is replaced by “\( a \)”, but the coefficients remain unchanged. The next improvement is to develop a three-body effective Hamiltonian, (\( a = 3 \)). This approach consists then of an approximation to a particular level of clustering, \( a \), with \( a \leq A \).

\[
\mathcal{H} = \mathcal{H}^{(1)} + \mathcal{H}^{(a)} = \sum_{i=1}^{A} h_i + \frac{\binom{A}{2}}{\binom{a}{2}} \sum_{i_1<i_2<...<i_a} V_{i_1i_2...i_a},
\] (2.12)

with

\[
\tilde{V}_{i_1i_2...i_a} = e^{-S^{(a)}} H_A^\Omega e^{S^{(a)}} - \sum_{i=1}^{a} h_i,
\] (2.13)

and \( S^{(a)} \) is an \( a \)-body operator; \( H_A^\Omega = h_1 + h_2 + h_3 + \ldots + h_a + V_a \), and \( V_a = \sum_{i<j} V_{ij} \).

Note, there is no sum over “\( a \)” in Eq. (2.12), so there is no coupling between clusters in this approach.

For the many-body basis, one can adopt Slater determinants that are eigenstates of the sum of one-body Hamiltonians, \( \sum_{i=1}^{A} h_i \). These one-body Hamiltonians are also taken to be harmonic oscillators.

The effective interaction discussed here is defined as an interaction that acts in a certain model space (or \( P \)-space) and yields some of the same eigenvalues as those of an original Hamiltonian. In this respect, the effective interaction should have a decoupling property between the model and the excluded spaces. In general, the effective interaction cannot be determined...
The possible effective interactions can be classified into some categories, according to $E$-dependence or hermicity. The $E$-dependent and non-Hermitian effective interaction have been used widely in nuclear many-body calculations. Non-hermitian effective interaction can be converted into a Hermitian form. It has been shown that a general effective interaction can be derived by means of similarity transformation and the variety of the effective interactions is due to the variety of possible transformations.

The full Hilbert space is divided into a finite model space ("$P$-space") and a complementary infinite space ("$Q$-space"), using projectors $P$ and $Q$ that project a state onto the model space and its complement, respectively. The operators, $P$ and $Q$, satisfy the relations $P^2 = P$, $Q^2 = Q$, $PQ = 0$, and $P + Q = 1$. One can introduce an operator, $\omega$, which acts as mapping between the $P$ and $Q$ spaces, such that $|\alpha_Q\rangle = \omega|\alpha_P\rangle$ ($\alpha_Q \in Q$, $\alpha_P \in P$), where $|\alpha_Q\rangle$ and $|\alpha_P\rangle$ are the model-space and the $Q$-space basis states, respectively. The operator $\omega$ satisfies $\omega = Q\omega P$, $\omega Q = 0$, $P\omega = 0$, and $\omega^2 = 0$. From here, also $\omega QP\omega = 0$.

Let’s discuss the meaning of operator $\omega$ in more detail. Let $d$ be the dimension of the $P$-space. Suppose that $|k\rangle$ is one of the $d$-eigenstates of the initial Hamiltonian, $H$, needed to be solved with the effective interaction. The vector, $|k\rangle$, can be decomposed into a $P$-space component and a $Q$-space component. It has been shown the $Q$-space component can be generated by the operation of the operator, $\omega$, onto $|k\rangle$, such that $Q|k\rangle = \omega|k\rangle$. Therefore, one can state the operator, $\omega$, induces a mapping of the model space onto a subspace of the $Q$-space states, which overlaps in the $d$-eigenstates $|k\rangle$.

One can determine the transformation operator $S_a$ from the decoupling condition

$$Q_a e^{-S^{(a)}} H_a^\Omega e^{S^{(a)}} P_a = 0 ,$$

(2.14)

and the simultaneous restrictions $P_a S^{(a)} P_a = Q_a S^{(a)} Q_a = 0$. The $a$-nucleon-state projectors $(P_a, Q_a)$ appear in Eq. (2.14). Their definitions follow from the definitions of the $A$-nucleon projectors $P$ and $Q$. The unitary transformation and decoupling conditions, introduced by Suzuki and Okamoto and referred to as the unitary-model-operator approach (UMOA) Ref. [38], have a solution that can be expressed in the following form,
\[ S^{(a)} = \text{arctanh}(\omega - \omega^\dagger), \quad (2.15) \]

with the operator, \( \omega \), satisfying \( \omega = Q_a \omega P_a \).

Let us also note that \( \tilde{H}_{a-\text{eff}} = P_a e^{-S^{(a)}} H_a^{\Omega} e^{S^{(a)}} P_a \) leads to the relation,

\[ \tilde{H}_{a-\text{eff}} = (P_a + \omega^\dagger \omega)^{-1/2} (P_a + P_a \omega^\dagger Q_a) H_a^{\Omega} (Q_a \omega P_a + P_a) (P_a + \omega^\dagger \omega)^{-1/2}. \quad (2.16) \]

Given the eigensolutions, \( H_a^{\Omega} |k\rangle = E_k |k\rangle \), in the infinite Hilbert space for the cluster, then, in terms of the states \( |k\rangle \) and a complete orthonormal set of states, \( |\alpha_P\rangle \), that span the model space, the operator, \( \omega \), can be determined from

\[ \langle \alpha_Q |\omega|\alpha_P \rangle = \sum_{k \in \mathcal{K}} \langle \alpha_Q |k\rangle \langle \tilde{k} |\alpha_P \rangle, \quad (2.17) \]

where the tilde stands for the inverted matrix of \( \langle \alpha_P |k\rangle \), i.e., \( \sum_{\alpha_P} \langle \tilde{k} |\alpha_P \rangle \langle \alpha_P |k'\rangle = \delta_{k,k'} \) and \( \sum_k \langle \alpha_P' |\tilde{k}\rangle \langle \tilde{k} |\alpha_P \rangle = \delta_{\alpha_P',\alpha_P} \), for \( k, k' \in \mathcal{K} \). In the relation (2.17), \( \mathcal{K} \) denotes a set of \( d_P \) eigenstates, whose properties are reproduced in the model space, with \( d_P \) equal to the dimension of the model space. Note, once \( \omega \) is determined, the effective interaction can be calculated, using the transformation (2.15).

In practice, the exact (to numerical precision) solutions for the \( a = 2 \) cluster are obtained in basis spaces of several hundred \( \hbar \Omega \) in each relative motion \( NN \) channel.

In the limit \( a \to A \), the exact solutions for \( d_P \) states of the full problem are obtained for any finite basis space, with flexibility for choice of physical states subject to certain conditions [40]. This approach has a significant residual freedom through an arbitrary residual \( P_a \)-space unitary transformation that leaves the \( a \)-cluster properties invariant. Of course, the \( A \)-body results obtained with the \( a \)-body cluster approximation are not invariant under this residual transformation. It may be worthwhile, in a future effort, to exploit this residual freedom to accelerate convergence in practical applications.

The model space, \( P_2 \), is defined by \( N_m \) via the maximal number of allowed HO quanta of the \( A \)-nucleon basis states, \( N_M \), where the sum of the nucleons’ \( 2n + l \leq N_m + N_{\text{spsm}} = N_M \), and
where $N_{\text{spsmin}}$ denotes the minimal possible HO quanta of the spectators, nucleons not involved in the interaction. For example, in $^{10}$B, one obtains $N_{\text{spsmin}} = 4$, since there are six nucleons in the $0p$-shell in the lowest HO configuration and $N_m = 2 + N_{\text{max}}$, where $N_{\text{max}}$ represents the maximum HO quanta of the many-body excitation above the unperturbed ground-state configuration. For $^{10}$B with $N_M = 12, N_m = 8$ for an $N_{\text{max}} = 6$ or “$6\hbar\Omega$” calculation. With the cluster approximation, a dependence of the results on $N_{\text{max}}$ (or equivalently, on $N_m$ or $N_M$) and on $\Omega$ arises. For a fixed cluster size, $a$, the smaller the basis space, the larger the dependence on $\Omega$. The residual $N_{\text{max}}$ and $\Omega$ dependences infer the uncertainty in the results arising from effects associated with increasing $a$ and/or effects with increasing $N_{\text{max}}$. For the $A = 47 - 49$ results, only the $N_{\text{max}} = 0$ basis space is retained and $\hbar\Omega = 10\text{MeV}$ employed also in Refs. [20] and [19].

At this stage the term $H_{CM}$ is added again with a large positive coefficient (the Lagrange multiplier) to separate the physically interesting states with $0s$ CM motion from those with excited CM motion. One can diagonalize the effective Hamiltonian with the m-scheme Lanczos method to obtain the $P$-space eigenvalues and eigenvectors [41]. All observables are then evaluated free of CM motion effects [41]. In principle, all observables require the same transformation as implemented for the Hamiltonian. One obtains small renormalization effects on long-range operators, such as the rms radius operator and the $B(E2)$ operator, when transforming them to $P$-space effective operators at the $a = 2$ cluster level [36, 42]. On the other hand, when $a = 2$, substantial renormalization is observed for the kinetic energy operator [43] and for higher momentum transfer observables [42].

2.2.2 SRG—example of application to JISP16

This subsection presents a simple model which shows how these renormalization group transformations consistently evolve two- and three-body interactions towards a band-diagonal form. The SRG approach was developed independently by Glazek and Wilson [44] and by Wegner [45]. The success of the SRG combined with advances in chiral effective field theory (EFT) opens the door to the consistent construction and RG evolution of many-body potentials
and other operators.

Wilsonian renormalization group transformations are designed to replace explicit coupling between disparate distances or energy scales with effective interactions in which disparate scales are decoupled \[46\]. Recent work by Bogner et al. \[31\] has employed a simple unitary renormalization group transformation to study the NN interaction. The transformation was a simplified version of Wegner’s flow equations \[45\] and one of a much larger class of SRG transformations developed by Glazek and Wilson \[44\]. This transformation led to NN potentials, where calculations of few-nucleon binding energies and other observables converge rapidly. However, further progress requires the consistent treatment of at least the three-nucleon interaction.

This subsection follows Wegner’s formulation in terms of a flow equation for the Hamiltonian \[45\], but with a different choice of generator. The basics of the unitary evolution are simply stated. The initial Hamiltonian in the center of mass, \( H = T_{rel} + V \), where \( T_{rel} \) is the relative kinetic energy, is transformed by the unitary operator \( U(s) \) according to

\[
H_s = U(s) H U^\dagger(s) \equiv T_{rel} + V_s ,
\]

(2.18)

where \( s \) is a continuous flow parameter. This also defines the evolved potential, \( V_s \), with \( T_{rel} \) taken to be independent of \( s \). Take \( s = 0 \) for the initial value with \( U_0 \) the identity transformation, so \( H \) is the input Hamiltonian. Choose \( U_s \) so that \( H_s \) is diagonalized (band-diagonalized in more realistic cases) within a specified basis as \( s \to \infty \), which will realize the desired decoupling of low- and high-energy states. A direct differentiation shows that \( H_s \) evolves according to

\[
\frac{dH_s}{ds} = [\eta(s), H_s] ,
\]

(2.19)

with

\[
\eta(s) = \frac{dU_s}{ds} U^\dagger(s) = -\eta^\dagger(s) .
\]

(2.20)

Choosing \( \eta(s) \) specifies the transformation. A simple choice is

\[
\eta(s) = [T_D, H_s] ,
\]

(2.21)
where $T_D$ is a fixed diagonal matrix (independent of $s$) in a partial-wave momentum basis, which gives the flow equation,

$$
\frac{dH_s}{ds} = [[T_D, H_s], H_s].
$$

(2.22)

In momentum representation, $\lambda = s^{-\frac{1}{2}}$, with units of [fm$^{-1}$], is a more useful flow variable that can be thought of as a cutoff on momentum transfers. This will be used exclusively in the results presented in this chapter. Therefore, the parameter $\lambda$ can be seen also as a measure of the resulting diagonal width of $V_s$ in momentum space.

As a simple initial choice, $T_D$ was chosen to be the kinetic energy operator $T_D \to T_{rel}$, like in the results of Refs. [39, 47, 48]; Ref. [31] chose the Hamiltonian for free particles in an infinite square well. For explicit calculations, they employed a basis in which $T_D$ was diagonal. In this representation, $H_s$ was driven towards band-diagonal form, as seen in Ref. [31]. A principal advantage of SRG transformations is that all operators are consistently transformed, which means that all observables are invariant. For the simple unitary transformation, this is obvious, simply because it is unitary. An additional advantage is that SRG transformations readily handle Fock space operators; indeed, Glazek and Wilson [44] designed them to address light-front quantum chromodynamics. Interactions that change particle numbers are not required for low-energy nuclear physics, but one requires the consistent evolution of all many-body operators. If one expresses the Hamiltonian in terms of creation and destruction operators, it is evident that the commutators in Eq. (2.22) will generate many-body interactions, even if $H$ includes only a two-body interaction. In principle, this could make practical calculations intractable, but in applications of interest (e.g., to nuclear physics), one can choose transformations that maintain a hierarchy of many-body forces, such that for sufficiently dilute many-body systems, we only need to evolve few-body operators.

This subsection illustrates how a unitary SRG consistently evolves two-body interactions, like JISP16. The particular choice of $\eta(s)$ for the evolution employed in this work is

$$
\eta(s) = [H_{rel}^{HO}, H_s],
$$

(2.23)

where $H_{rel}^{HO}$ stands for the relative HO Hamiltonian, defined as $H_{rel}^{HO} = \hbar\Omega(2n + l + 3/2)$. 


Therefore, one has to solve the new flow equation in a finite HO basis

\[
\frac{dH_s}{ds} = [(H_{rel}^{HO}, H_s), H_s] = \frac{dV_s}{ds},
\]

(2.24)

at \(\hbar \Omega = 40 \text{ MeV}\).

The potential in HO basis must satisfy the boundary condition, such that the potential at the initial \(s = 0\) (\(\lambda = \infty\)) is equal to the initial untransformed potential,

\[
V_s = V_{s=0} + \int_0^s \frac{dV_s}{ds} \times ds.
\]

(2.25)

The potential processed with the SRG approach presented above is then transformed to the momentum-space basis, referred as \(V_s(k, k')\). Since the SRG transformation is unitary, observables are unchanged at all energies, up to numerical errors.

This method is very general and can be applied to any potential. Particularly, this subsection presents results for JISP16 potential and compares them with Chiral N3LO interaction results processed with SRG by Bogner et al.'s group [49].

Figure 2.11 shows results for JISP16 interaction for \(^1S_0\) partial waves processed with SRG as a function of the cutoff renormalization scale, \(\lambda\), starting with \(\lambda = \infty\) (unprocessed JISP16) down to \(\lambda = 1.1 \text{ fm}^{-1}\). One can notice that very little happens down to \(\lambda = 1.1 \text{ fm}^{-1}\). This is due to the fact that JISP16 is a soft, non-local interaction and has minimum high-momentum components to begin with. Looking at the results obtained when applying SRG on Chiral N3LO interaction for the same partial waves performed by Bogner et al. [49], it is worth searching for the well-matched features as a function of the renormalization scale. In the N3LO case, there was a suppression of the off-diagonal strength as \(\lambda\) decreases and the interaction for \(^1S_0\) partial waves had significant strength on the diagonal.

Figure 2.12 presents results for the JISP16 interaction for the \(S\)-wave part of \(^3S_1-^3D_1\) coupled channel for the same set of the cutoff renormalization scale, \(\lambda\). Again, notice the same tendency that very little happens down to \(\lambda = 1.1 \text{ fm}^{-1}\), JISP16 is unchanged due to the fact that it is a soft enough interaction to begin with. Performing the same set of comparisons with Chiral N3LO results for these partial waves there was more far off-diagonal strength and weaker higher momentum strength on the diagonal for the N3LO case [49]. Particularly, one
could see a systematic suppression of off-diagonal strength, as anticipated, with the width of the diagonal scaling as $\lambda^2$. The same behavior was observed when evolving from conventional high-precision $NN$ potentials, such as Argonne V18, or other softer chiral potentials [50].

The goal of the SRG approach is to smooth the matrix elements, and thus, eliminate the high momentum components. In this way, one obtains a better convergence in the model space where one chose to work. Calculations on light nuclei in the NCSM have been done and improvements are noted in the convergence [39].

However, there is much more to explore, such as the nature of the decoupling of high and low-energy physics, and whether other choices of the generator $\eta(s)$ would be more effective in making the Hamiltonian diagonal. For example, the replacement $T_D \rightarrow H_D$, where $H_D$ is the diagonal part of the Hamiltonian, or some function of kinetic energy operator, $T_{\text{rel}}$, are easily implemented. More important is the consistent evolution of nuclear three-body operators.

In summary, the SRG applied to $NN$ potentials works as promised, even for a simple choice of transformation, driving the Hamiltonian in momentum space towards the diagonal, making it more perturbative and more convergent in few-body calculations.
Fig. 2.11 Momentum-space matrix elements contour plots for JISP16 $^1S_0$-partial waves potential processed with SRG running in $\lambda$ from $\infty$ to 1.1 $[fm^{-1}]$. See caption for Fig. 2.1 for more details on the color scale.
Fig. 2.12 Momentum-space matrix elements contour plots for JISP16 in the $^3S_1$ channel processed with SRG running in $\lambda$ from $\infty$ to $1.1 \ [fm^{-1}]$. See caption for Fig. 2.11 for color scale gradient details.
CHAPTER 3. AB-INITIO NCSM AND NCFC METHODS

Non relativistic quantum many-body theory plays a leading role in several areas of physics. Recent advances in the microscopic ab initio theory of light nuclei provide a computational foundation for evaluating properties of light nuclei, as well as properties of the hadrons and their interactions.

The “ab initio” problem in nuclear structure physics is to solve for nuclear properties with the best available NN potentials, supplemented by 3-body NNN potentials as needed, using a quantum many-particle framework that respects all known symmetries of the potentials. Therefore, the goal of any ab initio method is to describe nuclei from the first principles with nucleons interacting as non relativistic point-like particles via these fundamental interactions.

High quality NN potentials are difficult to use in many-body calculations. Therefore, one needs sophisticated approaches and significant computing power. For example, for $A = 3, 4$, there are many exact methods; but for $A > 4$, few methods are applicable, like Green’s Function Monte Carlo (GFMC), Effective Interaction for Hyperspherical Harmonics (EIHH), Coupled-Cluster Method (CCM), Full Configuration Interaction (FCI), and the ab initio NCSM and NCFC methods. No Core Shell Model (NCSM) and No Core Full Configuration (NCFC) are used to signify all nucleons are dynamically involved in the interactions and are treated on an equal footing. Among the few ab initio methods available for light nuclei beyond atomic number $A = 10$, the NCSM [36] and the NCFC [51] methods frame the problem as a large sparse Hamiltonian matrix eigenvalue problem.

NCSM and NCFC both employ a finite HO basis, defined as an $N_{max} \hbar \Omega$ model space, where $N_{max}$ defines a many-nucleon cutoff and all basis states consistent with this cutoff are retained. The NCSM and NCFC approaches are distinguished by their methods of treating the
realistic $NN$ and $NNN$ interactions. In the case of NCSM, there is a renormalization procedure to manage the strong pathological features of these interactions. In particular, repulsive core and/or short-range correlations in $NN$ (and also in $NNN$) interactions cannot be accommodated in a selected HO basis. Therefore, NCSM derives an effective interaction, $N_{\text{max}}$ and HO energy, $\hbar \Omega$, dependent. The effective interaction is derived using the Lee-Suzuki-Okamoto (LSO) renormalization procedure performing an $N_{\text{max}}$ truncation of the infinite matrix. Then, one can search for a converging sequence for each experimental observable. There is no extrapolation involved. NCSM uses a cluster approximation technique that performs an exact calculation with no $N_{\text{max}}$ truncation at the 2-body or 3-body cluster level. In this case, larger cluster sizes for the effective Hamiltonian may be employed to accelerate convergence.

The NCFC method adopts the HO (or WS) single-particle basis, which involves two parameters, $N_{\text{max}}$ and $\hbar \Omega$, and seeks results independent of these parameters either directly, in a sufficiently large basis, or via extrapolation to the infinite basis limit. Because of treating all nucleons equivalently and achieving convergence within evaluated uncertainties, this approach is referred to as the no-core full configuration (NCFC) method. This method uses either a bare $NN$ interaction [8] or a SRG, $V_{\text{lowk}}$, UCOM renormalization of the bare $NN$ interaction. With these renormalization procedures, the finite nucleus must still be solved in an infinite basis space. Therefore, there is a many-body basis space truncation, $N_{\text{max}}$, and one extrapolates to an infinite matrix limit.

The NCFC is both related to and distinct from the NCSM [36] that features a finite matrix truncation and an effective Hamiltonian renormalized to that finite space. The regulator, $N_{\text{max}}$, appears in the NCFC, where it is taken to infinity, and in the NCSM, where it also appears in the definition of the effective Hamiltonian.

In both NCFC and NCSM, this choice of a many-body basis regulator, $N_{\text{max}}$, is needed to preserve Galilean invariance—to factorize all solutions into a product of intrinsic and center-of-mass motion components. With $N_{\text{max}}$ as the regulator, both the NCFC and the NCSM are distinguished from the full configuration interaction (FCI) method in atomic and molecular physics that employs a cutoff in single-particle space. The NCFC results should agree with the
NCSM and no-core FCI results, when the latter results are obtained in sufficiently large basis spaces.

3.1 HO Single-particle Basis

The end goal of the MFDn code [41] is to solve for the low-lying eigenvalues of a nuclear Hamiltonian matrix. This is nontrivial, due to the strong nucleon-nucleon ($NN$) and three-nucleon ($NNN$) interactions between nucleons. The basic equation to solve is

$$H | \psi_\alpha \rangle = E_\alpha | \psi_\alpha \rangle,$$

(3.1)

where $H = H_0 + H_I$, $H_0$ is the unperturbed Hamiltonian, and $H_I$ is the interaction. The Hamiltonian can be defined in any convenient basis space. The harmonic oscillator (HO) basis space is one of the widely used examples. Due to the massive size and extreme sparsity of the matrix, the Lanczos algorithm is used to obtain the low-lying eigenvalues and eigenvectors.

To construct the HO basis space, consider the potential:

$$U(r) = \frac{1}{2}\mu\omega^2 r^2,$$

(3.2)

where $\mu$ represents the mass of the nucleon, taken as the average of the neutron and proton mass (938.92 MeV). Inserting this potential into the Schrödinger equation with the simplification, $\nu \equiv \frac{\mu\omega}{2\hbar}$, one obtains the wavefunction,

$$\psi_{nlm} = N_{nl} r^l e^{-\nu r^2} L_{(n-l)/2}^{l+\frac{1}{2}}(2\nu r^2) Y_{lm}(\theta, \phi),$$

(3.3)

where $L_{(n-l)/2}^{l+\frac{1}{2}}(2\nu r^2)$ represents an associated Laguerre Polynomial, defined by using the Rodrigues formula,

$$L_{\nu}^{q}(z) = \frac{e^z z^{-q}}{\nu!} \frac{d^\nu}{dz^\nu} (z^{\nu+q} e^{-z}),$$

(3.4)

and $Y_{lm}(\theta, \phi)$ is a spherical harmonic. The normalization factor, $N_{nl}$, given in Refs. [52, 53], is

$$N_{nl} = \sqrt{\frac{2(2\nu)^l 2^{l+\frac{3}{2}} \Gamma(n-l/2 + 1)}{\Gamma(l + \frac{3}{2}) \Gamma(n-l/2 + \frac{3}{2})}}.$$

(3.5)
To fully describe the particle, one must include a spinor which then leads, after coupling spin and orbital motion, to the full wavefunction,

$$\Psi_{nljm} = \sum_{m,s} \langle lmstm_s | jm \rangle \psi_{nlm} \chi_{sm}, \tag{3.6}$$

where $$\langle lmstm_s | jm \rangle$$ is a Clebsch-Gordon coefficient [54].

### 3.1.1 Terminology

For the purposes here, several inner products and operators are defined using the Dirac bra-ket notation and creation/destruction operators

$$H_0 | i \rangle = \epsilon_i | i \rangle, \tag{3.7}$$
$$a_i^\dagger | 0 \rangle = | i \rangle, \tag{3.8}$$
$$a_i^\dagger | i \rangle = | 0 \rangle, \tag{3.9}$$
$$a_i | i \rangle = | 0 \rangle, \tag{3.10}$$
$$a_i | 0 \rangle = 0, \tag{3.11}$$
$$\langle \vec{r} | i \rangle = \phi_i(\vec{r}), \tag{3.12}$$

and

$$\langle \vec{q} | i \rangle = \tilde{\phi}_i(\vec{q}), \tag{3.13}$$

where $$\vec{r}$$ represents a nucleon coordinate, $$\vec{q}$$ represents its momentum, and $$\tilde{\phi}_i$$ is the Fourier transform of $$\phi_i$$. Labels, such as $$i,j,k,...,n$$ represent single-particle states and are defined according to the chosen set of commuting observables, selected in several ways. For example, $$\{x,y,z\}$$ represents a spinless particle with discretized momenta in a coordinate box; $$\{k_x,k_y,k_z\}$$ represents a spinless particle in a momentum box; $$\{n,l,m\}$$ represents a spinless particle in a spherical potential; $$\{n,l,s,j,m_j\}$$ represents a particle with spin $$s$$ in a spherical potential, etc.
3.1.2 Second-quantized notation

Second quantization allows one to easily write down the Hamiltonian and represent the basis states

\[
H_0 = \sum_{i,j} \langle i | H_0 | j \rangle a_i^\dagger a_j ,
\]

\[
H_I = \frac{1}{4} \sum_{i,j,k,l} \langle ij | H_I | kl \rangle a_i^\dagger a_j^\dagger a_l a_k
\]

\[
+ \frac{1}{36} \sum_{i,j,k,l,m,n} \langle ijk | H_I | lmn \rangle a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l
\]

\[
+ \frac{1}{576} \sum_{i,j,k,l,m,n,o,p} \langle ijk| H_I | mnop \rangle a_i^\dagger a_j^\dagger a_k^\dagger a_p a_o a_n a_m ,
\]

\[
| \Phi_\alpha \rangle = \{ a_i^\dagger a_j^\dagger a_k^\dagger ... a_n^\dagger \}_\alpha | 0 \rangle = | i, j, k, ..., n \rangle .
\]

The first term in the expression given for \( H_I \), in Eq. (3.15) is the two-body term, the second term is the three-body term, and the third term is the four-body term. The fractional coefficients in front of the multi-body terms ensure no redundant counting and can be easily calculated as \( \frac{1}{(\text{rank})!} \).

3.1.3 Further conventions for second-quantized notation

Adopting a summation convention, the Hamiltonian becomes

\[
\hat{H} = \frac{1}{4} \sum_{i,j,k,l} \langle ij | \hat{H} | kl \rangle a_i^\dagger a_j^\dagger a_l a_k
\]

\[
= \sum_{i<j,k<l} \langle ij | \hat{H} | kl \rangle a_i^\dagger a_j^\dagger a_l a_k
\]

\[
= \frac{1}{4} H_{ijkl} a_i^\dagger a_j^\dagger a_l a_k ,
\]

\[
H_{ijkl} \equiv \langle ij | \hat{H} | kl \rangle .
\]

Note, in the \( m \)-scheme, the \( NN \) interaction conserves the angular momentum projection such that \( m_i + m_j = m_k + m_l \). The creation and destruction operators obey the anti-commutation
relation
\[ [a_i, a_j^\dagger]_+ = a_i a_j^\dagger + a_j^\dagger a_i = \delta_{ij} . \tag{3.19} \]

Define
\[ h_{ik} \equiv \sum_j \langle ij | \hat{H} | k j \rangle . \tag{3.20} \]

Due to Eq. (3.20), in combination with the above defined anti-commutation relation for second-quantization creation and annihilation operators, Eq. (3.19), the Hamiltonian can be expressed as
\[ \hat{H} = h_{ik} i^\dagger k - H_{ijkl} i^\dagger j^\dagger l^\dagger k . \tag{3.21} \]

The expectation value with respect to a particular eigenstate, \(|\Psi_\alpha\rangle\), becomes
\[ E_\alpha = \langle \Psi_\alpha | \hat{H} | \Psi_\alpha \rangle = h_{ik} \rho_{ik,\alpha\alpha} - H_{ijkl} \rho_{il,\alpha\beta} \rho_{jk,\beta\alpha} . \tag{3.22} \]

Note, in general, \(m_j \neq m_k, m_i \neq m_l\), and \(\rho\) represents the one-body density matrix and is defined as
\[ \rho_{ik,\alpha\beta} = \langle \Psi_\alpha | i^\dagger k | \Psi_\beta \rangle . \tag{3.23} \]

The following conditions are satisfied
\[ E_\alpha \delta_{\alpha\gamma} = E_\alpha (\rho) \]
\[ = \langle \Psi_\alpha | \hat{H} | \Psi_\gamma \rangle \]
\[ = h_{ik} \rho_{ik,\alpha\gamma} - H_{ijkl} \rho_{il,\alpha\beta} \rho_{jk,\beta\gamma} . \tag{3.26} \]

### 3.2 Construction of a Many-body Basis Space

The normalized wavefunction is given by a Slater determinant \([54],\)
\[ \Psi = \frac{1}{\sqrt{n!}} \begin{vmatrix} \psi_{a_1}(x_1) & \psi_{a_1}(x_2) & \cdots & \psi_{a_1}(x_n) \\ \psi_{a_2}(x_1) & \psi_{a_2}(x_2) & \cdots & \psi_{a_2}(x_n) \\ \vdots & \vdots & \ddots & \vdots \\ \psi_{a_n}(x_1) & \psi_{a_n}(x_2) & \cdots & \psi_{a_n}(x_n) \end{vmatrix} . \tag{3.27} \]
The many-body basis space is created with the destruction and creation operators from the second-quantization formalism of quantum mechanics. If $|\Phi_\alpha\rangle$ represents a Slater determinant of single-particle states, then

$$|\Phi_\alpha\rangle = a_i^\dagger a_j^\dagger a_k^\dagger ... a_n^\dagger |0\rangle \quad (3.28)$$

$$H_0 |\Phi_\alpha\rangle = \epsilon_\alpha |\Phi_\alpha\rangle \quad (3.29)$$

$$\epsilon_\alpha = \epsilon_i + \epsilon_j + \epsilon_k + ... + \epsilon_n . \quad (3.30)$$

Each index on a creation and destruction operator represents a specific orbit in which the single particle is located. Each state is orthonormal, as a result of the anti-commutation relation given in Eq. (3.19). The full Hamiltonian is diagonalized in this basis and produces the exact solutions expanded in this basis. Specifically, diagonalization yields

$$|\Psi_\alpha\rangle = \sum_\beta C_{\alpha,\beta} |\Phi_\beta\rangle , \quad (3.31)$$

where $\Psi_\alpha$ represents the exact solution, $\Phi_\beta$ is the many-body basis state in the representation used to approximate the exact wavefunction. The expansion coefficients can be easily computed by

$$C_{\alpha,\beta} = \langle \Psi_\alpha | \Phi_\beta \rangle . \quad (3.32)$$

### 3.2.1 Conventions for many-body basis states

When a many-body basis state is created, each unique $n$-fermion basis state is specified by a list $\{i, j, k, ..., n\}$ of $n$ occupied single-particle states, $|i, j, k, ..., n\rangle$. The single-particle states (sps) are ordered by their unperturbed energy, i.e., $\epsilon_1 \leq \epsilon_1 \leq \epsilon_3 \leq ... \leq \epsilon_M$. When the many-body basis states are generated, every possible state is enumerated and then checked to ensure that only states with a fixed value of the conserved quantum numbers specified by the magnetic projection,

$$\sum_{i=1}^N m_i = M_0 \quad (3.33)$$
and the total number of HO quanta less than or equal to the maximum number of allowed
HO quanta are stored. For NCSM the maximum number is \( N_{\text{max}} \) above the minimum quanta
needed to satisfy the Pauli principle.

Therefore, the many-body basis states are Slater determinants like Eq. (3.27) (e.g., in the
HO basis), and are limited by the imposed symmetries—parity and total angular momentum
projection \((M)\), rotational, translational, etc., invariance, as well as by a maximum number of
allowed HO quanta, \( N_{\text{max}} \), discussed next.

### 3.2.2 Many-body basis space cutoff \( N_{\text{max}} \)

To investigate the direct solution of the nuclear many-body problem, the initial choice
is a traditional HO basis. Therefore, there are two basis space parameters, the HO energy,
\( \hbar \Omega \), and the many-body basis space cutoff, \( N_{\text{max}} \). The goal is to obtain convergence in this
two-dimensional parameter space \((\hbar \Omega, N_{\text{max}})\), where convergence is defined as independence
of both parameters within evaluated uncertainties.

The first parameter, \( \hbar \Omega \), specifies the HO energy, the spacing between major shells. Each
shell is labeled uniquely by the quanta of its orbits, \( N = 2n + l \) (orbits are specified by quantum
numbers \( n, l, j, m_j \)), which begins with 0 for the lowest shell and increments in steps of unity.
Each unique arrangement of fermions (neutrons and protons) within the available HO orbits,
consistent with the Pauli principle, constitutes a many-body basis state. Many-body basis
states satisfying chosen symmetries are employed to evaluate the Hamiltonian, \( H \), in that
basis.

The second parameter is \( N_{\text{max}} \), which limits the total number of oscillator quanta allowed
in the many-body basis states and, thus, limits the dimension, \( D \), of the Hamiltonian matrix in
that basis space. \( N_{\text{max}} \) is defined as the maximum number of the total oscillator quanta allowed
in the many-body basis space above the minimum HO configuration for the specific nucleus
needed to satisfy the Pauli principle. Its use allows one to preserve Galilean invariance—
to factorize all eigenfunctions solutions into a product of intrinsic and center-of-mass motion
components. Because \( N_{\text{max}} \) is the maximum of the total HO quanta above the minimal HO
configuration, it is possible to have at most one nucleon in the highest HO single-particle state consistent with $N_{max}$.

Figure 3.1 presents an example for the proton and neutron energy level distributions in $^6$Li and shows one unit oscillator quanta is one unit of quantity $(2n + l)$. In this illustration, the lowest HO configuration is marked at the minimum $N_{max}$ value as, $MIN(N_{max}) = 0$. Neutrons are on the left side of the figure and protons are on the right side. Therefore, one observes this configuration has four excitation quanta for neutrons and two excitation quanta for protons above the minimum configuration. This distribution of protons and neutrons on the energy levels is referred to as $N_{max} = 6$ configuration or $6\hbar\Omega$ configuration in any *ab initio* calculation. In the NCSM, it is simply called a “$6\hbar\Omega$” calculation. The remaining states allowed with an $N_{max} = 6$ cutoff consist of all possible arrangements of the six nucleons in oscillator orbits leading to six quanta of excitation or fewer.

![Fig. 3.1 $^6$Li proton and neutron energy level distributions at $N_{max} = 6$ using an HO potential.](image-url)
3.3 M-scheme Basis

The “m-scheme” basis is defined with a simple unperturbed Hamiltonian in which total angular momentum projection is a good quantum number. For this symmetry to be a good symmetry, one usually selects a spherical central potential in which every nucleon is acted upon by the same potential that depends solely on the radial distance from the center of the nucleus. To obtain a basis with good total angular momentum projection, there are two types of coupling schemes used—LS-coupling and jj-coupling. When using an LS-coupling scheme, a group of single-particle states is specified by the orbits for each particle, denoted by \( n \), the principal quantum number, and \( l \), the orbital angular momentum. For the case of jj-coupling, \( n \) and \( l \) are used in combination with \( j \), the total angular momentum of the single particle. To completely describe the state, additional quantum numbers, such as \( m_s \), \( m_j \), and \( m_l \) are necessary, depending on whether LS-coupling or jj-coupling is utilized. For the many-body basis states, one assembles a set of single-particle states consistent with the chosen symmetries and cutoffs as seen in the second quantization scheme earlier in this chapter. When the \( NN \) and \( NNN \) interactions are not present, these basis states are degenerate.

The m-scheme is employed in this work, where each HO single-particle state has its orbital and spin angular momenta coupled to good total angular momentum, \( j \), and magnetic projection, \( m \). The many-body states are enumerated for a fixed value of the sum \( M \) of the single-particle \( m \)-values. Usually, \( M = 0 \) (\( M = \frac{1}{2} \)) for an even (odd) number of nucleons.

3.4 Lanczos Diagonalization

To evaluate the low-lying solutions of the full Hamiltonian, \( H \), a tridiagonal matrix, \( H_t \), is created. Define the scalar \( b_1 \equiv 0 \) and the initial pivot vector \( |\chi_0\rangle \equiv 0 \). For \( i = 1, ..., n \), it is possible to compute \( a_i, b_{i+1} \) and the Lanczos vector, \( \chi_i \), given that

\[
 b_{i+1} \chi_{i+1} = H \chi_{i} - a_i \chi_i - b_i \chi_{i-1} \\
 a_i \equiv \langle \chi_i \mid H \mid \chi_i \rangle .
\]
The tridiagonal Lanczos matrix, $H_t$, comprises $a_i$ as its diagonal elements and $b_{i+1}$ as the subdiagonal and superdiagonal elements giving

$$H_t = \begin{pmatrix} a_1 & b_2 & 0 & 0 & \cdots \\ b_2 & a_2 & b_3 & 0 & \cdots \\ 0 & b_3 & a_3 & b_4 & \cdots \\ 0 & 0 & b_4 & a_4 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$ (3.36)

The Lanczos diagonalization develops a dynamical basis in which the full Hamiltonian is tridiagonal. Actually, one diagonalizes the truncated $H_t$ after each Lanczos iteration until the desired precision is reached. In principle, the initial pivot vector, $\chi_0$, is arbitrary and we frequently adopt one generated by random numbers.

Lanczos recursion is ideal for the exploration of large sparse matrices for a variety of reasons, but principally due to the simple nature of the algorithm and the relatively low memory required to perform it. There is no manipulation of the original full Hamiltonian matrix, which saves an enormous amount of computation time for diagonalization. At most, the number of operations to diagonalize the matrix is of the order $n^2$. In practice, because of the need for only a few of the eigenvalues and the good convergence properties of the algorithm, the number of operations required to achieve the desired accuracy can be a few hundred times $n^2$, achievable for nuclear physics applications on large parallel computers with matrices of several billion basis states. It is also worth noting that only the two most recently calculated vectors need to be stored to continue the recursive algorithm. As a result, the memory required to perform the Lanczos algorithm is minimal compared to the size of the matrix [55].
CHAPTER 4. $A = 47 - 49$ APPLICATION WITH PHENOMENOLOGICAL ADJUSTMENT

Having introduced the theoretical frameworks for the “bare” [8] and the “renormalized” strong nuclear interactions, we can address a variety of applications in nuclei. However, as one increases the atomic number, $A$, of the nucleus, we will eventually hit a boundary where, due to computational limitations, precision results with realistic interactions are not achievable. At this stage, it would be valuable to have a semi-realistic path forward to heavier systems. To foster the development of this path, we address a set of systems in the $A = 47 - 49$ region, whose exact solution with realistic Hamiltonians is far beyond current computational capabilities. Also, we show a semi-realistic approach is promising and could lead to applications in heavier nuclei in the near term. This is the focus of the present chapter.

The low-lying levels of the $A = 47 - 49$ nuclei have long been of experimental and theoretical interest. On the one hand, extensive experimental information about these nuclei is available [56, 57] and, on the other hand, this is a suitable nuclear mass region for developing and testing effective $fp$-shell Hamiltonians. Numerous detailed spectroscopic calculations have been reported. For example, using a shell model approach, Martinez-Pinedo, Zuker, Poves, and Caurier have performed full $fp$-shell calculations for the $A = 47$ and $A = 49$ isotopes of Ca, Sc, Ti, V, Cr, and Mn [58]. They employed the KB3 interaction [59] with phenomenological adjustments and performed complete diagonalizations to obtain very good agreement with experimental level schemes, transition rates, and static moments. Extensive discussions of $fp$-shell effective Hamiltonians and nuclear properties can be found in recent shell model review articles [60–63].

Interest in these nuclei stems from the goal to extend the no-core shell model (NCSM)
applications to heavier systems than previously investigated. Until recently, the NCSM, which
 treats all nucleons on an equal footing, had been limited to nuclei up through \( A = 16 \). However,
in a recent paper \cite{20}, the first NCSM results for \(^{48}\text{Ca}, ^{48}\text{Sc}, \) and \(^{48}\text{Ti}\) isotopes, with derived
and phenomenological two-body Hamiltonians was reported. These three nuclei are involved
in double-beta decay of \(^{48}\text{Ca}\), and the interest in developing nuclear structure models for
describing them is also related to the need for accurate calculations of the nuclear matrix
elements involved in this decay. This initial application showed the limitations of such an
approach when applied to heavier systems and how much improvement one can obtain by
adding phenomenological two-body terms involving all nucleons. In brief, the results were the
following \cite{20}: i) the charge dependence of the bulk binding energy of eight \( A = 48 \) nuclei is
reasonably described with an effective Hamiltonian derived from CD-Bonn interaction \cite{3, 15}
in the very limited \( N_{\text{max}} = 0 \) basis space, while there is an overall underbinding by about
0.4 \( \text{MeV}/\text{nucleon} \); ii) the resulting spectra are too compressed compared with experiment; iii)
when isospin-dependent central terms plus a tensor interaction are added to the Hamiltonian,
one achieves accurate total binding energies for eight, \( A = 48 \), nuclei and reasonable low-lying
spectra for the three nuclei involved in double-beta decay. Only five input data were used
to determine the phenomenological terms—the total binding of \(^{48}\text{Ca}, ^{48}\text{Sc}, \) and \(^{48}\text{Ti}\) along
with the lowest positive and negative parity excitations of \(^{48}\text{Ca}\). Negative parity calculations
are performed in the \( N_{\text{max}} = 1 \) basis space. Since the NCSM effective 2-body interaction
is solely responsible for the spectroscopy and involves the interactions of all 48 nucleons, no
single-particle energies are employed.

In the present chapter, we extend the previous approach to the odd-\( A \) isotopes \(^{47}\text{Ca}, ^{49}\text{Ca},
^{47}\text{Sc}, \) and \(^{47}\text{K}\), which differ by one nucleon from \(^{48}\text{Ca}\). One of the goals is to test whether
the same modified effective 2-body Hamiltonian used for \( A = 48 \) isotopes is able to describe
these odd-\( A \) nuclei and whether experimentally-known single-particle properties emerge in a
natural manner. A particular feature of the spectroscopy of these odd nuclei is the spin-orbit
splitting gives rise to a sizable energy gap in the \( fp \)-shell between the \( f_{7/2} \) and other orbitals
\((p_{1/2}, p_{3/2}, f_{5/2})\). It is important to see if this feature is reproduced in the NCSM. Also, in
spite of the differences in frameworks with and without a core, it is important to compare selected aspects of the initial and modified Hamiltonian with a recent $fp$-shell interaction, the GXPF1, developed by Honma, Otsuka, Brown and Mizusaki [64]. It is valuable to compare various $fp$-shell interactions to understand better their shortcomings and their regimes of applicability. It is worth mentioning the NCSM interaction employed here and Honma et al. GXPF1 interactions were also tested recently within the framework of spectral distribution theory in Refs. [65, 66] to illustrate their similarities and differences.

One can note that direct comparisons of NCSM matrix elements with those of GXPF1 involve approximations. Three aspects of these comparisons are noted. First, the $A$-dependence of GXPF1 is $A^{-0.3}$, while the $A$-dependence of the derived NCSM effective interaction employed is not anticipated to be a simple scale factor. For this reason, it is better to focus on a narrow range of $A$ for the comparison. Second, a more precise comparison would involve the derivation of a pure ‘valence-only’ effective interaction and an appropriate scheme for doing this has recently been shown to yield important 3-body forces [67, 68]. Results presented here will help motivate this major undertaking. Third, the results presented here may also be compared with the earlier Brueckner-based matrix elements [69] for the same region, since phenomenological adjustments to the NCSM interaction may be expected to simulate the physics in the perturbative treatment of core-polarization.

### 4.1 Phenomenological Terms

To obtain NCSM spectroscopies fit to the data for the $A = 48$ nuclei, like $^{48}Ca$, $^{48}Sc$, and $^{48}Ti$ by means of additive phenomenological potentials, is a major undertaking. Hence, minimal approaches are investigated in Ref. [20] to modify the theoretical $H_{eff}$ to improve selected spectroscopic properties. This can be considered a baseline effort for future investigations in larger model spaces, where one expects a reduced need for phenomenological terms as one proceeds towards more complete treatments. The adopted overall fitting strategy emphasizes the total binding energy and the lowest lying excited states. Inspired by successful modifications found in Ref. [70], it was first investigated in Ref. [20] whether a phenomenological $S$-wave or
monopole interaction supplies the main missing ingredient from the NCSM realistic effective
two-body Hamiltonians. They choose to add simple $T = 0$ and $T = 1$ delta functions and find
they can produce greatly improved properties. However, they also found it necessary to adjust
the $T = 0$ and $T = 1$ strengths for each nucleus to obtain good agreement with experimental
properties. Thus, Ref. [20] concludes that, with this approach, six parameters are needed to
obtain reasonable results for the binding energies and the positive parity spectra of the three
$A = 48$ nuclei addressed. However, the spectrum of $^{48}\text{Sc}$ is still rather poor. A recent review
of the phenomenological shell model and the role of the monopole interaction [63] demonstrate
the ultimate source of the residual physics is contained in 3-body interaction effects—probably
a combination of core-polarization and realistic (bare [8]) 3-body forces.

Our own long-term goal is to include these additional contributions which are natural in
our NCSM approach but require next-generation computers. To appreciate the magnitude of
the effort needed and the potential success of including realistic $NN$ and $NNN$ interactions
in large basis spaces, refer to the recent investigation of $^7\text{Li}$ with a Hamiltonian derived from
chiral effective field theory [71]. In addition, a more detailed examination of the features of
our results (see below) and comparisons with NCSM results in light nuclei indicate the missing
physics is tied to larger basis spaces and to realistic $NNN$ interactions. The fact that a simple
monopole term in the conventional shell model with a core successfully approximates all this
complexity at the 2-body level is remarkable and deserves more extensive investigation. In
the hopes of obtaining a single, NCSM Hamiltonian for the binding energies and spectra of
these three nuclei, Ref. [20] explores the utility of two-body central plus tensor forces added
to the \textit{ab initio} $H_{\text{eff}}$. They achieve a reasonable description of a small set of the targeted
properties in these three nuclei by fitting the strengths and ranges of these three terms. The
specific forms of the finite range central and tensor potentials found acceptable are as follows:
\begin{equation}
V(r) = V_0 \exp\left(-\frac{(r/R)^2}{r^2}\right) + V_1 \exp\left(-\frac{(r/R)^2}{r^2}\right) + V_t S_{12}/r^3,
\end{equation}
where the central strengths, $V_0 = -14.40 \text{ MeV} - \text{fm}^2$ and $V_1 = -22.61 \text{ MeV} - \text{fm}^2$ with $R = 1.5 \text{ fm}$, the tensor strength $V_t = -52.22 \text{ MeV} - \text{fm}^3$, and $S_{12}$ is the conventional tensor operator.
4.2 \( A = 48 \) Results

The main goals of Ref. [20] were to present the first NCSM results for \( ^{48}Ca, \text{ }^{48}Sc, \) and \( ^{48}Ti \) with effective Hamiltonians derived directly from a realistic \( NN \) interaction and to investigate phenomenological improvements. The \textit{ab initio} results displayed the shortcomings of the limited model spaces presently available, as well as possible shortcomings from neglecting three-body forces. Hence, Ref. [20], addressing \( A = 48 \), as well as the present work, addressing \( A = 47 \text{ – } 49 \), adopted the NCSM approach and approximated the full \( H_{eff} \) with a two-body cluster truncation. To solve these systems, all nucleons were treated with the same two-body Hamiltonian derived from a realistic \( NN \) interaction, including Coulomb interaction between proton pairs. There were no single particle energies involved and the eigenenergies were the total binding energies. The results were initially obtained with the \textit{ab initio} NCSM, using the CD-Bonn interaction [3, 15] and \( \hbar \Omega = 10 \text{ MeV} \), a typical choice for this region.

Ref. [20] shows the trend of the even-even and odd-odd nuclear binding energies matches reasonably well with experiment, using \textit{ab initio} NCSM, except that theory consistently underbinds by about \( 20 \text{ MeV} \) (0.4 MeV/nucleon). In other words, except for this underbinding, the \textit{ab initio} NCSM already predicts some subtle features of the valley of stability. On the other hand, while all even-even nuclei have the correct \( J^{\pi} = 0^{+} \) ground-state spin and parity, the odd-odd nuclei generally have the incorrect ground-state spin Ref. [20].

Increasing \( \hbar \Omega \) leads to increased binding (and decreased rms radii) in this application of the \textit{ab initio} NCSM (\( \hbar \Omega = 10.5 \text{ MeV} \) would produce a good fit to the binding alone), but fails to improve the errors in ground-state spins and other deficiencies in the spectral properties.

The overall binding energy picture is considerably improved with the phenomenological additions described above. These additive terms are fit by hand to the ground-state energies of \( ^{48}Ca, \text{ }^{48}Sc, \) and \( ^{48}Ti \), as well as the first excited positive and negative parity states in \( ^{48}Ca \). This limited amount of data under-constrains the fit. It is reasonable to speculate the alternative parameterizations of the additive terms would yield equivalent fits to these limited data.

For \( ^{48}Ca \), Ref. [20] evaluated both the positive (0\( \hbar \Omega \)) and negative parity (1\( \hbar \Omega \)) spectra.
The main impression is the spectra in \(^{48}\text{Ca}\) is severely compressed relative to the experimental spreading. Inspecting the corresponding ground-state wavefunctions revealed an absence of the expected dominance by the \([0f_{7/2}]^8\) neutron configuration. Instead, the \(1p_{3/2}\) neutron state is significantly populated. Ref. [20] concludes the expected energy spacing between the \(0f_{7/2}\) and the \(1p_{3/2}\) state is not supported by the \textit{ab initio} NCSM in such a small model space. This means there is insufficient spin-orbit splitting in the effective interaction without phenomenological additive terms.

In light nuclei, the strategy has been to evaluate \(H_{\text{eff}}\) for each model space leading to a separate \(H_{\text{eff}}\) for positive and negative parity states. As one proceeds to heavier systems, a better strategy is to use the same \(H_{\text{eff}}\) for both positive and negative parities, e.g., use the \(1h\Omega\) \(H_{\text{eff}}\) in both the \(0h\Omega\) and \(1h\Omega\) model spaces. A more detailed discussion of the use of effective interactions created specifically for the \(0h\Omega\) and \(1h\Omega\) spaces separately—that is, they are different, model-space dependent, effective interactions—can be found in Ref. [20]. However, when using \(H_{\text{eff}}\) of the \(1h\Omega\) model space for both the positive and negative parity states at \(h\Omega = 10\text{ MeV}\), the relative spacings of the states within a given parity are essentially unchanged, while the lowest negative parity excitation above the ground-state is now at 6.9 MeV of excitation, a major improvement. In light of this result, the present applications retain the use of the effective interactions derived for the \(1h\Omega\) basis space.

A reasonable agreement of the \(^{48}\text{Ca}\) negative parity spectrum with experiment is significant, considering that only the position of the first \(3^-\) state was involved in the fit. It is also significant, since the negative parity spectrum is sensitive to a set of 2-body matrix elements considerably larger than the set controlling the positive parity spectrum. In particular, the negative parity spectrum is sensitive to matrix elements involving excitations from the \(sd\) states to the \(pf\) states, as well as from the \(pf\) states to the \(sdg\) states. These are negative parity 2-body matrix elements that complement the positive parity 2-body matrix elements for nucleons interacting entirely within the \(pf\) shell.

For \(^{48}\text{Sc}\), the interaction with additional terms produces correct ground-state spin and a reasonable low-lying positive parity spectrum. The resulting spectrum is slightly more spread
than the results of Caurier et al., [70]. The \textit{rms} energy deviations between theory and experiment (excluding states involved in the fit) indicate considerable room for improvement in the spectrum of $^{48}Ti$ and that future fits should include a representative excited state from this spectrum.

Ref. [20] answers the question of whether the NCSM can be adjusted to obtain reasonable fits with additive phenomenological two-body potentials for the $A = 48$ nuclei. In particular, Ref. [20] shows additive isospin-dependent central terms plus a tensor force can achieve accurate $BE/A$ and reasonable spectra for these three systems. In addition, accurate $BE/A$ are obtained for eight $A = 48$ nuclei, reproducing the experimental valley of stability. The net change of interaction energies is of the order of a few percent with the added phenomenological terms. More extensive searching could undoubtedly improve the fits to the low-lying spectra.

However, this work has a significant drawback. Due to the limited model space and the neglect of real and effective three-body interactions, one must resort to additive phenomenological terms to obtain a high quality description of selected experimental data. The dependence on the parameters introduced, including the basis space parameters, $N_{\text{max}}$ and $\hbar \Omega$, as well as dependence on the forms and strengths of the additive potential terms, severely limits the predictive power of this approach. On the other hand, the descriptions achieved with the initial choice of additive terms provides insight into the deficiencies of our current $H_{\text{eff}}$ in the $0\hbar \Omega$ and $1\hbar \Omega$ model spaces.

4.3 $A = 47 - 49$ Results

Many questions remain from the work of Ref. [20]. Chief among them is the range of validity of the Hamiltonian found successful for the $A = 48$ nuclei. It is natural to extend this work through NCSM applications to the $A = 47 - 49$ nuclei, the focus of the following subsections. Many of the results of the $A = 47 - 49$ applications have appeared in Ref. [19] and the additional results are presented in this thesis for the first time.
4.3.1 Binding energies

First, the calculated total interaction energies (Hamiltonian ground-state eigenvalues) in Fig. 4.1 are compared with experiment. Observe the ground-states calculated with the derived \textit{ab initio} CD-Bonn $H_{\text{eff}}$ (third column in Fig. 4.1) lie above the experimental values by approximately 20 MeV. This shift is similar to that observed in the case for all $A = 48$ isotopes [20]. Note, with CD-Bonn, there is nearly the same increase in binding from $^{47}\text{Ca}$ to $^{48}\text{Ca}$ as from $^{48}\text{Ca}$ to $^{49}\text{Ca}$, which signals a lack of subshell closure.

For the modified Hamiltonian (CD-Bonn + 3 terms), the NCSM produces reasonable agreement with experiment with deviations much less than 1% as seen in Fig. 4.1. There is a simple spreading of the theoretical ground-states relative to experiment. More importantly, we now observe the desired subshell closure condition, where the increased binding from $^{47}\text{Ca}$ to $^{48}\text{Ca}$ significantly exceeds that from $^{48}\text{Ca}$ to $^{49}\text{Ca}$. Thus, the modified Hamiltonian appears to pass the first major test of providing a reasonable spin-orbit splitting for the lowest-lying neutron and proton orbitals around the doubly-magic $^{48}\text{Ca}$ nucleus. Next, examination of a detailed $A = 47 - 49$ spectra follows to learn more about the subtleties of spin-orbit splittings involved in excited $A = 47 - 49$ states.

4.3.2 Excitation energy spectra

The excitation energy spectra for $^{49}\text{Ca}$, $^{47}\text{Ca}$, $^{49}\text{Sc}$, and $^{47}\text{K}$ are shown in Figs. 4.2 - 4.5, respectively. In every case, the \textit{ab initio} NCSM results with CD-Bonn are far too compressed relative to experiment—a feature also seen in the $A = 48$ results [20]. Here, trace this primary defect to the inferred properties of the neutron orbits. That is, the incorrect ground-state spin seen in Fig. 4.2 and the absence of a significant excitation energy gap in Fig. 4.3 indicate the spin-orbit splitting of the neutrons is insufficient to provide proper subshell closure at the neutron $0f_{7/2}$ orbit. This defect is rectified in the results with CD-Bonn + 3 terms as seen by the corresponding spectra in Figs. 4.2 and 4.3. Similar tendencies have been seen before with valence G-matrix interactions and identified as a problem with the $L^2$ dependence of the single-particle states [58, 63]. Since we generate our results without the use of single-particle
energies, the origin of the improved spectral spin-orbit properties lies with the three additive interaction terms.

The \textit{ab initio} NCSM results with CD-Bonn in Figs. 4.4 and 4.5 are more difficult to interpret, due to the glaring deficiencies just mentioned for the neutrons with the CD-Bonn Hamiltonian. Discussion below will show the proton shell closure is better established with CD-Bonn. This supports the assertion that the main deficiencies seen in the third columns of Figs. 4.4 and 4.5 are indeed likely to reside with the inferred neutron spin-orbit splitting problem.

The modified Hamiltonian provides greatly improved spectra for all four nuclei, as seen in the second columns of Figs. 4.2 - 4.5. Note, these nuclei are not involved in the fitting procedure used to determine the parameters of the added phenomenological terms. Perhaps the most significant remaining deficiency is the incorrect ground-state spin for $^{47}\text{K}$, as seen in Fig. 4.5. This is the first case of a nucleus in the region of $A = 47$ to $A = 49$ (12 nuclei studied to date), where we did not obtain the correct ground-state spin with CD-Bonn + 3 terms Hamiltonian.
4.3.3 Single-particle characteristics

To better understand the underlying physics of our NCSM results, we investigate the single-particle-like properties of our solutions. In a simple closed-shell nucleus, it is expected the leading configuration of the ground-state solution in the $m$-scheme treatment to be a single Slater determinant. Single-particle (or hole) excitations should be easily identified by the character of their leading configurations, i.e., a single-particle creation (or destruction) operator acting on the ground-state Slater determinant of the reference nucleus $^{48}Ca$. For our odd mass nuclei, this is the character we seek. That is, we take the standard phenomenological shell model configuration of a single Slater determinant with a closed $sd$-shell for the protons and a closed $f_{7/2}$ subshell for the neutrons, and look for the appropriate states which have a single nucleon added to (or subtracted from) this Slater determinant. We accept states as “single-particle-like”, when we find one with a leading configuration having more than a 50% probability to be in the simple configuration just described. When the majority weight is distributed over a few states, we use the centroid, as will be discussed in some detail below.

We were not successful in locating all the expected single-particle-like and single-hole-like states. That is, those absent from our presentation below were spread among a large number of eigenstates.
Fig. 4.3 Experimental and theoretical excitation energy levels for $^{47}Ca$. Both CD-Bonn and CD-Bonn + 3 terms results are presented.

For a closed-shell nucleus $(Z, N)$, the single-particle energies (SPE) for states above the Fermi surface are related to the binding energy differences

\[ e_p^> = BE(Z, N) - BE^*(Z + 1, N) \]

and

\[ e_n^> = BE(Z, N) - BE^*(Z, N + 1). \]

The SPE for states below the Fermi surface are given by

\[ e_p^< = BE^*(Z - 1, N) - BE(Z, N) \]

and

\[ e_n^< = BE^*(Z, N - 1) - BE(Z, N). \]

The BE are ground-state total binding energies (the difference between the sums of the masses of the neutrons and protons, and the mass of the ground-state of the nucleus), which are taken as positive values. $e$ is negative for bound states. $(BE^* = BE - E_x)$ is the ground-state binding energy minus the excitation energy of the excited states associated with the single-particle states.

Experimental SPE’s and the results of our analysis are shown in Fig. 4.6. The experimental
Fig. 4.4 Experimental and theoretical excitation energy levels for $^{49}$Sc. Both CD-Bonn and CD-Bonn + 3 terms results are presented.

SPE’s for protons and neutrons follow Brown’s analysis [60]. To guide the eye, a horizontal line indicates the vicinity of the Fermi surfaces for the protons and neutrons.

Figure 4.6 shows proton shell closure is established with both Hamiltonians, the CD-Bonn, and the CD-Bonn + 3 terms. The correct energy locations are better approximated with the modified Hamiltonian. Figure 4.6 also shows that neutron subshell closure only appears with the modified Hamiltonian. Here, the ordering is correct, but the states are considerably more spread out compared with experiment.

Consider some of the details underlying the single-particle-like states. The situation for the $1p_{3/2}$ or “$1p_3$” state in the left panel of Fig. 4.6, the proton single-particle state in $^{49}$Sc with the modified Hamiltonian, is quite interesting. It appears this state is mixed over several excited states in the spectrum. Take the strength spread over several states and construct a centroid for this $1p_3$ state by a weighted average over the states carrying this strength. Here are the relevant input ingredients.

The first excited state of $^{49}$Sc is a $3/2^-$, as seen in the second column of Fig. 4.4, with about 51% of the occupancy of the $1p_3$ state. Its eigenvalue is $-425.151$ MeV compared to a
Fig. 4.5 Experimental and theoretical excitation energy levels for $^{47}K$.
Both CD-Bonn and CD-Bonn + 3 terms results are presented.

ground-state of $-428.365 \text{ MeV}$. The 18th state in the $^{49}\text{Sc}$ spectrum is also a $3/2^-$ with 28% of the occupancy of the 1p3 state. Its eigenvalue is $-422.803 \text{ MeV}$. The 24th state is also a $3/2^-$ with 21% occupancy of the 1p3 state. Its eigenvalue is $-422.440 \text{ MeV}$.

Thus, to a good approximation, the 1p3 strength is spread over these three states. Identify the weighted average $[0.51 \times (-425.151) + 0.28 \times (-422.803) + 0.21 \times (-422.440)] = -423.79$ as the centroid of the single particle 1p3 state, which is included accordingly in the second column of Fig. 4.4.

For the proton hole states with the modified Hamiltonian, we perform a detailed search up to excitation energies of about 14 $\text{MeV}$ in the $^{47}K$ spectra. It appears the $0d_{5/2}$ single-hole state is spread among many states with the largest observed concentration on the $5/2^+$ state at $-386.17 \text{ MeV}$ ($13.36 \text{ MeV}$ of excitation energy). Here, a single $J^\pi = 5/2^+$ state in $^{47}K$ with 30% $0d_{5/2}$ vacancy is found. This state is assigned to our $0d_{5/2}$ single-hole state. Most of the $0d_{5/2}$ strength, however, is not observed among the limited number of converged eigenstates.

Consider the $^{49}\text{Ca}$ results with the modified Hamiltonian in the upper right panel of Fig. 4.6. The ground-state is approximately a pure $[(1p_{3/2})^1(0f_{7/2})^8]$ configuration. Note, the
Fig. 4.6  Experimental and theoretical levels dominantly single-proton and single-neutron particles or holes of $^{48}\text{Ca}$. The levels are labeled by $(n, l, 2j)$, and the dashed lines are the Fermi energies.

spacing for the subshell closure is in good agreement with experiment, while there is a shift of a couple $MeV$ towards more binding in the model, as previously indicated in Fig. 4.1. A nearly pure $1p_{1/2}$ single-particle state is obtained at 5.235 $MeV$ excitation energy and an extra low-lying $7/2^-$ appears with $2p - 1h$ character (see Fig. 4.2). The lowest-lying $5/2^-$ consists of $2p - 1h$ character relative to subshell closure.

Contrast the modified Hamiltonian’s results for the $^{49}\text{Ca}$ ground-state with those obtained using the $ab\ initio$ CD-Bonn, where $[(1p_{3/2})^1(1p_{1/2})^2(0f_{7/2})^3]_{3/2^-}$ is the dominant configuration, as opposed to the configuration expected from the simple shell model of $[(1p_{3/2})^1(0f_{7/2})^8]_{3/2^-}$, reflecting again the inadequacies of the neutron single-particle properties with the $ab\ initio$ CD-Bonn.

4.3.4 Monopole matrix elements $V(ab; T)$

Now that successes and deficiencies in the $A = 47 - 49$ spectra have been identified, we seek to determine the nature of the shortcomings in the underlying Hamiltonians. In this effort,
we will be guided by the successful phenomenological GXPF1 interaction [64], although it is defined only for the 0hΩ basis space. The GXPF1 interaction was developed to fit a significant range of fp-shell nuclei, including some of those addressed in this work. One of the main features identified for GXPF1, to distinguish it from microscopic G-matrix interactions, is its distinctive monopole character. This leads to investigation of the monopole character of the ab initio CD-Bonn and the semi-realistic CD-Bonn + 3 terms, at least for those matrix elements in the fp-shell or 0hΩ model space.

The monopole matrix element is defined by an angular momentum average of coupled doubly-reduced two-body matrix elements:

\[
V(ab; T) = \frac{\sum_J (2J+1)V(abab; JT)}{\sum_J (2J+1)}. \tag{4.1}
\]

For the NCSM Hamiltonians the, “V” appearing in Eq. (4.1) signifies the full 2-body intrinsic-coordinate Hamiltonian, \(T_{\text{rel}} + V_{\text{eff}}\), except we omit the Coulomb interaction from this analysis.

We examine the monopole character of the ab initio CD-Bonn Hamiltonian and note some
Fig. 4.8 (color online) Comparison between CD-Bonn+3 terms and GXPF1 of the monopole matrix elements $V(ab; T)(A = 48)$, shown by circles and squares, respectively. See the caption for Fig. 4.7.

similarities and differences from the GXPF1 interaction [64] as shown in Fig. 4.7. The see-saw shapes of the two Hamiltonians in Fig. 4.7 are similar, but our Hamiltonian is shifted towards less attraction. Given the many differences between the respective theoretical starting points, the ab initio $H_{\text{eff}}$ for the NCSM and the G-matrix for GXPF1, the different bare [8] $NN$ interactions, etc., the similarities observed in Fig. 4.7 are remarkable. Although the monopole characteristics were similar, it is worth mentioning the ambiguity of the role of the SPE’s. That is, one may shift some Hamiltonian components between SPE’s and two-body matrix elements (TBME’s) and this obscures direct comparisons of a subset of our TBME’s with the corresponding subset of GXPF1. To summarize a comparison of the underlying theoretical interactions, Table 4.1 provides a simplified overview of their differences and similarities.

For a sample comparison of the interactions, a small set of two-body $fp$-shell matrix elements applicable to the present investigation are given in Table 4.2. For convenience, we present two columns of key differences in the matrix elements—“diff1” represents the difference between the G-matrix and the GXPF1 interaction resulting from adjusting the G-matrix
Fig. 4.9 (color online) Comparison of the monopole matrix elements $V(\alpha\beta;T)(A = 48)$ between CD-Bonn and GXPF1 (shifted to have an overall average monopole the same as CD-Bonn), shown by circles and squares, respectively. See the caption for Fig. 4.7.

elements to fit spectra; and, “diff2” represents the difference between our \textit{ab initio} $H_{\text{eff}}$ and our modified $H_{\text{eff}}$. The scale for these changes from the respective starting solutions appears comparable, although one of the “diff2” values reaches $-1.2123$ MeV.

For a more detailed comparison of the interactions, we present the $fp$-shell matrix elements applicable to the present investigation in Tables 4.2 and A.1. For convenience in finding the major differences, we present two columns of key differences in the matrix elements—“diff1” represents the difference between our \textit{ab initio} $H_{\text{eff}}$ and our modified $H_{\text{eff}}$; and, “diff2” represents the difference between our modified $H_{\text{eff}}$ and the GXPF1 interaction. While “diff1” shows magnitudes that only occasionally exceed 1 MeV, “diff2” shows magnitudes approaching 2.6 MeV. This type of comparison suggests our solution for the modified Hamiltonian remains closer to our initial $H_{\text{eff}}$ derived from CD-Bonn, than it is to the fitted Hamiltonian, GXPF1.

Figure 4.8 presents a similar comparison of the monopole character in the $fp$-shell of the two phenomenological Hamiltonians, GXPF1 and CD-Bonn + 3 terms. Overall, the changes in the monopole character, due to the addition of the phenomenological terms to our $H_{\text{eff}}$ of
Fig. 4.10 (color online) Comparison of the monopole matrix elements $V(ab; T)(A = 48)$ between CD-Bonn + 3 terms and GXPF1 (shifted to have an overall average monopole the same as CD-Bonn + 3 terms), shown by circles and squares, respectively. See the caption for Fig. 4.7.

Fig. 4.7, appear somewhat larger for the $T = 1$ monopole than for $T = 0$. The effect of “+3 terms” is to increase the $T = 0$ and $T = 1$ splitting of six of the monopoles, while the 4 remaining $T = 0$ and $T = 1$ monopole splittings are reduced.

To better visualize the similarities of the $fp$-shell matrix elements, we present in Figs. 4.9 and 4.10 the same comparisons shown in Figs. 4.7 and 4.8, respectively, with an overall shift of the GXPF1 monopole matrix elements, so the average over all monopole matrix elements is the same for the two Hamiltonians. Specifically, the average shift of $T = 0$ and $T = 1$ monopoles for GXPF1 in Fig. 4.9 is $0.899768 \text{ MeV}$, while for GXPF1 in Fig. 4.10 it is $0.83485 \text{ MeV}$. It is now evident that both CD-Bonn and CD-Bonn + 3 terms have monopoles with less $T = 0$ and $T = 1$ splittings than GXPF1.
Fig. 4.11 (color online) Correlation of $V(\text{abcd}; JT)$ matrix elements between CD-Bonn + 3 terms and CD-Bonn. The matrix elements of $T = 0$ and $T = 1$ are shown by circles and squares, respectively. The filled circles and the filled squares are for all $V(\text{abab}; JT)$ matrix elements that contribute to the monopole $V(ab; T)$. The open circles and open squares are for the remaining matrix elements. There are no monopole shifts. The solid straight line represents a linear fit to all matrix elements. The diagonal dashed line represents the reference correlation line at 45-degrees.

4.3.5 Matrix element correlations

We present in Figs. 4.11 - 4.18 the correlations between pairs of $fp$-shell interaction matrix element sets. With Fig. 4.11, we observe the high degree of correlation between the 195 matrix elements of our starting Hamiltonian, CD-Bonn, and our modified Hamiltonian, CD-Bonn + 3 terms. This indicates, for the most part, our Hamiltonian is minimally modified by the addition of the phenomenological terms. Such a high correlation is reminiscent of the high correlations seen between GXPF1 and its starting interaction, the G-matrix [64]. It is interesting to see if certain groups of matrix elements appear to be more correlated than others. We distinguish the diagonal $V(\text{abab}; JT)$ matrix elements that contribute to the monopole by different symbols. Filled circles represent $V(\text{abab}; JT = 0)$ and filled squares represent $V(\text{abab}; JT = 1)$ matrix
Fig. 4.12 (color online) Correlation of $V(abcd; JT)$ between CD-Bonn + 3 terms and CD-Bonn, where we removed all $V(abab; JT)$ matrix elements that contribute to the monopole $V(ab; T)$. The solid straight line represents a linear fit to all the plotted points. The circles and the squares represent $T = 0$ and $T = 1$, respectively. The diagonal dashed line represents the reference correlation line at 45-degrees.

elements. All remaining matrix elements, $V(abcd; JT)$, where at least one single-particle-state (sps) of the bra is different from a sps of the ket are plotted as open circles for $T = 0$ and open squares for $T = 1$. We see the filled square points, that correspond to $V(abab; JT = 1)$ matrix elements, are farther from the linear fit, ranging between 1 and 2 $MeV$ away from the linear fit line. Therefore, these monopole matrix elements have received larger corrections than others in the process of fitting the $A = 48$ isotopes.

To see the stronger correlations more clearly, we next choose in Fig. 4.12 to eliminate all matrix elements contributing to the monopole. There are 135 remaining matrix elements out of a 195 total. The degree of correlation between the 135 matrix elements significantly improves with much less deviation from the linear fit. We can see another feature of the correlation by comparing the linear fit with the 45-degree line in Fig. 4.12 (similar pattern seen in Fig. 4.11). On the one hand, we see the CD-Bonn + 3 terms matrix elements are shifted towards greater
attraction, where CD-Bonn is already attractive. On the other hand, the CD-Bonn + 3 terms matrix elements are shifted towards greater repulsion, where CD-Bonn is already repulsive. Overall, we observe the larger differences between the CD-Bonn and CD-Bonn + 3 terms are coming from the monopole terms. This seems natural in light of the fact the phenomenological terms have the effect of adjusting the single particle features of the theory towards agreement with experiment. That is, the monopole terms receive the largest adjustments as required to achieve the needed single particle features.

It is then very interesting to observe in Fig. 4.13 the lack of correlation between our starting Hamiltonian, CD-Bonn, and the G-matrix underlying the GXPF1 interaction. Points are generally farther away from the fit line than in the correlation of CD-Bonn + 3 terms with the CD-Bonn case. Note, the G-matrix is a renormalization procedure and the specific results for GXPF1 are developed from the bare [8] CD-Bonn interaction. Since the underlying bare interaction [8] is the same, this lack of correlation in Fig. 4.13 reflects the major differences in the underlying effective interaction theories summarized in Table 4.1.

We now make the same set of comparisons between CD-Bonn and G-matrix in Figs. 4.13
Fig. 4.14 (color online) Correlation of $V(\text{abcd}; JT)$ between CD-Bonn and G. See the caption for Fig. 4.12.

and 4.14 as we performed in Figs. 4.11 and 4.12. The symbols used are the same as those in Figs. 4.11 and 4.12. Comparing Fig. 4.13 and Fig. 4.14, we can see how, after eliminating the matrix elements that contribute to the monopole, the correlation is significantly improved with the linear fit in Fig. 4.14. It now overlaps well with the 45-degree line. Again, this shows similarities between these two interactions with a difference arising primarily from the monopole part.

We can comment further about the comparison presented in Fig. 4.13 by observing the full Hamiltonian developed from the G-matrix includes single-particle energy (SPE) contributions. On the other hand, our \textit{ab initio} CD-Bonn does not have additional SPE contributions, since these contributions are already included in the 2-body matrix elements. In fact, these SPE contributions to our interactions are embedded in the monopole terms. This is one good reason why the correlations may be expected to improve when we proceed from Fig. 4.13 to Fig. 4.14, by removing the monopole terms.

Furthermore, we find minimal correlation between CD-Bonn + 3 terms and the full GXPF1 as seen in Fig. 4.15. This indicates the likely sensitivity to the starting Hamiltonians in the
fitting procedures and to the differences in the NCSM, compared to a valence shell model approach. In addition, we should note that neither Hamiltonian can claim to be unique given the number of parameters used to fit them to experiment. Therefore, one may also interpret the lack of correlation shown in Fig. 4.16 as an indication of a significant possibility for alternative improved fits along the lines of either approach.

To isolate the off-diagonal 2-body interaction effects from those that may contribute to the monopole, eliminate some of the matrix elements from the comparison. In Fig. 4.16, we present the correlation of $V(abcd;JT)(A = 48)$ between the remaining CD-Bonn + 3 terms and GXPF1 matrix elements. Clearly, the correlation improves.

If we represent all the matrix elements that can contribute to the monopole minus its own average monopole, then the correlation becomes significantly better. We can see this in Fig. 4.17 noticing that the solid line, that is a fit to all points, significantly approaches the diagonal dashed line. Note, however, that significant deviations from perfect correlation remain. From the residual lack of correlation, we may infer that improved fits to the spectra,
in either approach, are not likely to be limited to changes of the monopole character.

Finally, to focus as clearly as possible on the 2-body interaction effects, we present in Fig. 4.18 the correlation of matrix elements, $V(\text{abcd}; JT)$ ($A = 48$), between CD-Bonn + 3 terms and GXPF1, where we retain only those that cannot contribute to a single-particle Hamiltonian. That is, we eliminate all two-body matrix elements, where at least one single-particle-state (sps) of the bra equals a sps of the ket. There are 56 remaining two-body matrix elements. Differences ranging up to about 3 MeV are observed, which should lead to differences in experimental observables. Comparisons of spectra and other properties with these Hamiltonians, as one proceeds further from $A = 48$, may shed more light on their differences.

Fig. 4.16 (color online) Correlation of the matrix elements $V(\text{abcd}; JT)$ between CD-Bonn + 3 terms and GXPF1. See the caption for Fig. 4.12.
Fig. 4.17 (color online) Correlation of the matrix elements $V(abab;JT)$ between CD-Bonn + 3 terms and GXPF1, where we subtract the average monopole $V(ab;T)$ for each interaction. The circles and the squares represent $T=0$ and $T=1$, respectively. The thick solid line represents a linear fit to all plotted points. The diagonal dashed line represents the reference correlation line at 45-degrees.

Table 4.1 Overview of the differences and similarities of the two theoretical approaches that underlie the Hamiltonians whose matrix elements are compared in this work.

<table>
<thead>
<tr>
<th>Hamiltonian Property</th>
<th>G-matrix</th>
<th>NCSM cluster $H_{eff}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Oscillator parameter dependence</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Depends on the choice of P-space</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Requires effective multi-nucleon interactions as corrections</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Translationally invariant</td>
<td>No</td>
<td>Yes</td>
</tr>
<tr>
<td>Starting energy dependence</td>
<td>Yes</td>
<td>No</td>
</tr>
<tr>
<td>Single-particle spectra dependence</td>
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<td>No</td>
</tr>
<tr>
<td>$A$-dependence</td>
<td>No</td>
<td>Yes</td>
</tr>
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</table>
Fig. 4.18 (color online) Correlation of the matrix elements $V(abcd; JT)$ between CD-Bonn + 3 terms and GXPF1, where we retain only the off-diagonal matrix elements, i.e., the 56 matrix elements that cannot contribute to a single-particle Hamiltonian (see text). The filled circles and the filled squares represent $T = 0$ and $T = 1$, respectively. The thick solid line represents a linear fit to all the plotted points. The diagonal dashed line represents the reference correlation line at 45-degrees.

Table 4.2 Comparison of selected two-body matrix elements, $V(abcd; JT)$ ($MeV$) ($A = 48$), for which the difference between our interaction is large. “diff1” represents the difference between GXPF1 and G, while “diff2” is the difference between CD-Bonn + 3 terms and CD-Bonn.

<table>
<thead>
<tr>
<th>2j_a</th>
<th>2j_b</th>
<th>2j_c</th>
<th>2j_d</th>
<th>J</th>
<th>T</th>
<th>G</th>
<th>GXPF1</th>
<th>diff1</th>
<th>CD-Bonn</th>
<th>CD-Bonn</th>
<th>diff2</th>
</tr>
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<tbody>
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<td></td>
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<td></td>
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<td></td>
<td>+3 terms</td>
</tr>
<tr>
<td>7</td>
<td>3</td>
<td>7</td>
<td>3</td>
<td>5</td>
<td>0</td>
<td>-2.1167</td>
<td>-2.8504</td>
<td>-0.7337</td>
<td>-1.0390</td>
<td>-1.3413</td>
<td>-0.3023</td>
</tr>
<tr>
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<td>3</td>
<td>5</td>
<td>5</td>
<td>0</td>
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CHAPTER 5. EXTREME SINGLE PARTICLE SHELL MODEL (ESPSM)

One of the main objectives of the study of nuclear physics is understanding the structure of nuclei, including all aspects of the motion of nucleons—their paths in space, their momenta, the correlations between them, the energies binding them to each other, and their excited state properties including reaction cross sections. Mathematically, the complete description of the nuclear structure is contained in the total wavefunction of each state of the nucleus. Simplified models describing nuclei in terms of a number of parameters have been proposed. From a nuclear model, it must be possible to predict various observable properties of the nuclides. A simple nuclear model is the single-particle model, where individual nucleons are considered to move in stationary orbits, and have their spins and total angular momentum projection paired (e.g., two neutrons occupy the same orbit but with opposite magnetic projections), so the values of many nuclear parameters are determined solely by a single unpaired nucleon. This model contains no correlated or collective motion of several nucleons and has no explicit reference to 2-body forces or 3-body forces acting among the nucleons. These omissions, particularly the latter, suggest this model must have strictly limited applicability and, indeed, its predictions of quadrupole moments were completely erroneous. To describe quadrupole moments within the framework of a model, another extreme model has been proposed. In this model, the nucleus was seen as a distorted liquid drop, where fairly large fractions of the fluid move together to produce a nonspherical shape. A simple liquid-drop model contains little reference to the number of nucleons present and can hardly predict the discontinuities associated with the empirical “magic” numbers. It is clear, to incorporate even the main features of a nuclear structure, a model must be considerably more complicated than either of these extreme cases.
The more realistic models can be described as generalizations and extensions built on the single-particle model, where inter-nucleon forces are included.

### 5.1 Realistic Single-particle Basis—WS Example

A description of the nuclear many-body system by an effective mean field is a doorway to the understanding of atomic nuclei. The average single nucleon dynamics in the field of all other nucleons is a starting point in practically all many-body methods. In this context, a good choice of single-nucleon basis states is the key for success in any quantum many-body approach. A plethora of experimental observations, such as magic numbers, shell gaps, binding energies, nuclear radii, abundance of nuclei in nature, magnetic moments, and reaction properties, confirm the remarkable success of a very simple, pure mean field picture.

In a very simple approach, the mean field can be taken in the form of a 3-dimensional (3D) harmonic oscillator (HO), which provides an analytical set of basis states. The possibility of an exact translationally-invariant treatment with a full center of mass extraction is particularly appealing. Historically, the HO mean field with an added spin-orbit term was the first successful mean field treatment, by which the correct sequence of orbitals and the magic numbers were predicted [72].

In *ab initio* no core shell model (NCSM) calculations of finite nuclei in a HO basis (see Chap 3.1), the long distance tails of the wavefunctions are understood to be slowly convergent. This motivates us to develop new basis states with improved long distance properties. For observables sensitive to the long-range parts of the wavefunctions, like weakly bound-states, $rms$ radii, $B(E_L)$, $B(M_L)$, etc., convergence in the HO basis is slow, since the Gaussian tails of HO wavefunctions poorly represent the asymptotic exponential tails expected in the nuclear wavefunctions. Therefore, more realistic basis space methods would have a greater flexibility for solving these convergence challenges.

Although the single particle states of more realistic mean fields for nuclei must be determined numerically, such computations are trivial with today’s computers, making the numerical approach preferential over analytically solvable models, such as Ginocchio’s potential [73] or...
the square well. Other forms of potentials have been considered in the past [74]. With little exception, all modern theoretical techniques dealing with physics on the interface of structure and reactions have their roots in the Woods-Saxon (WS) potential [75, 76].

A number of parameterizations of the WS potential have been published, created with different objectives and relevant to different nuclear mass regions. Most commonly used is the so-called “Universal” parameterization [77], adjusted to reproduce the single-particle binding energies of proton and neutron orbitals around the doubly-magic nucleus $^{208}$Pb and correct ground-state spins for nuclei of masses around $A = 180$, but claimed to be applicable to lighter mass regions as well. Characteristic for the “Universal” parameterization is the choice of different radii for the proton and neutron potentials. It has been pointed out that this parameterization has shortcomings for applications to lighter nuclei. It predicts charge radii inconsistent with experiment [78]. The importance of a good starting parameterization of the mean field potential motivated an investigation here to reconsider the question of parameters in the WS potential.

This section presents the terms in the WS single-particle Hamiltonian from very general assumptions about the character of the nuclear mean field. One presents the conventional WS Hamiltonian, but the purpose here is to emphasize certain aspects of the mean field description and to recall some of the motivations for this construction.

Woods and Saxon [79] suggested to model the nuclear mean field i.e., the nucleon-core interaction, with a spherically-symmetric potential having a Fermi-function form $f(r, R, a)$

$$f(r, R, a) = \left[1 + \exp \left(\frac{r - R}{a}\right)\right]^{-1}, \quad (5.1)$$

where $r$ is the distance from the center of the nucleus, $R$ is the nuclear radius, $a$ is the diffuseness parameter representing the “surface thickness” of the nucleus, and all parameters have the same units of length. The nuclear radius, $R = r_0 A^{1/3}$, with $r_0 \approx 1.25 \text{ fm}$ and $A$ is the mass number. The total nuclear potential is defined as

$$u(r) = U_0 f(r, R, a), \quad (5.2)$$

where $U_0$ represents the total strength (potential well depth) and is intrinsically negative to
Fig. 5.1 Woods-Saxon (WS) central neutron potential and Harmonic Oscillator (HO) potential shifted to match the WS potential at a radius of 7.3 fm. The dashed red curve represents the HO potential and the solid blue curve represents the WS potential.

represent the attractive nature of the interaction. The typical values for the parameters are $U_0 \approx -50 \text{ MeV}$ and $a \approx 0.6 \text{ fm}$.

For large atomic number $A$ (see Fig. 5.1), this potential is similar to the density of the nucleus, with separate forms for neutrons and protons. It has the following desired properties:

- It is monotonically increasing with distance
- For large $A$, it is approximately flat in the center, signifying the empirical saturation property of nuclei
- Nucleons near the surface of the nucleus (i.e., having $r \sim R$ within a distance of order “$a$”) experience a large force towards the center
• It approaches zero fast as \( r \) goes to infinity \( (r - R \gg a) \), reflecting the short-distance nature of the strong nuclear force.

All these features can be seen in Fig. 5.1 for \(^{197}\text{Au}\), which presents the shape of the WS potential versus HO potential at \( \hbar \Omega = 7.5 \text{ MeV} \). The dashed red curve represents the HO potential and the solid blue curve represents the WS potential. For a better comparison of the two potentials, the potentials were matched at a radius, \( R = 7.3 \text{ fm} \), which required a shift of the HO potential downwards by 60 MeV.

The Coulomb potential is a second Hamiltonian component contributing to the proton-core interaction. This repulsive potential is fully determined with the assumption of a given nuclear charge distribution \( \rho(r) \). The solution of the corresponding electrostatics problem gives

\[
u_C(r) = 4\pi e \left( \frac{1}{r} \int_0^r r^2 \rho(r') dr' + \int_r^\infty r' \rho(r') dr' \right).
\] (5.3)

In the spirit of the WS parameterization, it is often assumed the nuclear charge distribution is proportional in shape to the same function from Eq. (5.1), \( \rho(r) \sim f(r, R_c, a_c) \), where the coefficient of proportionality must be determined from the normalization of density to the total nuclear charge. The integration in Eq. (5.3) along with a normalization of density must be achieved numerically. However, the influence of surface terms on the strength of the Coulomb interaction is weak. Since the Coulomb force is long-range, it smears fine details of the charge density and, for this reason, one conventionally takes the diffuseness of the charge distribution to be zero, when evaluating the proton-nucleus Coulomb potential \([80]\). Furthermore, for the same reason, this work assumed \( R_c = R \), which removes an extra unnecessary parameter that has little influence on the outcome. For the realistic single-particle Hamiltonian in Chapter 6, one adopts protons having the following form of the Coulomb potential

\[
u_C(r) = \begin{cases} \frac{Z e^2}{2 \pi} \left( 3 - \frac{r^2}{\pi^2} \right) & \text{for } r \leq R \\ \frac{Z e^2}{r} & \text{for } r \geq R \end{cases}.
\] (5.4)

which, as a result of the above assumptions, corresponds to a uniformly charged sphere of radius R.
In quantum physics, the spin-orbit interaction is any interaction of a particle's spin with its orbital motion. Due to the spin and orbital motion dependence of the strong inter-nucleon force, a mean field spin-orbit potential is experienced by the protons and neutrons moving inside the nucleus, leading to shifts in their energy levels.

In the phenomenologically successful Extreme Single Particle Shell Model (ESPSM), the spin-orbit potential is defined as follows

\[ u_{SO}(r) = \left( \frac{\hbar}{m \pi c^2} \right)^2 \vec{l} \cdot \vec{s} \frac{1}{r} \frac{\partial}{\partial r} [u(r)] , \]  

where \( \left( \frac{\hbar}{m \pi c^2} \right)^2 = 2.0 \text{ fm}^2 \). The total single-particle angular momentum is \( \vec{j} = \vec{l} + \vec{s} \), \( \vec{j}^2 = \vec{l}^2 + \vec{s}^2 + 2 \vec{l} \cdot \vec{s} \) and therefore,

\[ < lsj | \vec{l} \cdot \vec{s} | lsj > = \frac{1}{2} \left[ j(j+1) - l(l+1) - \frac{3}{4} \right] , \]  

where the spin is \( \frac{1}{2} \) for nucleons. Here, \( j \) and \( l \) represent the total angular momentum and the orbital angular momentum quantum numbers, respectively.

Due to the spin-orbit interaction, the energies of states of the same orbital angular momentum, \( l \), but with different \( j \) will no longer be identical. This arises from the fact that when \( \vec{l} \) is parallel to \( \vec{s} \), the spin-orbit interaction energy is attractive. In this case, \( j = l + s = l + 1/2 \). When \( \vec{l} \) is anti-parallel to \( \vec{s} \) (i.e., aligned oppositely), the interaction energy is repulsive. In this case, \( j = l - s = l - 1/2 \). Figure 5.2 illustrates the shifting of the energy levels due to the spin-orbit interaction within the nuclear shell model. Furthermore, the strength of the interaction is roughly proportional to \( l \).

\[ < lsj | \vec{l} \cdot \vec{s} | lsj > = \begin{cases} \frac{1}{2}; & \text{for } j = l + \frac{1}{2} \\ -\frac{1}{2}[l+1]; & \text{for } j = l - \frac{1}{2} \end{cases} . \]  

(5.6)

The higher \( j \) states have their energies shifted downwards by larger amounts due to Eq. (5.6). This is due to the negative spin-orbit interaction energy and to the reduction in energy resulting from deforming the potential to a more realistic one. The second-to-highest \( j \) states, on the contrary, have their energy shifted up by the first effect and down by the second effect, leading to a small overall shift. The shifts in the energy of the highest \( j \) states on one HO shell can
be shifted down sufficiently, through the spin-orbit interaction, to enter into the range of the energy of states of a lower HO shell.

One frequently-chosen convention is to assume a spin-orbit potential, as the gradient of the central mean field potential. However, it is phenomenologically more useful to have some additional freedom in the spin-orbit potential. Thus, the total effective Hamiltonian becomes

\[
H = \frac{p^2}{2\mu} + u(r) + u_C(r) + \frac{1}{2\mu^2r} \left[ \frac{\partial}{\partial r} \tilde{u}(r) \right] \vec{l} \cdot \vec{s},
\]

where, unlike for the charge distribution generating the Coulomb potential, the potential \( \tilde{u}(r) \) is not equal to the original central potential \( u(r) \). We allow it to have a different form factor. Therefore, the form factor of \( \tilde{u}(r) \) is another assumption that goes into the construction of our chosen WS Hamiltonian,

\[
\tilde{u}(r) = U_{SO} f(r, R_{SO}, a_{SO}).
\]

Here, \( R_{SO} \) and \( a_{SO} \) stand for the radius and the diffuseness of the spin-orbit term.

We also allow for orbital angular momentum \( l \)-dependence for the strength \( U \), radius \( R \), and parameter \( a \). The results presented next show the \( l \)-dependence for the strength, \( U \), is

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**Fig. 5.2** Spin-Orbit splitting of the energy levels illustrated
stronger than for $R$ and $a$, leading to improvements in the calculated binding energy (see Section 5.3).

In the conventional parameterization of the WS potential, as well as in this work, the radii of the form factors are taken to be proportional to the cubic root of the atomic number $A$. Specifically

$$R = R_C = R_0 A^{1/3} , R_{SO} = R_{0,SO} A^{1/3} ,$$

(5.9)
in terms of the parameters $R_0$ and $R_{0,SO}$, which, due to nuclear saturation, we expect to be approximately constant throughout the nuclear chart.

We considered four central $l$-dependent terms in the total Hamiltonian ($l = 0$, $l = 1$, $l = 2$ and $l \geq 3$). Each has its own radius $R = R_0 A^{1/3}$ and diffuseness parameter $a$. For $l \geq 3$ term, the radius and the diffuseness were taken to be the same as for $l = 2$ term. One introduces the following notation for the three parameters that determine the central WS potential, $U_0^l$, $R^l = R_0^l A^{1/3}$ and $a^l$ (e.g., $U_0^0$, $R_0^0$, $a^0$ refer to the $l = 0$ case, etc.). With our selections, then $R_0^{l \geq 3} = R_0^2$ and $a^{l \geq 3} = a^2$.

The many body (MB) basis states of the ESPM are taken to be simple Slater determinants, antisymmetrized product of single-particle solutions of a chosen mean field. Hence, the total nuclear energies may be approximated as a simple sum of single-particle energies (SPE) of the occupied orbits.

For the physically-meaningful properties of the nucleus, only the intrinsic motion of the nucleons is relevant. Spurious effects may result from the inclusion of the center-of-mass (CM) motion. To overcome this difficulty, in the fully interacting nuclear many-body problem, one could use as independent coordinates the CM position

$$\vec{R} = \frac{1}{A} \sum_{i=1}^{A} \vec{r}_i ,$$

(5.10)
plus $(A - 1)$ independent nucleon coordinates (intrinsic coordinates), e.g.,

$$\vec{r}^{\text{intr}}_j = \vec{r}_j - \vec{R} \quad (j = 1, \ldots, A - 1) ,$$

(5.11)
with “$i$”, “$j$” labelling the particles, $\vec{r}_i$ the particles’ spatial coordinates, and $\vec{r}^{\text{intr}}_j$ the intrinsic coordinates. The precise method of achieving factorization of the CM and the intrinsic co-
ponents of the many-body wavefunction follows a standard approach, sometimes referred to as Lawson-Lipkin projection method [81]. In this method, one adds a Lagrangian multiplier term, \( \lambda_{CM}(H_{CM}^{HO} - 3/2\hbar \Omega) \), to the fully interacting many-body Hamiltonian, where \( H_{CM}^{HO} \) is the harmonic oscillator Hamiltonian for the CM motion. With the Lagrangian multiplier, \( \lambda_{CM} \), chosen positive, one separates the states of lowest CM motion \((0s_{1/2})\) from the states with excited CM motion by a scale factor of order \( \lambda_{CM} \hbar \Omega \). Therefore, when working with the WS basis and employing this Lagrange multiplier term, the resulting low-lying states also have wavefunctions assured to have the desired factorized form,

\[
\langle \vec{r}_i | \Psi_\alpha \rangle = \langle \vec{R} | \Phi_{0s}^{CM} \rangle \langle \vec{r}_j^{\text{intr}} | \Psi_\alpha^{\text{intr}} \rangle ,
\]

where “\( \alpha \)” denotes the nuclear state, \( \Psi_\alpha \) and \( \Psi_\alpha^{\text{intr}} \) the many-body wavefunction and the intrinsic many-body wavefunction, respectively. In this manner, the CM motion could be separated as a function of \( \vec{R}, \Phi_{0s}^{CM} \) being “0s” HO wavefunction, a simple Gaussian (see Chapter 3). One would obtain intrinsic nuclear wavefunctions, depending only on the intrinsic coordinates \( \vec{r}_j^{\text{intr}} \). This factorization form of the total many-body wavefunction allows only internal motions to contribute to the evaluation of the \( B(E_2) \) electromagnetic transition operator between an initial and a final state, for example.

As an example, take the \(^{12}\text{C}\) case at \( \hbar \Omega = 25 \text{MeV} \). The many-particle basis space cutoff is \( N_{max} = 4 \) (see Chapter 3) and a cutoff of \( N_{shell} = 14 \) for the HO basis used to expand the WS single-particle states (see below for an extended discussion). Looking at the ground-state energies for \( \lambda = 0 \) and \( \lambda = 2 \), we obtain \( E_{gs}^{(\lambda=0)} = -82.706 \text{MeV} \) and \( E_{gs}^{(\lambda=2)} = -82.543 \text{MeV} \). Therefore, one concludes the “energy cost” of restricting the solutions to have CM motion as pure HO is about 150 \( \text{Kev} \), which is small if one compares it with the pure HO results at the same \( N_{max} \) and the same value of \( \hbar \Omega = 25 \text{MeV} \), \( E_{gs}^{(HO)} = -80.148 \text{MeV} \). To give a better understanding for these ground-state energy values, one must mention the experimental ground-state energy for \(^{12}\text{C}\) is \(-92.162\text{MeV}\). The gain in energy that one obtains when going from HO basis to the WS basis at \( \hbar \Omega = 25 \text{MeV} \) is about 2.5 \( \text{MeV} \), which appears to be significant, even at a lower value of \( N_{max} \) truncation.
5.2 Expansion in the HO Basis

The WS single-particle states (sps) are expanded in a finite HO basis, where we define the $N_{\text{shell}}$ as the cutoff in the number of HO shells used. Hence, one defines the following form of the expansion,

$$\psi_{nljm_\tau_z}^{\text{WS}}(\vec{r}) = \sum_{2n'+l=l}^{N_{\text{shell}}} a_{nn'ljm_\tau_z} \varphi_{nlljm_\tau_z}^{\text{HO}}(\vec{r}),$$

(5.13)

where $\psi_{nljm_\tau_z}^{\text{WS}}(\vec{r})$ is the total WS sps wavefunction with quantum numbers $n, l, j, m, \tau_z$ written as a linear combination of HO single-particle wavefunctions $\varphi_{nlljm_\tau_z}^{\text{HO}}(\vec{r})$ discussed in Chapter 3. Since $N_{\text{shell}}$ is finite, there may be some residual dependence on the chosen HO well for this expansion. This is the reason one quotes the $\hbar\Omega$-value for the WS basis results.

The WS wavefunctions have long-range exponential tails, in the case of a neutron orbit, compared to the Gaussian tail of the HO wavefunctions. This can be clearly seen in the semi-log plot of Fig. 5.3. The red color represents $\hbar\Omega = 13 \text{ MeV}$ and the blue color represents $\hbar\Omega = 25 \text{ MeV}$. The HO and WS bases are differentiated by a dashed line and a solid line, respectively. For the demonstration presented in Fig. 5.3, six conventional parameter values are used to describe the ground-state of $^{12}\text{C}$, with the following values: $U_0 = -32 \text{ MeV}$, $r_0 = 1.25 \text{ fm}$, $a_0 = 0.65 \text{ fm}$, $U_{SO} = 15 \text{ MeV}$, $R_{SO} = 1.25 \text{ fm}$, $a_{SO} = 0.47 \text{ fm}$. The WS parameters values are taken the same as the $^{12}\text{C}$ WS parameters used in Ref. [51]. Hence, the $l$-dependent terms are not considered and the WS wavefunctions are expanded up to 17 HO shells. Looking at the red curves corresponding to the $\hbar\Omega = 13 \text{ MeV}$ case, one notices how the HO and WS wavefunctions nicely overlap at smaller distances and spread apart at larger distances, where the WS wavefunctions have their exponential tail. The semi-log scale was chosen to emphasize these differences at larger distances. Using the same set of parameters for the central WS, one chooses to plot the WS neutron central potential and the HO potential for $^{12}\text{C}$ (see Fig. 5.4) and compare them with Fig. 5.1 for a heavier nucleus like $^{197}\text{Au}$.

One chooses the case for the similar WS and HO wavefunctions at small distances observed at $\hbar\Omega = 13 \text{ MeV}$ in Fig. 5.3. The dashed red curve represents the HO potential and the solid blue curve represents the WS potential. In this case, the potentials were matched at a radius,
Fig. 5.3 $^{12}$C wavefunctions for $0s_{1/2}$ neutrons for HO and WS basis at two values of $\hbar \Omega$, $\hbar \Omega = 13 \text{ MeV}$ and $\hbar \Omega = 25 \text{ MeV}$

$R = 2.85 \text{ fm}$, resulting in the HO potential shifted downwards by 32.255 MeV.

Comparing Figs. 5.1 and 5.4, one can see the shape of the WS potential is not as flat at the center in the $^{12}$C case and the WS potential, in the interior region, is closer to the HO potential than it was for the heavier nucleus, $^{197}$Au. The similarity of the two potentials for $^{12}$C (Fig. 5.4) at smaller distances is also reflected in the similarity of the wavefunctions up to the same distance range (Fig. 5.3).
Fig. 5.4 Woods-Saxon (WS) central neutron potential and Harmonic Oscillator (HO) potential for a commonly chosen value of $\hbar \Omega = 13\ MeV$ shifted to match the WS potential at a radius of 2.85 fm. The dashed red curve represents the HO potential and the solid blue curve represents the WS potential.
5.3 Search on WS Parameters—Newuoa

As a primary computational tool, we used codes that construct the $NN$ interaction matrix elements in a 2-particle WS basis via expansions in a HO basis and we input the resulting WS matrix elements into the Many-Fermion-Dynamics-nucleons (MFDn) code [41] discussed in Appendix B. The WS matrix element codes (“upstream codes”) run independently and prior to MFDn. Their output is then collected into a file that is the input for MFDn. The spectrum, radii, and many-body wavefunctions are evaluated, using these combined codes. With extrapolations to the infinite matrix limit, shown later, this constitutes our WS version of the no core full configuration method (NCFC), presented in Chapter 3. The upstream codes were modified to incorporate the changes to the WS parameterization introduced above in Section 5.1 and a WS potential or a HO potential is used for all calculations presented in Chapter 6.

The parameters of the WS single-particle Hamiltonian (Eq. (5.7)) were determined in a search for the minimum ground-state energy of the fully interacting system using a search program called Newuoa developed by Powell [82]. Newuoa initiates each iteration of the Woods-Saxon calculation through a shell command with the hypothetical fit parameters and reads back the calculated ground-state energy of the chosen nucleus. Hence, the relationship between the three codes can clearly be understood. After the upstream codes transform the needed operators from the HO basis into the WS basis and prepare the input for MFDn, then MFDn runs and produces the ground-state energy of the nucleus under consideration. This ground-state energy is further minimized by Newuoa until a desired precision for the minimum is obtained. This can be seen as an illustration in Fig. 5.5. The actual parameter optimization is realized through a derivative-free method [83], which minimizes the $\chi^2$ function of the calculated ground-state energy by systematically varying the potential parameters. Derivative-free methods were among the first numerical optimization methods. They rely on the ability to compute function values and make decisions for the next parameter sets, based on relationships among the values rather than the actual numeric value.

The search program allows for all presented parameters to vary for each individual nuclide.
This option was used to systematically investigate how to improve the dependence of certain parameters on the nuclide mass or the neutron-proton asymmetry.

Armed with a fitting procedure, one considers a structure of a WS potential presented above in Section 5.1 and fits its 13 parameters to minimize the ground-state energy of the interacting many-body system. These parameters, determined from searches which minimize the ground-state energy, will determine the WS optimal basis states used in nuclear spectra calculations.

The Hamiltonian of the basis states used in the NCFC calculations is defined in Eq. (5.7), where the central potential is determined in Eq. (5.2) and the spin-orbit term is given by Eq. (5.8). Both central and spin-orbit parts have a WS form factor given by Eq. (5.1). The Coulomb part is given by Eq. (5.4). However, for simplicity at the present time, we omit the Coulomb potential from the single-particle Hamiltonian, but retain it in the many-
body Hamiltonian. This is expected to be a very good approximation in light nuclei, where finite basis corrections are of second order in the Coulomb interaction. Considering also the $l$-dependent terms discussed above in Section 5.1, for each individual nucleus, the Hamiltonian is determined by the following list of parameters, $U^l_0, R^l_0, a^l, U_{SO}, R_{SO}, a_{SO}$, having $l = 0, 1, 2, 3$ with $R^{l=2} = R^{l=3}_0$ and $a^{l=2} = a^{l=3}$. These 13 parameters define the WS potential. One can also perform a 12 parameter search, eliminating the search on the strength parameter for $l \geq 3$ by setting, $U^{l=3}_0 = U^{2}_0$. The parameters of the potential change gradually and systematically as one proceeds to a different $N_{max}$ basis space truncation, to a different $N_{shell}$ value or to a different nucleus. The dependence of the above 13 parameters on small changes in the number of protons and neutrons in the many-body problem should also be systematic and gradual, but was not investigated here.

For initial applications, we chose a selected set of light nuclei where extensive investigations of the systematics are achievable, $^2$H, $^4$He, $^6$He and $^{12}$C. These systems were also chosen because there is a substantial amount of experimental data available, such as the assessed data in the NNDC database \[57\].

Our searches are done in the WS basis and a maximum of 13 parameters were used to minimize the ground-state energy of each nucleus. Then, one compares the new results with the HO results and with HO extrapolated results. Good improvements are obtained with 12 and 13 parameter searches and the results are presented in Tables 5.1, 5.2, and 5.3. The calculations are performed using the JISP16 interaction in the WS basis space using a HO expansion up to $N_{shell} = 10$. $\hbar \Omega$ and $N_{max}$ dependences are given, along with the number of function evaluations needed for each complete search. The ground-state energy and ground-state point proton $rms$ value at the WS optimal basis space are also presented. For comparison, one provides the ground-state energy and ground-state point proton $rms$ value in the HO basis space.

One chooses also to investigate $^6$He nucleus as it provides a more challenging test of the WS basis, being a halo nucleus. The results of $rms$ for this nucleus are presented in Chapter 6. Table 5.4 presents the set of WS parameters determined by the independent searches performed
for $^4\text{He}$ and $^6\text{He}$ for the 13 parameters search at $N_{\text{shell}} = 14$ HO shells using JISP16 interaction. Chapter 6 presents results from NCFC at WS optimal basis space for these nuclei.

One observes that, for the most part, the best fit basis state parameter values change smoothly with increasing $N_{\text{max}}$ and $N_{\text{shell}}$. However, this is not a requirement of the fits as each basis space is separately optimized. Also, there may be regions of nearly degenerate minima that are difficult to find and a full search for possible competitive minima has not been attempted.

In comparison with conventional phenomenological WS forms discussed above, the most significant new feature here is the rather deep central potential strength parameters. It appears that the best fits are producing WS shapes in the interior regions that approach that of the HO shape—i.e., a rounded, quadratic-like, bottom to the potential. This similarity to the HO oscillator potential in the interior region is also consistent with the feature that the minimum ground-state energies in the WS basis are only slightly improved over the minimum in the HO basis results (minimum with respect to $\hbar \Omega$). This is likely to be indirect evidence that the ground-state energy is controlled largely by shorter distance correlation effects that are already efficiently managed rather well in an optimized HO basis. Further results presented in the next chapter tends to support this viewpoint.
Table 5.1 $^2$H best results of Newuoa code for 12 parameters search. These calculations are performed using JISP16 interaction in the WS basis space up to $N_{shell} = 10$. $\hbar \Omega$ and $N_{max}$ dependences are given along with the number of function evaluations needed for each complete search. The ground-state energy and ground-state point proton $rms$ value at the WS optimal basis space are also presented. For comparison, one provides the ground-state energy and ground-state point proton $rms$ value obtained in the HO basis space.

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<td>$rms(p)^{HO}$</td>
<td>1.394</td>
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Table 5.2  $^4$He best results of Newuoa code for 12 and 13 parameters search.
See caption for Table 5.1.

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Table 5.3  $^{12}$C best results of Newuoa code for 13 parameters search. See caption for Table 5.1.

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</tr>
<tr>
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<td>$E_{gs}$</td>
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<tr>
<td>$rms(p)$</td>
</tr>
<tr>
<td>$E_{gs}^{HO}$</td>
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<tr>
<td>$rms(p)^{HO}$</td>
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Table 5.4 $^4$He and $^6$He best results of Newuoa code for 13 parameters search. The calculations are done using JISP16 interaction in the WS basis space up to $N_{shell} = 14$. See caption for Table 5.1.

<table>
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<th>Nucleus</th>
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<th>$^6$He</th>
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<td>25</td>
</tr>
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<tr>
<td>no. eval</td>
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<td>137, 153, 153</td>
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<tr>
<td>$U_0$</td>
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<td>-213.564, -166.969, -184.535</td>
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<td>2.261, 2.100, 2.239, 2.207</td>
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</tr>
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<td>$a_0$</td>
<td>0.834, 1.033, 0.992, 0.992</td>
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<td>-183.744, -189.248, -195.217</td>
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<td>1.247, 1.340, 1.479</td>
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<tr>
<td>$U_2$</td>
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</tr>
<tr>
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</tr>
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<tr>
<td>$rms(p)$</td>
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<tr>
<td>$rms(p)^{HO}$</td>
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<td>1.582, 1.625, 1.672</td>
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</table>
CHAPTER 6. APPLICATIONS OF THE NCFC METHOD WITH JISP16 IN WS BASIS

To carry out the NCFC calculations requires a realistic $NN$ interaction that is sufficiently weak at high-momentum transfers to obtain a reasonable convergence trend. The conventional Lee-Suzuki-Okamoto renormalization procedure of the $ab$ initio NCSM [36] develops soft, $N_{\text{max}}$ dependent, effective interactions, that provide answers close to experimental observations. However, the convergence trend of the results with increasing $N_{\text{max}}$ is often not uniform and leads to challenges for extrapolation to infinite model spaces. Nevertheless, there is also encouraging progress in extrapolating NCSM ground-state energies of light nuclei using different strategies [84, 85]. Of course, as the basis space increases, one expects the NCSM and NCFC methods to arrive at the same result. Thus, the choice of method, NCSM or NCFC, will ultimately depend upon the underlying Hamiltonian selected for the application. In the NCFC approach discussed in detail in Chapter 3, one seeks to obtain the ground-state energy of the original, or “bare” [8], Hamiltonian in the infinite model space with evaluated uncertainties. To this end, this chapter incorporates a systematic extrapolation tool for $rms$ radii as needed.

With JISP16 for the $NN$ interaction, one performs NCFC calculations of the ground-state energies and $rms$ radii of $^2$H, $^4$He, $^6$He, and $^{12}$C. The two lightest nuclei serve as test cases to demonstrate the extrapolation method, using results in limited basis spaces, is able to predict the fully converged results and to demonstrate the assessed uncertainties are realistic. The calculations are performed both in a harmonic oscillator (HO) and a Woods-Saxon (WS) basis, and convergence rates are compared for the ground-state energies, energies of selected excited states, $rms$ radii, and other observables. Convergence is obtained in this two-dimensional parameter space ($\hbar\Omega, N_{\text{max}}$), where convergence is defined as independence of both parameters
within evaluated uncertainties. All results include the Coulomb interaction between protons. Results for the binding energies and \( \text{rms} \) radii of the above mentioned nuclei will be presented in great detail in this chapter. The differences in the convergence rates of these results with increasing basis space size reflects the infra-red properties of the basis states, the properties of the \( NN \) interaction, and the binding energy of the nucleus in question. This chapter limits to examples for which a sufficient set of results could be achieved within the current computational resource limits to enable meaningful extrapolations.

The parallel-processor code Many-Fermion Dynamics-nuclear (MFDn) [41] that sets up the many-body basis space is employed to evaluate the many-body Hamiltonian matrix, obtain the low-lying eigenvalues and eigenvectors using the Lanczos algorithm, and evaluate a suite of experimental observables. Working in the single-particle HO or WS \( m \)-scheme basis, the lowest 10 states are usually obtained with 300-500 iterations, depending upon \( N_{\text{max}} \) and the nucleus involved. The required number of iterations grows slowly with \( N_{\text{max}} \).

While the description of the energy spectra is an important component of any model of single particle motion, the WS potential also strives to reproduce the geometry of the nucleus and properties sensitive to the long-range features of its wavefunctions. Especially, since the radial and potential depth parameters show strong correlations in their influence on the single-particle energy spectrum, it is important to study the long-range properties of the wavefunctions in an independent fashion.

The root-mean-square (\( \text{rms} \)) charge radii of the nuclei investigated here are expected to provide valuable tests of the saturation properties on the selected \( NN \) interaction. The \( \text{rms} \) radii are obtained from evaluation of the expectation value of the operator, \( r^2 \), where the 2-body operator \( r^2 = \sum_{i<j}^A | \vec{r}_i - \vec{r}_j |^2 \).

Using the parameters determined by searches at \( N_{\text{max}} = 4 \) and \( N_{\text{shell}} = 10 \) (see tables from Chapter 5.3), the \( \text{rms} \) radii of the corresponding nuclides are calculated by
\[ \text{rms} = \left[ \langle r^2 \rangle \right]^{1/2} \]
\[ = \left[ \langle \Psi_\alpha | r^2 | \Psi_\alpha \rangle \right]^{1/2} \]
\[ = \left[ \langle \Phi_{CM}^0 | \Phi_{CM}^0 \rangle \langle \Psi_{\text{intr}}^\alpha | r^2 | \Psi_{\text{intr}}^\alpha \rangle \right]^{1/2}, \]

where “\( \alpha \)” identify the nuclear state, and \( |\Psi_\alpha\rangle \) and \( |\Psi_{\text{intr}}^\alpha\rangle \) are the many-body and the intrinsic many-body state vectors, respectively.

The data on experimental \( \text{rms} \) charge radii is adopted from the NNDC database [57] and corrected for the finite proton charge radius contribution. The resulting experimental ground-state point proton \( \text{rms} \) radii and the extrapolated (converged) results are displayed in Table 6.1. This table also presents the experimental ground-state energies along with JISP16 extrapolated ground-state energies results [51] for the studied nuclei.

Overall, the agreement between theory and experiment is quite good by traditional measures, with the one exception that \( ^{12}\text{C} \) exhibits a slightly smaller \( \text{rms} \) radius than the experimental value. It is likely this deviation is due to inadequacies of the JISP16 \( NN \) interaction and improvements in this interaction, such as the possible addition of a small \( NNN \) potential, could significantly improve the results.

<table>
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<tr>
<th>Nucleus</th>
<th>( E_{gs}^{\text{exp}} )</th>
<th>( E_{gs}^{\text{conv}} )</th>
<th>( rms(p)^{\text{exp}} )</th>
<th>( rms(p)^{\text{conv}} )</th>
</tr>
</thead>
<tbody>
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<td>-2.225</td>
<td>1.971</td>
<td>1.964</td>
</tr>
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<td>-28.299</td>
<td>1.455</td>
<td>1.437</td>
</tr>
<tr>
<td>(^6\text{He})</td>
<td>-29.269</td>
<td>-28.760</td>
<td>1.912</td>
<td>1.844</td>
</tr>
<tr>
<td>(^{12}\text{C})</td>
<td>-92.162</td>
<td>-93.900</td>
<td>2.321</td>
<td>2.080</td>
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</tbody>
</table>

Direct data on the neutron radii are more difficult to obtain. However, some information on the relative radii of neutrons and protons can be deduced from isovector spin-dipole resonances,
e.g., as studied with the \(^{3}He, t\) reaction at intermediate energies. More discussions on \(rms\) radii and ground-state energies are presented for each nucleus studied.

6.1 Deuteron \(^{2}H\)

Deuteron consists of a proton and a neutron; it is the only bound two-nucleon system and is the lightest of all composite nuclei. It is also one of the fundamental systems of nuclear physics, and many experimental and theoretical studies have been devoted to it. One of the particular interests in \(^{2}H\) is the degree to which deuteron can be understood as a system of two point-like nucleons interacting via the non-relativistic \(NN\) potential. Deuteron properties are quantities of fundamental importance in nuclear physics. For example, electromagnetic properties provide crucial tests of the theory of electromagnetic currents. When addressing electromagnetic properties of the deuteron, the corresponding challenge concerns the ability to predict the three deuteron form factors starting from the calculated deuteron wavefunction and the nucleon form factors taken from electron-nucleon scattering. At very low momentum transfer, \(k\), the hope is to predict the electromagnetic properties. The form factors at very low \(k\) are dominated by parts of the deuteron wavefunction where the two nucleons are far apart. For this case, the electromagnetic properties of the deuteron should be determined by the known \(NN\) interaction (which has been tuned to give the correct deuteron binding energy) and the known nucleon form factors. This is true in particular for the quantity relevant at extremely low momentum transfer, the deuteron \(rms\) radius, one of the quantities of main interest. For these reasons, the deuteron \(rms\) radius has been a favorite observable used to compare experiment and theory. The interpretation of experimental data at low momentum transfer in terms of the \(rms\) radius appears to be simple and clean. The theoretical calculations of the \(rms\) radius are particularly reliable as the calculation is largely independent of the particular \(NN\) potential used, provided that potential fits the ground-state binding energy and quadrupole moment. Many authors \([86–88]\) paid special attention to deuteron observables, the observable \(rms\) radius, charge radius, and the related, but unobservable, \(rms\) matter radius. The main goal of this section is to introduce an extrapolation method to extract the value of
the deuteron point proton $rms$ radius by using the $NN$ interaction JISP16 in a sequence of basis space diagonalizations. This development of an extrapolation method will be useful for obtaining estimates of converged $rms$ radii from a sequence of basis space diagonalizations of other light nuclei.

Turning to the NCFC calculations for light nuclei using JISP16, one can achieve nearly exact results in large basis spaces, especially for nuclei with six or fewer nucleons. This and the following sections, investigate the convergence rates for the ground-state energies and $rms$ radii as a function of $N_{max}$ and $\hbar\Omega$.

Figure 6.1 presents the calculated ground-state energy of $^2$H using HO basis as a function of the oscillator energy, $\hbar\Omega$, for selected values of $N_{max}$ used in defining the basis states. The curve closest to experiment corresponds to the value $N_{max} = 20$ and successively higher curves are obtained with $N_{max}$ decreased by two units for each curve. The curves are formed by straight-line segments joining the calculated results.

The sequence of curves in Fig. 6.1 illustrates the trends when evaluating the ground-state energy in HO basis with JISP16. The purpose with $^2$H is only to illustrate convergence trends because the exact answer is also available from the direct solution of the Schrödinger equation [2] and agrees with experiment. The $N_{max} = 18$ curve reaches to within 9 $KeV$ of this exact result; the $N_{max} = 20$ curve reaches to within 5 $KeV$. Note, the weak binding of $^2$H leads to a slow progression of the curves toward independence of $\hbar\Omega$ and contrasts the stronger binding situation obtained for $^4$He, discussed in Sec. 6.2.

Figure 6.2 presents the calculated ground-state point proton $rms$ radii of $^2$H using the HO basis as a function of the oscillator energy, $\hbar\Omega$, for selected values of $N_{max}$. The curve closest to experiment corresponds to the value $N_{max} = 110$ and successively lower curves are obtained with $N_{max}$ decreased by six units for each curve. The $rms$ curves are also formed by straight-line segments joining the calculated results. The convergence is from below, contrary to the ground-state energy case, where the convergence pattern was from above, consistent with the variational principle.

To develop an impression of the effects of changing the basis representation, ground-state
Fig. 6.1 Calculated ground-state energy of $^2$H in the HO basis as a function of the oscillator energy, $\hbar\Omega$, for selected values of the basis space cutoff, $N_{\text{max}}$, increased in increments of two units, from $N_{\text{max}} = 2$ to $N_{\text{max}} = 20$. Energies and $\text{rms}$ radii are also evaluated using the WS basis for selected $N_{\text{max}}$ values, $N_{\text{max}} = 4, 6$ and $8$, in Figs. 6.3 and 6.4. The calculations are done using WS parameters determined from a 12-parameter search at $\hbar\Omega = 20 \text{ MeV}$, $N_{\text{max}} = 4$ and $N_{\text{shell}} = 10$ (see Table 5.1).

Figure 6.3 shows the ground-state energy of $^2$H versus $\hbar\Omega$, the energy gap between oscillator shells. The dashed lines with squares represent the calculations done in the HO basis and the solid lines with circles are the calculations done in the WS basis at $N_{\text{shell}} = 10$. Different colors are used for different $N_{\text{max}}$ truncations. Note, the solid black line is the experimental value, which, for this particular nucleus, coincides with the JISP16 NCFC (converged) result [51]. One observes the sequence starting from $N_{\text{max}} = 4$ to $N_{\text{max}} = 8$ approaches convergence from above to the exact result. The difference between the minimum of the $N_{\text{max}} = 8$ curve with the
WS basis and the NCFC converged result is about 200 KeV. Also, at a given \( N_{\text{max}} \) value, the results for the ground-state energy in the WS basis are less dependent on \( \hbar \Omega \) compared with the ones in HO basis, in agreement with expectations of a satisfactory expansion of the WS basis in the HO basis. That is, as \( N_{\text{shell}} \) is increased, one expects the WS results to become less dependent on \( \hbar \Omega \) at fixed \( N_{\text{max}} \), indicating an improved expansion of the WS single-particle states in terms of the HO single-particle states. A corresponding trend is observed for the \( \text{rms} \) radii in Fig. 6.4, where the convergence is from below instead of above. As specified earlier, \(^2\text{H}\) is well described using a sufficiently large HO basis and was only a test case to begin. Hence, the WS investigation for this nucleus stops here, motivating expansion of the WS basis more for the \(^4\text{He}\) case, where \( N_{\text{shell}} = 14 \) results are presented and compared with \( N_{\text{shell}} = 10 \) results. Higher \( N_{\text{shell}} \) results allow going to a higher basis space cutoff, \( N_{\text{max}} \), and
are expected to lead to improvement in the convergence patterns.

![Graph showing ground-state energy results for ²H in the HO and WS bases as a function of the oscillator energy, \( \hbar \Omega \), for selected \( N_{\text{max}} \) values of the many-body basis space cutoff and \( N_{\text{shell}} = 10 \).](image)

**Fig. 6.3** NCFC ground-state energy results for ²H in the HO and WS bases as a function of the oscillator energy, \( \hbar \Omega \), for selected \( N_{\text{max}} \) values of the many-body basis space cutoff and \( N_{\text{shell}} = 10 \).

To have a feeling for the results of different methods and truncations adopted for a no core \textit{ab initio} calculation, one presents results for ²H ground-state energy in Fig. 6.5 versus the Hamiltonian matrix dimension. The points represent different \( N_{\text{max}} \) cases that have been solved and correspond to those indicated in the legend. Solid blue color and solid magenta color represent the FCI truncation (see below for explanation of FCI) for WS search results at \( \lambda_{CM} = 0 \) and \( \lambda_{CM} = 2 \), respectively. The dashed blue line is an FCI calculation, using fixed WS at \( \lambda_{CM} = 0 \), while the solid green and red curves are the NCSM calculations in a fixed WS basis at \( \lambda_{CM} = 2 \) and the NCSM calculations in HO basis at \( \lambda_{CM} = 10 \), respectively. The fixed WS parameters used in these calculations are determined from searches at \( N_{\text{max}} = 4 \) and \( N_{\text{shell}} = 10 \).
Fig. 6.4  NCFC ground-state \textit{rms} radii results for $^2\text{H}$ in the HO and WS bases as a function of the inverse square root of the oscillator energy, $\hbar\Omega$, for selected $N_{\text{max}}$ values of the many-body basis space cutoff and $N_{\text{shell}} = 10$.

Looking in more detail at Fig. 6.5, it is clear that individual searches at each $N_{\text{max}}$ value further minimize the ground-state energy, compared with calculations performed with a set of parameters determined by minimizing the energy at a different $N_{\text{max}}$ value. Also, the green and the red curves are very similar, meaning that a calculation done at $\lambda_{CM} = 2$ in WS basis gives the same results for ground-state energies for $^2\text{H}$ as the NCSM calculations in the HO basis at $\lambda_{CM} = 10$. We do not expect sensitivity to $\lambda_{CM}$ once it is at least unity and above. A typical value, for $\lambda_{CM}$, used in NCSM calculations for the HO basis is $\lambda_{CM} = 10$ (see Chapter 4).

In both NCFC and NCSM, $N_{\text{max}}$ is the many-body basis regulator, needed to preserve Galilean invariance—to factorize all solutions into a product of intrinsic and center-of-mass motion components. With $N_{\text{max}}$ as the regulator, both the NCFC and the NCSM are distinguished from the full configuration interaction (FCI) method in atomic and molecular physics, that employs a cutoff in single-particle space. The NCFC results should agree with the NCSM
and no-core FCI results when the latter results are obtained in sufficiently large basis spaces.

Fig. 6.5  Ground-state energy of $^2\text{H}$ calculated using NCSM and FCI truncation methods as a function of the basis space dimension. The points represent sample $N_{\text{max}}$ cases that have been solved and correspond to those indicated in the legend. Solid blue color and solid magenta color represent the FCI WS search results at $\lambda_{CM} = 0$ and $\lambda_{CM} = 2$, respectively. The solid black curve is the experimental result. The other WS calculations are completed with fixed WS parameters, determined from searches at $N_{\text{max}} = 4$ and $N_{\text{shell}} = 10$. $\lambda_{CM}$, from the legend, is the Lagrangian multiplier term for the CM Hamiltonian term, defined in Chapter 5.

Figure 6.6(a) shows the calculated NCFC $rms$ $^2\text{H}$ results using the HO basis versus the basis space cutoff, $N_{\text{max}}$, for selected values of the oscillator energy, $\hbar\Omega = 5, 7.5, 10, 15$, and $20 \text{ MeV}$. Different colors are assigned for different $\hbar\Omega$ values results as shown in the figure’s legend.

There is a pronounced “odd-even” effect in the maximum principal quantum number used in the basis—especially at smaller $N_{\text{max}}$ values. These effects are most pronounced in weakly bound systems and may be attributed to the fact that HO wavefunctions fall off too fast—
wavefunctions of finite nuclei decrease exponentially at large distances. To mimic such an exponential decrease with HO basis functions, one needs HO basis functions with both even principle quantum number \( n \) (even number of nodes in the radial wavefunction) and with odd principle quantum number \( n \) (odd number of nodes in the radial wavefunction). One may understand this is due to the phase of the tail of the last HO basis state added. When it is in phase with the nodeless ground-state wavefunction, the results tend to be closer to the asymptotic value. As a consequence of the observed “odd-even” effect in Fig. 6.6(a), it seems more convenient for the fitting procedure presented next to separate the calculated results for \( N_{\text{max}}/2 = n = \text{odd} \) and \( N_{\text{max}}/2 = n = \text{even} \) on different curves as in Fig. 6.6(b).

Fig. 6.6 Calculated ground-state point proton \( r_{\text{rms}} \) of \(^2\text{H}\) in the HO basis as a function of the basis space cutoff, \( N_{\text{max}} \), for selected values the oscillator energy, \( \hbar \Omega = 5, 7.5, 10, 15, \) and 20 MeV. Different colors are assigned for different \( \hbar \Omega \) values results (see legend).

To further explore the \( r_{\text{rms}} \) extrapolation tools, the results of the ESPM are used to map the convergence pattern of the \( r_{\text{rms}} \) radii in the present work. Thus, Fig. 6.7 presents the calculated \(^2\text{H} \) \( r_{\text{rms}} \) radii as a function of \( N_{\text{max}} \) at fixed values of \( \hbar \Omega \) as in Fig. 6.6(b).

Due to the observed “odd-even” effect, separate exponential fits are conducted through the
results for odd $n$ and even $n$ results. Also, the first couple of $N_{\text{max}}$ points are ignored in the fitting procedure as they are less systematic compared to the smooth trends at higher $N_{\text{max}}$ values. The functional form fitted is an exponential plus a constant to each set of even or odd results as a function of $N_{\text{max}}$, excluding the first two points on each curve. The resulting fits are displayed in Fig. 6.7 as smooth curves. That is, for each set of points at fixed $\hbar\Omega$, the ground-state point proton $rms$ radii are fitted with three adjustable parameters using the relation

$$rms(N_{\text{max}}) = a \exp(-cN_{\text{max}}) + rms(\infty).$$ (6.2)

These fits are achieved, using Newuoa code described in Chapter 5, where each point has equal weight and a regression analysis is performed.

The smooth solid curves are fits by Eq. (6.2) to the four $N_{\text{max}}$ even data points—8, 12, 16, and 20—in Fig. 6.7 at each value of $\hbar\Omega$. The smooth dashed curves are fits by the same Eq. (6.2) to the four $N_{\text{max}}$ odd data points—10, 14, 18, and 22. The solid black line is the experimental $rms$ radius result.

Note, the exponential plus constant fits the results rather well. It appears the asymptote, in both even and odd cases, is very close to the experimental black line. More precisely, the converged $rms$ for the even $N_{\text{max}}/2$ case is $rms_{even}^{\text{conv}} = 1.944 \text{ fm}$, while the converged $rms$ for the odd $N_{\text{max}}/2$ case is $rms_{\text{odd}}^{\text{conv}} = 1.959 \text{ fm}$, compared with the experimental $rms^{\text{exp}} = 1.971 \text{ fm}$. Also, the exact solution of the Schrödinger equation yields an $rms$ of 1.9647 fm, which is within 1% of the extrapolated values. Thus, one observes the HO basis provides a rapidly converging sequence of $rms$ radii in the ESPM, one well-represented by exponential convergence in $N_{\text{max}}$ toward the asymptotic $rms$ radius, $rms(\infty)$. It appears reasonable to expect this convergence pattern of the HO basis treatment of the ESPM to be representative of the HO basis expansion behavior in the no core applications to light nuclei. Therefore, this functional form as an extrapolation tool is adopted for further investigations of the $rms$ radii convergence sequence of other nuclei presented in the following sections. This extrapolation form is further tested in light nuclei, where converged results are sometimes approached very closely in the direct calculations before extrapolation. Additional results are presented that shed further light on
the challenges of extracting \textit{rms} radii from the \textit{ab initio} no core approaches.

Fig. 6.7 Calculated ground-state point proton \textit{rms} of $^2\text{H}$ for JISP16 interaction as a function of $N_{\text{max}}$ in the HO basis. See caption for Fig. 6.6(b). The smooth solid curves are fits by Eq. (6.2) to the four $N_{\text{max}}$ even data points shown at each value of $\hbar \Omega$ with each point weighted equally. The smooth dashed curves are fits by the same Eq. (6.2) to the four $N_{\text{max}}$ odd data points shown. The solid black line is the experimental \textit{rms} radius result. The exact solution of the Schrödinger equation yields an \textit{rms} of 1.9647 fm, which is within 1\% of the extrapolated values.
6.2 Helium $^4$He

Another test case for the WS basis convergence pattern and $rms$ extrapolation method is $^4$He. Figure 6.8 presents the ground-state energy of $^4$He as a function of $\hbar\Omega$ for a sequence of basis states and with different basis functions. The dashed lines with circles represent the calculations performed in the HO basis, the dashed lines with squares are the calculations performed in the WS basis at $N_{shell} = 10$ and the solid lines with circles are the calculations in the WS basis at $N_{shell} = 14$. Different colors are used for different $N_{max}$ truncations. Note, the black line is the JISP16 NCFC (converged) result.

It is interesting to observe the sequence starting from $N_{max} = 2$ to $N_{max} = 12$, as it shows convergence to the NCFC result. The difference between the minimum of the $N_{max} = 12$ curve and the NCFC converged result is less than 1%. Also, for a given $N_{max}$ value, the results for the ground-state energy in the WS basis are less dependent on $\hbar\Omega$ compared with the ones in the HO basis. Comparing $N_{shell} = 10$ and $N_{shell} = 14$ for the same lower $N_{max}$ truncation, the curve corresponding to $N_{shell} = 14$ is less dependent on $\hbar\Omega$, bringing the ground-state energy corresponding to the lowest $\hbar\Omega$ value closer to the NCFC converged result. The curves corresponding to $N_{shell} = 10$ and $N_{shell} = 14$ for a higher $N_{max}$ truncation are mainly overlapping. Therefore, one can conclude the WS basis at $N_{shell} = 10$ is sufficient to obtain an accurate value for the ground-state energy in $^4$He.

For more details on the gaps between HO and WS basis space results, one may examine Fig. 6.9 to see the fractional improvement in the ground-state energy when going from HO to WS basis. The percentage ground-state energy gain is defined as the fractional form,

$$f = \frac{|E_{gs}^{WS} - E_{gs}^{HO}|}{|E_{gs}^{HO} - E_{gs}^{\infty}|}, \quad (6.3)$$

where $E_{gs}^{\infty}$ is the converged ground-state energy.

The green curve with crosses represents the energy gain when using the pure-central WS potential and the red square is the energy gain when using central WS + spin-orbit (SO) potential at $N_{max} = 4$. The calculations are done using the WS basis at $\hbar\Omega = 25\ MeV$ and $N_{shell} = 10$. Looking at the $N_{max} = 4$ results, the energy gain is about 13% for pure-central
WS and about 17% when adding the SO term over the HO result.

Figure 6.10 presents results for the $^4$He ground-state energy versus the Hamiltonian matrix dimension. The points represent different $N_{\text{max}}$ cases that have been solved and correspond to those indicated in the legend. Blue, red, and green represent the FCI results at $\lambda_{CM} = 10$, NCSM in the HO basis at $\lambda_{CM} = 10$ and NCSM in the WS basis at $\lambda_{CM} = 2$, respectively. The dashed blue curve is the FCI result at $\lambda_{CM} = 0$ and the black curve is the NCFC exact result. The WS calculations are with fixed WS parameters determined from searches at $N_{\text{max}} = 4$ and $N_{\text{shell}} = 10$ at $\hbar \Omega = 25$ MeV. Looking at Fig. 6.10, it is clear the WS basis space produces a slightly better minimum for the ground-state energy when compared with HO basis and FCI truncation results.

Figure 6.11 presents the shapes of the WS and HO potential for the $^4$He nucleus. Green represents the HO potential and red represents the WS potential. The two potentials have very similar shapes in the interior region. The similarity contrasts with a similar comparison of interior regions for the heavier nucleus, $^{197}$Au, presented in Fig. 5.1. The similarity of the two potentials for $^4$He at smaller distances, shown in Fig. 6.11, is also reflected in the similarity of the wavefunctions up to the same distance scale (see Fig. 6.14). Note, the calculated single-particle energy levels, $0S_{1/2}$ and $0P_{1/2}$, for nucleons inside the HO and WS potential wells. The calculations are performed with $\hbar \Omega = 25$ MeV, $N_{\text{max}} = 4$ and $N_{\text{shell}} = 10$. The green color represents the HO energy levels, and red signifies the WS energy levels as shown in the plot’s legend.

It is also important to check the convergence rates for the proton rms radii in the WS basis. Figure 6.12 presents WS basis rms radii results as a function of the oscillator energy, $\hbar \Omega$, for a sequence of $N_{\text{max}}$ values increased by two units for each curve. Colors are used to differentiate among $N_{\text{max}}$ values as shown in the plot’s legend. To guide the eye, the dashed magenta line represents the calculations performed in the HO basis at $N_{\text{max}} = 8$ and the solid lines are the calculations performed in the WS basis at $N_{\text{shell}} = 14$. The solid black line is the bare [8] JISP16 result at $N_{\text{max}} = 18$. The WS orange curve is closest to the converged result with deviations less than 1% and corresponds to $N_{\text{max}} = 12$ and $N_{\text{shell}} = 14$ results.
The Hamiltonian matrix dimension for the bare JISP16 result at $N_{\text{max}} = 18$ (black line) is over 16 million, where the dimension for the WS basis at $N_{\text{max}} = 10$ (green line) is about 200,000 and the dimension for the WS basis at $N_{\text{max}} = 12$ (orange line) is about 700,000. All three cases give very similar results for the $rms$ radii. The difference in the Hamiltonian matrix dimension is large (representing greatly increased computational effort) compared with the deviation in $rms$ results, less than 1%. Therefore, the WS basis gives $rms$ radii results closer to the converged answer with less computational resources compared to the HO basis.

The extrapolation technique is employed for the $^4$He ground-state point proton $rms$, evaluated in both the HO and WS bases. Figure 6.13 shows the calculated results and the exponential curves fitted with a common asymptote to determine the infinite basis result. The ground-state point proton $rms$ versus $N_{\text{max}}$ for different $\hbar \Omega$ values, 15, 20, 25, and 30 $MeV$, using the results from the HO basis and also the $\hbar \Omega = 25$ $MeV$ case using the WS basis are presented in Fig. 6.13(a). The region for the points involved in the fit is expanded for a closer inspection, as shown in Fig. 6.13(b).

The square points are the actual $rms$ values at different $N_{\text{max}}$ truncations and the colors are used to distinguished different $\hbar \Omega$ values. As seen in the plot’s legend, the HO basis results are dark blue squares for $\hbar \Omega = 15$ $MeV$, green squares for $\hbar \Omega = 20$ $MeV$, red squares for $\hbar \Omega = 25$ $MeV$, and purple squares for $\hbar \Omega = 30$ $MeV$. The magenta squares are the results in the WS basis for $\hbar \Omega = 25$ $MeV$. The $N_{\text{max}} = 0$ case was not plotted for the $^4$He case, but was included for the $^6$He and $^{12}$C cases (Figs. 6.17 and 6.22). The solid black line is the experimental value and the solid brown line is the converged fit result within assessed uncertainties. The dashed colored lines and the magenta continuous line represent the exponential fit curves of the functional form, like in Eq. (6.2) used for each $\hbar \Omega$ value by fitting the points from $N_{\text{max}} = 4$ to $N_{\text{max}} = 12$.

For this nucleus, the fits show the $N_{\text{max}} = 0$ and $N_{\text{max}} = 2$ points are far from the region of smooth behavior, seen in the dramatic drop in $\chi^2$ when the points fitted are taken only from $N_{\text{max}} = 4$ to $N_{\text{max}} = 12$. Therefore, dropping $N_{\text{max}} = 0$ and $N_{\text{max}} = 2$ points from fits may provide better fits in the future, as these two points appear to jump around by large amounts.
before the smooth pattern sets in.

There is a common trend that $N_{\text{max}} = 2$ points drop significantly when compared to $N_{\text{max}} = 0$ points (at low enough values of $\hbar\Omega$). Then $N_{\text{max}} = 4$ points rise again for $\hbar\Omega$ of 20 and 25 $MeV$. This does not occur at $\hbar\Omega$ of 15 $MeV$ and 30 $MeV$ (where the points drop to the converged line with increasing $N_{\text{max}}$).

$^4$He wavefunctions for $0s_{1/2}$ neutrons evaluated for the HO and WS bases at $\hbar\Omega = 25$ $MeV$ are shown in Fig. 6.14 for three consecutive $N_{\text{max}}$ values, 0, 2, and 4, on a semi-log scale. Red and green represent wavefunctions evaluated for the HO and WS basis, respectively. The WS wavefunctions have long-range exponential tails, in the case of a neutron orbit, compared to the Gaussian tail of the HO wavefunctions.

Figure 6.15 shows $^4$He wavefunctions for $0s_{1/2}$ neutrons evaluated for the WS basis at two different values of $\hbar\Omega$ for three consecutive $N_{\text{max}}$ values, 0, 2, and 4, on a semi-log scale. Red and green represent wavefunctions evaluated at $\hbar\Omega = 15$ $MeV$ and $\hbar\Omega = 25$ $MeV$, respectively. It is especially clear from these semi-log plots how expanding the HO basis representation improves the description of the exponential tails of the WS wavefunction.
Fig. 6.8 No core calculated ground-state energy of $^4$He using the JISP16 interaction in the HO and WS bases as a function of the oscillator energy, $\hbar\Omega$, for a sequence of $N_{\text{max}}$ values increased by two units for each curve. Colors are used to differentiate among $N_{\text{max}}$ values. The dashed lines are calculations performed in the HO basis, the dotted lines represent calculations performed in the WS basis at $N_{\text{shell}} = 10$ and the solid lines are calculations performed in the WS basis at $N_{\text{shell}} = 14$. The solid black line is the NCFC converged JISP16 result. The WS orange curve is closest to the converged result and corresponds to $N_{\text{max}} = 12$ and $N_{\text{shell}} = 14$. 
Fig. 6.9  The fractional ground-state energy gain in $^4$He calculated when changing from the HO basis to the WS basis. The green curve with crosses represents the energy gain when using the pure-central WS potential and the red square is the energy gain when using pure-central WS + spin-orbit (SO) potential at $N_{\text{max}} = 4$. The calculations are performed using the WS basis expanded in the HO basis at $\hbar \Omega = 25 \, \text{MeV}$ and $N_{\text{shell}} = 10$. 
Fig. 6.10  Ground-state energy of $^4$He calculated using NCSM and FCI truncation methods as a function of the basis space dimension. The points represent sample $N_{max}$ cases that have been solved and correspond to those indicated in the legend. Blue, red, and green represent the FCI results at $\lambda_{CM} = 10$, NCSM in the HO basis at $\lambda_{CM} = 10$, and NCSM in the WS basis at $\lambda_{CM} = 2$, respectively. The dashed blue curve is the FCI result at $\lambda_{CM} = 0$ and the black curve is the NCFC exact result. $\lambda_{CM}$, from the legend, is the Lagrangian multiplier term for the CM Hamiltonian term, defined in Chapter 5.
$^4$He potential energy using pure-central WS potential and HO potential for $0s_{1/2}$ and $0p_{1/2}$ nucleons’ energy levels. Green represents the HO potential and red represents the WS potential, as indicated in the legend. The WS calculations are for $\hbar\Omega = 25\ MeV$, $N_{max} = 4$ and $N_{shell} = 10$.
Fig. 6.12 No core calculated ground-state point proton rms radii of $^4$He using the JISP16 interaction in the HO and WS bases as a function of the oscillator energy, $\hbar\Omega$, for a sequence of $N_{\text{max}}$ values increased by two units for each curve. Colors are used to differentiate among $N_{\text{max}}$ values. The dashed magenta line represents the calculations for the HO basis at $N_{\text{max}} = 8$, and the solid lines are the calculations for the WS basis at $N_{\text{shell}} = 14$. The solid black line is the bare $^8$ JISP16 result at $N_{\text{max}} = 18$. The WS orange curve is closest to the converged result and corresponds to the value $N_{\text{max}} = 12$ and $N_{\text{shell}} = 14$. 
Fig. 6.13 Calculated ground-state point proton rms of $^4$He using the JISP16 interaction as a function of $N_{\text{max}}$ for different values of $\hbar\Omega$, 15-20 MeV in increments of 5 MeV. The magenta solid curve is a fit by Eq. (6.2) to the four $N_{\text{max}}$ data points, from 4 to 12 evaluated for the WS basis at $N_{\text{shell}} = 14$ and $\hbar\Omega = 25$ MeV. The smooth dashed curves are fits by Eq. (6.2) to the same four $N_{\text{max}}$ data points evaluated for the HO basis. The solid black line is the experimental rms radius result and the brown solid line is the converged result obtained in this work.

(a) All $N_{\text{max}}$ points from 2 to 12, except (b) Only $N_{\text{max}}$ points from 4 to 12 shown $N_{\text{max}} = 0$ points shown in the plot.

Fig. 6.14 $^4$He wavefunctions for 0$s_{1/2}$ neutrons evaluated in the HO and WS bases at $\hbar\Omega = 25$ MeV. Note the logarithmic scale. Red and green curves represent wavefunctions evaluated in the HO and WS bases, respectively.

(a) $N_{\text{max}} = 0$  
(b) $N_{\text{max}} = 2$  
(c) $N_{\text{max}} = 4$
Fig. 6.15 $^4\text{He}$ wavefunctions for $0s_{1/2}$ neutrons evaluated in the WS basis at two different values of $\hbar \Omega$. Note the logarithmic scale. Red and green curves represent wavefunctions evaluated at $\hbar \Omega = 15 \text{MeV}$ and $\hbar \Omega = 25 \text{MeV}$, respectively.
6.3 Helium $^6\text{He}$

$^6\text{He}$ represents another test for the $rms$ radii extrapolation method introduced earlier in this chapter, since it has two nucleons weakly bound to $^4\text{He}$. The calculations are performed using WS parameters determined by searches at $N_{\text{max}} = 8$ and $N_{\text{shell}} = 14$ for $\hbar\Omega = 20\ MeV$, presented in Table 5.4. Calculated ground-state point neutron $rms$ of $^6\text{He}$ as a function of $N_{\text{max}}$ for different values of $\hbar\Omega$—8, 15, 20, 25, and 30 $MeV$—are presented in Fig. 6.16. The fits are for four $N_{\text{max}}$ data points from 8-16 for each curve, constrained to have a common asymptote. The black line is the experimental result and the brown line is the converged result.

The same plot is presented for point proton $rms$ of $^6\text{He}$ as a function of $N_{\text{max}}$ for other selected values of $\hbar\Omega$—8, 15, 20, 25, and 30 $MeV$—in Fig. 6.17. The converged $rms$ is well reproduced when compared with experimental values in Table 6.1.

Fig. 6.16 Calculated ground-state point neutron $rms$ of $^6\text{He}$ using the JISP16 interaction as a function of $N_{\text{max}}$ for different values of $\hbar\Omega$—8, 15, 20, 25, and 30 $MeV$. See the caption for Fig. 6.13. This is a fit for four $N_{\text{max}}$ data points from 8-16 for each curve, constrained to have a common asymptote.
Fig. 6.17  Calculated ground-state point proton $r_{\text{rms}}$ of $^6\text{He}$ using the JISP16 interaction as a function of $N_{\text{max}}$ for different values of $\hbar\Omega$ from 10 $\text{MeV}$ to 30 $\text{MeV}$ in increments of 5 $\text{MeV}$. See the caption for Fig. 6.13. This is a fit for four $N_{\text{max}}$ data points from 8-16 for each curve, constrained to have a common asymptote.
6.4 Carbon $^{12}$C

The results for ground-state energy of $^{12}$C, using the JISP16 interaction, in finite basis spaces are presented in Fig. 6.18. It also shows uniform and monotonic convergence from above to the exact eigenenergy with increasing $N_{\text{max}}$. That is, the results for the energy of the lowest state of each spin and parity at any $N_{\text{max}}$ truncation are upper-bounds on the exact converged answers. The convergence is monotonic with increasing $N_{\text{max}}$. The representation for the line styles and colors is similar to $^{4}$He (Fig. 6.8) and is listed in the figure’s caption. Note, $N_{\text{max}} = 6$ is not sufficient to obtained a converged ground-state energy, which implies that one must proceed to higher model spaces to obtain a converged result.

Figure 6.19 presents the ground-state energy and the first excited 0$^{+}$, the “Hoyle-state”, energy for $^{12}$C in the HO and WS bases as a function of the oscillator energy, $\hbar \Omega$, at $N_{\text{max}} = 4$. The dashed lines represent the calculations performed in the HO basis, the dotted lines stand for the WS basis at $N_{\text{shell}} = 10$, and the solid lines represent the calculations performed in the WS basis at $N_{\text{shell}} = 14$. The shaded rectangles represent the experimental results with assessed uncertainties. The blue curves refer to the Hoyle-state results and the green curves are for the ground-state energy results. There is a small energy gain for the Hoyle-state, when using the WS basis at $N_{\text{max}} = 4$, where the gain does not exceed 2 MeV.

Calculated ground-state $r_{\text{rms}}$ radii of $^{12}$C in the HO and WS bases as a function of the oscillator energy, $\hbar \Omega$, for a sequence of $N_{\text{max}}$ values increased by two units for each curve are shown in Fig. 6.20. Colors are used to differentiate among $N_{\text{max}}$ values, similar to the ground-state energy plots. The dashed pink line represents the calculations performed in the HO basis at $N_{\text{max}} = 4$ and the solid lines are the calculations performed in the WS basis at $N_{\text{shell}} = 14$. The dotted lines represent the results in the WS basis at $N_{\text{shell}} = 10$.

Comparing the $N_{\text{shell}} = 10$ and $N_{\text{shell}} = 14$ curves from Fig. 6.20(b), the same trends are seen as in the $^{4}$He case (see Fig. 6.12), where the two curves were similar, except for low $\hbar \Omega$ values. The sequence pattern for $r_{\text{rms}}$ radii indicates the theory tends to converge to a value rather far from the experimental $r_{\text{rms}}$ value, which is at about 2.32 fm, as seen in Fig. 6.20(a).

Therefore, is interesting to see how the extrapolation $r_{\text{rms}}$ results emerge. The $^{12}$C calcu-
lated ground-state point proton \textit{rms} as a function of $N_{max}$, for different values of $\hbar \Omega$, from 15 MeV to 30 MeV, in increments of 5 MeV are presented in Figs. 6.21 and 6.22. In Fig. 6.21, the dashed curves are formed by straight-line segments joining all $N_{max}$ calculated results for the HO basis and solid curves are for the WS basis results. In Fig. 6.22, each dotted line represents the fit for four $N_{max}$ data points from 2-8 constrained to have a common asymptote. A smaller $N_{max}$ region is selected for a better visualization of the points on the fit lines. Contrary to the $^4$He case (Fig. 6.13), $N_{max} = 2$ points were included in the fit, since they appear to follow the systematics better in $^{12}$C. A second figure with a larger $N_{max}$ region shows in finer detail how the exponential fits converge at the common asymptote, Fig. 6.23.
Fig. 6.18  No core calculated ground-state energy of $^{12}$C in HO and WS bases as a function of the oscillator energy, $\hbar \Omega$, for a sequence of $N_{\text{max}}$ values increased by two units for each curve. Colors are used to differentiate among $N_{\text{max}}$ values. The dashed lines are calculations for the HO basis, the dotted lines represent calculations for the WS basis at $N_{\text{shell}} = 10$ and the solid lines are calculations for the WS basis at $N_{\text{shell}} = 14$. The solid black line is the experimental result. The WS dark green curve is closest to the converged result and corresponds to $N_{\text{max}} = 6$ and $N_{\text{shell}} = 14$. 
Fig. 6.19 No core calculated ground-state energy and Hoyle-state $0^+$ energy for $^{12}$C in the HO and WS bases as a function of the oscillator energy, $\hbar\Omega$, at $N_{\text{max}} = 4$, using the JISP16 interaction. The dashed lines represent the calculations for the HO basis, the dotted lines stand for the WS basis at $N_{\text{shell}} = 10$ and the solid lines represent calculations for the WS basis at $N_{\text{shell}} = 14$. The shaded rectangles represent experimental results with evaluated uncertainties. The blue curves refer to the Hoyle-state results and the green curves are the ground-state energy results.
Fig. 6.20 NCFC calculated ground-state rms radii of $^{12}$C in the HO and WS bases as a function of the inverse square root of the oscillator energy, $\hbar \Omega$, for a sequence of $N_{max}$ values increased by two units for each curve. Colors are used to differentiate among $N_{max}$ values. The dashed pink line represents calculations for the HO basis at $N_{max} = 4$ and the solid lines are calculations for the WS basis at $N_{shell} = 14$. The dotted lines represent the results for the WS basis at $N_{shell} = 10$. 

(a) $N_{shell} = 14$

(b) $N_{shell} = 10$ and $N_{shell} = 14$ comparison. Note the difference in the scale from part a).
Fig. 6.21 Calculated ground-state point proton $rms$ of $^{12}$C in the HO and WS bases as a function of the basis space cutoff, $N_{max}$. Selected values the oscillator energy, $\hbar \Omega$ from 15-30 $MeV$ in increments of 5 $MeV$ are chosen for the HO basis calculations and two $\hbar \Omega$ values, $\hbar \Omega = 15$ and 25 $MeV$, are chosen for the WS basis calculations. Different colors are assigned for different $\hbar \Omega$ values as seen in the legend. The dashed curves are formed by straight-line segments joining all $N_{max}$ calculated results for the HO basis and solid curves are for the WS basis results.
Fig. 6.22  Calculated ground-state point proton RMS of $^{12}\text{C}$ as a function of $N_{\text{max}}$ for different values of $\hbar\Omega$ from 15 to 30 MeV in increments of 5 MeV, using the JISP16 interaction. See caption for Fig. 6.13. Each dotted line represents the fit for four $N_{\text{max}}$ data points from 2-8 constrained to have a common asymptote.
Fig. 6.23  The same figure as Fig 6.22, plotted at a larger $N_{\text{max}}$ scale. See caption for Fig. 6.22.
To check the ability of the \textit{ab initio} theory to predict large scale collective motion, one may compare with the energy of the quantum rotator defined as,

\[ E_J = \frac{j^2}{2I} = \frac{J(J + 1)\hbar^2}{2I}, \]

where \( J \) is the total angular momentum quantum number. Theoretically, using the formula from Eq. (6.4), the ratio \( \frac{E_4}{E_2} = \frac{20}{6} = 3.33 \). The experimental ratio \( \frac{E_4}{E_2} = 3.17 \), which is conventionally considered to be close to that of the quantum rotator and far from a quantum vibrator, which would have the ratio 2.0.

\(^{12}\text{C} \) excitation energy levels, \( E_2 \) and \( E_4 \), are calculated using HO and WS bases at \( \hbar \Omega = 25 \text{ MeV} \) as in Fig. 6.24. Red represents the \( J = 2 \) excited energy levels and green represents the \( J = 4 \) excited energy levels. The solid lines refer to energies for the HO basis and the dotted lines refer to energies for the WS basis. Results from \( N_{\text{max}} = 0 \) to \( N_{\text{max}} = 10 \) are presented for the HO basis. Results for \( N_{\text{max}} = 4 \) and \( N_{\text{max}} = 6 \) are presented using the WS basis. Figure 6.24 clearly shows an energy gain for the excited energy levels, \( E_2 \) and \( E_4 \), when using the WS basis. Note, this is an extra energy gain obtained apart from the ground-state energy gain in \(^{12}\text{C} \), about 2.5 \text{ MeV} \), presented in Chapter 5.1 for the \( N_{\text{max}} = 4, N_{\text{shell}} = 14, \) and \( \hbar \Omega = 25 \text{ MeV} \) case.

The theory HO ratio result is \( \frac{E_4}{E_2} = 3.27 \) at \( N_{\text{max}} = 4 \) and \( \frac{E_4}{E_2} = 3.54 \) at \( N_{\text{max}} = 10 \). For the WS basis space calculations, the ratio is \( \frac{E_4}{E_2} = 3.36 \) at \( N_{\text{max}} = 4 \) and \( \frac{E_4}{E_2} = 3.43 \) at \( N_{\text{max}} = 6 \). All these results can be considered to fall within a reasonable range of the experimental ratio and indicate quantum rotator behavior in the results.
Fig. 6.24 Quantum rotator for $^{12}$C at $\hbar \Omega = 25$ MeV for the WS and HO bases. Red represents the $J = 2$ excited energy levels and green represents the $J = 4$ excited energy levels. The solid lines refer to the HO basis results, where dotted lines refer to the WS basis results. Results from $N_{\text{max}} = 0$ to $N_{\text{max}} = 10$ are presented for the HO basis and results for $N_{\text{max}} = 4$ and 6 are presented using the WS basis for $N_{\text{shell}} = 14$. 
CHAPTER 7. CONCLUSIONS AND OUTLOOK

The rapid development of \textit{ab initio} methods for solving finite nuclei has opened a range of nuclear phenomena that can be evaluated to high precision using realistic nucleon-nucleon (NN) and three-nucleon (NNN) interactions. Total binding energies, spin-dependent structure effects, and electroweak properties of light nuclei play major roles in pinpointing properties of the underlying strong interaction.

Such advances define a path for testing fundamental properties of the strong interaction, such as their origins from QCD via chiral effective field theory [4, 21, 89]. Eventually, one anticipates a theory bridge with immense predictive power from QCD through nuclear forces to nuclear structure and nuclear reactions.

This thesis gives a brief description of the inter-nucleon interactions that fit two-body scattering and bound state data. It also introduces NNN interactions. Major new progress, including the goal of applying these interactions to solve for properties of nuclei, is limited by the challenge to assure convergence. That is, with the goal of obtaining high precision solutions of the nuclear many-body Hamiltonian with no core methods (all nucleons treated on the same footing), one needs to proceed to very large basis spaces to achieve a convergence pattern suitable for extrapolation to the exact result.

Progress on the nuclear many-body problem has been hindered for decades because NN potentials typically exhibit strong short-range repulsion, as well as a strong tensor force. This leads to strongly correlated many-body wavefunctions and highly non-perturbative few- and many-body systems. The more perturbative potentials induce weaker short-range correlations in few- and many-body wavefunctions, which leads to greatly improved convergence in variational calculations. However, to obtain more perturbative interactions, one usually begins
with a strongly correlated interaction and introduces a program of renormalization.

This work presents a simple method called the similarity renormalization group (SRG) approach to softening the $NN$ interaction, while preserving its phase shift properties. SRG is a set of unitary transformations that consistently evolve two- and three-body interactions towards the band-diagonal form. The SRG approach is demonstrated by applying it to a realistic $NN$ interaction, JISP16, in a harmonic oscillator (HO) representation. The degree of interaction softening achieved through a regulator parameter, $\lambda$, is examined. Particularly, results for the JISP16 potential are compared with Chiral N3LO interaction results processed with SRG by Bogner et al.’s group [49].

The method is very general and can be applied to any potential. There is much more to explore, such as the nature of decoupling of high- and low-energy physics, and whether other choices of the generator, $\eta(s)$, would be more effective in making the Hamiltonian diagonal. In general, SRG applied to $NN$ potentials works as promised, even for a simple choice of transformation, driving the Hamiltonian in momentum space towards the diagonal, making it more perturbative and more convergent in few-body calculations. The more the Chiral N3LO interaction is softened, the more it appears to resemble the JISP16 interaction at comparable values of $\lambda$, as judged from 2D contour plots of the interaction in momentum space.

The direct solution of the nuclear many-body problem is obtained by diagonalization in a sufficiently large basis space, where converged binding energies are accessed—either directly or by simple extrapolation. The choice is either a traditional harmonic oscillator (HO) basis or a Woods-Saxon (WS) basis. The features of results within the WS basis are a major focus of this investigation.

In no core calculations of finite nuclei in a HO basis, the long distance tails of the wavefunctions are understood to be slowly convergent. This motivates this work to develop new basis states with improved long distance properties. For observables sensitive to the long-range parts of the wavefunctions, like weakly bound-states, $rms$ radii, $B(E_L)$, $B(M_L)$, etc., convergence in the HO basis is slow, since the Gaussian tails of HO wavefunctions poorly represent the asymptotic exponential tails. Therefore, the more realistic basis space methods would
have a greater flexibility for solving these convergence challenges. This work adopts a realistic single-particle basis space using a WS potential. Other forms of potentials may be considered to determine the realistic single-particle basis, such as Ginocchio’s potential.

New sets of parameters are established for the WS potential by conducting searches over several conventional cases. Its thirteen parameters are determined by minimizing the ground-state energy of the interactive many-body system within the truncated NCFC. The parameter set is intended to enable the use of the WS potential as a basis for no core calculations and a pathway to connect the physics of bound and unbound nuclear states. These are numerically intensive many-body calculations. There is plenty of room for additional progress—e.g., departing from the limitations of a WS parametrization for the single-particle potential.

No core full configuration (NCFC) calculations are performed for a set of light nuclei, $^2$H, $^4$He, $^6$He, and $^{12}$C, using the realistic $NN$ interaction, JISP16. The calculations are performed both in a HO and WS basis, and convergence rates are compared for the ground-state energies, energies of selected excited states, $rms$ radii, and other observables. The differences in the convergence rates of these results with increasing basis space size reflects the infra-red properties of the basis states. The factorization of the center-of-mass (CM) motion is discussed and is shown how insuring factorization minimally affects the results in the WS basis space.

An exponential plus a constant extrapolation tool for $rms$ radii is presented. One observes the HO basis provides a rapidly converging sequence of $rms$ radii in the ESPM, one well-represented by exponential convergence in $N_{max}$ toward the asymptotic $rms$ radius, $rms(\infty)$. It appears reasonable to expect this convergence pattern of the HO basis treatment of the ESPM to be representative of HO basis expansion behavior in no-core applications. This functional form may be adopted as a foundation for further developing extrapolation methods. Initially, this extrapolation tool is tested in light nuclei, where converged results are obtained directly.

Table 6.1 is a summary of the results, using extrapolations for $rms$ radii performed with the methods introduced, comparing them with the experimental results. All cases used calculated results to the highest $N_{max}$ available with the bare [8] JISP16 interaction. In the cases of the
lightest nuclei, the extrapolations were rather modest as nearly converged results were obtained directly. The overall conclusion is that these results demonstrate sufficient convergence is achieved for ground-state energies of light nuclei to allow extrapolations to the infinite basis limit with the chosen Hamiltonian. The extrapolations of NCFC results with the JISP16 interaction agree with experimental results rather well with the exception of $^{12}C$, where the $rms$ radius is about 10% too small.

The convergence rate reflects the short-range properties of the nuclear Hamiltonian. Fortunately, new renormalization schemes have been developed and applied that show promise for providing suitable nuclear Hamiltonians with good convergence properties [39]. Additional work is needed to develop the corresponding $N_{NN}$ interaction. Also, further work is in progress to improve the extrapolation tools for the $rms$ radii. Of course, the $rms$ radii present a greater challenge because they are more sensitive than the energies to the asymptotic properties of the wavefunctions.

A similar exponential behavior for HO basis space calculations of a cold trapped Fermi gas has been observed [90]. In that case, the same type of single-particle space regulator was employed as in this thesis in the ESPM application. The exponential plus constant was also employed as an extrapolation tool in more conventional shell-model studies [91]. In these applications, the variable is the matrix dimension rather than $N_{max}$.

To gain insight into the CD-Bonn potential for no core investigations of heavier nuclei, initial investigation of the odd mass $A = 47 - 49$ region nuclei straddling $^{48}Ca$ is presented. The motivation for selecting these nuclei, with one nucleon away from doubly-magic $^{48}Ca$, stems from the aim of preparing for nuclear double beta-decay studies of $^{48}Ca$. In these heavier systems, phenomenological additions to the realistic $NN$ interaction determined by previous fits to $A = 48$ nuclei are needed. The modified Hamiltonian produces reasonable spectra for these odd mass nuclei.

Shell closure and single-particle spectral properties are obtained indicating a path has been opened for multi-shell investigations of these nuclei within the NCSM. This work underpins such additional investigations.
Also, for a better understanding of various $fp$-shell interactions, a comparison between the initial and modified $fp$-shell matrix elements in the HO basis with the GXPF1 interaction [64] is presented. The initial and modified NCSM $H_{eff}$ matrix elements in the $fp$-shell are strongly correlated [19]. Evidence is obtained suggesting that significant differences in single-particle properties may underly some of the distinctions between our $H_{eff}$ and the GXPF1 interaction. The differences were reduced when comparing the purely off-diagonal matrix elements in Fig. 4.18. Additional applications to other observables and other nuclei reveal the importance of these distinctions in greater detail.

There is considerable freedom with both the method of renormalization and the choice of basis space. This work has improved the convergence of the ab initio NCFC results in $^4$He, $^6$He, and $^{12}$C. Advances in computers and algorithms will help expand the range of applications of the methods introduced here to heavier nuclei. Such advances appear very likely in the near future and will greatly enhance the capability to capitalize further on the developments presented in this work.
APPENDIX A. TWO-BODY MATRIX ELEMENTS

A set of comparisons of the $fp$-shell two-body matrix elements (TBME) $V(abcd; JT) \ (MeV)$ for $A = 48$ nuclei employed in this work are presented. The interaction GXPF1 is taken from Ref. [64]. “diff1” represents the difference between CD-Bonn+3 terms and CD-Bonn, while “diff2” is the difference between CD-Bonn + 3 terms and GXPF1. Since all matrix elements involve orbitals (“a”, “b”, “c” and “d”) in the $fp$-shell, we abbreviate the orbital label in the first four columns by specifying twice the angular momentum of the orbital (e.g., “$2j_a$”, etc.).
Table A.1 Comparison of the $fp$-shell TBME $V(\text{abcd}; JT)$ (MeV) ($A = 48$) between CD-Bonn + 3 terms and GXPF1 interactions.

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APPENDIX B. MANY-FERMION DYNAMICS – NUCLEONS (MFDn)

Let us outline the steps for a calculation using the code, MFDn, developed at Iowa State University \[41]\, to solve the quantum many-nucleon problem in a basis constructed from 3-dimensional (3D) harmonic oscillator (HO) single-particle states (sps). Input files include matrix elements of the Hamiltonian expressed as a rank-2 operator and/or a rank-3 operator evaluated in the HO basis. These notes are also useful for MFDq (Many-Fermion Dynamics - quarks).

- Specify proton number (Z) and neutron number (N) for the nucleus.
- Input/generate sps quantum numbers \(nljm_tz\), where \(t_z\) is isospin projection (+1/2 for protons and -1/2 for neutrons) and \(m_j\) is the magnetic projection \((-j \leq m_j \leq +j)\) of the total sps angular momentum \(\vec{j} = \vec{l} + \vec{s}\).
- Input “symmetries” for many-body (MB) states, such as parity \((\pm)\), total angular momentum projection, \(M_j\), total isospin projection, \(T_j\), and the cutoff in the total number of HO excitation quanta above the lowest configuration, \(N_{\text{max}}\), where \(M_j = \sum_i m_j^i\). The symmetries are identified from the chosen maximal set of commuting observables. Represent these observables by the Hermitian operators \(Q_q\):
  \[ [H, Q_q] = 0, [Q_q, Q_{q'}] = 0. \]
- Input or generate/store/output MB basis states (half billion-billion or more in some applications) consistent with parts 2 and 3. For example, restrict the \(A = N + Z\) particle basis states to satisfy:
  \[ \sum (2n_i + l_i) \leq N_{\text{max}} + N_0, \] where \(N_0\) is the sum of the single-particle HO quanta for the lowest configuration for this nucleus.
• Evaluate/store $H + \lambda_{CM} H_{CM}$ in the MB basis, where $H_{CM}$ is the pure HO Hamiltonian acting on the center of mass (CM) of the system and $\lambda_{CM} H_{CM}$ is a Lagrange multiplier term that restricts the low-lying solutions to obtain a pure $0S$ state of CM motion. Note, the Hamiltonian may conserve additional quantities (such as total angular momentum), not explicit in the MB basis space. Thus, a cross check of the precision of a calculation is to evaluate these quantities to check if they are indeed conserved via the dynamics of $H$. For example, in this “m-scheme”, where total angular momentum, $J$, is not explicitly conserved, we evaluate the expectation value of total angular momentum squared, $J^2$: $\langle \Psi_i | J^2 | \Psi_i \rangle = J(J+1) = 0, 2, 6...$ both to obtain the observable and to verify $J$ is an integer (or half-odd integer in the case of an odd number of nucleons).

It is known that all even-even (even $Z$ and even $N$) nuclei, have $J^\pi = 0^+$ for the ground state and frequently one finds $2^+$ for the first excited state.

It is convenient to view the Hamiltonian operator for the rank-2 case as:

$$\hat{H} = \sum_{\alpha\leq\beta,\gamma\leq\delta} <\alpha\beta|H|\gamma\delta> a_\alpha^+ a_\beta^+ a_\delta a_\gamma,$$

where, for a local interaction (with antisymmetrization understood for the initial and final two-nucleon states),

$$<\alpha\beta|H|\gamma\delta> = \int \varphi_\alpha^*(\vec{r}_1) \varphi_\beta^*(\vec{r}_2) H(\vec{r}_1 - \vec{r}_2) \varphi_\gamma(\vec{r}_2) d^3 r_1 d^3 r_2$$

and

$$\int \varphi_\alpha^*(\vec{r}) \varphi_\beta(\vec{r}) d^3 r = \delta_{\alpha\beta}.$$

The Kronecker delta, $\delta_{\alpha\beta}$, implies all quantum numbers of state “$\alpha$” are restricted to be the same as all quantum numbers of state “$\beta$”. Here, we have represented the 3D HO single-particle wavefunctions as $\varphi_\alpha^*(\vec{r}_1)$.

$\text{MFDn}$ evaluates the MB matrix elements from the input rank-2 matrix elements (in this case) by carrying out the operator contractions dictated by the MB basis space. For $C^{12}$ for example, $\text{MFDn}$ evaluates the contractions for a string of 12 annihilation operators, 2-creation and 2-annihilation operators, and a string of 12 creation operators (28 operators in total), using the anti-commutation relations, and produces a result of $+1, -1, \text{or zero}$. That is, the quantity $\langle 0| ... a_j^+ a_i^+ a_\alpha^+ a_\beta^+ a_\gamma a_\delta a_i^+ a_j^+ ... |0 \rangle$ results in such
a value. The resulting value multiples the matrix element \( <\alpha|H|\gamma\delta> \) and is added to the MB matrix element. Note, there can be more contributions to a particular MB matrix element when, for example, the bra and ket differ by one sps.

- Diagonalize \( H \) using the Lanczos iteration scheme. The Lanczos iteration scheme produces a tridiagonal \( H \) that depends on the chosen initial pivot vector. \( H \) is tridiagonal in a dynamically-generated MB basis founded on the initial pivot vector. This tridiagonal \( H \) is diagonalized, using a standard procedure after the selected number of iterations are complete, to produce the Lanczos values for eigenvalues of \( H \). The lowest eigenvalues converge from above to the exact answer satisfying the variational principle.

As a general rule, one needs about 20 Lanczos iterations/converged eigenstate.

Represent the MB basis states by \( |\Phi_j\rangle \). The initial pivot vector is some superposition of these \( |\Phi_j\rangle \)

\[
|\psi_1\rangle = \sum_j A_{ij} |\Phi_j\rangle \quad \text{and} \quad H|\psi_1\rangle = \alpha|\psi_1\rangle + \beta|\psi_2\rangle.
\]

The diagonalization of the tridiagonal \( H \) produces the eigenvalues and eigenvectors:

\[
H|\Psi_i\rangle = E_i|\Psi_i\rangle,
\]

where

\[
|\Psi_i\rangle = \sum_j C_{ij} |\psi_j\rangle.
\]

From this result, one can recast the converged wavefunctions in terms of the original basis functions to obtain:

\[
|\Psi_i\rangle = \sum_j D_{ij} |\Phi_j\rangle.
\]

The resulting amplitudes \( D_{ij} \) for the converged eigenstates are stored in a file, “mfdne.smwf”, where “smwf” stands for “shell model wavefunction”.

- Evaluate/output matrix elements for a set of electromagnetic operators:

\[
<\Psi_i | O_q | \Psi_j >
\]

for comparison with experiment, where available.
Notes

A typical path for an investigation begins with the selection of a nucleon-nucleon (NN) interaction, such as “JISP16”. One proceeds to renormalize the rank-2 Hamiltonian for the selected basis space ($N_{\text{max}}$ and $h\Omega$ dependent) to obtain the rank-2 “effective Hamiltonian” for input to MFDn. The resulting smwf’s may also be used with Navrátil’s code called “TR-DENS” to evaluate additional observables.

JISP16 $\rightarrow$ $H_{\text{eff}}$(2-body) $\rightarrow$ MFDn. $\rightarrow$ TRDENS(Navrátil)

producing $\beta$ decay rates, 1-body and 2-body density matrices, overlap matrices, etc.

A 1-body density matrix is defined by:

$$ f_{ij}^{\alpha\beta} = \langle \Psi_{A,N,Z}^i | a_\alpha^+ a_\beta | \Psi_{A,N',Z'}^j \rangle. $$

It is useful to store the 1-body and 2-body density matrices for rapid evaluation of additional observables using, for example, in the case of a rank-1 observable:

$$ \langle \Psi_{A,N,Z}^i | O_q | \Psi_{A,N',Z'}^j \rangle = \sum_{\alpha\beta} f_{ij}^{\alpha\beta} \langle \alpha | O_q | \beta \rangle. $$

Using additional codes developed by Navrátil, it is also possible to develop input Hamiltonians rank-2 or rank-3 operators, based on the $V_{NN}$ interactions: AV18, AV8’, Idaho, Nijmegen, CD-Bonn, and others, plus $V_{NNN}$ interactions from chiral effective field theory or TM’.
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