Comment on "p-shell nuclei in a $(0+2)\hbar\omega$ model space. I. Method" and on "p-shell nuclei in a $(0+2)\hbar\omega$ model space. II. Results."

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We point out that the shell-model calculations of Wolters, van Hees, and Glaudemans for the p-shell nuclei in a $(0+2)\hbar\omega$ basis have several serious consistency problems, and we use the case of ^{16}O to illustrate these problems. We discuss some limitations of the parametrization used for the effective interaction, criticize the choice of experimental data used in the least-squares fit, and demonstrate that the resultant interaction exhibits some peculiar features which make it differ considerably from realistic interactions.

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In two recent publications [1,2] Wolters, van Hees and Glaudemans (WvHG) have reported on $(0+2)\hbar\omega$ shell-model calculations for normal-parity states of nuclei in the mass range A =4–16. A mass-independent interaction, universal for all active orbits, was obtained by fitting the Talmi integrals of a translationally invariant interaction to experimental data (the fit actually included static moment data, with four effective g factors and two effective charges as additional parameters). A final parameter was the spacing between the harmonic oscillator major shells which, to compensate for the strong mutual repulsion between $0\hbar\omega$ and certain $2\hbar\omega$ states, took the small value of $\hbar\omega$ = 9.78 MeV compared to $\hbar\omega$ = 13.54 MeV (b = 1.75 fm) required to fit rms charge radii.

A disturbing feature of the calculations of WvHG is that radial excitations, i.e., states with large $0p \rightarrow 1p$ and $0s \rightarrow 1s$ components, occur at low excitation energies in all nuclei. For the lighter even-even p-shell nuclei, the first excited 0^+ states are of this type and have a large overlap with the isoscalar giant monopole resonance (see Table VI of Ref. [1] and Table I of Ref. [2]). In addition, there tend to be substantial $1p1h$ admixtures in the ground-state wave functions. Toward the end of the p-shell, the 0_2^+ states are predicted to result predominantly from $p^2 \rightarrow (sd)^2$ excitations but states with large monopole matrix elements still occur at low excitation energies.

One purpose of this comment is to point out that the appearance of radial excitations in the low-lying spectrum is unphysical. Another is to examine the consistency of the way in which WvHG have handled the strong $\Delta\hbar\omega$=2 interaction. When empirical or realistic Hamiltonians which give a reasonable description of $0\hbar\omega$ and $1\hbar\omega$ spectra are used in full $(0+2)\hbar\omega$ spaces, the $\Delta\hbar\omega$=2 interaction pushes the ground state down by several MeV producing a spectrum in poor agreement with experiment. This was noticed in the first full $(0+2)\hbar\omega$ calculation [3] for ^{16}O and has been commented on many times since [4–9]. WvHG have restored the spectrum by starting with the *pure* $0\hbar\omega$ state well above the lowest $2\hbar\omega$ state prior to configuration mixing. In this way the excitation energy of the dominantly $0\hbar\omega$ states in the mixed $(0+2)\hbar\omega$ calculations are reproduced reasonably well. However, we are critical of the philosophy behind these procedures and point out that in consequence the fitted interaction exhibits a number of unphysical features. We discuss below general features of the problems with radial excitations and then go on to discuss a calculation for ^{16}O which illustrates these and other problems with $(0+2)\hbar\omega$ calculations.

The excitation energy of the giant monopole resonance (GMR) is directly related to the compressibility of the nucleus, and thus can be determined only by self-consistent calculations using saturating effective interactions. Self-consistent RPA calculations, which generally use density-dependent interactions, predict [10] the GMR to lie above 20 MeV of excitation in ^{16}O. On the other hand, as documented by Kirson [11], if harmonic oscillator wave functions are used with standard shell-model effective interactions the GMR is shifted strongly downwards from its unperturbed position. This is the situation that applies in the calculations of WvHG and in our example for ^{16}O. In self-consistent calculations, self consistency for the single-particle energies and wave functions (the $1p0f$ orbits are unbound), together with density dependence of the effective interaction, play important roles in determing the energy of the monopole state. A further difficulty arises because the matrix element between a $2\hbar\omega$ $1p1h$ state and the $0\hbar\omega$ state generally contains contributions from both the kinetic and potential energy operators. The matrix elements of these two operators are large but of opposite sign, so that the resulting values of $\langle 1p1h|T+V|0\hbar\omega\rangle$ cannot be determined reliably in non-self-consistent calculations [12]. If no constraints are introduced in full $(0+2)\hbar\omega$ calculations

to avoid these problems, the GMR is invariably predicted to lie very low in the spectrum and large percentages of $1p1h$ excitations are predicted in the ground-state wave functions. An analogous situation arises when diagonalizing full $(0+2)\hbar\omega$ spaces for higher-J states. On the other hand, if there is no $0\hbar\omega$ state of a given J, there is no monopole excitation and the low-lying $2\hbar\omega$ states will have a dominant $2p2h$ structure. For example, the class-A intruder states of WvHG are often dominantly $1p1h$ excitations and the corresponding $0\hbar\omega$ state has large admixtures of $1p1h$ configurations, while class-B intruder states are mostly $2p2h$ states.

We illustrate some of the problems with monopole states, and isolate the source of the strong $\Delta\hbar\omega=2$ mixing, by reference to a $(0+2)\hbar\omega$ calculation for ^{16}O. The configurations which are essential to describe the monopole state and to understand the $\Delta\hbar\omega=2$ mixing are listed in Table I. Results from full $(0+2)\hbar\omega$ diagonalizations are given in Table II. From Table I, we note the low energy of the monopole state (as expected from the discussion above) and that the large off-diagonal matrix element with the closed shell is concentrated in the $2p2h$ (2 0) configuration $|2\rangle$. The small values of the off-diagonal matrix elements for the L=S=0 $1p1h$ states are deceptive since $\langle\sqrt{5/6}(0p^{-1}1p) + \sqrt{1/6}(0s^{-1}1s)|T|0\rangle = 3\hbar\omega$ and the cancellation for the Millener-Kurath interaction [13] is fortuitous (for $\hbar\omega$=14 MeV). The qualitative similarity between our $(0+2)\hbar\omega$ diagonalization and that of WvHG is evident from Table II. However, if matrix elements of the saturating SGII interaction[14] evaluated with Hartree-Fock wave functions are used in our calculation, the monopole state is centered around 24 MeV relative to the closed shell and plays little role in the low-lying states. This does not mean that the monopole matrix elements for low-lying states should be very small. The monopole state as we, and WvHG, have used the term is the state created by operating on the closed shell with $\sum_i (r_i - R_{\rm c.m.})^2$ when using harmonic-oscillator wave functions, and monopole matrix elements are attributed entirely to these $\Delta\hbar\omega=2$ excitations. When more realistic radial wave functions are used, $\Delta\hbar\omega=0$ contributions to monopole matrix elements no longer vanish since the orbits of a major shell no longer have identical rms radii. However, delicate cancellations are inevitable and it is not clear that reliable estimates of monopole matrix elements can be made from conventional shell-model calculations.

WvHG have put considerable emphasis on the appearance of radial excitations at low-excitation energies and on the agreement between measured and calculated monopole matrix elements (Table VII of Ref. [1]). On the basis of the preceding discussion, this emphasis is unfortunate and the problem is exacerbated by the misidentification of model states with experimental counterparts. In the spirit of the venerable Brown and Green model [15], we would identify the lowest dominantly $2\hbar\omega$ 0^+ state with the 12.05 MeV level of ^{16}O and take the 6.05 MeV level to be the bandhead of a mostly $4p4h$ band. If the giant monopole state is centered where self-consistent calculations put it, little monopole strength remains at low excitation energy and we are left with another $2p2h$ state of mainly (0 4) symmetry, which is mixed with the monopole state to form the 0^+_3 and 0^+_4 states of Table II, and another $4p4h$ state, crudely speaking ^{12}C$(gs)\otimes^{20}$Ne(0^+_2), as candidates for the known 0^+ states at 14.03 and 15.10 MeV in ^{16}O. These conclusions regarding the structure of ^{16}O are consistent with the results of a calculation by Haxton and Johnson [9] who use the complete $(0+2+4)\hbar\omega$ shell-model space and address a number of the points referred to in this Comment. In the case of ^{12}C, the famous 7.65 MeV 0^+ state is usually described as a loose agglomeration of α particles and the entire monopole form factor can be beautifully described in calculations which treat it as such [16]. In this calculation, and in the ^{12}C plus α calculation [17] referred to below, configurations up to $20\hbar\omega$ and beyond are required to describe the radial structure of the excited states. It is inappropriate to attempt such a description in conventional shell-model calculations.

The question of the proper identification of $2\hbar\omega$ in-

TABLE I. Model $(0+2)\hbar\omega$ problem for $J=0$, $T=0$ states of ^{16}O. The basis consists of the closed shell and the [f]=[4444] $2\hbar\omega$ configurations with (4 2) and (2 0) SU(3) symmetry which, for a translationally invariant central interaction and harmonic-oscillator wave functions, are the only $2\hbar\omega$ configurations which have nonzero matrix elements with the closed shell. The expansions, in terms of shell-model basis states (columns 2 through 6), of 5 states which span the (2 0) space are given in the first five rows. The doubly and singly spurious states are denoted by $|D\rangle$ and $|S\rangle$. The important nonspurious states, for our purposes, are the monopole state $|M\rangle$ and the purely $2p2h$ state $|2\rangle$. The remaining nonspurious state $|1\rangle$ is given for completeness. The off-diagonal matrix elements (in MeV) of the basis states with the closed shell are given in the final row. Those of the nonspurious (2 0) states, with $\langle 1p1h|T+V|0\rangle$ set to zero, and of the (4 2) symmetry state are given in column 7. The corresponding diagonal matrix elements relative to the energy of the closed shell are given in column 8.

State	$p^{-2}(sd)^2$ (02)×(40)	$p^{-2}(sd)^2$ (02)×(02)	$p^{-2}(sd)^2$ (10)×(21)	$p^{-1}pf$ (01)×(30)	$s^{-1}sd$ (00)×(20)	Off-diag.	Diag.
$\|D\rangle$	$\sqrt{30/64}$	$-\sqrt{3/64}$	$\sqrt{25/64}$	$\sqrt{5/64}$	$-\sqrt{1/64}$		
$\|S\rangle$	$\sqrt{6/32}$	$\sqrt{15/32}$	$-\sqrt{5/32}$	$\sqrt{1/32}$	$-\sqrt{5/32}$		
$\|M\rangle$	$-\sqrt{30}/8\sqrt{23}$	$\sqrt{3}/8\sqrt{23}$	$-5/8\sqrt{23}$	$15\sqrt{5}/8\sqrt{23}$	$17/8\sqrt{23}$	-2.53	13.29
$\|2\rangle$	$\sqrt{10/62}$	$-\sqrt{25/62}$	$-\sqrt{27/62}$			10.42	22.36
$\|1\rangle$	$86/8\sqrt{23.31}$	$19\sqrt{10}/8\sqrt{23.31}$	$-\sqrt{30}/8\sqrt{23.31}$	$-31\sqrt{6}/8\sqrt{23.31}$	$31\sqrt{30}/8\sqrt{23.31}$	2.28	31.52
$\|(4\,2)\rangle$	1					-4.34	13.97
Off-diag	12.85	-10.14	1.78	-2.19	-1.31		

TABLE II. Full $(0+2)\hbar\omega$ basis results for $J=0$, $T=0$ states of ^{16}O. Case 1: No $\Delta\hbar\omega=2$ mixing. Case 2: $\Delta\hbar\omega=2$ mixing allowed (energies are given relative to the closed shell of case 1). Case 3: Wolters *et al.* (energies read from Fig. 25 of Ref. [2], $1p1h$ intensities from Table I of Ref. [2] and Table VI of Ref. [1]). The intensity of the closed shell in the case-2 ground state would decrease to a value closer to that of case 3 if an energy shift were applied to compensate for the $\Delta\hbar\omega=2$ mixing. The 0_2^+ state in cases 1 and 2 has a dominant (4 2) component (> 60%); in contrast, Wolters *et al.* obtain a dominant (2 0) component (Ref. [2]).

Case	Quantity	0_1^+	0_2^+	0_3^+	0_4^+
1	E (MeV)	0.0	9.5	12.4	13.7
	% $1p1h$	0.0	1.6	55.5	43.5
2	E (MeV)	−9.9	10.8	13.7	14.7
	% $1p1h$	3.1	18.7	48.5	29.0
	% $0p0h$	72.5	1.7	0.0	7.2
3	E (MeV)	0.0	7.8	11.1	13.5
	% $1p1h$	6.7	19.4	20.6	30.4
	% $0p0h$	55.7	0.1	a	a

[a]Not given by Wolters *et al.* (Refs. [1] and [2]).

truder states is clearly crucial when an interaction is to be obtained empirically by fitting energy-level data. However, WvHG include the 0^+, 2^+, and 4^+ of the $4p4h$ band in ^{16}O and the excited 0^+ level of ^{12}C in their fit. Other questions that one might raise about their fitting procedure are

(i) Is it wise to use a mass independent interaction to fit levels from $A=4$ to $A=16$ and is it wise to include very light nuclei, many of which exhibit pronounced cluster structures, in such a fit?

(ii) Is the use of a translationally invariant interaction too restrictive? In a fit in which the independent two-body matrix elements and the single-particle energies are varied, certain linear combinations of the parameters are well determined by the data. There is no guarantee, however, that these combinations can be reproduced within the restrictions imposed by a potential. In any case, medium and model-space renormalization effects, and the need to absorb the effects of real or effective 3-body forces, spoil the translational invariance of the G-matrix in the passage to an effective two-body interaction.

(iii) Should one allow the two-body interaction to determine the single-particle energies? Within the framework of the WvHG model at the $0\hbar\omega$ level, the spin-orbit splittings for the $0p$ hole states and the $0d$ particle states are given by $-(54I_1^o+30I_2^e)/8$, and $-(75I_1^o-30I_2^o+105I_3^o+30I_2^e)/8$, respectively, where the superscripts e and o refer to even- and odd-state spin-orbit forces. Thus, for short-range spin-orbit forces, there is a serious difficulty in reconciling the observed splittings at $A=15$ and $A=17$. Indeed, the interaction of WvHG gives 11.9 MeV for the splitting of the $0d$ orbits, to be compared with 5.08 MeV under the assumption of pure single-particle states in ^{17}O.

Our answers to the above questions are no, yes, and no, respectively. One might also ask what one gains by including the high-lying $2\hbar\omega$ states (after diagonalization of the $2\hbar\omega$ space) with the concomitant need to adjust so drastically the relative separation of the $0\hbar\omega$ and $2\hbar\omega$ configurations. This adjustment is necssary because $4\hbar\omega$, $6\hbar\omega$, ... configurations are not present to push on the $2\hbar\omega$, $4\hbar\omega$, ... configurations. This is a slowly convergent process as is well illustrated by ^{12}C plus α cluster calculations [17], which use a subset of the [4444] symmetry shell-model configurations for ^{16}O. Here, one is basically improving the ^{12}C-α relative wave function, and, as we observed in connection with monopole excitations, this is not something that can be handled well in limited-space shell-model calculations.

To understand better the nature of the $2p2h$ correlations in the ^{16}O ground state, we note that the strongly admixed $|2\rangle$ configuration of Table I has a large overlap with the $2\hbar\omega$ state which is formed by operating on the closed shell with two successive $E3$ operators, the dominance of such correlations having been demonstrated in early RPA calculations [18]. As indicated above, it would be very difficult to include such correlations consistently in all low-lying excited states. However, the concept of an effective charge for $E3$ transitions, to take into account these correlations and $1p1h$ excitations through $3\hbar\omega$, works well throughout the mass region of interest. The same is true for $E2$ transitions, where the effective charge takes into account $1p1h$ excitations through $2\hbar\omega$. We would argue that it is best to subsume the influence of high-lying configurations into effective one-body operators and to concentrate on getting a good description of the mutual mixing of low-lying configurations (of whatever nominal $\hbar\omega$ excitation energy). In this regard, we observe that the wave functions of the low-lying intruder states can generally be expressed in terms of relatively few weak-coupling configurations [19], so that it would make sense to start with such a basis (large shell-model codes can be used to generate all the matrix elements needed for such a calculation), giving up only the ability to eliminate spurious states exactly (in the usual har-

monic oscillator sense).

We turn now to the interaction obtained by WvHG (Table III of Ref. [1]) and compare it with other A-independent interactions. The p-shell two-body matrix elements, which depend only on the low-order Talmi integrals, are qualitatively similar to those from previous fits [20]. One would hope that this would be the case, albeit with some refinements due to the explicit inclusion of $2\hbar\omega$ intruder states, since many $0\hbar\omega$ states are included in the data set fitted. The other important sets of matrix elements for $p^2 \rightarrow (sd)^2$ excitations relate to the sd-shell interaction and the cross-shell $p(sd)$ interaction. We would argue that the sd-shell interaction should differ little from Wildenthal's universal sd-shell interaction [21] at $A = 18$ and that the cross-shell interaction would be a refinement of the Millener-Kurath interaction [13]. To see that this is far from the case, we observe that some of the higher order Talmi integrals are large and, in some cases, alternate in sign within a particular channel. This happens for the odd-state tensor force and to see the consequences we look at the tensor force contribution to the diagonal $0p_{1/2}1s_{1/2}$ matrix element for $J^\pi=0^-$ and $T = 1$, given by $-\frac{9}{2}I_1 + \frac{25}{3}I_2 - \frac{35}{6}I_3$, and find a contribution of 12.35 MeV. Taking now the full interaction, we find that the diagonal $0p_{1/2}^{-1}1s_{1/2}$ matrix element for $J^\pi=0^-$ and $T = 0$ has the value +18.5 MeV, compared with the small and attractive matrix element that, in a simple model, is necessary to shift the state from its unperturbed position of $\sim$ 12.4 MeV to 10.95 MeV excitation energy in ^{16}O. In fact, the entire tensor force obtained by WvHG is basically of the opposite sign to, and very much stronger than, that found in G matrices based on realistic NN interactions. To take an example for the sd-shell interaction, the diagonal $d_{5/2}^2$ matrix element for $J = 1$, $T = 0$ has the value -7.12 MeV compared with -1.63 MeV for Wildenthal's interaction. The difference comes almost entirely from the singlet-odd channel, another channel for which the Talmi integrals alternate in sign (these Talmi integrals are poorly determined in the fit but have large effects on important matrix elements). On the other hand, the $J = 5$, $T = 0$ matrix element, which is determined largely by the triplet-even central force differs from Wildenthal's value of -4.23 MeV by only 0.3 MeV. Clearly, the basic $(sd)^2$ spectrum obtained from the interaction of WvHG differs greatly from what one would expect on physical grounds, the more so because of the very large difference in their $d_{5/2}$ and $d_{3/2}$ single-particle energies. The same can be said of the simple $1\hbar\omega$ particle-hole spectrum which forms a basic building block in describing excitations across the major shell gap.

The pathological behavior of the effective interaction of WvHG arises in part because of the constraint that all matrix elements be derived from the same underlying potential, in part because the data set for cross-shell excitations is far too limited (basically to the excitation of a few pairs of particles) and in part to poor choices for the correspondence between experimental and theoretical states (this includes the problems with radial excitations).

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