Ab Initio Nuclear Structure – Recent Developments

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Abstract

The goals of *ab initio* theory of nuclear structure and nuclear reactions are to preserve the predictive power of strong interactions based on QCD, to test fundamental symmetries with the nucleus as laboratory and to develop new understandings of the vast array of nuclear phenomena. Recent progress includes the derivation, within chiral perturbation theory (ChPT), of the leading terms of the nucleon-nucleon (NN), three-nucleon ($3N$) and four-nucleon ($4N$) potentials. Additional substantial progress includes using these ChPT interactions to solve nuclear structure and reactions in light nuclei and some heavier nuclei around closed shells and closed subshells. Advances in theoretical frameworks (renormalization and many-body methods) as well as in computational resources (new algorithms and leadership-class supercomputers) signal a new generation of theory simulations that will yield valuable insights into origins of nuclear shell structure, collective phenomena and complex reaction dynamics. I outline some recent achievements that, with additional research, will strengthen the links between nuclear theory and nuclear experiment, between nuclear physics and astrophysics, and between nuclear physics and its practical applications.

Keywords: *Nuclear theory; microscopic many-body theory; chiral interactions; light nuclei*

1 Introduction

A long-standing goal of nuclear theory is to predict nuclear structure and nuclear reactions from knowledge of the underlying strong interactions based on the accepted theory of the strong interactions, Quantum Chromodynamics (QCD). With this foundation, we may address many fundamental questions of nuclear physics such as:

1. What controls nuclear saturation?
2. How do the nuclear shell and collective models emerge from the underlying theory?
3. What are the properties of nuclei with extreme neutron/proton ratios?
4. Can we predict useful cross sections that cannot be measured?
5. Can nuclei provide precision tests of the fundamental laws of nature?
6. Under what conditions do we need explicit quark and gluon degrees of freedom to describe nuclear properties?

Traditionally, we pursued this goal with meson-theoretical nucleon-nucleon (NN) interactions that were tuned to provide high-quality descriptions of the NN scattering phase shifts and the deuteron bound state properties. We also employed three-nucleon forces ($3N$Fs) that were derived from meson theory and then tuned to the properties of $A = 3$ nuclei and/or other nuclear properties. The Argonne V18 [1] NN interaction

plus the Tucson–Melbourne [2, 3] 3NF or Urbana IX [4] 3NF represent popular choices of this genre and we continue to use these interactions.

More recently, concerted efforts have led to the development of realistic NN and 3NF based upon QCD. Chiral perturbation theory (ChPT) within effective field theory (EFT) [5] provides us with a promising bridge between QCD and the hadronic systems [6]. In this approach one works consistently with systems of increasing nucleon number [7, 8, 9] and makes use of the explicit and spontaneous breaking of chiral symmetry to systematically expand the strong interaction in terms of a dimensionless constant, the ratio of a generic small momentum divided by the chiral symmetry breaking scale (about 1 GeV/c). The resulting NN and 3NFs [10, 11, 12] provide a high-quality fit to the NN data and the $A = 3$ ground state properties. Continuing world-wide efforts are expected to provide next-generation interactions within the coming year or two.

To solve for the properties of finite nuclei with these realistic microscopic Hamiltonians, one faces immense theoretical and computational challenges. Recently, *ab initio* approaches have been developed that preserve all the underlying symmetries and they converge to the exact result. If we limit our discussions to nuclei heavier than $A = 6$, there are two main approaches that have proven successful with these realistic interactions. The first approach, called No-core Shell Model (NCSM) [13, 14] or No-core Full Configuration (NCFC) [15], diagonalizes the Hamiltonian in a suitable basis. The second approach, called Coupled Cluster (CC) [16, 17] solves coupled equations that emerge from a representation of the nuclear eigenstate as a correlation operator acting on a representative Slater determinant (SD). The primary advantages of these *ab initio* no core methods are their flexibility for choosing (1) the Hamiltonian; (2) the method of renormalization/regularization; and (3) the single-particle basis. These advantages also support the adoption of these same techniques in light-front quantum field theory [18].

Recent developments in other *ab initio* approaches show additional promise for addressing fundamental questions posed above. These include the Green's Function Monte Carlo (GFMC) approach [19, 20, 21, 22] using meson exchange interactions and a lattice-simulation approach with nucleons using effective field theory [23].

Additional notable advances attempt to retain advantages of a configuration interaction (CI) basis while overcoming the explosion in the basis space that occurs with the original *ab initio* NCSM when one addresses collective modes such as clusters or proceeds to heavier systems. These advances include the "Importance-truncated" NCSM [24], the "Symmetry-adapted" NCSM [25], the "Monte-Carlo" NCSM [26], and the NCSM with a core [27] (based on ideas presented in Ref. [28]). For a more complete recent review of the *ab initio* NCSM and its connections with some of these other methods one may consult Ref. [29].

2 *Ab initio* No-core Shell Model (NCSM) and Full Configuration (NCFC) methods

The starting point of *ab initio* nuclear theory is the non-relativistic many-body Hamiltonian:

$$H_A = T_{\rm rel} + \mathcal{V} = \frac{1}{A}\sum_{i<j}\frac{(\vec{p}_i - \vec{p}_j)^2}{2m} + \sum_{i<j}^{A} V_{ij} + \sum_{i<j<k}^{A} V_{ijk} + \dots \,, \tag{1}$$

where m is the nucleon mass, V_{ij} is the NN interaction including the Coulomb interaction between protons, V_{ijk} is the three-nucleon interaction, and we allow for higher-body interactions as well. Note that the Hamiltonian does not involve the nuclear center of mass (CM) motion.

We obtain solutions in a basis of Slater determinants (SDs) constructed with single-particle states, usually from the harmonic oscillator (HO) but not exclusively. To force the many-body eigenstates to factorize into a CM component times an intrinsic component, we add the "Lawson projection term" [30] $\beta(H_{\rm CM} - \frac{3}{2}\hbar\Omega)$ to the Hamiltonian (1) to shift the spurious CM excitations. The center-of-mass Hamiltonian can be written as $H_{CM} = T_{\rm CM} + U_{\rm CM}$, where $U_{\rm CM} = \frac{1}{2}Am\Omega^2\vec{R}^2$, $\vec{R} = \frac{1}{A}\sum_{i=1}^{A}\vec{r}_i$, and Ω the HO frequency. With β chosen large and positive (a typical value is 10) the eigenenergies of physical states are the low-lying solutions and are independent of the parameter β. When a basis other than the HO is used or a many-body truncation other than the preferred N_{max} truncation is used within the HO basis, this factorization may not be precise to within numerical precision. In that event, additional investigation is needed to measure the extent of the factorization in each eigenstate.

Realistic nuclear NN interactions, such as those mentioned in the Introduction, fit the NN phase shift data and deuteron properties to high precision. This implies that these NN interactions have components that strongly couple low nucleon momentum regions (regions typical of the nuclear Fermi momentum ≈ 1 fm^{-1} with higher momentum regions ≈ 3 fm^{-1} and above. This strong coupling, which is a likely feature of $3N$Fs as well, requires us to "soften" these interactions using renormalization techniques that preserve the exact many-body solutions in suitable limits that are achievable with current computational methods and resources. An outline of selected renormalization methods is presented in Section 5.

Refs. [13, 14, 31, 32, 33, 34, 35] and [15, 36, 37, 38] provide examples of the recent advances in the *ab initio* NCSM and NCFC, respectively. The NCSM adopts a renormalization method that provides an effective interaction dependent on the chosen many-body basis space cutoff (N_{max} for example discussed below). The NCFC either retains the un-renormalized interaction or adopts a basis-space-independent renormalization so that the exact results are obtained either by using a sufficiently large basis space or by simple extrapolation to the infinite matrix limit. For a more complete discussion of nomenclature and relationships to other methods, see Section 3 below.

Recent results for the NCSM employ realistic NN and $3N$Fs derived from ChPT to solve nuclei with atomic numbers 10–13 [31]. Recent results for the NCFC feature a realistic NN interaction that is sufficiently soft that binding energies and spectra from a sequence of finite matrix solutions may be extrapolated to the infinite matrix limit as in the case of results for the Li isotopes [38]. Experimental binding energies, low-lying spectra, magnetic moments and Gamow–Teller transitions are well-reproduced in both the NCSM and NCFC approaches. Convergence of long range observables such as the rms charge radius and the electric quadrupole moment are more challenging. A sample of recent results is presented in Section 6 below.

In a NCSM or NCFC application, one typically adopts a 3D HO for all the particles in the nucleus (with harmonic oscillator energy $\hbar\Omega$) as mentioned above, treats the neutrons and protons independently, and generates a many-fermion basis space that includes the lowest oscillator configurations as well as all those generated by allowing up to N_{max} oscillator quanta of excitations. Alternatives to the HO basis space such as a Woods–Saxon basis [39] and a Coulomb–Sturmian basis [40] have recently been investigated with promising results. The single-particle states specify the orbital angular momentum projection and the basis is referred to as the m-scheme basis. For the NCSM one also selects a renormalization scheme linked to the basis truncation while in the NCFC the renormalization is either absent or of a type that retains an infinite matrix problem.

It is important to note three recent analytical and technical advances. First, non-perturbative renormalization has been developed to accompany these basis-space methods and their success is impressive. Several schemes have emerged and current research focuses on understanding the scheme-dependence of convergence rates (differ-

ent observables converge at different rates) [36]. For an introduction to two of these methods see Section 5. Second, impressive new extrapolation tools have emerged [41, 42] with indications they are the forerunners of even more powerful tools based on improved theory of the infra-red and ultra-violet properties of the interactions and basis spaces. Third, large scale calculations are performed on leadership-class parallel computers to solve for the low-lying eigenstates and eigenvectors and to evaluate a suite of experimental observables. Low-lying solutions for matrices of basis-space dimension 10-billion on 215,000 cores with a 5-hour run is the current record. However, one expects these limits to continue growing as the techniques are evolving rapidly [33] and the computers are growing dramatically. Matrices with dimensions in the several tens of billions will soon be solvable with strong interaction Hamiltonians. It remains to be seen if the higher degree of parallelism offered by the newest technological advances, Graphics Processor Units (GPUs) adapted for numerical simulations, can be efficiently exploited by the many-body methods described here.

Additional advances in physics and algorithm developments are well underway and offer additional promise. One of the current ambitious undertakings seeks to develop a symmetry-adapted no core shell model approach [25]. In this approach, called the Symplectic No-core Shell Model (Sp-NCSM), one augments the conventional spherical harmonic oscillator basis with the physically relevant symplectic Sp(3,R) symmetry-adapted configurations of the symplectic shell model that describe naturally the monopole–quadrupole vibrational and rotational modes, and also partially incorporate α-cluster correlations. The potential savings in basis space dimensions are enormous but there is a price — increased complexity of the Hamiltonian matrix elements. Current projections indicate a net large gain in the scope of physics problems that may be addressed with the Sp-NCSM.

Another ambitious program extends the Monte Carlo Shell Model (MCSM) to the no-core regime and greatly increases the number of active shells [26]. Since the MCSM has superior scaling properties with the number of nucleons, once validated, we envision this will be a very fruitful avenue for addressing heavier nuclei — possibly the entire periodic table. However, there are daunting challenges to overcome such as developing a load-balanced and scalable code.

3 Relationships among many-body methods

There are several quantum many-body methods that are closely related to the methods we have developed and applied. The associated nomenclatures require some discussion as well.

The term Configuration Interaction (CI) is the broadest term that seems widely recognized across physics disciplines. In general any method that uses a basis space developed from Slater Determinants (SDs) of single-particle wave functions (configurations) is referred to as a CI method. It covers all the methods discussed here except the Coupled Cluster, Greens Function Monte Carlo and lattice simulation methods mentioned above.

The term Full Configuration Interaction (FCI) was introduced by the quantum chemists and used widely by them. FCI signifies the use of all many-body configurations consistent with a chosen set of symmetries and a defined finite set of single-particle states. Most often there is an inert core of filled single-particle states in these calculations. An FCI calculation is considered the "gold standard" in quantum chemistry to which, for example, Coupled Cluster and Density Functional Theory (DFT) approaches are often benchmarked.

The use of no-core model spaces for solving light nuclei in Hamiltonian matrix formulations has a long history. Some of that history is summarized, including the distinction between the FCI truncation and the N_{max} truncation in Ref. [43]. For a more recent summary, see Ref. [29].

The term "No-core Shell Model" (NCSM) first appeared in the title of a paper in Ref. [44] where the renormalization scheme was the Brueckner G-matrix approach adapted to the no-core basis. Limitations to this approach included the presence of spurious CM motion in the effective NN interaction, the G-matrix, and in the occurrence of a free parameter, the "starting energy". While the first limitation remains to this day, the starting-energy dependence of this approach could be removed by including sufficiently large sets of higher-order processes formed with the G-matrix as building block, including effective $3N$Fs and beyond.

To accurately preserve all the symmetries of the underlying strong interactions and include sufficient renormalization to achieve accurate results, we developed the "*Ab Initio* No-core Shell Model" [13, 14]. Indeed, the terminology "*Ab Initio* No-core Shell Model" first appeared in a title in Ref. [14] while the term "*ab initio* no-core nuclear shell model" appears in the first sentence of the abstract of Ref. [13]. At the time of its introduction, we adopted the "Okubo–Lee–Suzuki" (OLS) method [45, 46] of renormalizing the Hamiltonian (see Section 5 below for an introduction) since it enabled us to preserve the factorization of the CM and internal motion which is important especially in light nuclei.

It is important to note that both the Brueckner G-matrix and the OLS approaches evaluate effective Hamiltonians specific to the many-body basis space for that application. That is, they are dependent on the many-body basis truncation and may also have dependence on the atomic number. More importantly, there is no variational upper bound property of the resulting eigensolutions and this limits the ability to extrapolate to the infinite matrix limit.

As a guide to our recent papers where a more extensive presentation of the methods and results may be found, it is useful to note that we have used the following terminology:

1. No-core Shell Model (NCSM) — follows the original NCSM papers where the interaction is derived for the chosen many-body model space. This could be any renormalization scheme such as the Brueckner approach or the OLS approach that has a dependence on the model space cutoff. It is "*ab initio* NCSM" if it respects all the symmetries of the original nuclear Hamiltonian so this includes OLS renormalization but not Brueckner G-matrix applications.

2. No-core Full Configuration (NCFC), first introduced in the title of Ref. [15], — signifies we use interactions independent of the basis space and achieve converged eigenenergies within numerical error estimates or we extrapolate to the infinite matrix limit with error estimates. The interactions may be either the "bare" interactions of Eq. (1) or interactions softened via methods that are independent of the many-body basis space. Thus, the NCFC results are independent of all basis parameters (N_{max}, N_{shell} (number of HO shells), $\hbar\Omega$, Woods–Saxon parameters, Coulomb–Sturmian parameters, etc). This newer terminology emerged in response to the criticism that the NCSM was not so much of a "Shell Model" as a CI approach which did not assume a shell model structure for the solutions. In other words, the approach was general and should, if successful, be able to derive the "Shell Model" from first principles. One colleague even refers to the NCSM as the "no-core no-shell no-model" approach to underscore that criticism. Additionally, quantum chemists have adopted the terminology of CI and FCI which are widely understood in physics so we should include the term "Configuration" as we do with NCFC.

3. No-core Configuration Interaction (NCCI), introduced in the text of Ref. [40], — for a more general case where the variational upper bound is obtained for an arbitrary finite basis (i. e. includes FCI, N_{max} truncation, N_{shell} truncation, Coulomb–Sturmian, etc.) — i. e. without the extrapolation and error estimation of the NCFC.

With this newer terminology, results from basis-space independent interactions, therefore allowing for some forms of renormalization, with extrapolation and error estimates would be be called NCFC calculations. Without extrapolation and error estimates, they would be called NCCI calculations according to our current usage.

This usage has evolved since we earlier used NCSM more liberally (prior to introducing "NCFC" in early 2009) to include both truncated calculations preserving variational limits as well as extrapolations with error estimates in Ref. [36].

Due to the flexibility of renormalization procedures, choice of truncations, choice of basis, etc., it may be that the above nomenclature does not cover all cases uniquely. That is, it is easy to see there are possible overlaps in the use of these terminologies.

4 Realistic Hamiltonians

We began our no-core investigations in the 1980s and 1990s with the best available interactions that were meson-theoretical nucleon-nucleon interactions, tuned to provide high-quality descriptions of the NN scattering phase shifts and the deuteron bound state properties. For example, we introduced and employed no-core spectral distribution methods [47, 48, 49] with realistic NN interactions in advance of the current era where direct diagonalization in large basis spaces became feasible. Those early results produced favorable comparisons with Coupled Cluster results [50] for total binding energies.

As mentioned earlier, we also employed $3N$Fs that were derived from meson theory and then tuned to the properties of $A = 3$ nuclei and/or other nuclear properties such as the binding energy of nuclear matter. The Argonne V18 [1] NN interaction plus the Tucson–Melbourne [2, 3] $3N$F or Urbana IX [4] $3N$F represent popular choices of this class of interactions. Many current investigations continue to use these interactions. When these interactions are employed, it is possible to include a consistent treatment of meson-exchange currents in the development of effective operators for other observables such as electromagnetic moments and transition rates. There is an increasing trend to using these theoretically consistent operators.

More recently, concerted efforts have led to the development of realistic NN and $3N$F based upon QCD using chiral perturbation theory (ChPT) within effective field theory (EFT) [5]. This EFT approach provides us with a promising bridge between QCD and the hadronic systems [6]. In this approach one works consistently with systems of increasing nucleon number [7, 8, 9] and makes use of the explicit and spontaneous breaking of chiral symmetry to systematically expand the strong interaction in terms of a dimensionless constant, the ratio of a small momentum (characteristic of the low-energy application such as nuclear structure) divided by the chiral symmetry breaking scale of QCD (taken to be about 1 GeV/c). The resulting NN and $3N$Fs [10, 11, 12] have the appearance of a pion-exchange theory (no higher mass mesons appear explicitly nor do baryon resonances) and they provide a high-quality fit to the NN data and the $A = 3$ ground state properties. The ChPT is characterized by the appearance of low-energy constants (LECs)which are, in principle, calculable with non-perturbative methods from QCD itself. However, since they are not calculable with current computer resources, these constants are fit to NN data and three-nucleon systems (for the new constants that appear in the $3N$Fs). One hallmark of this approach is the natural hierarchy that places NN interactions at lower order than $3N$Fs. In addition, a cross check that ChPT is producing a convergent series, i. e. one that is "under control", is that these LECs all turn out to be of order unity. The appearance of an LEC of order 10, for example, would signal the potential need to rearrange the series. Such a rearrangement is under development with a "deltafull" version of ChPT where where the delta-resonance is included explicitly as intermediate state excitations with the ChPT graphs.

At present we employ NN interactions complete through "next-to-next-to-next-to

leading order" (N3LO). However, the 3NFs we use are only available in the useful partial-wave decomposed form through N2LO. Fortunately, world-wide efforts are expected to provide ChPT interactions for both NN and 3NFs complete through N3LO within the coming year or two. At about the same time, we expect the deltafull versions of ChPT to become available.

We also adopt the NN interaction JISP16, a realistic NN interaction initially developed from NN data using inverse scattering techniques [32, 51, 52]. It is then adjusted with phase-shift equivalent unitary transformations to describe light nuclei without explicit 3NFs. One major advantage of JISP16 is that it is considerably softer (reduced high-momentum components) relative to the meson-exchange or ChPT NN interactions. Since JISP16 incorporates some of the 3NF effects of the other interactions, and is sufficiently soft, we can achieve NCFC results in light nuclei and the results are in remarkably good agreement with experiment [15, 37, 38, 41, 53].

With all these interaction developments, we can expect an era of vigorous scientific activity testing these improved interactions in nuclear structure and nuclear reactions. With the emerging predictive power, we expect to be able to reliably predict quantities that cannot be measured directly in the laboratory but have practical significance such as in the design of advanced nuclear reactors.

5 Renormalization and regularization

Given that the NN interaction and 3NFs couple strongly the low-momentum regions of phase space with the high-momentum regions, we require methods to soften these interactions (reduce those couplings) while maintaining the full predictive power of the microscopic theory. This leads to the introduction of renormalization and regularization methods. When properly used, these methods allow the exact results (results from the original input interactions) to be obtained in a systematic and controllable approach. Different methods have been introduced and each has its advantages and disadvantages. Here, I will summarize two of those methods that we have been using extensively. The first is the Okubo–Lee–Suzuki (OLS) method [45, 46] and the second is the Similarity Renormalization Group (SRG) method [54, 55, 56, 57, 58, 59]. There is considerable freedom in each of these renormalization methods and there is ongoing research that investigates the potential utility of these freedoms. For the subsections of this section, I will follow our descriptions presented in Ref. [29] that should be consulted for additional details and key references.

The topic of regulators is one that requires its own discussion. For the present paper, I will simply mention that regulators appear at all levels of the development of effective Hamiltonians. These occur in the choices of form factors regulating vertices in the underlying interactions all the way up to the choice of basis space parameters such as N_{max} and $\hbar\Omega$. Ultimately, the test of a good theory is to obtain converged results that agree with experiment as regulators are removed. These challenges are addressed, at least in part, by the ChPT approach of EFT and by the NCFC method discussed above.

5.1 Okubo–Lee–Suzuki method

For pedagogical purposes, we outline the OLS approach with NN interactions alone and point the reader to the literature [29] for the extensions to include 3NFs. We begin with the simplified purely intrinsic Hamiltonian for the A-nucleon system, i. e. we retain only the first two terms of Eq. (1) to write

$$H_A = T_{\rm rel} + \mathcal{V} = \frac{1}{A}\sum_{i<j}^{A}\frac{(\vec{p}_i - \vec{p}_j)^2}{2m} + \sum_{i<j}^{A} V(\vec{r}_i - \vec{r}_j), \tag{2}$$

where m is the nucleon mass and $V(\vec{r}_i - \vec{r}_j)$, the NN interaction, with both strong and electromagnetic components. Note the absence of a phenomenological single-particle potential. We may use either coordinate-space or momentum-space NN potentials. They may also be non-local interactions.

Next, we add the center-of-mass HO Hamiltonian to the Hamiltonian (2) $H_{\rm CM} = T_{\rm CM} + U_{\rm CM}$, where $U_{\rm CM} = \frac{1}{2}Am\Omega^2\vec{R}^2$, $\vec{R} = \frac{1}{A}\sum_{i=1}^{A}\vec{r}_i$. In the full Hilbert space the added $H_{\rm CM}$ term has no influence on the intrinsic properties. However, when we introduce our cluster approximation below, the added $H_{\rm CM}$ term facilitates convergence to exact results with increasing basis size. The modified Hamiltonian, with a pseudo-dependence on the HO frequency Ω, can be cast into the form

$$H_A^\Omega = H_A + H_{\rm CM} = \sum_{i=1}^{A}\left[\frac{\vec{p}_i^{\,2}}{2m} + \frac{1}{2}m\Omega^2\vec{r}_i^{\,2}\right] + \sum_{i<j=1}^{A}\left[V_{\rm N}(\vec{r}_i - \vec{r}_j) - \frac{m\Omega^2}{2A}(\vec{r}_i - \vec{r}_j)^2\right]. \tag{3}$$

In the spirit of Da Providencia and Shakin [60] the OLS method [45, 46] introduces a unitary transformation, which is able to accommodate the short-range two-body correlations in a nucleus, by choosing an antihermitian operator S, acting only on intrinsic coordinates, such that

$$\mathcal{H} = e^{-S}H_A^\Omega e^S. \tag{4}$$

In our approach, S is determined by the requirements that $\mathcal{H}$ and H_A^Ω 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. Our 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 with $a \leq A$,

$$\mathcal{H} = \mathcal{H}^{(1)} + \mathcal{H}^{(a)} = \sum_{i=1}^{A} h_i + \frac{\binom{A}{2}}{\binom{A}{a}\binom{a}{2}} \sum_{i_1<i_2<\ldots<i_a}^{A} \tilde{V}_{i_1 i_2 \ldots i_a}, \tag{5}$$

with

$$\tilde{V}_{12\ldots a} = e^{-S^{(a)}}H_a^\Omega e^{S^{(a)}} - \sum_{i=1}^{a} h_i, \tag{6}$$

and $S^{(a)}$ is an a-body operator; $H_a^\Omega = h_1 + h_2 + h_3 + \ldots + h_a + V_a$, and $V_a = \sum_{i<j}^{a} V_{ij}$. Note that there is no sum over "a" in Eq. (5). Also, we adopt the HO basis states that are eigenstates of the one-body Hamiltonian $\sum_{i=1}^{A} h_i$.

If the full Hilbert space is divided into a finite model space ("P-space") and a complementary infinite space ("Q-space"), using the projectors P and Q with $P + Q = 1$, it is possible to determine the transformation operator S_a from the decoupling condition

$$Q_a e^{-S^{(a)}}H_a^\Omega e^{S^{(a)}}P_a = 0, \tag{7}$$

and the simultaneous restrictions $P_a S^{(a)} P_a = Q_a S^{(a)} Q_a = 0$. Note that a-nucleon-state projectors (P_a, Q_a) appear in Eq. (7). Their definitions follow from the definitions of the A-nucleon projectors P, Q. The net effect of the OLS renormalization procedure is to develop a finite P-space effective Hamiltonian decoupled from the infinite complementary Q-space as illustrated in Fig. 1.

The unitary transformation and decoupling condition, introduced by Suzuki and Okamoto and referred to as the unitary-model-operator approach (UMOA) [61], has a solution that can be expressed in the following form

$$S^{(a)} = \text{arctanh}(\omega - \omega^\dagger), \tag{8}$$

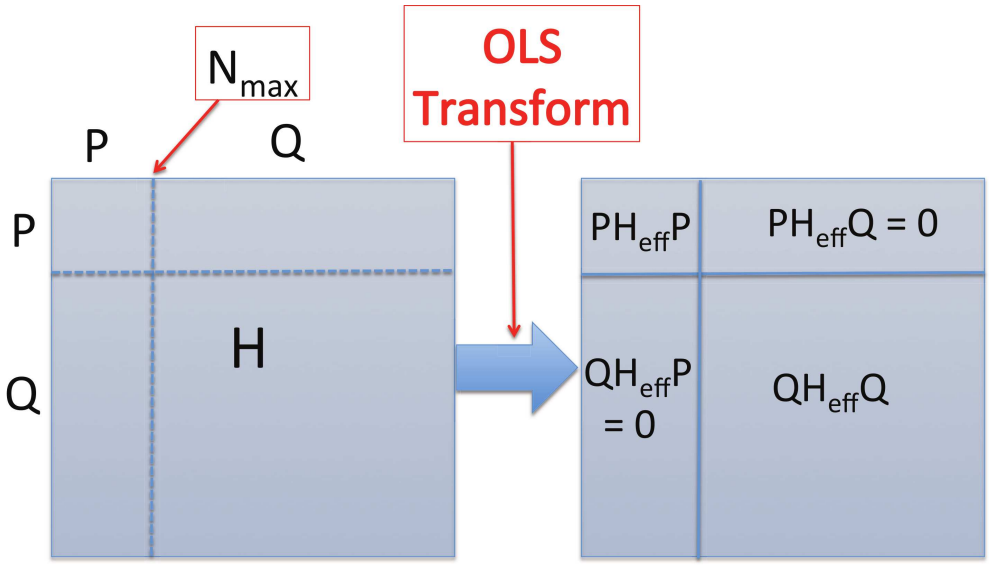

Figure 1: Schematic illustration on how Okubo–Lee–Suzuki (OLS) similarity transformation yields an $\bar{H}_{\rm eff}$ in a finite model space P decoupled from the infinite complementary Q-space.

with the operator ω satisfying $\omega = Q_a \omega P_a$, and solving its own decoupling equation,

$$Q_a e^{-\omega} H_a^\Omega e^\omega P_a = 0. \tag{9}$$

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

$$\bar{H}_{\rm a-eff} = (P_a + \omega^\dagger\omega)^{-1/2}(P_a + P_a\omega^\dagger Q_a) H_a^\Omega (Q_a\omega P_a + P_a)(P_a + \omega^\dagger\omega)^{-1/2}. \tag{10}$$

Given the eigensolutions, $H_a^\Omega|k\rangle = E_k|k\rangle$, then the operator ω can be determined from

$$\langle\alpha_Q|\omega|\alpha_P\rangle = \sum_{k\in\mathcal{K}} \langle\alpha_Q|k\rangle\langle\tilde{k}|\alpha_P\rangle, \tag{11}$$

where we denote by tilde 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 $\sum_k \langle\alpha'_P|\tilde{k}\rangle\langle k|\alpha_P\rangle = \delta_{\alpha'_P,\alpha_P}$, for $k, k' \in \mathcal{K}$. In the relation (11), $|\alpha_P\rangle$ and $|\alpha_Q\rangle$ are the model-space and the Q-space basis states, respectively, and $\mathcal{K}$ 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.

With the help of the solution for ω (11) we obtain a simple expression for the matrix elements of the Hermitian effective Hamiltonian

$$\langle\alpha_P|\bar{H}_{\rm a-eff}|\alpha'_P\rangle = \sum_{k\in\mathcal{K}}\sum_{\alpha''_P}\sum_{\alpha'''_P}\langle\alpha_P|(P_a+\omega^\dagger\omega)^{-1/2}|\alpha''_P\rangle\langle\alpha''_P|\tilde{k}\rangle E_k\langle\tilde{k}|\alpha'''_P\rangle \times \langle\alpha'''_P|(P_a+\omega^\dagger\omega)^{-1/2}|\alpha'_P\rangle. \tag{12}$$

For computation of the matrix elements of $(P_a + \omega^\dagger\omega)^{-1/2}$, we can use the relation

$$\langle\alpha_P|(P_a+\omega^\dagger\omega)|\alpha''_P\rangle = \sum_{k\in\mathcal{K}}\langle\alpha_P|\tilde{k}\rangle\langle\tilde{k}|\alpha''_P\rangle. \tag{13}$$

We note that in the limit $a \to A$, we obtain the exact solutions for d_P states of the full problem for any finite basis space, with flexibility for choice of physical states subject to certain conditions [62].

On account of our cluster approximation a dependence of our results on $N_{\rm m}$ and on Ω arises. For a fixed cluster size, the smaller the basis space, the larger the dependence on Ω. The residual $N_{\rm m}$ and Ω dependences can be used to infer the uncertainty in our results.

The model space P_2 is defined by the maximal number of allowed HO quanta of the A-nucleon basis states $N_{\rm m}$ from the condition $2n + l \leq N_{\rm m} - N_{\rm spsmin}$, where $N_{\rm spsmin}$ denotes the minimal possible HO quanta of the spectators, i. e., nucleons not affected by the interaction process. For example, ^{10}B, $N_{\rm spsmin} = 4$ as there are 6 nucleons in the $0p$-shell in the lowest HO configuration and, e. g., $N_{\rm m} = N_{\rm spsmin} + 2 + N_{\rm max}$, where $N_{\rm max}$ represents the maximum HO quanta of the many-body excitation above the unperturbed ground-state configuration. For ^{10}B, $N_{\rm m} = 12$ for an $N_{\rm max} = 6$ or "$6\hbar\Omega$" calculation.

In order to construct the operator ω (11) we need to select the set of eigenvectors $\mathcal{K}$. We select the lowest states obtained in each two-body channel. It turns out that these states also have the largest overlap with the model space for the range of $\hbar\Omega$ we have investigated and the P-spaces we select. Their number is given by the number of basis states satisfying $2n + l \leq N_{\rm m} - N_{\rm spsmin}$.

We input the effective Hamiltonian, now consisting of a relative 2-body operator and the pure H_{CM} term introduced earlier, into an m-scheme Lanczos diagonalization process to obtain the P-space eigenvalues and eigenvectors. At this stage we also add the term H_{CM} again with a large positive coefficient (referred to as β above) to separate the physically interesting states with $0s$ CM motion of the HO from those with excited CM motion according to the Lawson method [30]. We retain only the states with pure $0s$ CM motion when evaluating observables.

All observables that are expressible as functions of relative coordinates, such as the rms radius and radial densities, are then evaluated free of CM motion effects. In addition, all observables that are not spherically symmetric such as electromagnetic multipole operators receive no contribution from the $0s$ CM motion component of state vectors so they are correctly dependent only on the internal motion though they may be evaluated within the full SD basis.

We close our presentation on the theoretical framework with the observation that all observables require the same transformation as implemented on the Hamiltonian. To date, we have found rather small effects on the rms radius operator when we transformed it to a P-space effective rms operator at the $a = 2$ cluster level [13, 14]. On the other hand, substantial renormalization was observed for the kinetic energy operator when using the $a = 2$ transformation to evaluate its expectation value [63].

5.2 Similarity Renormalization Group method

The Similarity Renormalization Group (SRG) method also develops effective two-, three- (and even higher-) body forces (induced many-body interactions) while reducing the strong couplings of the available initial interactions across large regions of momentum space. This will also aid convergence in many-body calculations provided the induced interactions are retained to the level needed. One perceived advantage of SRG is that it retains the effective interactions in the full (infinite) Hilbert space. With a given SRG-evolved effective Hamiltonian, the variational principle allows smooth extrapolations to the ground state energy from above as a function of the many-body truncation. Thus NCFC results are, in principle, obtainable with SRG-evolved effective Hamiltonians. This advantage is absent in the OLS approach.

The SRG is a continuous unitary transformation of the free-space Hamiltonian H (2) ($H \equiv H_{\lambda=\infty}$),

$$H_\lambda = U_\lambda H_{\lambda=\infty} U_\lambda^\dagger, \tag{14}$$

labeled by a momentum parameter λ that runs from ∞ toward zero, which keeps track of the sequence of Hamiltonians ($s = 1/\lambda^4$ has been used elsewhere [54, 64, 65]). These

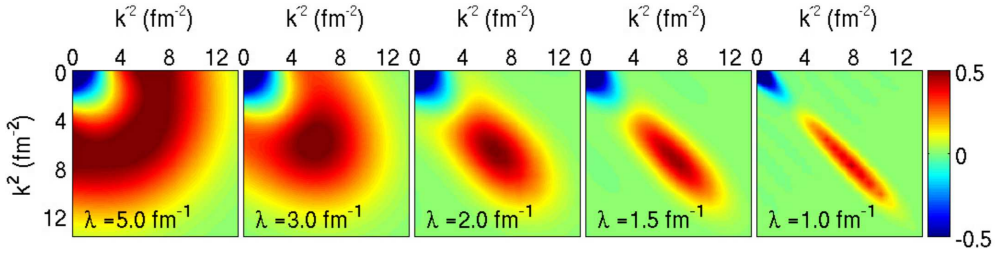

Figure 2: Illustration of how the SRG procedure [64, 66, 65, 67] weakens the strong off-diagonal couplings of the $^1S_0$ chiral N^{3}LO NN potential [11, 12] in momentum space as the flow proceeds to smaller values of λ (left to right panels). The flow increasingly concentrates the non-vanishing potential strength to an attractive region near the origin and a repulsive region at higher momenta with both regions lying along the diagonal.

transformations are implemented as a flow equation in λ (in units where $\hbar^2/M = 1$),

$$\frac{dH_\lambda}{d\lambda} = -\frac{4}{\lambda^5}[[T_{\rm rel}, H_\lambda], H_\lambda] \ , \tag{15}$$

whose form guarantees that the H_λ's are unitarily equivalent [54, 55, 56, 66].

The utility of the nucleon relative kinetic energy $T_{\rm rel}$ in Eq. (15) is that it reduces the coupling of the high- and low-momentum parts of H_λ, which means softer and more convergent may-body calculations [36, 57]. This is evident in a partial-wave momentum basis, where matrix elements $\langle k|H_\lambda|k'\rangle$ connecting states with (kinetic) energies differing by more than λ^2 are suppressed by $e^{-(k^2-k'^2)^2/\lambda^4}$ factors and, therefore, the states decouple as λ decreases. (Decoupling also results from replacing $T_{\rm rel}$ in Eq. (15) with other generators [54, 56, 58, 59] where the common feature is a generator having diagonal or nearly diagonal structure in the relative HO basis.) The decoupling between the high-momentum and low-momentum parts of the NN interaction is illustrated in Fig. 2.

To see how the two-, three-, and higher-body potentials are identified, it is useful to decompose H_λ in second-quantized form. Schematically (suppressing indices and sums),

$$H_\lambda = \langle T\rangle a^\dagger a + \langle V_\lambda^{(2)}\rangle a^\dagger a^\dagger aa + \langle V_\lambda^{(3)}\rangle a^\dagger a^\dagger a^\dagger aaa + \cdots \ , \tag{16}$$

where $a^\dagger$, a are creation and destruction operators with respect to the vacuum in some (coupled) single-particle basis. This *defines* $\langle T\rangle$, $\langle V_\lambda^{(2)}\rangle$, $\langle V_\lambda^{(3)}\rangle$, ... as the one-body, two-body, three-body, ... matrix elements at each λ. Upon evaluating the commutators in Eq. (15) using H_λ from Eq. (16), we see that even if initially there are only two-body potentials, higher-body potentials are generated with each step in λ. Thus, when applied in an A-body subspace, the SRG will "induce" A-body forces. But we also see that $\langle T\rangle$ is fixed, $\langle V_\lambda^{(2)}\rangle$ is determined only in the $A = 2$ subspace with no dependence on $\langle V_\lambda^{(3)}\rangle$, $\langle V_\lambda^{(3)}\rangle$ is determined in $A = 3$ given $\langle V_\lambda^{(2)}\rangle$, and so on.

While it may seem natural to solve Eq. (15), in momentum representation, it is an operator equation, so we can use any convenient basis. In our applications, we evolve in a *discrete* HO basis, where spectators are handled without a decomposition and induced many-body forces can be directly identified. Having chosen such a basis, we obtain coupled first-order differential equations for the matrix elements of the flowing Hamiltonian H_λ, where the right side of Eq. (15) is evaluated using simple matrix multiplications.

Calculations may be performed in the Jacobi coordinate HO basis. We start by evolving H_λ in the $A = 2$ subsystem, which completely fixes the two-body matrix

elements $\langle V_\lambda^{(2)} \rangle$. Next, by evolving H_λ in the $A = 3$ subsystem we determine the combined two-plus-three-body matrix elements. We can isolate the three-body matrix elements by subtracting the evolved $\langle V_\lambda^{(2)} \rangle$ elements in the $A = 3$ basis [68]. Having obtained the separate NN and NNN matrix elements, *we can apply them unchanged to any nucleus*. We are also free to include any initial three-nucleon force in the initial Hamiltonian without changing the procedure. If applied to $A \geq 4$, four-body (and higher) forces will not be included and so the transformations will be only approximately unitary.

Once the evolved interactions are determined in the Jacobi HO basis, transformations to the SD basis are performed, in particular, when nuclei with $A > 4$ are studied. The transformations of two-body interactions are standard. The correspondent $3N$F transformations were derived and implemented in Refs. [69, 70] with recent advances presented in Ref. [71], where a JT-coupled representation was developed with a highly efficient storage scheme, which allows us to handle $3N$F matrix-element sets up to $N_{\max} = 12$ model spaces for p-shell nuclei.

6 Recent NCSM and NCFC results

In this section, I present a selection of NCSM and NCFC results. First, recall that in the NCFC case [15], one extrapolates to the continuum limit (infinite matrix result) illustrated in Fig. 3.

Here, I show results for the ground state (gs) of ^{12}C as a function of N_{max} obtained with the realistic NN interaction, JISP16 [32, 51, 52]. The smooth curves portray exponential fits that achieve asymptotic independence of N_{max} and $\hbar\Omega$. The NCFC gs energy (the common asymptote) of -94.5 MeV indicates overbinding of $\sim 2.5\%$ leading us to conclude that $3N$Fs must play a role. The assessed uncertainty

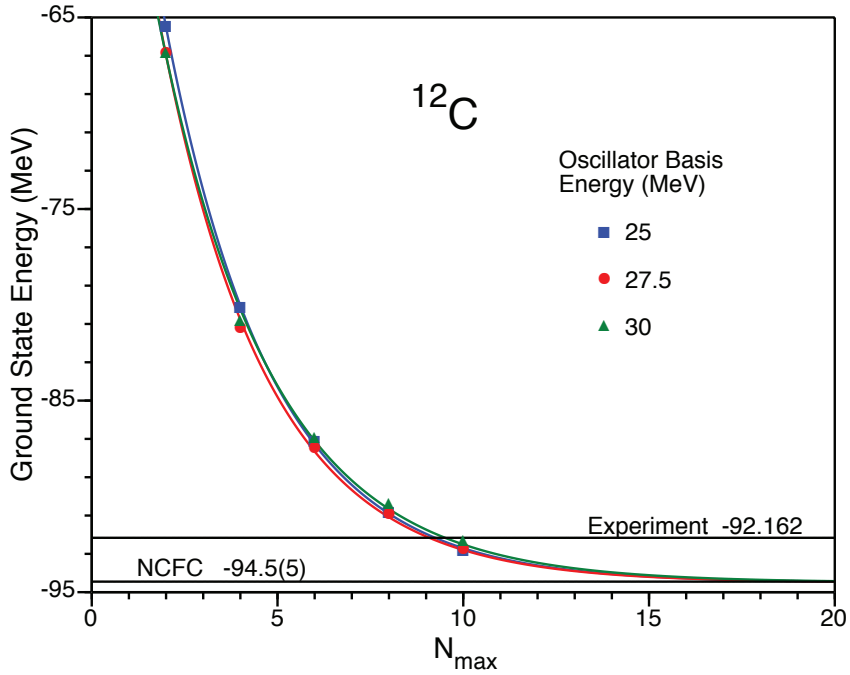

Figure 3: Calculated ground state (gs) energy of ^{12}C for $N_{max} = 2{-}10$ (symbols) at selected values of $\hbar\Omega$. For each $\hbar\Omega$, the results are fit to an exponential plus a constant, the asymptote, constrained to be the same for all $\hbar\Omega$ [15]. Horizontal lines indicate the experimental gs and the NCFC result (uncertainty = 0.5 MeV).

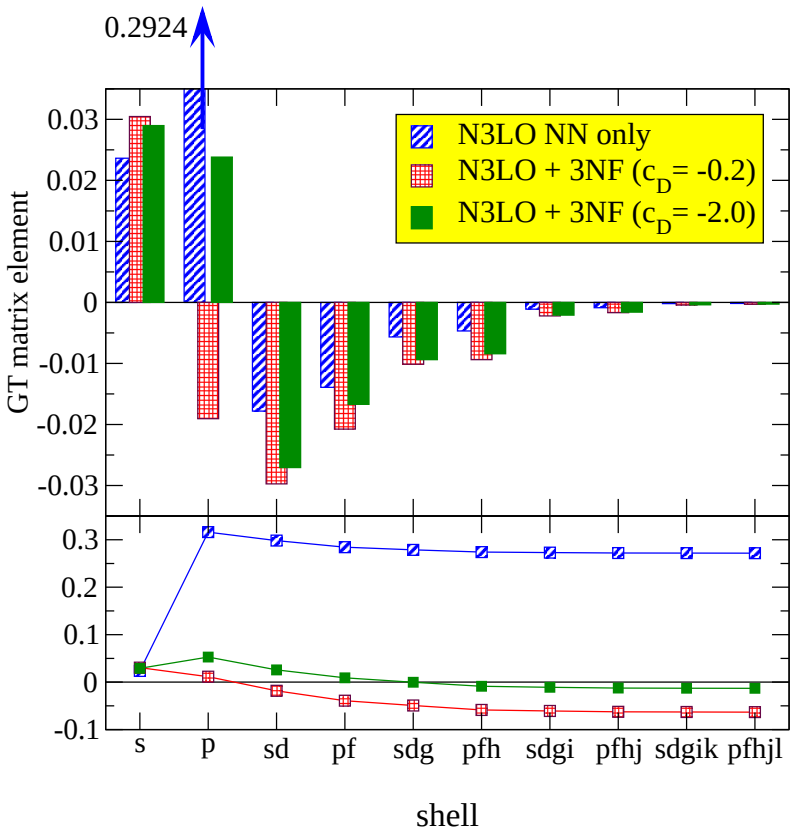

Figure 4: *Ab-initio* NCSM calculations the Gamow–Teller (GT) matrix element for the beta decay of ^{14}C [34]. Contributions to the ^{14}C beta decay matrix element are displayed as a function of the HO shell in the $N_{max} = 8$ basis space using interactions from ChPT. The top panel displays the contributions without and with the 3NF with two reasonable choices for the 3NF parameter c_D. Contributions are summed within each shell to yield a total for that shell. The bottom section displays the running sums of the GT contributions over the shells. Two choices for for c_D in the 3NF lead to similar strong suppression of the GT matrix element where the final sums are closer to zero. $c_D = -2.0$ yields the final sum closest to zero. Note, in particular, the order-of-magnitude suppression of the 0p-shell contributions arising from the 3NF.

in the NCFC result is 0.5 MeV shown in parenthesis in the figure. The largest calculations correspond to $N_{max} = 10$, with an m-scheme matrix dimension near 8 billion. $N_{max} = 12$ produces an m-scheme matrix dimension near 81 billion which we hope to solve in the future.

A particular example of the recent NCSM accomplishments stands out and that is the demonstration that the anomalous long half life of ^{14}C is a consequence of ChPT 3NFs strongly quenching the Gamow-Teller (GT) matrix element [34]. The results without and with 3NFs are shown in Fig. 4. In the top of Fig. 4 one observes that, without 3NFs there is a large contribution to the GT matrix element coming from the 0p-shell single particle spin flip as a neutron converts to a proton. This is the conventional shell-model single-particle GT transition and it leads to a "normal" beta decay halflife of a light nucleus which is not suppressed.

Inclusion of 3NFs shows little effect on the contribution of most shells to the GT matrix element. However, the contribution of the 0p-shell terms becomes strongly suppressed — by more than an order of magnitude in the two examples shown. The two examples differ by changes in the LECs of the 3NF that are allowed within the

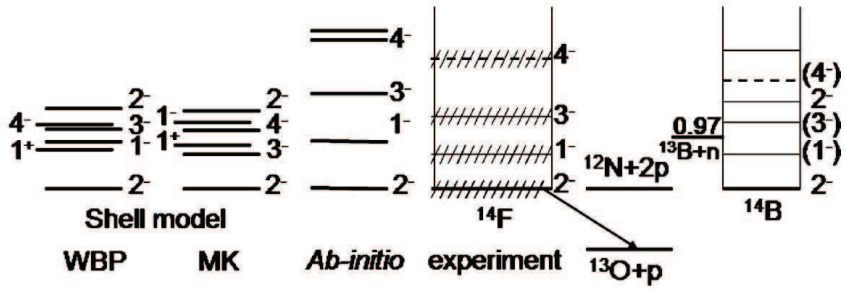

Figure 5: Comparison of the ^{14}F theoretical spectra with the Texas A&M Cyclotron experiment showing excellent agreement between *ab initio* predictions of Ref [37] and experiment [53]. This figure also shows comparisons with predictions of traditional phenomenological shell model calculations with a core labelled by "WBP" and "MK" (see Ref [53] for details).

range that is "natural" as discussed above. The conclusion is that one may easily fit the exact experimental halflife with an allowed adjustment of the LECs for the $3N$Fs. However, we did not carry out this fine tuning since there remain additional corrections from enlarging the basis and including ChPT corrections to the weak decay matrix element. These additional small corrections will not change the main conclusion (large suppression due to $3N$Fs) but will effect the fine tuning of the LECs.

As another example of NCFC achievements, we successfully predicted the spectra for the proton unstable nucleus ^{14}F [37] before it was measured using JISP16 [32, 51, 52] as shown in Fig. 5. This figure is adapted from the paper [53] reporting the experimental results and presenting the comparison with our published *ab initio* NCFC predictions.

As a final example illustrating recent NCSM progress in light nuclei, I select the example of ^{7}Li calculated with NN + $3N$Fs from ChPT. The resulting excitation spectra is shown in Fig. 6 at $N_{max} = 4{-}6{-}8$ [35] and compared with experiment shown in the leftmost column. The HO energy is chosen, where the g.s. energy of ^{7}Li is a minimum in the $8\hbar\Omega$ basis space. Note that our NN +$3N$F (also referred to as "NNN" in the legend) spectral ordering is in agreement with experiment for the 9 lowest states in ^{7}Li and the excitation spectra is rather stable with increasing $N_{\rm max}$. We also obtain theoretical excitation spectra showing comparable agreement with experiment for ^{7}Be.

7 Summary

The *ab initio* NCSM and NCFC approaches treat all A nucleons equally with modern NN + $3N$F interactions and successfully describe properties of nuclei throughout the $0p$-shell. Collaborations with computer scientists and applied mathematicians as well as the use of supercomputers is critical to the progress achieved to date. Several investigations are underway to extend these *ab initio* methods to nuclei with $A > 16$ and to more completely unify these *ab initio* structure approaches with a corresponding predictive theory of nuclear reactions [72]. The outlook is very promising for resolving many long-standing problems in microscopic nuclear theory.

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I would like to thank my collaborators who have worked diligently over many years to accomplish the key results summarized here. They are most easily identified by the papers I have cited in this work. I also thank the sponsors of this workshop, Pacific

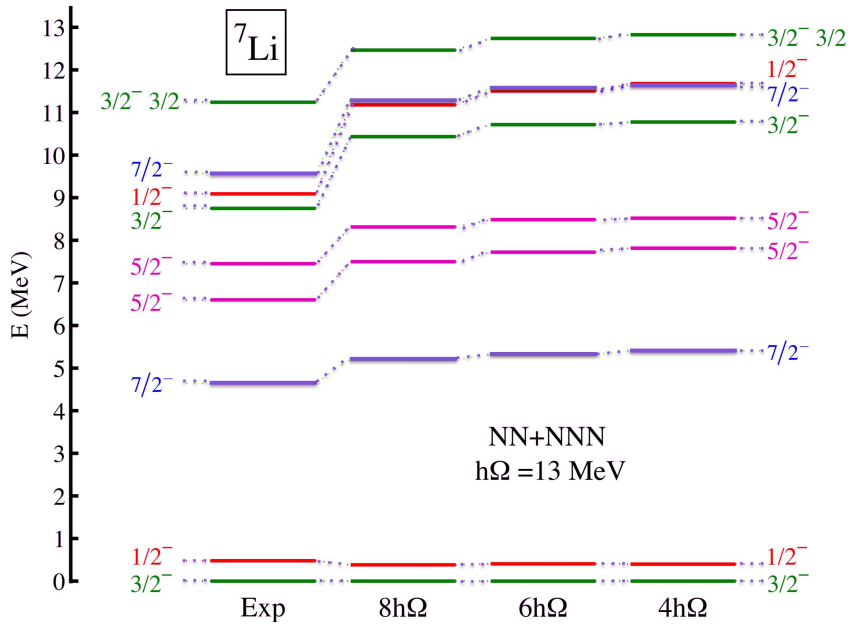

Figure 6: Calculated and experimental excitation energies of ^{7}Li from Ref. [35]. Dependence on the size of the basis is presented. The chiral EFT NN and NNN interaction was used and $\hbar\Omega = 13$ MeV. The isospin of the states is $T = 1/2$ unless shown otherwise as in the example of the highest lying experimental state which is $T = 3/2$.

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