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Large-basis shell-model treatment of $A=16$

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A recently constructed shell-model interaction is used to calculate wave functions for the 0^+ states of ^{16}O in a six-shell $(0+2+4)\hbar\omega$ model space. Several different methods of dealing with problems arising from truncation of the model space at $4\hbar\omega$ are described. The preferred is to lower the $4\hbar\omega$ components by the same energy shift as occurs for the ground state when changing from $0\hbar\omega$ to $(0+2+4)\hbar\omega$. The strong role of the SU3(20) component of the interaction is described. it is shown that a clear and sensitive test of the wave functions of the ground state and 6049 keV deformed state is the ^{16}N 2^- unique first-forbidden decay rates to them. Good agreement is found for these observables.

^{16}O has a fascinating and complex structure since $0\hbar\omega$, $2\eta\omega$, and $4\hbar\omega$ excitations are manifestly apparent amongst the low-lying levels. The $(0+2+4)\hbar\omega$ model of Brown and Green [1] was an early, successful, and important description of these states. Although simple, the essential truth of the Brown–Green model remains as was emphasized in a recent study [2] similar to this one and as will also be reaffirmed here.

There are two severe problems encountered in mixed $(0+2+...)\hbar\omega$ calculations. These are (a) the difficulty of obtaining the mixing between the different $n\hbar\omega$ configurations correctly, and (b) the difficulty of respecting the Hartree–Fock condition vis-a-vis one-particle–one-hole (1p-1h) excitations through two oscillator shells. The first of these problems is the most difficult. As has been commented on at length [3–5] it has its basic cause in the fact that the low-lying $n\hbar\omega$ states interact most strongly with those higher-lying $(n+2)\hbar\omega$ states which mix via the (20) SU3 tensor part of the $2\hbar\omega$ interaction $V^{2\hbar\omega}$ and are thereby depressed by a considerable amount; ~ 10 MeV in ^{16}O. For example, the $2\hbar\omega$ (20) states commence ~ 20 MeV above the $0\hbar\omega$ ground state so that after the mixing they commence at ~ 30 MeV. Mixing of $(n+4)\hbar\omega$ is needed to restore the proper energy relationship between the $n\hbar\omega$ and $(n+2)\hbar\omega$ states. Hence truncation of the slowly-varying series $n\hbar\omega$, $(n+2)\hbar\omega$, ... will badly distort the relative energies of the different $n\hbar\omega$ configurations and thereby give incorrect mixing between them. Here we explore three approximations designed to handle the truncation problem: (1) a lowering of the energy gap between the 0p and 1s0p shells, (2) a lowering of the $4\hbar\omega$ excitations alone, and (3) a removal of the SU3(20) symmetry component from the $V^{2\hbar\omega}$ interaction used in the diagonalization in the $(0+2+4)\hbar\omega$ model space, and a compensation for this omission by including perturbatively the (20) component in the effective operators used to calculate electroweak observables.

The second problem is that single-particle excitations through two oscillator shells must be included for the proper elimination of spurious center-of-mass motion, but one must maintain a proper balance between the potential and kinetic energy contributions to the off-diagonal matrix elements connecting the $(n+2)\hbar\omega$ and $n\hbar\omega$ excitations. Also, single-particle self-consistency and the use of a saturating effective interaction are important to place the centroid of the monopole strength at a reasonable position ($\sim$20–30 MeV) [5,6]. For many applications, an adequate solution to this problem is to suppress these excitations except for that part needed to insure removal of spuriosity. This is the approach adopted by Haxton and Johnson [2] and by us.

Shell-model calculations were performed with the shell-model code OXBASH [7]. With OXBASH, spurious center-of-mass motion is removed by the usual method [8] of adding a center-of-mass hamiltonian H_{cm} to the interaction. The shell-model studies use the recently constructed WBT and WBP hamiltonians of Warburton and Brown [9]. These hamiltonians are based on interactions for the 0p1s0d shells determined by a least-squares fit to 216 energy levels in the $A=10$–22 region assuming no mixing of $n\hbar\omega$ and $(n+2)\hbar\omega$ configurations. The 0p1s0d part of the WBT interaction results from a fit to two-body matrix elements (TBME) and single-particle energies (SPE) while the 0p1s0d part of the WBP interaction was determined from a fit to TBME and SPE for the p-shell and a potential representation of the cross-shell 0p-(1s0d) interaction. The 1s0d part of the hamiltonian is the W interaction of Wildenthal [10]. Then the model space was expanded to include the 0s and 0f1p major shells by adding the appropriate 0f1p and cross-shell 1s0d–0f1p TBME of the WBMB interaction [4] and all the other necessary matrix elements from the bare G matrix potential of Hosaka, Kubo, and Toki [11]. The 0s, 0f, and 1p SPE were determined as described in ref. [9]. Thus the WBT and WBP interactions are constructed in a similar manner to the four-shell (i.e., 0s–0p–1s0d–0f1p) interaction MK3 described in ref. [12], but reproduce the binding energies of low-lying $\geqslant 1\hbar\omega$ levels in the $A=16$ region with 2–3 times greater accuracy.

With the $0\hbar\omega$ ^{16}O ground state taken as $0s_{1/2}^4 0p^{12}$ in the zeroth-order approximation, a $4\hbar\omega$ excitation involves the six lowest oscillator shells. Consequently interactions based on the four-shell WBT and WBP interactions were constructed in a six-shell model space. Our approach to the construction of this model space is essentially identical to that of Haxton and Johnson [2]. Namely, all $\Delta Q>1$ TBME were set equal to zero. For ^{16}O this is equivalent to setting all $\Delta Q>0$ TBME outside the basic 0p1s0d model space equal to zero. Thus the Hartree–Fock condition is satisfied and the 0s and 4th–6th shells are present for the sole purpose of allowing accurate removal of spurious center-of-mass motion. We began our shell-model studies by diagonalizing the 0^+ $T=0$ and 0^-–3^- $T=1$ states of ^{16}O in both six-shell and four-shell model spaces. Negligible difference was found in the wave functions and observables of interest here as calculated within these two model spaces. This is not unexpected since the four-shell space is complete for $2\hbar\omega$ excitations and the $4\hbar\omega$ components in the low-lying states are largely $(0p)^{-4}(1s, 0d)^4$, and these 4p–4h excitations as well as $2\times(\Delta Q=2)$ excitations are also allowed in the four-shell model space. The dimension $D(J^\pi)$ of the 0^+ states in the two model spaces differ negligibly – 4340 and 4255, respectively – but the four-shell model space is convenient in other ways. Thus some of the calculations reported here were performed in a four-shell model space – but, we emphasize that the results in a six-shell model space would be essentially identical.

The energy-gap method. Haxton and Johnson [2] used a variant of the Millener–Kurath interaction [13] for the 0p1s0d model space and adjusted the four single-particle variables of this space to fit six low-lying $T=0$ states in ^{16}O. These four variables can be taken as the $0p_{3/2}$–$0p_{1/2}$, $0d_{3/2}$–$0d_{5/2}$, $1s_{1/2}$–$0d_{5/2}$ and $0p_{1/2}$–$0d_{5/2}$ energy splittings. The last of these we term the 0p–1s0d energy gap Δ_{psd}. In our variant of the Haxton–Johnson method we keep the first three of these splittings fixed at the WBT values and vary Δ_{psd} so as to place the 0_2^+ state ~ 6050 keV above the 0_1^+ state. We believe this one-parameter model contains the essence of the Haxton–Johnson four-parameter method. The necessary change in Δ_{psd} was from 11632 keV in the four-shell WBT interaction to $11632-3020=8612$ keV. The odd-parity $T=1$ states were calculated in a $(1+3)\hbar\omega$ model space using the same value of Δ_{psd}. This places the lowest predominantly $3\hbar\omega$ states ~ 5 MeV above the yrast states.

The $\Delta_{4\hbar\omega}$ method. One obvious fault in the energy-gap method is that the $2\hbar\omega$ states receive a double lowering, first by $2\times(11.632-\Delta_{psd})$ and again via the repulsive interaction with the $4\hbar\omega$ states. An obvious method which avoids this weakness is to lower the $4\hbar\omega$ components only. Then, this lowering can be viewed as the collective repulsive effect of $>4\hbar\omega$ excitations and should be roughly equal to the difference in binding of the ^{16}O ground state between $0\hbar\omega$ and $(0+2+4)\hbar\omega$ calculations. For the WBT interaction, it is found that a shift $\Delta_{4\hbar\omega}$ of -10.90 MeV places the 0_2^+ state at 6.05 MeV excitation at the same time as the ground state is lowered 10.60 MeV from the $0\hbar\omega$ value. The close agreement in these shifts is evidence for the consistency of this method. The $\Delta_{4\hbar\omega}$ found for the WBP interaction is -10.10 MeV. Be-

cause diagonalization in a $5\hbar\omega$ space is beyond our capabilities, the odd-parity states cannot be treated in as logical a fashion and we simply use the same produce for the odd-parity states as described for the energy-gap method.

The SU3(20) method. This method takes advantage of the fact that for a translationally invariant interaction and HO wave functions only the (20) and (42) SU3 tensor components of the central $\langle (\mathrm{sd})^2 | V | \mathrm{p}^2 \rangle$ interaction are non-zero and that, to a good approximation, the (42) component mixes low=lying states with $\Delta\hbar\omega = 2$ and the (20) component connects low-lying $n\hbar\omega$ states with high-lying $(n+2)\hbar\omega$ states. The SU3(20) component of $V^{2\hbar\omega}$ was set equal to zero by transforming from the *jj*-coupling basis used in OXBASH to an SU3 basis, setting all (20) TBME equal to zero and transforming back again. With all other TBME the same as in the WBT interaction, diagonalization in the four-shell model space produced a $(0+2+4)\hbar\omega$ ground state depressed by 2.7 MeV relative to a $0\hbar\omega$ calculation as compared to a depression of 10.6 MeV with the (20) symmetry included. With $\Delta_{4\hbar\omega} = -2.7$ MeV, the $4\hbar\omega$ first-excited state lies at 6005 keV.

The Δ_{4p4h} method. Although a complete $(0+2+4)\hbar\omega$ calculation is possible for ^{16}O, the dimensions are much larger for $A = 11$–15 nuclei for which an investigation of the role of $4\hbar\omega$ admixtures would also be of interest. In order to include $4\hbar\omega$ admixtures in these states a truncation of the $(0+2+4)\hbar\omega$ model space is necessary. We seek a truncation which preserves the essence of the $4\hbar\omega$ component. We test one here which appears to work rather well for ^{16}O at least. This truncation consists of the complete $(0+2)\hbar\omega$ model space coupled with a truncation of the $4\hbar\omega$ model space to a 4p–4h excitation of $0\mathrm{p}^{12}(1\mathrm{s}0\mathrm{d})^0$. With this truncation the *J*-dimension for 0^+ states is 2381. Calculations performed with this truncation are labeled $\Delta^{\mathrm{P}}_{4\mathrm{p}4\mathrm{h}}$. For simplicity, we shift the $4\hbar\omega$ components downward by the same amount, 10.10 MeV, as was used in the $\Delta^{\mathrm{P}}_{4\hbar\omega}$ method.

Comparison of results for the 0^+ states of ^{16}O. The spectrum of states calculated with the WBT-based interaction is illustrated in fig. 1. Our interest is in matrix elements involving the $T=0$ 0^+ states of ^{16}O and we have not considered other even-parity states. Haxton and Johnson [2] have shown that the present approach gives reasonable results for $J^\pi > 0^+$ states. The $\hbar\omega$ composition of the 0^+ states of ^{16}O obtained in the present calculations are compared to each other and to those reported by Haxton and Johnson [2] and Brown and Green [1] in table 1. Direct overlaps of the 0^+_1 and 0^+_2 states are compared in table 2. For preciseness we label the various calculations by superscripts T or P for a WBT or WBP basis, respectively. We note some relevant comparisons (a) The full $(0+2+4)\hbar\omega$ results of Haxton and Johnson are quite similar to the present energy gap results. (b) The energy gap method gives more $0\hbar\omega$ and $2\hbar\omega$ mixing in the ground state than the $\Delta_{4\hbar\omega}$ method. This is expected because of the explicit lowering of 2p–2h configurations in the energy gap method. (c) The SU3(20) method is closest to the Brown–Green method. This is expected because both are truncated so as to emphasize mixing between the

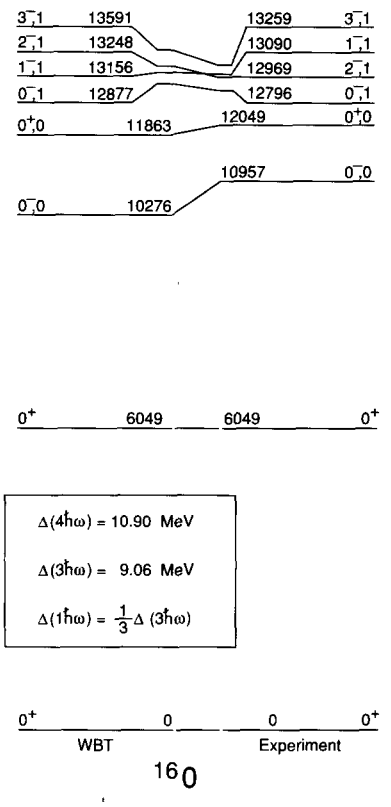

Fig. 1. The energy levels of ^{16}O pertinent to the present study. The theoretical levels were calculated with the WBT interaction with the indicated downward shifts to the different $n\hbar\omega$ components relative to the unshifted $0\hbar\omega$ and $2\hbar\omega$ components.

Table 1
The percentage of $0\hbar\omega$, $2\hbar\omega$, and $4\hbar\omega$ components in the wave functions of the first four ($k=1, ..., 4$) 0^+ states of ^{16}O for the five calculations described in the text. Results of the Brown–Green (BG) and Haxton–Johnson (HJ) calculations are also given. The first entry for the $k=2, ..., 4$ states is the excitation energy E_x (in keV).

Calculation	$k=1$ state			$k=2$ state				$k=3$ state				$k=4$ state			
	$0\hbar\omega$	$2\hbar\omega$	$4\hbar\omega$	E_x (keV)	$0\hbar\omega$	$2\hbar\omega$	$4\hbar\omega$	E_x (keV)	$0\hbar\omega$	$2\hbar\omega$	$4\hbar\omega$	E_x (keV)	$0\hbar\omega$	$2\hbar\omega$	$4\hbar\omega$
HJ	42	45	13	6050	4	5	90	12290	3	68	30	12800			
gap^P	48	41	11	6049	4	4	92	11101	11	62	27	12046	1	43	56
$\Delta^T_{4\hbar\omega}$	56	33	11	6046	4	3	93	11863	7	31	62	13090	3	25	72
$\Delta^P_{4\hbar\omega}$	55	33	12	6049	4	3	93	11932	9	37	54	12778	2	30	68
$SU3(20)^T$	85	14	1	6005	2	6	92	9682	4	81	15	12577	1	26	73
BG	76	22	2	6070	7	5	88	11260	17	73	10				
Δ^P_{4p4h}	60	31	9	5944	4	2	94	12597	2	13	85	13807	8	48	44

Table 2
Direct overlaps of the three $n\hbar\omega$ components (taken separately and normalized) in the ^{16}O 0^+_1 and 0^+_2 states. The amplitudes of the three components are in phase for the 0^+_1 state so that the sign of the fractional overlap is the phase of the given component in the 0^+_2 state.

Calculation	$n\hbar\omega$ component		
	$0\hbar\omega$	$2\hbar\omega$	$4\hbar\omega$
BG	+1.00	−1.00	−1.00
$SU_3(20)^T$	+1.00	−0.72	−0.72
$\Delta^T_{4\hbar\omega}$	+1.00	−0.01	−0.46
$\Delta^P_{4\hbar\omega}$	+1.00	−0.03	−0.49
gap^P	+1.00	+0.02	−0.47
Δ^P_{4p4h}	+1.00	−0.01	−0.50

first few 0^+ states, i.e., the SU3(20) method is the microscopic equivalent of the schematic Brown–Green model, in which only the SU3(42) tensor part of $V^{2\hbar\omega}$ acts between states with $\Delta\hbar\omega=2$. (d) The $2\hbar\omega$ components of the 0^+_1 and 0^+_2 states bear little resemblance to each other in either the $\Delta_{4\hbar\omega}$ or the gap calculation. This is because the main $2\hbar\omega$ admixture in the ground state is of SU3(20) character while that in the $4\hbar\omega$ states is of SU3(42) character [the SU3(20) states have no matrix element with the "deformed" 4p–4h state which has (84) symmetry in the SU3 limit]. (e) The SU3(20) method gives much less configuration mixing than is obtained in the full $(0+2+4)\hbar\omega$ diagonalizations. From this we conclude that a first-order perturbation treatment does not work well in this case. However, we fell that the SU3(20) method may be useful in other nuclei where $4\hbar\omega$ excitations are not so important.

We now test these wave functions by consideration of the unique first-forbidden β^- decay of the ^{16}N 2^- ground state to the first two states of ^{16}O – both with $J^\pi=0^+$. These decays are unique first-forbidden with only one matrix element M^z_2 entering in normal order [14]. The usual shell-model procedure is followed of forming single-particle matrix elements of the operator $r[Y_1, \sigma]^2\tau$ and combining them with the one-body transition densities which contain all the information on the initial and final wave functions [14]. The single-particle matrix elements are calculated with either harmonic oscillator (HO) or a combination of HO and Woods–Saxon (WS) wave functions. For the latter we use the geometrical parameters

of Streets, Brown and Hodgson [15] which reproduce the root-mean-square charge radii $\langle r^2\rangle^{1/2}$ of stable nuclei in the $A\sim 16$ region. For HO wave functions we use $\hbar\omega = 45A^{-1/3} - 25A^{-2/3} = 13.92$ MeV which gives closely the same $\langle r^2\rangle^{1/2}$ for ^{16}O as the WS value. One prescription to determine the WS wave functions is to vary the depth of the well to bind the nucleons to each specific parent state of the core at the separation energies $S(\mathrm{n})$ for ^{16}N and $S(\mathrm{p})$ for ^{16}O for the orbits involved in the transition. The value of the single-particle matrix element for a given pair of orbits then depends on the excitation energy of the core state. This dependence can be adequately represented by a linear dependence of the matrix element on the separation energy, or equivalently the excitation energy of the core. This assumption leads to our prescription for determining the separation energies $S(\mathrm{p}) - S(\mathrm{n}) = Q(\beta^-) - 0.782$ MeV, $S(\mathrm{n}) = 2.492 - E_x(^{16}\mathrm{N}) + \bar{E}_x$ MeV, $S(\mathrm{p}) = 12.128 - E_x(^{16}\mathrm{O}) + \bar{E}_x$ MeV, where $\bar{E}_x$ is an *effective* excitation energy [16] of the common parent state in the ^{15}N core and $Q(\beta^-) = 10419$ keV. In the simple $(0+1)\hbar\omega$ model, for example, $\bar{E}_x = 0$ for the dominant $\nu 0\mathrm{d}_{5/2} \rightarrow \pi 0\mathrm{p}_{1/2}$ transition. For all transitions other than $\nu(1\mathrm{s}, 0\mathrm{d}) \rightarrow \pi 0\mathrm{p}$ the $\bar{E}_x$ lie at quite high energy and thus the separation energies are large enough so that one might as well use HO wave functions and this we do.

For the two decays at hand the experimental data [17,18] yield $M^z_2(0^+_1) = 3.04 \pm 0.02$ fm and $M^z_2(0^+_2) = 1.09 \pm 0.18$ fm (table 2). For the wave functions obtained in the SU3(20) method, the theoretical $M^z_2(0^+)$ were calculated with effective operators designed to correct for the omission of the SU3(20) symmetry contribution in the 0^+ wave functions. The effective operators were derived as described in ref. [19] but using a pure SU3(20) $\mathrm{V}^{2\hbar\omega}$. The effective operators resulted in quenching of the bare nucleon $M^z_2(0^+)$ by $\sim 20\%$. For the other three sets of wave functions, the operator appropriate to bare nucleons was used. This is so because, to first order, the model space contains all possible contributions to the matrix elements.

Table 3
Matrix elements for the unique first-forbidden β decay of ^{16}N to the first two 0^+ states of ^{16}O.

Calculation	$M^z_2(0^+_1)$ (fm)		$M^z_2(0^+_2)$ (fm)	
	HO	WS	HO	WS
$\Delta^{\mathrm{I}}_{4\hbar\omega}$	3.51	3.53	0.84	0.84
$\Delta^{\mathrm{P}}_{4\hbar\omega}$	3.15	3.16	0.79	0.80
$\mathrm{gap}^{\mathrm{P}}$	2.84	2.86	0.80	0.80
$\mathrm{SU3(20)}^{\mathrm{P}}$	3.72	3.74	0.38	0.38
$\Delta^{\mathrm{P}}_{4\mathrm{p4h}}$	3.26	3.28	0.70	0.69
exp.	3.04(2)		1.09(18)	

A decomposition of the M^z_2 into the four possible $n\hbar\omega \rightarrow (n\pm 1)\hbar\omega$ transitions of which it is constituted is shown in fig. 2. The $n\hbar\omega$ contributions to the ground-state matrix element follows the classic pattern found for de-excitation of E1-like particle–hole configurations in a previous study of first-forbidden decays in the $A=40$ region [14]. In particular, the $1\hbar\omega \rightarrow 0\hbar\omega$ and $3\hbar\omega \rightarrow 2\hbar\omega$ matrix elements and the $1\hbar\omega \rightarrow 2\hbar\omega$ and $3\hbar\omega \rightarrow 4\hbar\omega$ matrix elements are closely equal and the latter two are out of phase with the former two. Because the particle–hole interaction is repulsive, configuration mixing within a specific $n\hbar\omega \rightarrow (n\pm 1)\hbar\omega$ transition is also destructive. For the ground-state $(n+1)\hbar\omega \rightarrow n\hbar\omega$ transitions, e.g., the sum of all other contributions are out of phase with

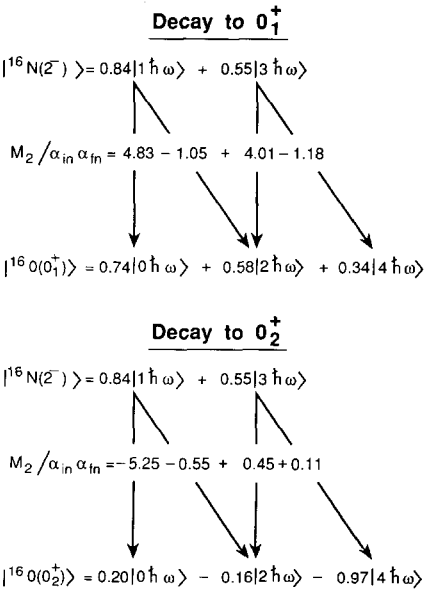

Fig. 2. Schematic showing the contributions of $n\hbar\omega \rightarrow (n\pm 1)\hbar\omega$ transitions to rank-two $2^- \rightarrow 0^+_{1,2}$ decays calculated with WS wave functions.

the dominant one giving a total $(n+1)\hbar\omega \rightarrow n\hbar\omega$ contribution ($n=0$ and 2) to $M_2^z(0_1^+)$ for $\Delta_{4\hbar\omega}^{\mathrm{T}}$ of 4.79–0.60 fm, where the first term is the dominant $\nu 0d_{5/2} \rightarrow \pi 0p_{1/2}$ contribution and the second is the remainder. In spite of the destructive interference which is a characteristic of these decays, the calculated M_2^z are in quite good agreement with experiment for all but the SU3(20) calculation. It was found that the first three results were very insensitive to changes of several MeV or less in the energy shifts adopted in the calculations. Thus the differences in the calculated M_2^z are mainly due to the differences in the WBT and WBP interactions.

As can be inferred from fig. 2, $M_2^z(0_2^+)$ is dominated by the $1\hbar\omega \rightarrow 0\hbar\omega$ contribution. For this reason it provides a very good test of the $0\hbar\omega$ admixture in the 0_2^+ wave function. Thus, we would say that this admixture is quite well predicted for all but the SU3(20) calculation and, indeed, the poor prediction in this case can be traced to the very small amount of $0\hbar\omega$ in the 0_2^+ wave function.

It is to be expected that the improvement in the 0p–1s0d cross-shell interaction [9] coupled with the ability to perform large-basis shell-model calculations illustrated here, will result in a significant improvement in our understanding of nuclear structure and electroweak observables in light nuclei.

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