A 21st Century View of Nuclear Structure

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Abstract. Exploiting exact and special symmetries to unmask simplicity within complexity, which remains the “holy grail” of nuclear physics, will be considered within its historical context and as evolving through 21st century *ab initio* methods, including emerging results linked to the internal structure of nucleons. Some exemplar results for very light to medium mass nuclei will be presented, and what these may portend for heavier systems, including species beyond known lines of stability, will be proffered.

1 Introduction

This contribution is organized as follows: after this introduction (Sec. 1), we discuss the development of various nuclear models which could capture collective and cluster features in atomic nuclei in Sec. 2. This includes an introduction to the symmetry-adapted no-core shell model (SA-NCSM). We then apply the SA-NCSM to study a number of different nuclei in Sec. 3, including intermediate and medium mass nuclei from an *ab initio* perspective. Afterwards, we discuss and summarize key findings in our conclusions (Sec. 4).

2 Historical Overview

Mayer and Jensen’s independent particle model (IPM) [1, 2] and its ability to reproduce the so-called ‘magic’ numbers lead to the first microscopic theory of nuclear structure. Many modern nuclear structure techniques can trace their initial underpinning to more sophisticated versions of the IPM. These models, when combined with the breath of high-performance computing resources available today, have allowed for good descriptions of the structure of many low-lying states in light nuclei, including descriptions starting from an *ab initio* perspective. Principle among these is the no-core shell model (NCSM) [3, 4] and its extensions, e.g. Refs. [5–7].

The NCSM takes all of the nucleons in a nucleus and uses them to begin filling shells in a harmonic oscillator (HO) potential. Notably, it treats all nucleons as active and allows any of them to be excited to higher shells by an amount $N_{\max}$, where $N_{\max}$ is the total number of HO quanta available above the ground state configuration. Each of these HO shells is separated in energy by a value $\hbar\Omega$ and in the full, infinite space, i.e. a real nucleus, independence

must be shown for both $\hbar\Omega$ and $N_{\max}$ since both are external parameters.

Further, and of particular relevance here, was the development of Elliott’s SU(3) model [8, 9]. Starting from a microscopic perspective, it was able to realize the ability of the SU(3) symmetry to describe deformation in nuclei. The multi-shell generalization of this approach, the symplectic shell model [10, 11], uses the Sp(3, $\mathbb{R}$) symmetry (of which SU(3) is a subgroup) to study the one-particle-one-hole/ $2\hbar\Omega$ excitations of the underlying equilibrium deformation, thereby allowing us to study a variety of collective phenomena.

The *ab initio* symmetry-adapted no-core shell model (SA-NCSM) builds on the advantages of the NCSM and these symmetry-informed shell models to study this underlying collectivity (as well as clustering) starting from first principles. It generally employs a Hamiltonian of the form

$$H = T_{\text{rel}} + V_{\text{NN}} + V_{\text{Coul}}, \quad (1)$$

where T_{rel} is the relative kinetic energy of the nucleons, V_{NN} is the nucleon-nucleon interaction, and V_{Coul} is the Coulomb interaction between the protons. This V_{NN} includes the use of realistic nuclear interactions which start from the underlying quark-gluon dynamics. To control the growth of the model space for heavier systems, e.g. intermediate and medium mass nuclei, the SA-NCSM selects only the most physically-relevant basis states and thus can construct a model space whose dimension is significantly smaller than the complete NCSM model space for the same number of total HO excitations ($N_{\max}$). The ability to naturally truncate the model space to its most physically-relevant components arises from the emergent fact that realistic nuclear interactions have a preference for a smaller subset of all possible SA-NCSM basis states available. Previous *ab initio* studies of light nuclei have illustrated this fact, regardless of the specific nucleus chosen

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(e.g. ${}^6\text{Li}$, ${}^6\text{He}$, ${}^8\text{Be}$, ${}^{12}\text{C}$) and the choice of realistic interaction, including interactions based on chiral effective field theory. This emergent feature again points to the importance of these symmetries to describing nuclear structure.

3 Exemplary Results

We have performed *ab initio* SA-NCSM calculations for intermediate and medium mass nuclei. Further details on the structure results discussed here can be found in Refs. [12, 13, 15]. For the intermediate mass region, we present results for odd- A nuclei with negative parity states (e.g. Fig. 1a) ${}^{19}\text{Ne}$ in 12 HO major shells [12]) and nuclei near the dripline (e.g. Fig. 1b) ${}^{32}\text{Ne}$ in 7 HO major shells [13]). Medium mass nuclei (e.g. ${}^{48}\text{Ti}$ in 8 HO major shells [13]) are also within the reach of the SA-NCSM. These results use realistic chiral interactions and can include contributions from higher HO major shells than previously achievable, thus allowing for the development of the most important configurations in each nucleus. They show good agreement with experiment, particularly with regards to collectivity, which is a traditionally challenging feature for *ab initio* models to reproduce. For example, the quadrupole moment for the first 2^+ state in ${}^{48}\text{Ti}$ from experiment is known to be -17.7 e fm^2 [14] and SA-NCSM calculations, without the use of effective charges, show a value of -19.3 e fm^2 [15] based on the chiral NNLO_{opt} NN interaction [16] in 8 HO major shells. This indicates that the symmetry-adapted basis is capable of allowing the necessary collectivity to develop while also controlling the combinatorial growth associated with standard NCSM model spaces.

To further study collectivity, especially with respect to the isospin symmetry breaking effects in mirror nuclei, we also present results for $B(E2)$ values in mirror nuclei. Isospin symmetry breaking has traditionally been studied by comparing the energy levels in mirror nuclei or their masses, but we can also use a variety of spectroscopic data, including $B(E2)$ values. In Fig. 2, we present *ab initio* SA-NCSM calculation results for the mirror nuclei ${}^{21}\text{Mg}$ and ${}^{21}\text{F}$. The $B(E2)$ strengths were calculated using various symmetry-based selections of the SA-NCSM model space and various $\hbar\Omega$ values, and only the results with the most optimal parameters that show the fastest convergence trend are depicted in Fig. 2. Variations in the size of the model space and the HO parameter $\hbar\Omega$ are accounted for the extrapolated values and their uncertainties. These results compare to the recent experimental values [17] reasonably well, demonstrating the SA-NCSM capability to describe collectivity in these challenging mirror nuclei. See Refs. [15, 17] for further discussions.

In addition to being able to describe the structure of intermediate and medium mass nuclei, recent work with the SA-NCSM has illustrated its ability to capture other important characteristics of nuclei, including dynamic properties. For example, starting from the symmetry-adapted wave functions, we can calculate response functions via the Lanczos response function method [18, 19], which tell us about how a nucleus responds to an external probe. If a probe is able to excite the ground state, the final states it

Figure 1. *Ab initio* SA-NCSM calculations using the chiral NNLO_{opt} NN interaction [16] for excitation spectra in (a) ${}^{19}\text{Ne}$ with 12 HO major shells and (b) ${}^{32}\text{Ne}$ with 7 HO major shells. Simulations were performed on the Blue Waters system.

then connects to and the strength of those transitions can also tell us something about the similarity of those two states.

More specifically, a typical response function can be expressed as

$$R(\omega) = \sum_f \left| \langle \psi_f | \hat{O} | \psi_0 \rangle \right|^2 \delta(E_f - E_0 - E_x), \quad (2)$$

where E_0 (E_f) and $|\psi_0\rangle$ ($|\psi_f\rangle$) are the energy and wave function for the ground (final) state, E_x is the energy transferred between the nucleus and the external probe, and $\sum_f$ indicates a sum over all possible discrete and continuum final states. The operator $\hat{O}$ describes the external probe – here, we will use the monopole operator, though any operator could be employed. In the Lanczos response function method, this response function $R(\omega)$ is folded with a Lorentzian of width Γ and the wave function information

Figure 2. *Ab initio* SA-NCSM calculations using the chiral NNLO_{opt} NN interaction in ultra-large model spaces ($\hbar\Omega = 15$ MeV). (a) Energy spectrum of ^{21}Mg and ^{21}F in 11 HO major shells, and (b) convergence of the $B(E2: \frac{1}{2}^+ \rightarrow \frac{5}{2}^+)$ (top) and $B(E2: \frac{5}{2}^+ \rightarrow \frac{9}{2}^+)$ (bottom) strengths with increasing model space, and the extrapolated values with uncertainties from model space and $\hbar\Omega$ variance. Simulations were performed on the Blue Waters system. Experimental values for the $B(E2)$ are from Ref. [17].

Figure 3. *Ab initio* SA-NCSM calculations using the chiral NNLO_{opt} NN interaction for monopole response functions in (a) ^{16}O at $\hbar\Omega = 16$ MeV in 12 HO shells and (b) ^{20}Ne at $\hbar\Omega = 15$ MeV in 11 HO major shells. The response are folded with a Lorentzian of width $\Gamma = 2$ MeV. Simulations were performed on NERSC systems.

is included from solving the many-body Hamiltonian via the Lanczos algorithm.

Given the SA-NCSM's connection to the symplectic symmetry (and subsequently giant resonances [11]), we can use this approach to study the structure of giant resonances from first principles. For example, in Fig. 3a), we can see a single, strong peak in the monopole response function of ^{16}O , as calculated with the NNLO_{opt} chiral interaction. This peak is dominated ($> 60\%$) by a $(2\ 0)$ state of correlated $2\hbar\Omega$ one-particle excitations, which is inline with expectations we would have for a giant monopole resonance based on previous work with the symplectic shell model [20]. Similarly, in Fig. 3b), we can see the monopole response function for ^{20}Ne , as calculated with NNLO_{opt} . Unlike the ^{16}O case, here the giant resonance peak is fragmented and signatures of it are found in various amounts in a few different peaks in this response function. See Ref. [21] for further analysis of these results.

4 Conclusions

We presented a short historical overview of the development of (no-core) shell model techniques capable of properly describing the observed collectivity in nuclei in Sec. 2. We focused on the development of the *ab initio* SA-NCSM, which can use realistic nuclear interactions and study nuclei from a first principles perspective. Through the use of emergent symmetries and high performance computing, the SA-NCSM has been able to control the growth of the model space and study up to, and including, intermediate and medium mass nuclei. In Sec. 3, we discussed results for the structure of neon isotopes, including the odd-*A* nucleus ^{19}Ne and a nucleus near the dripline, ^{32}Ne . We also examined collectivity in ^{21}F and ^{21}Mg through their associated $B(E2)$ values. Lastly, we also discussed recent work with the SA-NCSM to examine giant monopole resonances in ^{16}O and ^{20}Ne . These results, through calculations of the response function, point to the SA-NCSM's unique applicability to study giant resonances (and their fragmentation) from first principles.

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