the U.S. Department of Energy under Grant Nos. DE-FG02-96ER40963 (University of Tennessee) and DE-AC05-00OR22725 with UT-Battelle, LLC (ORNL), and by the Natural Sciences and Engineering Research Council of Canada (NSERC). Computational resources were provided by the National Center for Computational Sciences at Oak Ridge and the National Energy Research Scientific Computing Facility.

References:

SYMPLECTIC NO-CORE SHELL MODEL

JERRY P. DRAAYER, TOMÁŠ DYTRYCH, KRISTINA D. SVIRATCHEVA, AND CHAIRUL BAHRI

Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803, USA

JAMES P. VARY

Department of Physics and Astronomy, Iowa State University, Ames, IA 50011, USA

Results from a full 6fω No-Core Shell Model (NCSM) calculation for low-lying states in \(^{12}\)C and \(^{16}\)O using a realistic nucleon-nucleon interaction are found to project at approximately the 90% level onto a few of the leading \(6p-0h\) and \(2p-2h\) symplectic representations. The latter spans a symplectic space that is typically only a very small fraction (under 1%) of the NCSM model space, and grows slowly with increasing \(M1\) oscillator strength parameter. The results are nearly independent of \(M1\) and whether bare or renormalized effective interactions are used in the analysis.

Keywords: ab-initio no-core shell model, symplectic Sp(3,R) shell model, model space truncation scheme, \(^{12}\)C, \(^{16}\)O.

1. Introduction

A unified microscopic description of low-lying states in light nuclei requires a theory that can incorporate diverse degrees of freedom, ranging from single-particle effects, pairing correlations and a few particle-hole excitations, to \(0\)-clustering phenomena and enhanced shape deformations. Furthermore, if such a theory is designed to employ realistic interactions, it could relate to the fundamental strong interaction as well as quark constituents and be applicable in regions of the nuclear chart where experimental data necessary to adjust effective interactions might not be available.

We propose the Symplectic No-Core Shell Model (SpNCSM)\(^1\) as the first ab initio approach capable of meeting those criteria. It combines the NCSM,\(^2\) which uses modern realistic interactions and yields a good description of the low-lying states in few-nucleon systems\(^3\) as well as in more complex nuclei like \(^{12}\)C,\(^4\) with the symplectic Sp(3, R) model\(^5,6\) that can
yield a dramatic reduction of the NCSM space and hence serve as a powerful basis space reduction (truncation) scheme. This approach allows one to advance \textit{ab initio} calculations to heavier nuclei and to account for even higher $\hbar \Omega$ configurations required to realize experimentally measured $\text{B}(E2)$ values without an effective charge, and to accommodate highly deformed spatial configurations including $\alpha$-cluster structures,\textsuperscript{7} which may be essential for modeling, e.g., the second $0^{+}$ state in $^{12}\text{C}$ and $^{16}\text{O}$.

We recently showed in a 'proof-of-principle' study\textsuperscript{1} that realistic eigenstates for low-lying states determined in NCSM calculations for light nuclei with the JISP16 realistic interaction,\textsuperscript{5,6} project predominantly on a few of the most deformed $\text{Sp}(3, \mathbb{R})$-symmetric basis states that are free of spurious center-of-mass motion. This suggests the presence of an underlying symplectic structure, which is not \textit{a priori} imposed on the interaction and furthermore that is found to remain essentially unaltered after a Lee-Suzuki similarity transformation is introduced to accommodate the truncation of the infinite Hilbert space through a renormalization of the bare interaction. This in turn provides insight into the physics of a nucleon system and its geometry since collective states shaped by monopole/quadrupole-vibrational and rotational modes are described naturally by irreducible representations (irreps) of $\text{Sp}(3, \mathbb{R})$.

We focus on the $0^{+}_{gs}$ ground state and the lowest $2^{+}$ and $4^{+}$ states in the deformed $^{12}\text{C}$ nucleus as well as the $0^{+}_{gs}$ in the `closed-shell' $^{16}\text{O}$ nucleus. The corresponding NCSM eigenstates are reasonably well converged in the $N_{\text{max}} = 6$ (or $6\hbar \Omega$) model space with an effective interaction based on the JISP16 realistic interaction. In addition, calculated binding energies as well as other observables for $^{12}\text{C}$ such as $\text{B}(E2; 2^{+}_{gs} \rightarrow 0^{+}_{gs})$, $\text{B}(M1; 1^{+}_{gs} \rightarrow 0^{+}_{gs})$, ground-state proton rms radii and the $2^{+}$ quadrupole moment all lie reasonably close to the measured values. While symplectic algebraic approaches achieve a good reproduction of low-lying energies and $\text{B}(E2)$ values in light nuclei\textsuperscript{9-13} using phenomenological or semi-microscopic interactions, here, for the first time, we establish the dominance of the symplectic symmetry in light nuclei, and hence their propensity towards the development of collective motion as unveiled through \textit{ab initio} NCSM calculations.

2. Symplectic $\text{Sp}(3, \mathbb{R})$ Basis

The symplectic shell model\textsuperscript{5,6} based on the noncompact symplectic $\text{sp}(3, \mathbb{R})$ algebra\textsuperscript{6}, is known to underpin the successful Bohr-Mottelson collective model and has also been shown to be a multiple oscillator shell generalization of Elliott's $\text{SU}(3)$ model. The significance of the symplectic symmetry for a microscopic description of a quantum many-body system of interacting particles emerges from the physical relevance of its 21 generators. For $A$ nucleons the bilinear products of the particle momentum $(p_{\alpha})$ and coordinate $(x_{\alpha})$ operators, $T_{\alpha\beta} = \sum_{\alpha} p_{\alpha} p_{\beta}$, $I_{\alpha\beta} = \sum_{\alpha} (x_{\alpha} p_{\beta} - 2 \delta_{\alpha\beta} p_{\alpha})$, $S_{\alpha\beta} = \sum_{\alpha} (x_{\alpha} x_{\beta} + p_{\alpha} p_{\beta})$, and $Q_{\alpha\beta} = \sum_{\alpha} x_{\alpha} x_{\beta}$ with $\alpha, \beta = 1, 2, 3$ for the 3 spatial directions and $s = 1, \ldots, A$, realize the symplectic $\text{sp}(3, \mathbb{R})$ algebra. Hence, the many-particle kinetic energy, the mass quadrupole moment operator, and the angular momentum are all elements of the $\text{sp}(3, \mathbb{R}) \supset \text{su}(3) \supset \text{so}(3)$ algebraic structure. It also includes monopole and quadrupole collective vibrations reaching beyond a single shell to higher-lying and core configurations, as well as vorticity degrees of freedom for a description of the continuum from rotational to rigid rotor flows. Alternatively, the elements of the $\text{sp}(3, \mathbb{R})$ algebra can be represented as bilinear products in harmonic oscillator (HO) raising and lowering operators, which means the basis states of a $\text{Sp}(3, \mathbb{R})$ irrep can be expanded in a 3-D HO ($m$-scheme) basis which is the same basis used in the NCSM, thereby facilitating calculations and symmetry identification.

The basis states within a $\text{Sp}(3, \mathbb{R})$ irrep are built by applying multiples of the symplectic raising operators to a $n$-particle-$n$-hole ($n$-particle-$n$-hole, $n = 0, 2, 4, \ldots$) lowest-weight $\text{Sp}(3, \mathbb{R})$ state (symplectic bandhead), which by definition is annihilated by the symplectic lowering operator. The raising operator induces a $2\hbar \Omega$ $1p-1h$ monopole or quadrupole excitation (one particle raised by two shells) together with a $2\hbar \Omega$ $2p-2h$ correction for eliminating the spurious center-of-mass motion. If one were to include all possible lowest-weight $n$p-$n$h starting state configurations ($n \leq N_{\text{max}}$), and allowed all multiples thereof, one would span the full NCSM space.

3. Results and Discussions

3.1. Reproduction of NCSM results in a $\text{Sp}(3, \mathbb{R})$ subspace

The lowest-lying eigenstates of $^{12}\text{C}$ and $^{16}\text{O}$ were calculated using the NCSM\textsuperscript{6} as implemented through the Many Fermion Dynamics (MFD) code\textsuperscript{14} with an effective interaction derived from the realistic JISP16 NN potential\textsuperscript{8} for different $\hbar \Omega$ oscillator strengths. For both nuclei we considered

\textsuperscript{8}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 total norm.
structed all of the 0p-0h and 2\(\Omega\) 2p-2h symplectic bandheads and generated their \(Sp(3, R)\) irreps up to \(N_{\text{max}} = 6\) (6\(\Omega\) model space). Analysis of overlaps of the symplectic states with the NCSM eigenstates in the 0, 2, 4 and 6\(\Omega\) subspaces reveals the dominance of the 0p-0h \(Sp(3, R)\) irreps [Fig. 1(a,b,c)]. For the 0\(_{\text{p}}^+\) and the lowest 2\(_{\text{p}}^+\) and 4\(_{\text{p}}^+\) states in \(^{12}\text{C}\) there are nonnegligible overlaps for only 3 of the 13 0p-0h \(Sp(3, R)\) irreps, namely, the leading (most deformed) representation specified by the shape deformation of its symplectic bandhead, (0 4), and spin \(S = 0\) together with two (1 2) \(S = 1\) irreps with different bandhead constructions for protons and neutrons. For the ground state of \(^{16}\text{O}\) there is only one possible 0p-0h \(Sp(3, R)\) irrep, (0 0) \(S = 0\) (Fig. 1d). In addition, among the 2\(\Omega\) 2p-2h \(Sp(3, R)\) irreps only a small fraction of the most deformed configurations contributes significantly to the overlaps accounting for 5\% (10\%) in \(^{12}\text{C}\) (\(^{16}\text{O}\)) (Fig. 2). The results reveal that approximately 85-90\% of the NCSM eigenstates fall within a subspace spanned by the few most significant 0p-0h and 2\(\Omega\) 2p-2h \(Sp(3, R)\) irreps.

![Fig. 1. Probability distribution for the (a) 0\(_{\text{p}}^+\), (b) 2\(_{\text{p}}^+\), and (c) 4\(_{\text{p}}^+\) states in \(^{12}\text{C}\) and (d) 0\(_{\text{p}}^+\) in \(^{16}\text{O}\) over 0\(\Omega\) (blue, lowest) to 6\(\Omega\) (green, highest) subspaces for the 3 0p-0h \(Sp(3, R)\) irrep case (left) and NCSM (right) together with the (0 4) irrep contribution (black diamonds) in \(^{12}\text{C}\) as a function of the \(\hbar\Omega\) oscillator strength in MeV for \(N_{\text{max}} = 6\).](image)

The largest contribution comes from the leading \(Sp(3, R)\) irrep (Fig. 2, black diamonds), growing to 80\% of the NCSM wavefunctions for the lowest \(\Omega\). The results can be also interpreted as a strong confirmation of Elliott’s SU(3) model since the projection of the NCSM states onto the 0\(\Omega\) space [Fig. 2, blue (lowest) bars] is a projection of the NCSM results onto the SU(3) shell model. Clearly, 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\(\Omega\) model space or richer multi-\(\Omega\) NCSM model spaces.

The 0\(_{\text{p}}^+\), 2\(_{\text{p}}^+\), and 4\(_{\text{p}}^+\) states in \(^{12}\text{C}\), constructed in terms of the three \(Sp(3, R)\) irreps with probability amplitudes defined by the overlaps with the NCSM wavefunctions for \(N_{\text{max}} = 6\) case, were also used to determine \(B(E2; 2_{\text{p}}^+ \rightarrow 0_{\text{p}}^+;\) transition rates. The \(Sp(3, R)\) \(B(E2; 2_{\text{p}}^+ \rightarrow 0_{\text{p}}^+;\) values reproduce almost exactly (∼100\%) the NCSM results.

3.2. **Large reduction of model space dimension**

As \(N_{\text{max}}\) is increased the dimension of the \(J = 0, 2\), and 4 symplectic space built on the 0p-0h \(Sp(2, R)\) irreps for \(^{12}\text{C}\) grows very slowly compared to the NCSM space dimension (Fig. 3a). The dominance of only three irreps additionally reduces the dimensionality of the symplectic model space, which remains a small fraction of the NCSM basis space even when the most dominant 2\(\Omega\) 2p-2h \(Sp(3, R)\) irreps are included. The space reduction is even more dramatic in the case of \(^{16}\text{O}\) (Fig. 3b). This means that a space
spanned by a set of symplectic basis states is computationally manageable even when high-$\Omega$ configurations are included.

In short, the symplectic subspace for the low-lying states in $^{12}$C and $^{16}$O that achieves large overlaps with the realistic NCSM eigenstates and reproduction of the NCSM estimates for the B(E2) transition rates comprises only a small fraction of the full NCSM model space.

3.3. Sp(3, R) invariance within NCSM spin components

Another striking property of the low-lying eigenstates is revealed when the spin projections of the converged NCSM states are examined. Specifically, as shown in Fig. 4, their Sp(3, R) symmetry and hence the geometry of the nucleon system being described is nearly independent of the $\Omega$ oscillator strength. The symplectic symmetry is present with equal strength in the spin parts of the NCSM wavefunctions for $^{12}$C as well as $^{16}$O regardless of whether the bare or the effective interactions are used. This suggests that the Lee-Suzuki transformation, which effectively compensates for the finite space truncation by renormalization of the bare interaction, does not affect the Sp(3, R) symmetry structure of the spatial wavefunctions. Hence, the symplectic structure detected in the present analysis for $6\Omega$ model space is what would emerge in NSCM evaluations with a sufficiently large model space to justify use of the bare interaction.

4. Conclusions

We have shown that ab initio NCSM calculations with the JISP16 nucleon-nucleon interaction display a very clear symplectic structure, which is unaltered whether the bare or effective interactions for various $\Omega$ strengths are used. The NCSM results are reproduced remarkably well by only a few 0p-0h and 2$\Omega$ 2p-2h spurious center-of-mass free symplectic irreps with dimensionality that is only $\approx 10^{-3}$% that of the NCSM model space. Specifically, these symplectic states account for 85-90% of the NCSM wavefunctions for the lowest 0$_2^+$, 2$^+_1$ and 4$^+_1$ states in $^{12}$C and the ground state in $^{16}$O and they closely reproduce the NCSM B(E2) estimates.

The comparisons with NCSM results open the path for consequent studies as the results suggest either the effective nucleon-nucleon interaction possesses a heretofore unappreciated symmetry, namely Sp(3, R) and the complementary (spin-isospin) supermultiplet symmetry, or the nuclear many-body system acts as a filter that allows the symplectic symmetry to propagate in a coherent way into the many-body dynamics while reducing the effects of symplectic symmetry breaking terms.

In short, the results confirm for the first time the validity of the Sp(3, R) approach when realistic interactions are invoked in a NCSM space. This demonstrates the importance of the Sp(3, R) symmetry in light nuclei while reaffirming the value of the simpler Elliott SU(3) model upon which it is
based. The results further suggest that a Sp-NCSM extension of the ab-initio NCMS may be a practical scheme for reaching heavier nuclei and achieving convergence to measured $B(E2)$ values without the need for introducing an effective charge.

**Acknowledgments**

Discussions with many colleagues, but especially Bruce R. Barrett, are gratefully acknowledged. This work was supported by the US National Science Foundation, Grant Nos 0140300 & 0500291, and the Southeastern Universities Research Association, as well as, in part, by the US Department of Energy Grant No. DE-FG02-87ER40371. TD acknowledges supplemental support from the Graduate School of Louisiana State University.

**References**


**ROLE OF DEFORMED SYMPLECTIC CONFIGURATIONS in AB INITIO NO-CORE SHELL MODEL RESULTS**

T. DYTRYCH$^1$, K. D. SVIRATCHEVA$^1$, C. BAHRI$^1$, J. P. DRAAYER$^2$, AND J. P. VARY$^2$

$^1$Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana 70803, USA
$^2$Department of Physics and Astronomy, Iowa State University, Ames, IA 50011, USA

A set of methods for the construction of an arbitrary n-particle-n-hole (np-nh) translationally invariant symplectic irreducible representation in a spherical harmonic oscillator basis is presented. The methods are used to construct all possible 2p-2h as well as the most deformed 4p-4h irreducible representation of Sp(3, R) in $^{12}$C and in $^{16}$O. We use the results to demonstrate the significant role these 2p-2h Sp(3, R) states plays in a description of the low-lying states calculated within the framework of the no-core shell model using the realistic JISP16 nucleon-nucleon interaction.

1. **Introduction**

The ab initio no-core shell model (NCSM)$^1$ approach has emerged as a prominent method for modeling properties of light nuclei at the microscopic level. Utilizing modern realistic intranucleon interactions, the NCSM has achieved favorable agreement between theory and experiment for various low-lying states of light nuclei.

Despite its success, the NCSM with the largest model spaces currently attainable, i.e. $N_{max} = 6$ for the upper p-shell nuclei, is still not capable of reproducing the observed excitation energies of low-lying states dominated by multiple-particle-multiple-hole modes.$^{1,5}$ Examples of the latter are the $2^+_2$ states in $^{12}$C and $^{16}$O, both highly deformed with dominating multiple-particle-multiple-hole configurations$^6$ and a pronounced $\alpha$-cluster structure.$^7$ The intrinsic structure of these states essentially requires yet larger NCSM model spaces$^3$ in order to accurately reproduce their excitation energies. However, the dimensionalities of such model spaces are well beyond present computing capabilities. Clearly, physically relevant schemes