NUCLEAR THEORY, Vol. 38 (2019)
eds. M. Gaidarov, N. Minkov, Heron Press, Sofia

Current and Next-Generation Features of the Symmetry-Adapted No-Core Shell Model

G.H. Sargsyan[1], **J.P. Draayer**[1], **K.D. Launey**[1], **T. Dytrych**[1,2], **O. Molchanov**[1], **D. Kekejian**[1], **R.B. Baker**[1], **A. Mercenne**[1], **A.C. Dreyfuss**[1]

[1]Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803-4001, USA

[2]Nuclear Physics Institute, 250 68 Řež, Czech Republic

Abstract. Exploiting exact and partial symmetries to unmask simplicity within complexity, which remains the 'holy grail' of nuclear structure physics, is considered within its historical context and as now being advanced through modern *ab initio* methods. Some results for light to medium mass nuclei are shown, as well as a possible path forward for consideration of even heavier nuclei is proffered.

1 Introduction

A central challenge of nuclear physics is to describe nuclei in terms of the fundamental strong force, and especially by gaining a deeper understanding of emergent patterns found within many-nucleon systems. To this end, we employ the *ab initio* (from 'first principles') symmetry-adapted no-core shell model (SA-NCSM) [1, 2] that links the structure of a nucleus to its fundamental building blocks; namely, the properties of two or three nucleons that are consistent with the underlying symmetries and symmetry-breaking patterns of quantum chromodynamics (QCD) of quarks and gluons.

Within the NCSM framework, a complete model space is organized into levels of the harmonic oscillator (HO), each of which is separated in energy from its neighbors by $\hbar\Omega$. Interactions among particles within a level, as well as between particles in neighboring levels, is accounted for up to some $N_{\max}$ cutoff which is the maximum total number of oscillator quanta above the lowest HO configuration for a nucleus. This cutoff is used to throttle the infinite model space down to a finite size, for which convergence of results needs to be ensured within the memory constraints of a computer on which the calculations are being performed. In the $N_{\max}\rightarrow$ infinity limit, the theory encompasses the entire shell-model space.

Here, we present a symmetry-guided strategy that utilizes exact as well as partial symmetries to move beyond the $N_{\max}$ truncation concept; thereby, enabling an exploitation of *ab initio* concepts through a deeper appreciation for

the role emergent symmetries play in determining microscopic structures over a broad range atomic nuclei. Specifically, our symmetry-adapted no-core shell-model is a novel framework that capitalizes on symmetries - exact and partial - that when fully appreciated and applied can be used to extend the reach of the NSCM to heavier nuclei. The SA-NCSM is governed by two special symmetries that are key to understanding the structure and dynamics of atomic nuclei; namely, the symplectic $\mathrm{Sp}(3,\mathbb{R})$ group and its deformation-related $\mathrm{SU}(3)$ subgroup. Further, as also illustrated below, these symmetries can be used to identify dominant features of QCD-inspired interactions.

2 Dominant Features of Realistic Interactions

Basic building blocks of *ab initio* models are QCD-inspired realistic interactions. A nuclear interaction is considered realistic if it reproduces low-energy nucleon-nucleon scattering data to high precision, and precisely describes the properties of the two-nucleon deuteron system. Additionally, the theory shows that weaker three-nucleon (*3N*) interactions become necessary for a description of $A > 2$ systems; however, their inclusion results in an explosive growth of computational resources necessary for many-body calculations. To address this difficulty, various two-nucleon interactions have been designed, which partially account for *3N* effects. Examples of such interactions include JISP16 [5], INOY [6] and $\mathrm{NNLO}_{\mathrm{opt}}$ [7].

Two-body interactions that are used in various shell models (*e.g.*, NCSM [11,12]) are typically represented in a JT-coupled HO basis $|rsJMTT_Z\rangle$ where r and s label two interacting nucleons and represent the set of single-particle quantum numbers $\{\eta(l\frac{1}{2})jt = \frac{1}{2}\}$ with $\eta = 0,1,2,...$ being the oscillator shell number. Any interaction can be transformed from the JT-coupled basis representation into a basis for the SA-NCSM, the $\mathrm{SU}(3)$-coupled HO basis, $|\eta_r\eta_s(\lambda\mu)(LS)JMTT_Z\rangle$, via a unitary transformation [8]. When using the $\mathrm{SU}(3)$-basis, the significance of various interaction terms can be estimated by the norm of the corresponding interaction $\mathrm{SU}(3)$ tensor (analogous to the norm of a matrix A defined as $||A|| = \sqrt{\sum_{ij} A_{ij}A_{ji}}$). This transformation allows one to decompose the interaction into its $\mathrm{SU}(3)$ components, each possessing a certain strength. Figure 1 shows the decomposition of the realistic JISP16 interaction. As can be seen from these results, only a small number of $\mathrm{SU}(3)$ tensors dominate the interaction, with the vast majority of the components having less than 1% of the total strength. Similar pictures can be seen for other interactions. It should be noted that in the JT-coupled basis, no such dominance of interaction matrix elements is apparent. This exercise demonstrates a long-standing principle that holds across all of physics; namely, one should work within a framework that is as closely aligned with the dynamics as possible.

Using the decomposition of the interaction in the $\mathrm{SU}(3)$ basis we can choose sets of major components to construct new 'selected' interactions. These interactions can be used for calculations of various nuclear properties that can be

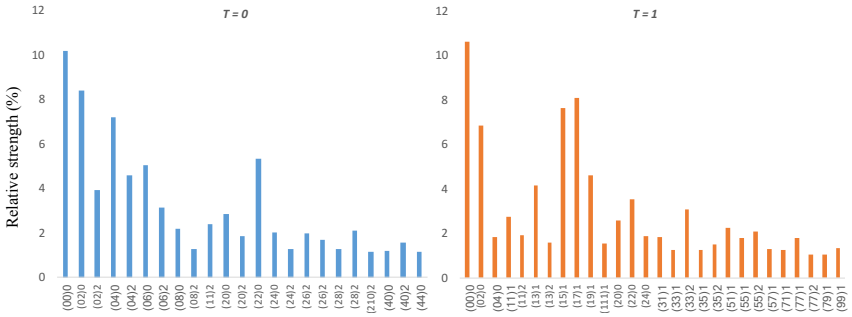

Figure 1. Relative strengths for the SU(3)-coupled JISP16 *NN* interaction with $\hbar\Omega = 15$ MeV in the $N_{\max}$= 12 model space. T is the isospin of the two nucleon system. Each component is specified along the abscissa by a set of $(\lambda\mu)S$ quantum numbers. Only components that have more than 1% of the relative strength of the interaction are shown in the plots; there are 242 more components with less than 1% for T=0 and 212 more for $T = 1$.

compared to the results from the initial interaction. In this way, we can examine how sensitive specific nuclear properties are to the interaction components.

Figure 2 shows excitation energies of ^{12}C calculated with the JISP16 $\hbar\Omega = 15$ MeV interaction (corresponding to the ratio of interaction components being

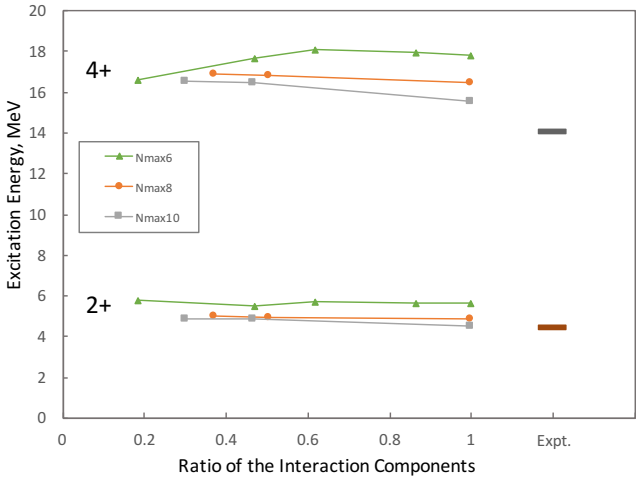

Figure 2. First 2^+ and 4^+ excitation energies for ^{12}C from SA-NCSM calculations (connected lines) compared with experiment [9] (horizontal bars on the far right). Results for $N_{\max}$= 6, 8 and 10 are shown for various truncations of the JISP16 interaction with $\hbar\Omega = 15$ MeV. Specifically, the value 1 on the abscissa indicates the full interaction (100%) was used, while an abscissa value of 0.4 implies that only the most significant (and structurally the simplest) 40% of the tensors were retained, etc.

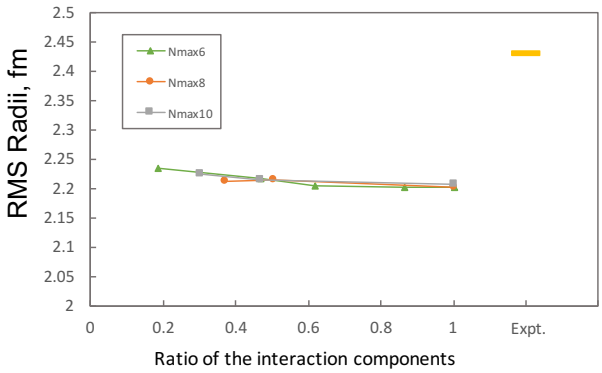

Figure 3. RMS radius (fm) of the ^{12}C ground state (experimental value from Ref. [10]) calculated using JISP16 interaction with $\hbar\Omega = 15$MeV and the corresponding selected interactions.

unity) and several selected truncations of the interaction. As the plot shows, with only half of the interaction terms the excitation energies essentially do not differ from the corresponding full interaction results, and even with less than 30% of the interaction components the deviation for most of the values is insignificant. The comparatively large deviation in 4^+ energy for $N_{\max}$= 6 that happens when about 20% of the $\mathrm{SU}(3)$ components are used is likely due to the small model space. This issue disappears in higher $N_{\max}$ values, and even $N_{\max}$= 6 results for the 2^+ state compare remarkably well to the initial interaction for all selections.

The selected interactions yield very close results to the initial one for other observables as well. Figure 3 shows the results for ^{12}C rms radius of the ground state using the same interactions as for the excitation energies. Specifically, the values are essentially the same when half of the interaction components are used. With less than 30% of interaction components, the difference from the initial interaction results is less than 2%.

In summary, the $\mathrm{SU}(3)$ coupling scheme can be used to pare down an interaction to a relatively small subset of terms that are responsible for the bulk of the underlying low-energy physics. And this, in turn, suggests a potentially powerful tool for constructing new realistic interactions.

3 Exploiting New Patterns in the SA-NCSM

The SA-NCSM framework has enabled a major breakthrough; namely, discovering highly organized patterns in the nuclear wavefunctions that emerge from first principles [1]. To take a full advantage of these ordered substructures, one can utilize neural networks and their ability to detect patterns. The SA-NCSM wavefunctions can be decomposed in terms of $\mathrm{SU}(3)$ basis states each possessing a certain probability. The neural network can be trained on these wavefunctions and then be applied to predict probabilities of basis states for another nucleus.

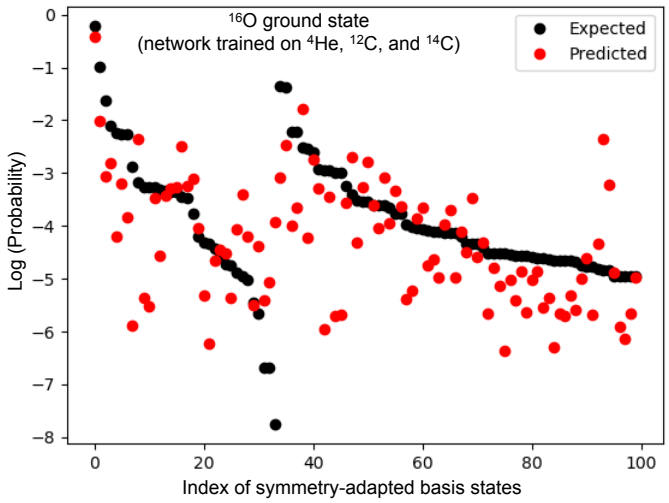

Figure 4. Neural network predictions for the structure of ^{16}O ("predicted"), as compared to complete SA-NCSM nuclear simulations ("expected"), with the aim to predict heavier nuclei inaccessible to SA-NCSM calculations.

Figure 4 shows preliminary predictions for the important basis states needed for SA-NCSM calculations of ^{16}O ground state, with a neural network trained on ^{4}He, ^{12}C and ^{14}C wavefunctions. This method intends to additionally broaden the reach of SA-NCSM to larger model spaces and heavier nuclei.

Complementary to this, it is also possible to extend the computational capabilities of SA-NCSM to heavier nuclei by incorporating deformation into the construction of the basis states. This is carried out by canonical transformations that preserve the commutation relations between coordinates and momenta [13]. This, in turn, allows us to use the full capabilities of algebraic methods and group symmetries when utilizing deformed basis, since the canonical transformations preserve not only the Heisenberg algebra but also the $\mathrm{Sp}(3,\mathbb{R})$ algebra. Since nuclei have intrinsic deformation, a basis tailored to capture deformation would allow us to treat calculations conducted in smaller model spaces equivalently to those done in large model spaces with non deformed basis.

4 Reactions with Symmetry-Adapted Basis

Ab initio SA-NCSM calculations have now been extended into and even beyond the intermediate mass region, including odd-A nuclei and negative parity states. In addition to being able to describe the structure of intermediate and medium mass nuclei, recent work with the SA-NCSM has also illustrated an ability to capture other important features of nuclei, including dynamic properties. For example, starting from the symmetry-adapted wave functions, we can calculate

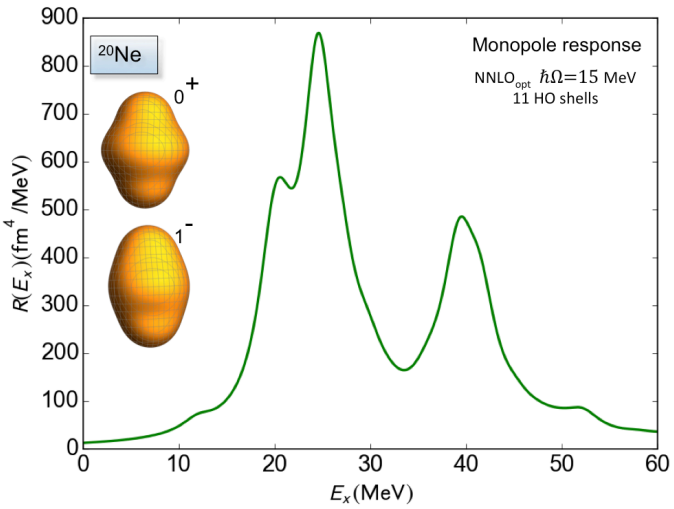

Figure 5. *Ab initio* SA-NCSM calculations with the chiral NNLOopt NN interaction for the monopole response functions in ^{20}Ne at $\hbar\Omega$ = 15 MeV in 11 HO major shells. The responses are folded with a Lorentzian of 2 MeV width. The insets show one-body density (in the intrinsic frame) for the ground state (0^+) and the lowest 1^- excited state.

response functions via the Lanczos response function method [14, 15], which describes the nuclear response to an external probe. If a probe is able to excite the ground state, the final states to which it connects and the strength of those transitions can provide information about how those states are related to one another. We can use this approach to study, for example, the structure of giant resonances from first principles. In Figure 5 we show the monopole response function for ^{20}Ne, as calculated with NNLO$_{\rm opt}$. In this case the peak in the giant resonance peak is fragmented in a few different peaks. Moreover, in some cases it is beneficial to calculate the energy moments of the response functions also known as electromagetic sum rules. Various electromagnetic sum rules have been calculated for ^{4}He in the SA-NCSM using the JISP16 interaction as well as some others and successfully benchmarked against the Hyperspherical Harmonics method [16], which provides exact solutions for this nucleus [17].

Additionally, the symmetry-adapted framework combined with the resonating group method (RGM) is also being employed for developing a new *ab initio* approach for nuclear reactions involving nuclei up to the medium-mass region [19, 20]. The use of the SU(3) symmetry in this model enables a reorganization of the large-scale model space into physically relevant basis states and allows us to study *ab initio* reactions involving heavier and more exotic nuclei of astrophysical interest than heretofore. The formalism describes the target-projectile composite system within an SU(3) RGM framework by using an SA-NCSM target wave function with SU(3) basis states coupled with the pro-

jectile states. The model has been applied to phase shifts for proton scattering off ^{4}He and ^{20}Ne, with the view toward calculating proton-capture reaction rates of intermediate-mass nuclei of importance to x-ray burst nucleosynthesis [20].

For microscopic calculations of alpha widths and alpha capture reaction rates, a new formalism has been developed that begins with first-principles structure calculations to describe alpha-clustering. It can be used to provide a description of alpha-capture reaction rates with impacts on abundance patterns from x-ray burst (XRB) nucleosynthesis. For narrow resonances, coupling to the continuum is weak and the number of competing channels is greatly reduced, so most of the physics of the system is described through the overlap of a wave function for the composite many-particle system, computed with a single symplectic configuration (consisting of several hundreds of basis states), and a cluster (few-body) basis for a single cluster partitioning. This proves to be a very powerful tool for estimating spectroscopic amplitudes, decay widths, and nuclear reaction rates, with the ability to push toward nuclear reactions involving exotic nuclei that cannot currently be measured.

5 Conclusion

We discussed applications of the symmetry-adapted basis within an *ab initio* framework. Decomposing nuclear realistic interactions in terms of $\mathrm{SU}(3)$ components allowed us to determine that only a fraction of those components is sufficient to describe most nuclear properties. Additionally, we presented some of the recent advances of the SA-NCSM that include calculations of electromagnetic response functions and sum rules, development of a new *ab initio* reaction theory along with the implementation of neural networks for predictions of nuclear wave functions and deformed symmetry-adapted basis for reaching heavier nuclear species. These results point to the ability of a symmetry-adapted basis to proffer a simpler view of nuclear structure.

Acknowledgements

Support from the U.S. National Science Foundation (ACI -1713690, OIA-1738287, PHY-1913728), the Czech Science Foundation (16-16772S) and the Southeastern Universities Research Association are all gratefully acknowledged. This work benefitted from computing resources provided by NSF's Blue Waters computing system (NCSA), LSU (www.hpc.lsu.edu), and the National Energy Research Scientific Computing Center (NERSC). This work was also supported in part by an undergraduate LSU Discover Grant award.

References

[1] T. Dytrych, K.D. Launey, J.P. Draayer, P. Maris, J.P. Vary, E. Saule, U. Catalyurek, M. Sosonkina, D. Langr, and M.A. Caprio, *Phys. Rev. Lett.* **111** (2013) 252501.

[2] K.D. Launey, T. Dytrych, and J.P. Draayer, *Prog. Part. Nucl. Phys.* **89** (2016) 101 (review).

[3] A.C. Dreyfuss, K.D. Launey, T. Dytrych, J.P. Draayer, and C. Bahri, *Phys. Lett. B* **727** (2013) 511.

[4] A.C. Dreyfuss, K.D. Launey, T. Dytrych, J.P. Draayer, R.B. Baker, C. Deibel, and C. Bahri, *Phys. Rev. C* **95** (2017) 044312.

[5] A.M. Shirokov, V.A. Kulikov, P. Maris, A.I. Mazur, E.A. Mazur, and J.P. Vary. NN interaction JISP16: Current status and prospect. In *EPJ Web of Conferences*, volume 3, pp. 515 (EDP Sciences, 2010).

[6] P. Doleschall, *Phys. Rev. C* **69** (2004) 054001.

[7] A. Ekström, G. Baardsen, C. Forssén, G. Hagen, M. Hjorth-Jensen, G.R. Jansen, R. Machleidt, W. Nazarewicz, T. Papenbrock, J. Sarich, and S. M. Wild, *Phys. Rev. Lett.* **110** (2013) 192502.

[8] G.H. Sargsyan, *et al.* "SU(3)-guided Realistic Nucleon-nucleon Interactions for Large-scale Calculations", *Phys. Rev. C*. (to be submitted).

[9] F. Ajzenberg-Selove and J.H. Kelley, *Nucl. Phys. A* **506** (1990) 1.

[10] I. Tanihata, *et al.*, *Phys. Rev. Lett.* **55** (1985) 2676.

[11] P. Navrátil, J.P. Vary, and B.R. Barrett, *Phys. Rev. Lett.* **84** (2000) 5728.

[12] B. Barrett, P. Navrátil and J. Vary, *Prog. Part. Nucl. Phys.* **69** (2013) 131.

[13] D. Kekejian, J.P. Draayer, K.D. Launey, *Proceedings of the Symmetries and Order: Algebraic Methods in Many Body Systems: A symposium in celebration of the career of Professor Francesco Iachello*, 56 October, 2018, Connecticut, USA, ed. Reina Maruyama (AIP Conference Proceedings 2150, 040002, 2019)

[14] V.D. Efros, W. Leidemann, G. Orlandini, N. Barnea, *J. Phys. G: Nucl. Part. Phys.* **34** (2007) R459.

[15] R.B. Baker, K.D. Launey, N. Nevo Dinur, S. Bacca, J.P. Draayer, and T. Dytrych, *Proceedings of the 4th International Workshop on "State of the Art in Nuclear Cluster Physics" (SOTANCP4)*, May 2018, Galveston, Texas, Volume 2038 (AIP Conf. Proc., 2018).

[16] N. Barnea, W. Leidemann, and G. Orlandini, *Phys. Rev. C* **61** (2000) 054001.

[17] R.B. Baker, "Electromagnetic Sum Rules and Response Functions from the Symmetry-Adapted No-Core Shell Model," Ph.D. Dissertation, Physics and Astronomy Dept., Louisiana State University, Baton Rouge, LA (2019).

[18] K.D. Launey, A. Mercenne, G.H. Sargsyan, H. Shows, R.B. Baker, M.E. Miora, T. Dytrych, and J.P. Draayer, *Proceedings of the 4th International Workshop on "State of the Art in Nuclear Cluster Physics" (SOTANCP4)*, May 2018, Galveston, Texas, Volume 2038 (AIP Conf. Proc., 2018).

[19] A. Mercenne, K.D. Launey, J.E. Escher, T.Dytrych and J.P. Draayer, *Proceedings of the XXII International Conference on Few-Body Problems in Physics*, July 2018, Caen, France (Springer Proceedings in Physics) (to be published).

[20] A. Mercenne, K.D. Launey, J.E. Escher, T. Dytrych and J.P. Draayer, *Proceedings of the 6th International Workshop on Compound-Nuclear Reactions and Related Topics*, September 2018, Berkley, California (Springer Proceedings in Physics) (to be published).