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Evidence for Symplectic Symmetry in *Ab Initio* No-Core Shell Model Results for Light Nuclei

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Clear evidence for symplectic symmetry in low-lying states of ^{12}C and ^{16}O is reported. Eigenstates of ^{12}C and ^{16}O, determined within the framework of the no-core shell model using the JISP16 NN realistic interaction, typically project at the 85-90% level onto a few of the most deformed symplectic basis states that span only a small fraction of the full model space. The results are nearly independent of whether the bare or renormalized effective interactions are used in the analysis. The outcome confirms Elliott's SU(3) model which underpins the symplectic scheme, and above all, points to the relevance of a symplectic no-core shell model that can reproduce experimental B(E2) values without effective charges as well as deformed spatial modes associated with clustering phenomena in nuclei.

Recently developed realistic interactions, such as J-matrix inverse scattering potentials [1] and modern two- and three-nucleon potentials derived from meson exchange theory [2] or by using chiral effective field theory [3], succeed in modeling the essence of the strong interaction for the purpose of input into microscopic shell-model calculations that target reproducing characteristic features of light nuclei. The *ab initio* No-Core Shell Model (NCSM) [4] which employs such modern realistic interactions, yields a good description of the low-lying states in few-nucleon systems [5] as well as in more complex nuclei like ^{12}C [4, 6]. In addition to advancing our understanding of the propagation of the nucleon-nucleon force in nuclear matter and clustering phenomena [7, 8], modeling the structure of ^{12}C, ^{16}O and similar nuclei is also important for gaining a better understanding of other physical processes such as parity-violating electron scattering from light nuclei [9] and results gained through neutrino studies [10] as well as for making better predictions for capture reaction rates that figure prominently, for example, in the burning of He in massive stars [11].

In this letter we report on investigations that show that realistic eigenstates for low-lying states determined in NCSM calculations for light nuclei with the JISP16 realistic interaction [1], predominantly project onto few of the most deformed $\mathrm{Sp}(3,\mathbb{R})$-symmetric basis states that are free of spurious center-of-mass motion. This reflects the presence of an underlying symplectic $\mathfrak{sp}(3,\mathbb{R}) \supset \mathfrak{su}(3) \supset \mathfrak{so}(3)$ algebraic structure [22], which is not *a priori* imposed on the interaction and furthermore is found to remain unaltered after a Lee-Suzuki similarity transformation used to accommodate the truncation of the infinite Hilbert space by renormalization of the bare interaction. This in turn provides insight into the physics of a nucleon system and its geometry. Specifically, nuclear collective states with well-developed quadrupole and monopole vibrational modes and rotational modes are described naturally by irreducible representations (irreps) of $\mathrm{Sp}(3,\mathbb{R})$.

The present study points to the possibility of achieving convergence of higher-lying collective modes and reaching heavier nuclei by expanding the NCSM basis space beyond its current limits through $\mathrm{Sp}(3,\mathbb{R})$ basis states that span a dramatically smaller subspace of the full space. In this way, the symplectic no-core shell-model (Sp-NCSM) with realistic interactions and with a mixed $\mathrm{Sp}(3,\mathbb{R})$ irrep extension will allow one to account for even higher $\hbar\Omega$ configurations required to realize experimentally measured B(E2) values without an effective charge, and to accommodate highly deformed spatial configurations [12] that are required to reproduce α-cluster modes, which may be responsible for shaping, e.g., the second 0^+ state in ^{12}C and ^{16}O [8].

We focus on the 0^+_{gs} ground state and the lowest $2^+(\equiv 2^+_1)$ and $4^+(\equiv 4^+_1)$ states in the oblate ^{12}C nucleus as well as the 0^+_{gs} in the 'closed-shell' ^{16}O nucleus. The NCSM eigenstates for these states are reasonably well converged in the $N_{max} = 6$ (or $6\hbar\Omega$) model space with an effective interaction based on the JISP16 realistic interaction [1], which typically leads to rapid convergence in the NCSM evaluations, describes NN data to high accuracy and is consistent with, but not constrained by, meson exchange theory, QCD or locality. In addition, calculated binding energies as well as other observables for ^{12}C such as B(E2;$2^+_1 \to 0^+_{gs}$), B(M1;$1^+_1 \to 0^+_{gs}$), ground-state proton rms radii and the 2^+_1 quadrupole moment all lie reasonably close to the measured values. While symplectic algebraic approaches have achieved a very good reproduction of low-lying energies and B(E2) values in light nuclei [13, 14] and specifically in ^{12}C using phenomenological interactions [15] or truncated symplectic basis with simplistic (semi-) microscopic interactions [16, 17], here, for the first time, we establish, the dominance of the symplectic $\mathrm{Sp}(3,\mathbb{R})$ symmetry in light nuclei, and hence their propensity towards development of collective motion, as unveiled through *ab initio* calculations of the NCSM type starting with realistic two-nucleon interactions.

The symplectic shell model [18, 19] is based on the noncompact symplectic $\mathfrak{sp}(3,\mathbb{R})$ algebra. The classical realization of this symmetry underpins the dynamics of rotating bodies and has been used, for example, to describe the rotation of deformed stars and galaxies [20]. In its quantal realization it 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 SU(3) model. Consequently, symplectic basis states bring forward important information about nuclear shapes and deformation in terms of (λ,μ), which serve to label the SU(3) irreps within a given $\mathrm{Sp}(3,\mathbb{R})$ irrep, for example, $(0,0)$, $(\lambda,0)$ and $(0,\mu)$ describe spherical, prolate and oblate shapes, respectively.

The significance of the symplectic symmetry for a microscopic description of a quantum many-body system emerges from the physical relevance of its 21 generators constructed as bilinear products of the momentum (p_α) and coordinate (q_β) operators, e.g. $p_\alpha p_\beta$, $p_\alpha q_\beta$, and $q_\alpha q_\beta$ with α, $\beta = x$, y, and z for the 3 spatial directions. Hence, the many-particle kinetic energy, the mass quadrupole moment operator, and the angular momentum are all elements of the $\mathfrak{sp}(3,\mathbb{R}) \supset \mathfrak{su}(3) \supset \mathfrak{so}(3)$ 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 irrotational to rigid rotor flows. Alternatively, the elements of the $\mathfrak{sp}(3,\mathbb{R})$ algebra can be represented as bilinear products in harmonic oscillator (HO) raising and lowering operators, which means the basis states of a $\mathrm{Sp}(3,\mathbb{R})$ 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 $\mathrm{Sp}(3,\mathbb{R})$ irrep are built by applying symplectic raising operators to a np-nh (n-particle-n-hole, $n = 0, 2, 4, \ldots$) lowest-weight $\mathrm{Sp}(3,\mathbb{R})$ state (symplectic bandhead), which is defined by the usual requirement that the symplectic lowering operator annihilates it. The raising operator induces a $2\hbar\Omega$ 1p-1h monopole or quadrupole excitation (one particle raised by two shells) together with a smaller $2\hbar\Omega$ 2p-2h correction for eliminating the spurious center-of-mass motion. If one were to include all possible lowest-weight np-nh starting state configurations ($n \leq N_{max}$), and allowed all multiples thereof, one would span the full NCSM space.

The lowest-lying eigenstates of ^{12}C and ^{16}O were calculated using the NCSM as implemented through the Many Fermion Dynamics (MFD) code [21] with an effective interaction derived from the realistic JISP16 NN potential [1] for different $\hbar\Omega$ oscillator strengths. For both nuclei we constructed all of the 0p-0h and $2\hbar\Omega$ 2p-2h (2 particles raised by one shell each) symplectic bandheads and generated their $\mathrm{Sp}(3,\mathbb{R})$ irreps up to $N_{max} = 6$ ($6\hbar\Omega$ model space). Analysis of overlaps of the symplectic states with the NCSM eigenstates for $2\hbar\Omega$, $4\hbar\Omega$, and $6\hbar\Omega$ model spaces ($N_{max} = 2, 4, 6$) reveals the dominance of the 0p-0h $\mathrm{Sp}(3,\mathbb{R})$ irreps. For the 0^+_{gs} and the lowest 2^+ and 4^+ states in ^{12}C there are nonnegligible overlaps for only 3 of the 13 0p-0h $\mathrm{Sp}(3,\mathbb{R})$ irreps, namely, the leading (most deformed) representation specified by the shape deformation of its symplectic bandhead, (0 4), and carrying 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}O there is only one possible 0p-0h $\mathrm{Sp}(3,\mathbb{R})$ irrep, (0 0) $S = 0$. In addition, among the $2\hbar\Omega$ 2p-2h $\mathrm{Sp}(3,\mathbb{R})$ irreps only a small fraction contributes significantly to the overlaps and it includes the most deformed configurations that correspond to oblate shapes in ^{12}C and prolate ones in ^{16}O.

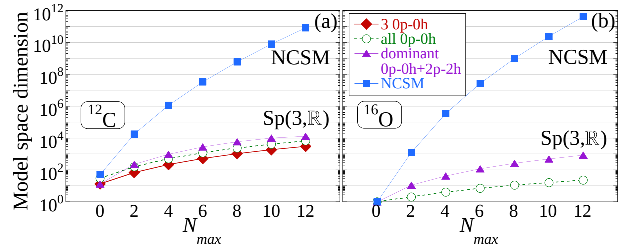

FIG. 1: NCSM space dimension as a function of the maximum $\hbar\Omega$ excitations, N_{max}, compared to that of the $\mathrm{Sp}(3,\mathbb{R})$ subspace: (a) $J = 0, 2$, and 4 for ^{12}C, and (b) $J = 0$ for ^{16}O.

The typical dimension of a symplectic irrep 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 for ^{12}C grows very slowly compared to the NCSM space dimension (Fig. 1a). 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 $2\hbar\Omega$ 2p-2h $\mathrm{Sp}(3,\mathbb{R})$ irreps are included. The space reduction is even more dramatic in the case of ^{16}O (Fig. 1b). This means that a space spanned by a set of symplectic basis states is computationally manageable even when high-$\hbar\Omega$ configurations are included.

The overlaps of the most dominant symplectic states with investigated NCSM eigenstates for the ^{12}C and the ^{16}O in the 0, 2, 4 and $6\hbar\Omega$ subspaces are given in Table I and II. 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. The results show that approximately 85% of the NCSM eigenstates for ^{12}C (^{16}O) fall within a subspace spanned by the few most significant 0p-0h and $2\hbar\Omega$ 2p-2h $\mathrm{Sp}(3,\mathbb{R})$ irreps, with the $2\hbar\Omega$ 2p-2h $\mathrm{Sp}(3,\mathbb{R})$ irreps accounting for 5% (10%) and with the leading irrep, (0 4) for ^{12}C and (0 0) for ^{16}O, carrying close to 70% (75%) of the NCSM wavefunction.

Furthermore, the $S=0$ part of all three NCSM eigenstates for ^{12}C is almost entirely projected (95%) onto only six $S=0$ symplectic irreps included in Table I, with as much as 90% of the spin-zero NCSM states accounted for solely by the leading (0 4) irrep. The $S=1$ part is also remarkably well described by merely two $\mathrm{Sp}(3,\mathbb{R})$ irreps. Similar results are observed for the ground state of ^{16}O.

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. 2, their $\mathrm{Sp}(3,\mathbb{R})$ symmetry and hence the geometry of the nucleon system being described is nearly independent of the $\hbar\Omega$ 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 $\mathrm{Sp}(3,\mathbb{R})$ symmetry structure of the spatial wavefunctions. Hence, the symplectic structure detected in the present analysis for $6\hbar\Omega$ model space is what would emerge in NSCM evaluations with a sufficiently large model space to justify use of the bare interaction.

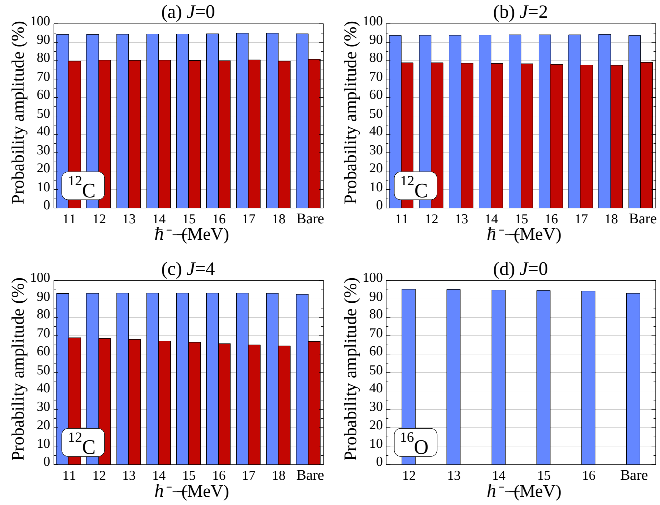

FIG. 2: Projection of the $S=0$ (blue, left) [and $S=1$ (red, right)] $\mathrm{Sp}(3,\mathbb{R})$ irreps onto the corresponding significant spin components of the NSCM wavefunctions for (a) 0^+_{gs}, (b) 2^+_1, and (c) 4^+_1 in ^{12}C and (d) 0^+_{gs} in ^{16}O, for effective interaction for different $\hbar\Omega$ oscillator strengths and bare interaction.

In addition, as one varies the oscillator strength $\hbar\Omega$, the projection of the NCSM wavefunctions onto the symplectic subspace changes only slightly (see, e.g., Fig. 3 for the 0^+_{gs} state of ^{12}C and ^{16}O). The symplectic structure is preserved, only the $\mathrm{Sp}(3,\mathbb{R})$ irrep contributions change because the $S=0$ ($S=1$) part of the NCSM eigenstates decrease (increase) towards higher $\hbar\Omega$ frequencies. Clearly, the largest contribution comes from the leading $\mathrm{Sp}(3,\mathbb{R})$ irrep (black diamonds), growing to 80% of the NCSM wavefunctions for the lowest $\hbar\Omega$. These results can be interpreted as a strong confirmation of Elliott's SU(3) model since the projection of the NCSM states onto the $0\hbar\Omega$ space [Fig. 3, blue (lowest) bars] is a projection of the NCSM results onto the SU(3) shell model. The outcome is consistent with what has been shown to be a dominance of the leading SU(3) symmetry for SU(3)-based shell-model studies with realistic interactions in $0\hbar\Omega$ model spaces. It seems the simplest of

TABLE I: Probability distribution of NCSM eigenstates for ^{12}C across the dominant 0p-0h and $2\hbar\Omega$ 2p-2h $\mathrm{Sp}(3,\mathbb{R})$ irreps, $\hbar\Omega$=15 MeV.

		$0\hbar\Omega$	$2\hbar\Omega$	$4\hbar\Omega$	$6\hbar\Omega$	Total
		$J=0$				
$\mathrm{Sp}(3,\mathbb{R})$	$(0\ 4)S=0$	46.26	12.58	4.76	1.24	64.84
	$(1\ 2)S=1$	4.80	2.02	0.92	0.38	8.12
	$(1\ 2)S=1$	4.72	1.99	0.91	0.37	7.99
	$2\hbar\Omega$ 2p-2h		3.46	1.02	0.35	4.83
	Total	55.78	20.05	7.61	2.34	85.78
NCSM		56.18	22.40	12.81	7.00	98.38
		$J=2$				
$\mathrm{Sp}(3,\mathbb{R})$	$(0\ 4)S=0$	46.80	12.41	4.55	1.19	64.95
	$(1\ 2)S=1$	4.84	1.77	0.78	0.30	7.69
	$(1\ 2)S=1$	4.69	1.72	0.76	0.30	7.47
	$2\hbar\Omega$ 2p-2h		3.28	1.04	0.38	4.70
	Total	56.33	19.18	7.13	2.17	84.81
NCSM		56.18	21.79	12.73	7.28	98.43
		$J=4$				
$\mathrm{Sp}(3,\mathbb{R})$	$(0\ 4)S=0$	51.45	12.11	4.18	1.04	68.78
	$(1\ 2)S=1$	3.04	0.95	0.40	0.15	4.54
	$(1\ 2)S=1$	3.01	0.94	0.39	0.15	4.49
	$2\hbar\Omega$ 2p-2h		3.23	1.16	0.39	4.78
	Total	57.50	17.23	6.13	1.73	82.59
NCSM		57.64	20.34	12.59	7.66	98.23

TABLE II: Probability distribution of the NCSM eigenstate for the $J=0$ ground state in ^{16}O across the 0p-0h and dominant $2\hbar\Omega$ 2p-2h $\mathrm{Sp}(3,\mathbb{R})$ irreps, $\hbar\Omega$=15 MeV.

		$0\hbar\Omega$	$2\hbar\Omega$	$4\hbar\Omega$	$6\hbar\Omega$	Total
$\mathrm{Sp}(3,\mathbb{R})$	$(0\ 0)S=0$	50.53	15.87	6.32	2.30	75.02
	$2\hbar\Omega$ 2p-2h		5.99	2.52	1.32	9.83
	Total	50.53	21.86	8.84	3.62	84.85
NCSM		50.53	22.58	14.91	10.81	98.83

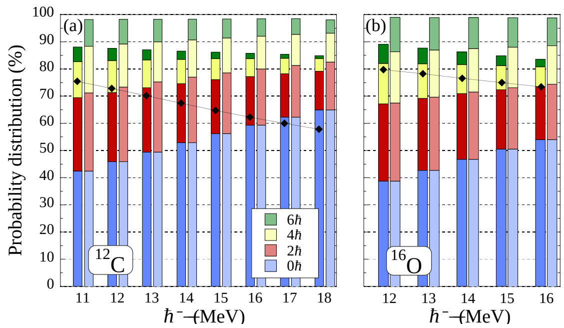

FIG. 3: Ground 0^+ state probability distribution over $0\hbar\Omega$ (blue, lowest) to $6\hbar\Omega$ (green, highest) subspaces for the most dominant 0p-0h + $2\hbar\Omega$ 2p-2h Sp$(3,\mathbb{R})$ irrep case (left) and NCSM (right) together with the leading irrep contribution (black diamonds), $(0\,4)$ for ^{12}C (a) and $(0\,0)$ for ^{16}O (b), as a function of the $\hbar\Omega$ oscillator strength, $N_{max} = 6$.

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 richer multi-$\hbar\Omega$ NCSM model spaces.

The 0^+_{gs} and 2^+_1 states in ^{12}C, constructed in terms of the three Sp$(3,\mathbb{R})$ irreps with probability amplitudes defined by the overlaps with the NCSM wavefunctions for $N_{max} = 6$ case, were also used to determine $B(E2 : 2^+_1 \to 0^+_{gs})$ transition rates. The latter, increasing from 101% to 107% of the corresponding NCSM numbers with increasing $\hbar\Omega$, clearly reproduce the NCSM results.

In summary, 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 $\hbar\Omega$ strengths are used. Specifically, NCSM wavefunctions for the lowest 0^+_{gs}, 2^+_1 and 4^+_1 states in ^{12}C and the ground state in ^{16}O project at the 85-90% level onto a few 0p-0h and $2\hbar\Omega$ 2p-2h spurious center-of-mass free symplectic irreps. Furthermore, while the dimensionality of the latter is only $\approx 10^{-3}$% that of the NCSM space, they closely reproduce the NCSM $B(E2)$ estimates. The wavefunctions for ^{12}C are strongly dominated by the three leading 0p-0h symplectic irreps, with a clear dominance of the most deformed $(0\,4)S = 0$ collective configuration. The ground state of ^{16}O is dominated by the single 0p-0h irrep $(0\,0)S = 0$. The results confirm for the first time the validity of the Sp$(3,\mathbb{R})$ approach when realistic interactions are invoked in a NCSM space. This demonstrates the importance of the Sp$(3,\mathbb{R})$ symmetry in light nuclei while reaffirming the value of the simpler 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. In short, the NCSM with a modern realistic interaction supports the development of collective motion in nuclei which is realized through the Sp-NCSM and as is apparent in its $0\hbar\Omega$ Elliott model limit.

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[1] A. M. Shirokov, A. I. Mazur, S. A. Zaytsev, J. P. Vary, and T. A. Weber, Phys. Rev. C **70**, 044005 (2004); A. M. Shirokov, J. P. Vary, A. I. Mazur, S. A. Zaytsev, and T. A. Weber, Phys. Letts. B **621**, 96(2005); A. M. Shirokov, J. P. Vary, A. I. Mazur, and T. A. Weber, Phys. Letts. B **644**, 33 (2007).
[2] R. Machleidt, F. Sammarruca, and Y. Song, Phys. Rev. C **53**, R1483 (1996); R. Machleidt, Phys. Rev. C **63**, 024001 (2001).
[3] D. R. Entem and R. Machleidt, Phys. Rev. C **68**, 041001 (2003).
[4] P. Navrátil, J. P. Vary, and B. R. Barrett, Phys. Rev. Lett. **84**, 5728 (2000); Phys. Rev. C **62**, 054311 (2000).
[5] P. Navrátil and B. R. Barrett, Phys. Rev. C **57**, 562 (1998); **59**, 1906 (1999); P. Navrátil, G. P. Kamuntavičius, and B. R. Barrett, Phys. Rev. C **61**, 044001 (2000).
[6] P. Navrátil and W. E. Ormand, Phys. Rev. C **68**, 034305 (2003).
[7] S. Karataglidis *et al.*, Phys. Rev. C **52**, 861 (1995).
[8] Y. Funaki *et al.*, Phys. Rev. C **67**, R051306 (2003).
[9] M. J. Musolf and T. W. Donnelly, Nucl. Phys. A**546**, 509 (1992).
[10] A. C. Hayes, P. Navrátil, and J. P. Vary, Phys. Rev. Lett. **91**, 012502 (2003).
[11] C. R. Brune *et al.*, Phys. Rev. Lett. **83**, 4025 (1999).
[12] K. T. Hecht and D. Braunschweig, Nucl. Phys. A**295**, 34 (1978); Y. Suzuki, Nucl. Phys. A**448**, 395 (1986).
[13] G. Rosensteel and D. J. Rowe, Ann. Phys. N.Y. **126**, 343 (1980).
[14] J. P. Draayer, K. J. Weeks and G. Rosensteel, Nucl. Phys. A**413**, 215 (1984).
[15] J. Escher and A. Leviatan, Phys. Rev. C **65**, 054309 (2002).
[16] F. Arickx, J. Broeckhove, and E. Deumens, Nucl. Phys. A**377**, 121 (1982).
[17] S. S. Avancini and E. J. V. de Passos, J. Phys. G **19**, 125 (1993).
[18] G. Rosensteel and D. J. Rowe, Phys. Rev. Lett. **38**, 10 (1977).
[19] D. J. Rowe, Reports on Progr. in Phys. **48**, 1419 (1985).
[20] G. Rosensteel, Astrophys. J. **416** 291, (1993).
[21] J. P. Vary, "The Many-Fermion-Dynamics Shell-Model Code," Iowa State University, 1992 (unpublished); J. P. Vary and D. C. Zheng, *ibid* 1994 (unpublished).
[22] We use lowercase (capital) letters for algebras (groups).