Light Nuclei in the Framework of the Symplectic No-Core Shell Model

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Abstract. A symplectic no-core shell model (Sp-NCSM) is constructed with the goal of extending the *ab-initio* NCSM to include strongly deformed higher-oscillator-shell configurations and to reach heavier nuclei that cannot be studied currently because the spaces encountered are too large to handle, even with the best of modern-day computers. This goal is achieved by integrating two powerful concepts: the *ab-initio* NCSM with that of the $\mathrm{Sp}(3,\mathbb{R}) \supset \mathrm{SU}(3)$ group-theoretical approach. The NCSM uses modern realistic nuclear interactions in model spaces that consists of many-body configurations up to a given number of $\hbar\Omega$ excitations together with modern high-performance parallel computing techniques. The symplectic theory extends this picture by recognizing that when deformed configurations dominate, which they often do, the model space can be better selected so less relevant low-lying $\hbar\Omega$ configurations yield to more relevant high-lying $\hbar\Omega$ configurations, ones that respect a near symplectic symmetry found in the Hamiltonian. Results from an application of the Sp-NCSM to light nuclei are compared with those for the NCSM and with experiment.

1 Introduction

The concept of an *ab initio* no-core shell-model (NCSM) [1], which yields a good description of the low-lying states in few-nucleon systems as well as in more complex nuclei [1,2], has taken center stage in the development of microscopic tools for studying the structure of atomic nuclei. The architecture for the NCSM capitalizes on computational efficiencies that can be realized when many-particle Slater determinant basis states are mapped onto an integer bit string representation of that state on a computer. In addition, in the framework of the NCSM one can employ modern realistic interactions that reflect on the essence of the strong interaction. Recently developed realistic NN potentials include J-matrix inverse scattering potentials [3], high-precision NN potentials derived from meson exchange theory [4] and nuclear two- and many-body forces based on chiral effective field theory [5].

The symplectic no-core shell-model (Sp-NCSM) [6] amplifies on this concept by recognizing that deformed configurations often dominate and these, while typically described by only few collective $\mathrm{Sp}(3,\mathbb{R})$ basis states, correspond to a special linear combination of a large number of NCSM basis states. Hence, the effective size of the model space can be significantly reduced and constrained to respect a near symplectic symmetry, that within a $0\hbar\Omega$ space reduces to SU(3), of the model Hamiltonian. In this way, the Sp-NCSM will allow one to account for even higher $\hbar\Omega$ configurations required to realize experimentally measured B(E2) values without an effective charge, and especially highly deformed spatial configurations required to reproduce α-cluster modes in heavier nuclei.

As a 'proof-of-principle' study, results for no-core and symplectic no-core calculations up to $6\hbar\Omega$ are compared for two nuclei, namely, the deformed ^{12}C and the closed-shell ^{16}O. The analysis of the results shows that the 0^+_{gs} and the lowest 2^+ and 4^+ states in ^{12}C as well as the 0^+_{gs} in ^{16}O, which are derived in the framework of the NCSM with the JISP16 realistic interaction [3] and are well converged, reflect the presence of an underlying symplectic $\mathfrak{sp}(3,\mathbb{R})$ algebraic structure [1]. This is achieved through the projection of realistic NCSM eigenstates onto $\mathrm{Sp}(3,\mathbb{R})$-symmetric basis states of the symplectic shell model.

The symplectic shell model [7, 8] is a multiple oscillator shell generalization of Elliott's $\mathrm{SU}(3)$ model and as well, a microscopic realization of the successful Bohr-Mottelson collective model. Symplectic algebraic approaches have achieved a very good reproduction of low-lying energies in ^{12}C using phenomenological interactions [9] or truncated symplectic basis with simplistic (semi-) microscopic interactions [10, 11]. Here, we establish, for the first time, the dominance of the symplectic $\mathrm{Sp}(3,\mathbb{R})$ symmetry in nuclei as unveiled through *ab initio* calculations of the NCSM type with realistic interactions. This in turn opens up a new and exciting possibility for representing significant high-$\hbar\Omega$ collective modes by extending the NCSM basis space beyond its current limits through $\mathrm{Sp}(3,\mathbb{R})$ basis states, which yields a dramatically smaller basis space to achieve convergence of higher-lying collective modes. In this regard, it may be interesting to understand the importance of a larger model space beyond the $6\hbar\Omega$ limit and its role in shaping other low-lying states in ^{12}C and ^{16}O such as the second 0^+, which is likely to reflect a cluster-like behavior (e.g., see [12]). This task, albeit challenging, is feasible for the no-core shell model with the symplectic $\mathrm{Sp}(3,\mathbb{R})$ extension.

2 Symplectic Shell Model

The symplectic shell model is based on the noncompact symplectic $\mathfrak{sp}(3,\mathbb{R})$ algebra that with its subalgebraic structure unveils the underlying physics of a microscopic description of collective modes in nuclei [7, 8]. The latter follows from the fact that the mass quadrupole and monopole moment operators, the many-particle kinetic energy, the angular and vibrational momenta are all elements of the $\mathfrak{sp}(3,\mathbb{R}) \supset \mathfrak{su}(3) \supset \mathfrak{so}(3)$ algebraic structure. Hence, collective states of a nucleus with well-developed quadrupole and monopole vibrations as well as collective

[1] We use lowercase (capital) letters for algebras (groups).

rotations are described naturally in terms of irreducible representations (irreps) of $\mathrm{Sp}(3,\mathbb{R})$. Furthermore, the elements of the $\mathfrak{sp}(3,\mathbb{R})$ algebra are constructed as bilinear products in the harmonic oscillator (HO) raising and lowering operators that in turn are expressed through particle coordinates and linear momenta. This means the basis states of a $\mathrm{Sp}(3,\mathbb{R})$ irrep can be expanded in a HO (m-scheme) basis, the same basis used in the NCSM, thereby facilitating symmetry identification.

The symplectic basis states are labeled (in standard notation [7,8]) according to the reduction chain

$$\begin{array}{ccccc} \mathrm{Sp}(3,\mathbb{R}) & \supset & \mathrm{U}(3) & \supset & \mathrm{SO}(3) \\ \Gamma_\sigma & \Gamma_n\rho & \Gamma_\omega & \kappa & L \end{array} \tag{1}$$

and are constructed by acting with polynomials $\mathcal{P}$ in the symplectic raising operator, $A^{(2\,0)}$, on a set of basis states of the symplectic bandhead, $|\Gamma_\sigma\rangle$, which is a $\mathrm{Sp}(3,\mathbb{R})$ lowest-weight state[2],

$$|\Gamma_\sigma\Gamma_n\rho\Gamma_\omega\kappa(LS)JM_J\rangle = \left[\mathcal{P}^{\Gamma_n}(A^{(2\,0)}) \times |\Gamma_\sigma\rangle\right]^{\rho\Gamma_\omega}_{\kappa(LS)JM_J}, \tag{2}$$

where $\Gamma_\sigma \equiv N_\sigma\,(\lambda_\sigma\,\mu_\sigma)$ labels $\mathrm{Sp}(3,\mathbb{R})$ irreps with $(\lambda_\sigma\,\mu_\sigma)$ denoting a $\mathrm{SU}(3)$ lowest-weight state, $\Gamma_n \equiv n\,(\lambda_n\,\mu_n)$, and $\Gamma_\omega \equiv N_\omega\,(\lambda_\omega\,\mu_\omega)$. The $(\lambda_n\,\mu_n)$ set gives the overall $\mathrm{SU}(3)$ symmetry of $\frac{n}{2}$ coupled raising operators in $\mathcal{P}$, $(\lambda_\omega\,\mu_\omega)$ specifies the $\mathrm{SU}(3)$ symmetry of the symplectic state, and $N_\omega = N_\sigma + n$ is the total number of oscillator quanta related to the eigenvalue, $N_\omega\hbar\Omega$, of a HO Hamiltonian that is free of spurious modes.

The symplectic raising operator $A^{(2\,0)}_{lm}$, which is a $\mathrm{SU}(3)$ tensor with $(\lambda\,\mu) = (2\,0)$ character, can be expressed as a bilinear product of the HO raising operators,

$$A^{(20)}_{lm} = \frac{1}{\sqrt{2}}\sum_i \left[b^\dagger_i \times b^\dagger_i\right]^{(20)}_{lm} - \frac{1}{\sqrt{2}A}\sum_{s,t}\left[b^\dagger_s \times b^\dagger_t\right]^{(20)}_{lm}, \tag{3}$$

where the sums are over all A particles of the system. The first term in (3) describes $2\hbar\Omega$ one-particle-one-hole (1p-1h) excitations (one particle raised by two shells) and the second term eliminates the spurious center-of-mass excitations in the construction (2). For the purpose of comparison to NCSM results, the basis states of the $|\Gamma_\sigma\rangle$ bandhead in (2) are constructed in a m-scheme basis,

$$\begin{aligned} &|\Gamma_\sigma\kappa(L_0S_0)J_0M_0\rangle = \\ &\left[\mathcal{P}^{(\lambda_\pi\,\mu_\pi)}_{S_\pi}(a^\dagger_\pi)\times\mathcal{P}^{(\lambda_\nu\,\mu_\nu)}_{S_\nu}(a^\dagger_\nu)\right]^{(\lambda_\sigma\,\mu_\sigma)}_{\kappa(L_0S_0)J_0M_0}|0\rangle, \end{aligned} \tag{4}$$

where $|0\rangle$ is a vacuum state, $\mathcal{P}^{(\lambda_\pi\,\mu_\pi)}_{S_\pi}$ and $\mathcal{P}^{(\lambda_\nu\,\mu_\nu)}_{S_\nu}$ denote polynomials of proton ($a^\dagger_\pi$) and neutron ($a^\dagger_\nu$) creation operators coupled to good $\mathrm{SU}(3)\times\mathrm{SU}(2)$ symmetry.

[2] A $\mathrm{Sp}(3,\mathbb{R})$ lowest-weight state, $|\Gamma_\sigma\rangle$, is defined as $A^{(0\,2)}|\Gamma_\sigma\rangle = 0$, where the symplectic lowering operator $A^{(0\,2)}$ is the adjoint of $A^{(2\,0)}$.

3 Results and Discussions

The lowest-lying states of ^{12}C and ^{16}O were calculated using the NCSM as implemented through the Many Fermion Dynamics (MFD) code [13]. For ^{12}C we used an effective interaction derived from the realistic JISP16 *NN* potential [3] for different $\hbar\Omega$ oscillator strengths, while for ^{16}O the bare JISP16 interaction was employed. We are particularly interested in the $J = 0^+_{gs}$ and the lowest $J = 2^+(\equiv 2^+_1)$ and $J = 4^+(\equiv 4^+_1)$ states of the ground-state (gs) rotational band in ^{12}C and the $J = 0^+_{gs}$ state in ^{16}O that appear to be well converged in the $N_{max} = 6$ NCSM basis space.

Here we report on an analysis that is restricted to 0p-0h configurations. It is important to note that $2\hbar\Omega$ 2p-2h (2 particles raised by one shell each) and higher rank np-nh excitations and allowed multiples thereof can be included by building them into an expanded set of lowest-weight $\mathrm{Sp}(3,\mathbb{R})$ starting state configurations. The same "build-up" logic, (2), holds because by construction these additional starting state configurations are also required to be lowest-weight $\mathrm{Sp}(3,\mathbb{R})$ states. Note that if one were to include all possible lowest-weight np-nh starting state configurations ($n \leq N_{max}$), and allowed multiples thereof, one would span the entire NCSM space. The addition of $2\hbar\Omega$ 2p-2h, $4\hbar\Omega$ 4p-4h, and higher configurations, which build upon more complex starting states, will be the subject of a follow-on investigation.

3.1 Ground-State Rotational Band in the ^{12}C Nucleus

For ^{12}C there are 13 unique 0p-0h $\mathrm{Sp}(3,\mathbb{R})$ irreps which form the symplectic bandhead basis states, $|\Gamma_\sigma\rangle$ with $N_\sigma = 24.5$. For each 0p-0h $\mathrm{Sp}(3,\mathbb{R})$ irrep we generated basis states according to (2) up to $N_{max} = 6$ ($6\hbar\Omega$ model space). The typical dimension of a symplectic irrep basis in the $N_{max} = 6$ space is on the order of 10^2 as compared to 10^7 for the full NCSM m-scheme basis space.

As N_{max} is increased the dimension of the $J = 0, 2,$ and 4 symplectic space built on the 0p-0h $\mathrm{Sp}(3,\mathbb{R})$ irreps grows very slowly compared to the NCSM space dimension (Figure 1). This means that a space spanned by a set of symplectic basis states may be computationally manageable even when high-$\hbar\Omega$ configurations are included.

Analysis of overlaps of the symplectic states with the NCSM eigenstates for the 0^+_{gs} and the lowest 2^+ and 4^+ states reveals nonnegligible overlaps for only 3 of the 13 0p-0h $\mathrm{Sp}(3,\mathbb{R})$ ($N_\sigma = 24.5$) irreps, specifically, the leading (most deformed) representation $(\lambda_\sigma\, \mu_\sigma) = (0\ 4)$ carrying spin $S = 0$ together with two $S = 1$ representations with identical labels (1 2) but different bandhead constructions for protons and neutrons (4), namely, $\{(\lambda_\pi\, \mu_\pi)S_\pi,\ (\lambda_\nu\, \mu_\nu)S_\nu\}$ is $\{(0\ 2)0,\ (1\ 0)1\}$ and $\{(1\ 0)1,\ (0\ 2)0\}$. The dominance of only three irreps additionally reduces the dimensionality of the symplectic model space (Figure 1, red diamonds).

The overlaps of the most dominant symplectic states with the NCSM eigenstates for the 0^+_{gs}, 2^+_1 and 4^+_1 states in the 0, 2, 4 and $6\hbar\Omega$ subspaces are given in Table 1. The results show that approximately 80% of the NCSM eigenstates fall within a subspace spanned by the 3 leading 0p-0h $\mathrm{Sp}(3,\mathbb{R})$ irreps, with the most deformed

Table **1.** Probability distribution of NCSM eigenstates for ^{12}C across the leading 3 0p-0h $\mathrm{Sp}(3,\mathbb{R})$ irreps, $\hbar\Omega$=15 MeV.

		$0\hbar\Omega$	$2\hbar\Omega$	$4\hbar\Omega$	$6\hbar\Omega$	Total
			J=0			
	$(0\ 4)S=0$	46.26	12.58	4.76	1.24	64.84
$\mathrm{Sp}(3,\mathbb{R})$	$(1\ 2)S=1$	4.80	2.02	0.92	0.38	8.12
	$(1\ 2)S=1$	4.72	1.99	0.91	0.37	7.99
	Total	55.78	16.59	6.59	1.99	80.95
NCSM		56.18	22.40	12.81	7.00	98.38
			J=2			
	$(0\ 4)S=0$	46.80	12.41	4.55	1.19	64.95
$\mathrm{Sp}(3,\mathbb{R})$	$(1\ 2)S=1$	4.84	1.77	0.78	0.30	7.69
	$(1\ 2)S=1$	4.69	1.72	0.76	0.30	7.47
	Total	56.33	15.90	6.09	1.79	80.11
NCSM		56.63	21.79	12.73	7.28	98.43
			J=4			
	$(0\ 4)S=0$	51.45	12.11	4.18	1.04	68.78
$\mathrm{Sp}(3,\mathbb{R})$	$(1\ 2)S=1$	3.04	0.95	0.40	0.15	4.54
	$(1\ 2)S=1$	3.01	0.94	0.39	0.15	4.49
	Total	57.50	14.00	4.97	1.34	77.81
NCSM		57.64	20.34	12.59	7.66	98.23

irrep, $(0\,4)$, carrying about 65% of the 80%. In order to speed up the calculations, we retained only the largest amplitudes of the NCSM states, those sufficient to account for at least 98% of the norm which is quoted also in the table.

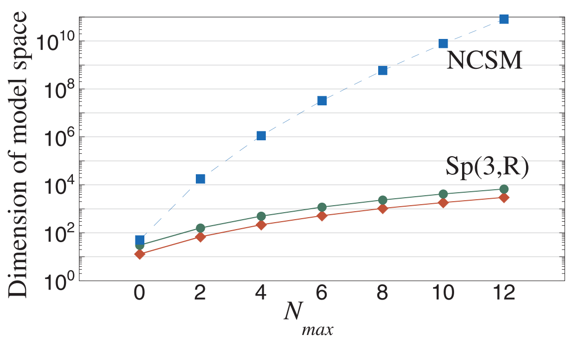

Figure **1.** Dimension of the NCSM (blue squares) and $J = 0, 2,$ and 4 $\mathrm{Sp}(3,\mathbb{R})$ (red diamonds for the 3 most significant 0p-0h irrep case and green circles for when all 13 0p-0h irreps are included) model spaces as a function of maximum allowed $\hbar\Omega$ excitations, N_{max}.

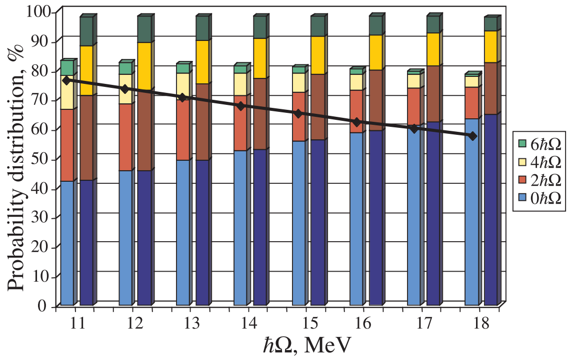

Figure **2.** ^{12}C ground 0^+ state probability distribution over $0\hbar\Omega$ (blue, lowest) to $6\hbar\Omega$ (green, highest) subspaces for the 3 0p-0h $\mathrm{Sp}(3,\mathbb{R})$ irrep case (left) and NCSM (right) together with the $(0\,4)$ irrep contribution (black diamonds) as a function of the $\hbar\Omega$ oscillator strength in MeV for $N_{max} = 6$.

In addition, the 0^+_{gs} analysis of the $S = 0$ ($S = 1$) part of the NCSM wavefunction reveals that within each $\hbar\Omega$ subspace only about $1 - 1.5\%$ of the NCSM 0^+_{gs} are not accounted for by the $S = 0$ ($S = 1$) $\mathrm{Sp}(3,\mathbb{R})$ irrep(s) under consideration. In the $N_{max} = 6$ model space the $S = 0$ symplectic irrep and the two $S = 1$ irreps account for 91% and 80%, respectively, of the corresponding $S = 0$ and $S = 1$ parts of the NCSM realistic eigenstate for the $J = 0^+_{gs}$ in ^{12}C. In summary, the $S = 0$ plus $S = 1$ part of the NCSM wavefunction is very well explained by only the three $\mathrm{Sp}(3,\mathbb{R})$ collective configurations.

How the results presented in Table 1 change as a function of the oscillator strength $\hbar\Omega$ is shown in Figure 2 for the case of the 0^+_{gs} state. Clearly, the projection of the NCSM wavefunctions onto the symplectic space slightly changes as one varies the oscillator strength $\hbar\Omega$. The 3 $\mathrm{Sp}(3,\mathbb{R})$ irreps, $(0\,4)S = 0$ and the two $(1\;2)S = 1$, remain dominant, only their contributions change. The overall overlaps increase towards smaller $\hbar\Omega$ HO frequencies and, for example, for 0^+_{gs} it is 85% in the $N_{max} = 6$ and $\hbar\Omega = 11$MeV case. Clearly, the largest contribution comes from the leading, most deformed, $(0\;4)S = 0$ $\mathrm{Sp}(3,\mathbb{R})$ irrep, growing to 91% of the total $\mathrm{Sp}(3,\mathbb{R})$-symmetric part for $\hbar\Omega$ =11 MeV. As expected, Figure 2 also confirms that with increasing $\hbar\Omega$ the higher $\hbar\Omega$ excitations contribute less while the lower $0\hbar\Omega$ configurations grow in importance.

In short, the low-lying states in ^{12}C are well described in terms of only three $\mathrm{Sp}(3,\mathbb{R})$ irreps with total dimensionality of 514, which is only 0.001% of the NCSM space, with a clear dominance of the most deformed $(0\,4)S = 0$ collective configuration. It is important to note that our results suggest that overlaps can be further improved by the inclusion of the most important $2\hbar\Omega$ 2p-2h $\mathrm{Sp}(3,\mathbb{R})$ irreps. In this way it may be possible to achieve overlaps of more then 90% while keeping the size of the basis space small, possibly much less than 1% of the NCSM result. This is the subject of ongoing investigations and will be addressed in a subsequent study.

The 0^+_{gs}, 2^+_1 and 4^+_1 states, constructed in terms of the three $\mathrm{Sp}(3,\mathbb{R})$ irreps with probability amplitudes defined by the overlaps with the NCSM wavefunctions, were also used to determine B(E2) transition rates. The $B(E2 : 2^+_1 \to 0^+_{gs})$ value, for example, turns out to be ≈110% of the corresponding NCSM number for the $\hbar\Omega = 15$MeV and $N_{max} = 4$ case. While this ratio decreases slightly for smaller $\hbar\Omega$ oscillator strengths, it is significant that this estimate for the dominant $\mathrm{Sp}(3,\mathbb{R})$ configurations exceeds the corresponding full NCSM results and therefore lies closer to the experimental $B(E2 : 2^+_1 \to 0^+_{gs})$ value.

3.2 Ground State in the ^{16}O Nucleus

The Sp-NCSM is also applied to the ground state of a closed-shell nucleus like ^{16}O. There is only one 0p-0h $\mathrm{Sp}(3,\mathbb{R})$ irrep with spin $S = 0$ and Γ_σ specified by $N_\sigma = 34.5$ and $(\lambda_\sigma\ \mu_\sigma) = (0\,0)$. As in the ^{12}C case, for the 0p-0h $\mathrm{Sp}(3,\mathbb{R})$ irrep we generated basis states according to (2) up to $N_{max} = 6$ ($6\hbar\Omega$ model space), which yields a symplectic model space that is only a fraction ($\approx 0.1\%$) of the size of the NCSM space. Consistent with the outcome for ^{12}C, the projection of the NCSM eigenstates onto the symplectic basis reveals a large $\mathrm{Sp}(3,\mathbb{R})$-symmetric content in the ground-state wavefunction (Figure 3). Furthermore, the overall overlap increases by $\approx 10\%$ when the most significant $2\hbar\Omega$ 2p-2h are included.

While the focus here has been on demonstrating the existence of $\mathrm{Sp}(3,\mathbb{R})$ symmetry in NCSM results for ^{12}C and ^{16}O, and therefore a possible path forward for extending the NCSM to a Sp-NCSM scheme, the results can also be interpreted as a further strong confirmation of Elliott's $\mathrm{SU}(3)$ model since the projection of the NCSM states onto the $0\hbar\Omega$ space [Figure 2 and Figure 3, blue (right) bars] is a projection of the NCSM results onto the $\mathrm{SU}(3)$ shell model. For ^{16}O the $0\hbar\Omega$ $\mathrm{SU}(3)$ symmetry is $\approx 60\%$ of the NCSM 0^+_{gs} [Figure 3, blue (left) bars]. For ^{12}C the $0\hbar\Omega$ $\mathrm{SU}(3)$ symmetry ranges from just over 40% of the NCSM 0^+_{gs} for $\hbar\Omega$ = 11 MeV

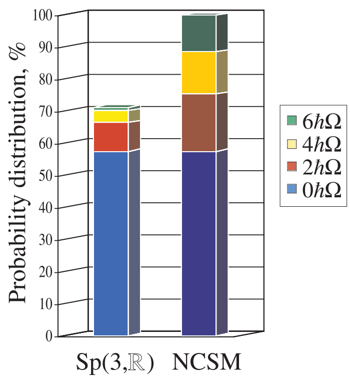

Figure **3.** ^{16}O ground 0^+ state probability distribution over $0\hbar\Omega$ (blue, lowest) to $6\hbar\Omega$ (green, highest) subspaces for the leading 0p-0h (0 0) $\mathrm{Sp}(3,\mathbb{R})$ irrep case (left) and NCSM (right) for $N_{max} = 6$ and bare JISP16 interaction.

to nearly 65% for $\hbar\Omega$ =18 MeV [Figure 2, blue (left) bars] with 80%-90% of this symmetry governed by the leading (0 4) irrep. These numbers are consistent with what has been shown to be a dominance of the leading $\mathrm{SU}(3)$ symmetry for $\mathrm{SU}(3)$-based shell-model studies with realistic interactions in $0\hbar\Omega$ model spaces. It seems the simplest of Elliott's collective states can be regarded as a good first-order approximation in the presence of realistic interactions, whether the latter is restricted to a $0\hbar\Omega$ model space or the richer multi-$\hbar\Omega$ NCSM model spaces.

4 Conclusions

Wavefunctions, which are obtained in a NCSM analysis with the JISP16 realistic interaction, project at approximately the 80% level onto the leading (three) 0p-0h irreps of the corresponding Sp-NCSM for the lowest 0^+_{gs}, 2^+_1 and 4^+_1 states in ^{12}C and at more than 70% level for the ground state in the closed-shell ^{16}O nucleus. (While not part of the current analysis, preliminary results indicate that when the space is expanded to include the most important $2\hbar\Omega$ 2p-2h irreps the percentage grows by approximately 10%.) The results confirm for the first time the validity of the $\mathrm{Sp}(3,\mathbb{R})$ approach when realistic interactions are invoked and hence demonstrate the importance of the $\mathrm{Sp}(3,\mathbb{R})$ symmetry in light nuclei as well as reaffirm the value of the simpler $\mathrm{SU}(3)$ model upon which it is based.

The results further suggest that a Sp-NCSM extension of the NCSM may be a practical scheme for achieving convergence to measured B(E2) values without the need for introducing an effective charge and even for modeling cluster-like phenomena as these modes can be accommodated within the general framework of the $\mathrm{Sp}(3,\mathbb{R})$ model if extended to large model spaces (high N_{max}), but with a size that is typically only a fraction of the NCSM size. This suggests that a Sp-NCSM code could allow one to extend no-core calculations to higher $\hbar\Omega$ configurations and heavier nuclei that are currently unreachable because the model space is typically too large to handle, even on the best of modern day computers.

Acknowledgments

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