Analysis of shell-model calculations for low-lying levels in ¹⁶C

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I have compared results of different shell-model calculations for the low-lying states of ¹⁶C. Comparisons include excitation energies, neutron occupancies, calculated matter radius of ¹⁶C, and the energy difference between mirrors ¹⁶C and ¹⁶Ne. I find that an older, simple calculation produces quite good agreement with experimental quantities.

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I. INTRODUCTION AND HISTORY

The structure of the low-lying states of ¹⁶C is a topic of current interest [1-5]. These levels themselves are of interest, but they are also useful as cores in certain calculations [3-8]of the low-lying states of ¹⁷C. Some time ago, we reported a shell-model calculation [9] (hereinafter referred to as Fo78) of these ¹⁶C levels in a simple model that has worked very well in predicting excitation energies and (t,p) reaction strengths in several light nuclei. We presented excitation energies and wave functions, along with the results of the ${}^{14}C(t, p){}^{16}C$ reaction. The model consists of two sd-shell neutrons coupled to the ground state (g.s.) of a p-shell core. It uses "local" singleparticle energies (spe's) and global two-body matrix elements (2BME's) [10]. Here I use the term "global" merely to indicate that the 2BME's do not change with A, in contrast to some other interactions and my spe's, which do. The 2BME's were derived for ¹⁸O [10], where the main accomplishment was the separation of the two-neutron structure from other structures involving core excitation. In Ref. [10] and in Fo78, the 2^+ and 4^+ states contained small amounts of configurations involving the $d_{3/2}$ orbital, but this orbital was omitted for the 0^+ states. It is present at some level, but the bulk of its strength lies 10–14 MeV above the first $(sd)^2 0^+$ state (see Table I). Furthermore, the 0⁺ 2BME's were derived [10] for the $d_{5/2}$ $s_{1/2}$ space. A later evaluation [11], which included the $1d_{3/2}$ orbital in the g.s., reduced the $2s_{1/2}$ occupancy from 1.07 to 0.96. I return to this point below.

Maddelena et al. [12] also performed calculations in a similar model, as did Bohlen et al. [13], who allowed excitation of the ¹⁴C core. In Ref. [12], the active neutrons were restricted to the *sd* shell, and active proton holes to the 1*p* shell. They presented two sets of shell-model calculations, using two different interactions from Warburton and Brown [14]. One interaction, called WBT, started with matrix elements derived from a bare G matrix and varied 28 linear combinations of the 95 p-sd 2BME's in a fit to energies of 165 states in several light nuclei. The other, called WBP, originated from one-boson exchange plus a long-range monopole interaction. It varied ten quantities in a fit to the same 165 energies. The root-mean-square (rms) deviations for these fits were 330 keV for WBT and 389 keV for WBP. For the in-shell parts, both used the universal *sd*-shell interaction (USD) [15], and a standard *p*-shell interaction [14]. The WBP calculations gave $C^2S(2s_{1/2}) = 0.60$, $C^2S(1d_{5/2}) = 1.23$; those with WBT gave 0.78, 1.07. They favored the latter on excitation energy

grounds, but the former from comparison to neutron knockout cross sections, which they were able to reproduce using overlap factors of 0.948 and 0.897 for $1/2^+$ and $5/2^+$, respectively. Experimental values of spectroscopic strengths derived from a comparison of experimental and calculated cross sections were 0.56(10) and 1.28(20) for $1/2^+$ and $5/2^+$, respectively.

Fujii *et al.* [1] performed a microscopic no-core shell-model calculation for ¹⁶C, using all orbitals up to and including 2p1f. They restricted excitations of the ¹⁴C core to two nucleons and allowed, at most, two nucleons in the 2p1f shell. Their two-body interaction was derived microscopically from the CD-Bonn potential [16] [The authors of Ref. 16 use CD to denote charge-dependent.] They found it necessary to refine their spe's in an orbit-dependent way to get the correct level ordering. These are their "dressed" calculations and are the ones discussed here. They found that their results support the decoupling of the two valence neutrons from the core.

Amos et al. [4] (hereinafter referred to as Am13) also recently presented results of shell-model calculations for ¹⁶C. They are inconsistent in their use of the term " $n\hbar\omega$ ". They did not cite our early paper [9], but they referred to a paper [5] that does cite it. They call our calculation a "simple $0\hbar\omega$ shell model" and theirs a "complete $(0+2)\hbar\omega$ shell model," even though their space is also $v(sd)^2 \pi (1p)^{-2}$. They stated that all their ¹⁶C states are "purely of $2\hbar\omega$ character". Am13 criticized our ¹⁶C calculation because "only neutrons were active." Their calculation allowed excitation of the ¹⁴C core, but only within the 1p shell. They assumed no *sd*-shell occupation of protons and no 1*p*-shell neutron vacancies—unlike the authors of Ref. [1] who allowed both. In fact, the $p_{1/2}$ proton occupancies in Am13 for the first 0^+ , 2^+ , and 4^+ are virtually identical-0.29, 0.30, and 0.32, respectively. They did not state the amount of excited ¹⁴C in their wave functions.

TABLE I. For each J^{π} in the $(sd)^2$ space, the excitation energy of the lowest state with a large $1d_{3/2}$ occupancy.

J^{π}	E_x (MeV)
0+	14.1
1+	10.8
2+	9.5
3+	10.6
4+	8.8

TABLE II. Excitation energies and J^{π} of low-lying states of ¹⁶C.

Source	Ref.	Exc	itation e	Ave. deviation ^a		
		2^{+}_{1}	$0^{+}{}_{2}$	$2^{+}{}_{2}$	4+	
Fo78	[<mark>9</mark>]	2.244	3.338	3.942	4.163	175 ^b
No core	[1]	1.67	3.82	4.31	4.98	465
Am13 Exp	[4] [15]	2.369 1.766	3.41 3.027	4.934 3.986	5.036 4.142	707

^aAverage of the absolute values of the deviations (in keV) between experimental and calculated excitation energies.

^bIncludes the contribution arising from the fact that our absolute energy for the g.s. is missed by 110 keV.

Am13 stated "The (proton) *p*-shell occupancies are less than what a packed model assumes." Yet their *p*-shell proton occupancies sum to 4.0000. I am not familiar with the term "packed model." If Am13 intended "packed" to imply a filled $1p_{3/2}$ orbital that certainly did not apply to our calculation. Our calculations [9] are for ${}^{14}C(g.s.) \ge (sd)^2$, where ${}^{14}C(g.s.)$ is the *p*-shell ${}^{14}C g.s.$, as given (for example) by Cohen-Kurath (CK) [17]. It is not an idealized subshell closure. In Cohen-Kurath, the $p_{1/2}$ occupancy is 0.3288.

Wuosmaa *et al.* [2] investigated the ¹⁵C(*d,p*) ¹⁶C reaction, in reverse kinematics, and analyzed the data with distorted-wave Born-approximation (DWBA) calculations. They used their experimental relative spectroscopic factors for the g.s. and excited 0⁺ state (plus closure) to deduce the s^2 occupancy in the g.s. Their result was 29% s^2 , 71% d^2 —considerably less s^2 than in most shell-model calculations. If they had normalized the DWBA curves to the data at forward angles, as is customarily done for direct reactions, their s^2 parentage in the g.s. would have been larger, but still less than most predictions. Their spectroscopic factors are in approximate agreement with the knockout results, and with one of the calculations found in Ref. [12].

As noted above, Maddelena *et al.* [12] investigated neutron knockout from ¹⁶C and deduced spectroscopic factors of 0.56 and 1.28 for the $1/2^+$ and $5/2^+$ states, respectively. This s^2 occupancy is also less than in most shell-model calculations, though in agreement with their WBP results. One non-shell-model (three body *n*-*n*⁻¹⁴C) calculation [18] produced even smaller 2*s* occupancy of about 0.20, and poor agreement with excitation energies. As the focus of the present paper is on

an analysis of shell-model calculations, I do not discuss this reference further.

Another shell-model calculation [19] is a major work, but I did not find there any numerical values of the quantities being compared here. From an inspection of their energy level diagram for ¹⁶C, it did not appear to be an improvement over the others I do cite.

II. COMPARISONS AND ANALYSIS

For various calculations of ¹⁶C, Table II lists the calculated excitation energies of the first and second 2⁺, second 0⁺, and first 4⁺ states. Also listed there are the experimental energies [20]. Each of these calculations also contains a 3⁺ state, whose structure is nearly pure $d_{5/2}s_{1/2}$. These four states, plus the 3⁺ and ground state, are all the six states that exist in a space of two $d_{5/2}$, $s_{1/2}$ neutrons plus a *p*-shell ¹⁴C g.s. Even with inclusion of the $d_{3/2}$ orbital, these six are the only low-lying states. This feature can be understood by an inspection of Table I, which lists the lowest state of each J^{π} that has an appreciable $d_{3/2}$ component.

In Fo78, the energies of the second 2^+ state and the 4^+ state are very well reproduced, but the calculated 2^+_1 and 0^+_2 energies are too large. The no-core calculations have very good agreement with the first 2^+ , but worse agreement for the other states. The Am13 energies are somewhat higher than those of Fo78 (which were already too high) for the first two excited states, but about 1 MeV too high for the other two. As a figure of merit, I have computed the average of the absolute values of the deviations between experimental and calculated excitation energies. These are listed in the last column of Table II. It can be seen that Fo78 energies provide the best agreement, with the no-core calculations second, and Am13 poorest, despite the statement of Am13 that the agreement "is quite reasonable for a shell-model calculation."

Neutron occupancies of *sd*-shell orbitals for the first 0^+ , 2^+ , and 4^+ states are listed in Table III for these three sets of calculations. For the g.s., I also list a later evaluation [11] of the Fo78 results that included the $d_{3/2}$ orbital, along with the results of the ${}^{15}C(d,p)$ ${}^{16}C$ reaction [2] and shell-model results of Maddelena *et al.* [12]. A comparison of the g.s. numbers suggests that the Am13 results are nearly identical to those of the second set from Maddelena *et al.* Also, for the g.s., the $2s_{1/2}$ occupancy is significantly larger in Fo78 and the no-core calculations than in the others. For the 2^+ state, Am13 and

TABLE III. Neutron occupancies of sd-shell orbitals in ¹⁶C.

Source	g.s.			2+			4+		
	$1d_{5/2}$	$2s_{1/2}$	$1d_{3/2}$	$1d_{5/2}$	$2s_{1/2}$	$1d_{3/2}$	$1d_{5/2}$	$2s_{1/2}$	$1d_{3/2}$
Fo78	0.930	1.070	_	1.308	0.630	0.063	1.978	0	0.022
Fo78 + $d_{3/2}$	0.837	0.963	0.20		As above			As above	
No core	1.01	0.97	≤0.17	1.17	0.81	≤0.18		Not given	
Am13	1.079	0.778	0.143	1.198	0.655	0.147	1.818	0.011	0.171
${}^{15}C(d,p)$	1.42	0.58	_						
Maddelena1	1.23,	0.60,	≼0.17,						
Maddelena2	1.07	0.78	≼0.15						

TABLE IV. Proton p-shell occupancies in ¹⁶C.

Source	State	$1 p_{3/2}$	$1 p_{1/2}$
Am13	g.s.	3.7118	0.2882
	2+	3.7026	0.2974
	4+	3.6799	0.3201
CK ^a	¹⁴ C (g.s.)	3.6712	0.3288
Exp. ^b	$^{14}C(g.s.)$	3.70	0.30

^aReference [17].

^bReference [21].

Fo78 are closer to one another than no-core is to either. For all these states in all the calculations the $d_{3/2}$ contribution is seen to be small.

As noted above, Am13 claimed that the excitation of the ¹⁴C core is important for the low-lying states of ¹⁶C. They considered only proton excitations within the 1*p* shell. Table **IV** lists their *p*-shell proton occupancies for the three states of Table **II**. They can be seen to be nearly identical for the three states, and about the same as in the g.s. of Cohen-Kurath. In fact, CK has slightly more $p_{1/2}$ occupancy than does Am13. The experimental numbers [21] (Table **IV**) are in agreement with CK.

Earlier, we calculated the matter radius of 16 C (along with those of several other neutron-excess C nuclei) [22]. We also computed the mass excess of the g.s. of 16 Ne in a potential model that assumed mirror symmetry [23]. I have redone those calculations with the other g.s. wave functions given above. The results are listed in Table V. All the computed radii are in the range of 2.57–2.62 fm, all slightly smaller than the matter radii of 2.76(6) [24] and 2.70(3) [25] fm extracted from measurements of reaction cross sections. We see that the matter radius is not sufficiently sensitive to the configuration admixtures to differentiate among the models on the basis of calculated radii. We do note, however, that those of Fo78 are closest to the experimental values.

The calculated energy of 16 Ne(g.s.) is much more sensitive, as is well known from the so-called Thomas-Ehrman effect:

TABLE V. Matter radius (fm) of ¹⁶C and energy of ¹⁶Ne (keV) calculated with the wave functions compared herein, and compared with experimental quantities.

Calc	$P(s^2)$	R_m	$E_x(\text{calc})^{c}$
Fo78	0.53	2.62	- 33
Fo78 + d3/2	0.48	2.61	+21
No core	0.45-0.49	2.61-2.62	12 to 52
Am13	0.389	2.59	116
$^{15}C(d,p)$	0.29	2.57	217
Maddelena1	0.30-0.32	2.57-2.58	184 to 207
Maddelena2	0.39-0.42	2.59-2.60	12 to 82
Exp.	_	2.76(6) ^a , 2.70(3) ^b	0.0

^aFrom Ref. [24].

^bFrom Ref. [25].

^cUsing an experimental mass excess of 23.986(20) MeV from Ref. [26].

the Coulomb energies of the $2s_{1/2}$ orbital are quite different from those for $1d_{5/2}$. This phenomenon is well reproduced in potential-model calculations. Table V lists the difference between the calculated and experimental mass excess of 23.986(20) MeV in the latest mass evaluation [26]. We see that the Fo78 calculations do best, with the no-core results a close second, and Maddelena2 not very far behind. Results with the other wave functions are unsatisfactory.

III. SUMMARY

I have compared the results of several shell-model calculations for the low-lying states of ${}^{16}C$. Comparisons include excitation energies, neutron occupancies, matter radius of ${}^{16}C(g.s.)$, and mirror energy difference between the ground states of ${}^{16}C$ and ${}^{16}Ne$. In all aspects, the simplest (and oldest) calculation [9] is found to provide the best agreement with experimental quantities. No-core calculations [1] give fair agreement. For the others agreement is unsatisfactory.

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