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Shell-Model Spectroscopy of f-p-Shell Nuclei with $A \leq 44$*

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The properties of all f-p-shell nuclei with $42 \leq A \leq 44$ have been calculated from one consistent shell model. The model space includes all Pauli-allowed states for all configurations of two, three, or four particles distributed among the four f-p shell orbits. The model Hamiltonian is a one-body plus two-body operator very similar to the "realistic" effective Hamiltonian of Kuo and Brown. Calculated results are given for excitation energies, single-particle transfer spectroscopic factors, electric-quadrupole and magnetic dipole moments, and $B(M1)$'s and $B(E2)$'s for transitions between low-lying states. The calculated results are in fair agreement with experimental information on these various observables. The results suggest that core-excitation effects are more important in the lower half of the $f_{7/2}$ shell than in the s-d shell.

I. INTRODUCTION

Among the earliest systematic studies of nuclei in terms of the nuclear shell model were the studies of nuclei in the $f_{7/2}$ region above ^{40}Ca reported by McCullen, Bayman, and Zamick (MBZ)[1] and by Ginocchio and French (GF).[2] They assumed an inert ^{40}Ca core, and restricted active particles to the $f_{7/2}$ shell. They were able to correlate a large amount of the then-known experimental data on many of the nuclei between ^{40}Ca and ^{56}Ni in terms of this model. There were, however, some states which clearly could not be described in terms of such a model. Since these early papers, there have been studies of some of the lightest of the nuclei in this region in a larger shell-model space. Most of these calculations have involved the calcium isotopes.[3-6] For these isotopes the most significant improvement, insofar as enlarging the model space within the f-p shell is concerned, occurred with the addition of the $p_{3/2}$ orbit to the active model space. There have also been some full f-p-shell calculations for ^{43}Sc reported.[7] The expansion of the shell-model space led to some significant improvement in the theory-experiment agreement for this nucleus. There have been no shell-model calculations reported for nuclei with $A \geq 44$ in which the full f-p shell is included in the model space, and which simultaneously considered energies, single-particle transfer strengths, and electromagnetic properties. There has been a significant increase in the amount of experimental information available on these nuclei in recent years with which the shell-model results can be compared. For these reasons, it seems worthwhile to make a systematic shell-model study of the light f-p-shell nuclei, using one model Hamiltonian and treating all f-p-shell orbits as active orbits. In this paper, the energy levels, single-particle transfer strengths, magnetic and quadrupole moments, and $B(M1)$ and $B(E2)$ values for transitions in nuclei with $A = 42$ to $A = 44$ are discussed.

This paper represents one part of a larger calculation of light f-p-shell nuclei. With the programs[8] used in these calculations, it is still impractical to carry out a complete f-p-shell model calculation for $A \geq 45$, but it is possible to treat nuclei with $A \geq 45$ in the space in which only the $f_{7/2}$ and $p_{3/2}$ orbits are active. In a forthcoming paper, the results obtained in the full f-p-shell calculations discussed here will be used as "experimental data" to determine effective operators which reproduce these "data" in an $f_{7/2}$-$p_{3/2}$ space. These operators will then be used to study nuclei with $A = 45$ and 46.

In Sec. II we discuss the model we use in some detail. In Sec. III we discuss the calculated energies and spectroscopic factors for the $A = 42$–44 nuclei, and in Sec. IV we discuss the electromagnetic observables in these same nuclei. Section V is a summary of these results. Some preliminary results of the calculations discussed here have been reported previously.[9]

II. DISCUSSION OF THE MODEL

In all the calculations discussed here, an inert ^{40}Ca core is assumed, and the $0f_{7/2}$, $1p_{3/2}$, $0f_{5/2}$, and $1p_{1/2}$ orbits are included in the active space. For nuclei with n active particles, all Pauli-allowed states of all configurations of the form $(\frac{7}{2}^{n_1}, \frac{3}{2}^{n_2}, \frac{5}{2}^{n_3}, \frac{1}{2}^{n_4})$ with $n_1 + n_2 + n_3 + n_4 = n$ are included in the basis space. Within this model space we diagonalize an effective one-body plus two-body Hamiltonian. We identify the resulting eigenvalues with observed energy levels, and we use the eigenvectors as wave functions to calculate various observables. We assume that the one-body part of the Hamiltonian operator is a diagonal operator which introduces effects due to the interaction of the active particles with the ^{40}Ca core. The eigenvalues of this operator are suggested by the observed spectrum of ^{41}Ca. The values used here, in MeV, are:

$$\tfrac{7}{2}=-8.36\,,\quad \tfrac{3}{2}=-6.26\,,\quad \tfrac{5}{2}=-1.86\,,\quad \tfrac{1}{2}=-4.46\,.$$

These values represent best guesses for the centroids of the single-particle strengths. The $^{40}Ca(d,p)^{41}Ca$ reaction has been studied experimentally.[10] The results suggest that in ^{41}Ca, the $f_{7/2}$ strength is almost entirely in the ground state, the $p_{3/2}$ strength is fragmented over two states, and the $p_{1/2}$ and $f_{5/2}$ strengths are even more highly fragmented.

In the first calculations we made, we used the matrix elements of the f-p shell effective interaction published by Kuo and Brown.[11] These matrix elements were determined by reaction matrix techniques from the Hamada-Johnston nucleon-nucleon potential. The interaction was designed for a model space which includes the orbits we include in our active model space, plus the $g_{9/2}$ orbit. There would be problems if we included this latter orbit in the model space. One is the practical problem that the resulting matrices would become prohibitively large. Further, the inclusion of the $g_{9/2}$ orbit would introduce states with spurious center-of-mass motion, and we do not have a practical way of handling such problems. From experiment,[10] we know that the orbit is at least 6 MeV above the $f_{7/2}$ orbit in ^{41}Ca. It has opposite parity from the f-p-shell orbits. For the latter reason, the f-p-shell states would admix only with states which contained at least two $g_{9/2}$ particles. Such states would be at a very high energy. In a previous study of the calcium isotopes,[5] this $g_{9/2}$ orbit was omitted, and the results suggested there that the omission was not significant.

TABLE I. List of matrix elements of model Hamiltonian (model H) used in calculations discussed in the text. Only the matrix elements involving $f_{7/2}{}^2, J, T$ states are shown. Also shown are the same matrix elements in the Kuo-Brown interaction.

J, T	Model H	Kuo-Brown
0,1	−2.22	−1.81
1,0	−1.45	−0.52
2,1	−1.15	−0.78
3,0	−1.07	−0.21
4,1	−0.36	−0.09
5,0	−1.10	−0.50
6,1	0.29	0.23
7,0	−2.42	−2.20

We have renormalized the Kuo-Brown interaction for the omission of the $g_{9/2}$ orbit in the following empirical way. We assumed that the most important matrix elements in the calculation were those involving the eight $|f_{7/2}{}^2, J, T\rangle$ states. That this is so is strongly suggested by the success of the MBZ and GF results. Thus, we treated the eight matrix elements involving these states as free parameters. The parameters were adjusted to optimize the agreement between calculation and observation for the excitation energies of 29 states, and for 7 ground-state binding energies. The resulting interaction is the one used in all calculations discussed here. The differences between the results obtained with this semiempirical interaction and those obtained with the Kuo-Brown interaction are not sufficient to warrant presenting both sets of results. The values of these eight adjusted matrix elements are given in Table I. The values of the same

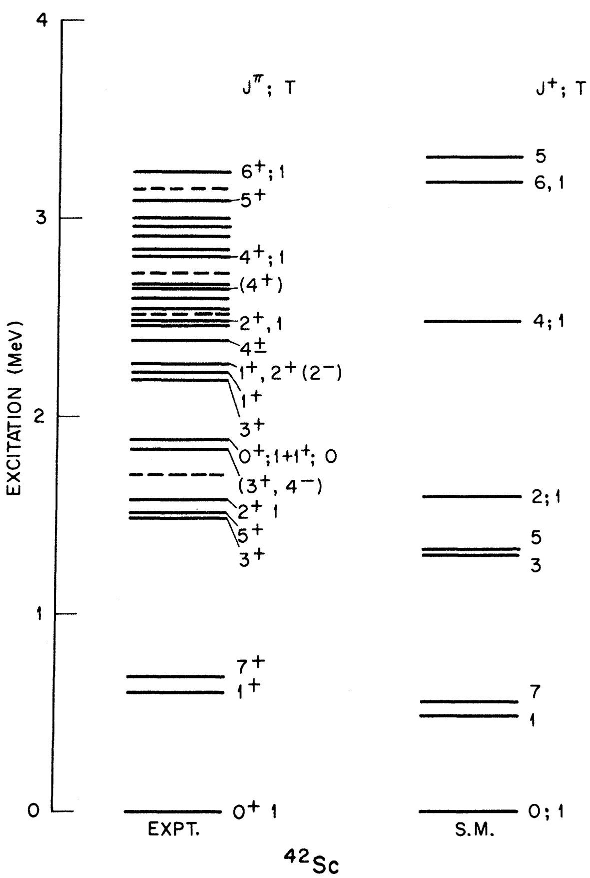

FIG. 1. Observed experimental and calculated shell-model excitation energies of low-lying $T=0$ and $T=1$ states in ^{42}Sc. All known levels below the highest level shown are included in the experimental spectrum. States for which a T label is omitted are $T=0$ states.

eight matrix elements as calculated by Kuo and Brown are also listed in Table I.

The effective operators used to calculate the electromagnetic observables will be discussed in the section on those calculations. The Oak Ridge-Rochester shell-model computer programs[8] were used for all these calculations. The searches made to determine the final effective interaction were made with programs written by Glaudemans and Wildenthal.[12]

III. ENERGY LEVELS AND SINGLE-PARTICLE STRENGTHS

A. A=42

The calculated and observed excitation energies[13] of $T=0$ and $T=1$ states in $A=42$ nuclei are shown in Fig. 1, and listed in Table II. The observed levels are those seen in ^{42}Sc. In this case, the $T=1$ states are also seen in ^{42}Ca. The single-particle strengths[14] for the neutron pickup reaction leading from ^{43}Ca to states in ^{42}Ca are also given in Table II. The energy levels of the $A=42$ system have been discussed[1-4, 15, 16] at some length several times, so we only briefly review the results here. There are nine $T=0$ levels in the calculated spectrum below 5.0 MeV. There are 13 positive-parity states observed below 4.0 MeV known to have $T=0$. For six of the calculated $T=0$ states, there are good experimental partners. There are also possible partners for the remaining three calculated $T=0$ states below 5 MeV. The lowest four of these, with $J=1$, 3, 5, and 7, are predominantly $f_{7/2}{}^2$ levels. There are six $T=1$ levels calculated to be below 5.0 MeV excitation. Four of these are the $f_{7/2}{}^2$ $T=1$ states with $J=0$, 2, 4, and 6, and for these there are excellent experimental partners. There are several levels of unknown spin in the observed spectrum which could be partners to the remaining two cal-

TABLE II. Calculated and observed excitation energies of and single-particle strengths to states in $A=42$ system. All states calculated to be below 5 MeV are listed, plus the first state of each J above 5.0 MeV in the calculated spectrum. The levels are listed in ascending order in both the calculated and observed columns, and the fact that levels in each column appear on same line does *not* imply these levels are partners. This is true in Figs. 3–6.

	Excitation (MeV)		Spectroscopic factors for $^{43}Ca \rightarrow {}^{42}Ca$			
	Calculated		Calculated		Observed[b]	
J,T	(MeV)	Observed[a]	$l=3$	$l=1$	$l=3$	$l=1$
1, 0	0.48	0.61				
1, 0	4.27	1.89				
1, 0	6.94	2.22				
2, 0	3.99	(2.27)				
2, 0	6.64	3.39				
3, 0	1.29	1.49				
3, 0	3.67	2.19				
3, 0	5.50	3.31				
4, 0	4.85	(2.39)				
4, 0	5.08	(2.65)				
5, 0	1.31	1.51				
5, 0	3.32	3.09				
5, 0	9.23					
6, 0	7.26					
7, 0	0.56	0.62				
0, 1	0	0	0.8	0.0		0.5
0, 1	5.72	1.83	0.0	0.0		0.1
1, 1	9.08		0.0	0.0		
2, 1	1.59	1.59	0.4	0.0		0.2
2, 1	4.16	2.48	0.0	0.0		0.1
2, 1	6.67	3.39	0.0	0.0		
3, 1	5.05	···	0.0	0.0		
4, 1	2.48	2.81	0.7	0.0		0.5
4, 1	4.87		0.0	0.0		
4, 1	6.74		0.0	0.0		
5, 1	5.23		0.0	0.0		
6, 1	3.18	3.24	1.0	0.0		1.0
6, 1	8.68		0	0.0		

[a] Reference 13. [b] Reference 14.

culated $T=1$ levels. There are at least 13 $T=1$ levels below 5.0 MeV in the observed spectrum. Thus, most of the calculated levels are accounted for in the experimental spectrum, but there are a large number of observed states unaccounted for. The lowest states not accounted for by the shell model are the $T=1$ states with $J=0^+$ and 2^+ at 1.88 and 2.48 MeV. These are now generally assumed to be 4p-2h states. They have been studied extensively in terms of core-excited or deformed-state bases by Zuker,[6] Gerace and Green,[15] and Flowers and Skouras.[16]

In Table II, the calculated spectroscopic factors (S factors) for the neutron pickup reaction are listed, as are numbers extracted from experimental cross sections for the $^{43}Ca(t,\alpha)^{42}Ca$ reaction by conventional distorted-wave analyses.[14] The agreement of calculated with experimental results is typical for these sorts of calculations. The strength calculated for the ground state is apparently split between the observed 0^+ states at 0 and 1.83 MeV. A similar situation holds for the lowest calculated 2^+ states. We consider the agreement for the absolute strengths between calculation and experiment to be acceptable when the uncertainties in the distorted-wave techniques are considered. Other conventional shell-model calculations[3-5] of ^{42}Ca and ^{42}Sc give results similar to these. The lowest eight calculated states are predominantly $f_{7/2}{}^2$ states. The MBZ and GF calculation used the energies of these states for the values of the matrix elements of their effective interaction.

B. $A=43$, $T=\frac{3}{2}$

In Table III and Fig. 2, the calculated excitation energies for negative-parity states in ^{43}Ca below 4.0 MeV are presented. Some of the observed[17] levels below 3.0 MeV are also shown. There are 19 levels known between 1.9 and 3.0 MeV in ^{43}Ca from γ-decay studies. We show only those with some spin assignment or which are seen in strip-

TABLE III. Calculated and observed excitation energies for states in the $A=43$, $T=\frac{3}{2}$ system, and calculated and measured single-particle strengths for neutron transfer to such states. All calculated and observed states below 4.0 MeV are listed, plus the first state of each J above 4.0 MeV in the calculated spectrum. (See also last lines of caption of Table II.)

	Excitation (MeV)			$(2J+1)S(42\to43)$		$S(44\to43)$	
$2J$	Calculated	Observed[a]	Δl	Calculated	Observed[b]	Calculated	Observed[c]
1	3.05	(2.61)	1	1.0	0.3	0.0	
1	4.06	(2.87)	1	0.9	0.2	0.0	
3	0.68	0.59	1	0.0	0.2	0.0	
3	1.69	2.04	1	3.6	3.0	0.1	0.1
3	3.19	2.94	1	0.1	0.2	0.0	
3	5.17		1	0.1		0.0	
5	0.41	0.37	3	0.0		0.1	0.1
5	3.28		3	0.0		0.0	
5	3.89		3	0.0		0.0	
5	5.02		3	0.0		0.0	
7	0	0	3	6.0	5.5	3.6	2.8-4.0
7	3.38			0.1		0.0	
7	3.63			0.0		0.0	
7	5.29			0.0		0.0	
9	1.72	(2.09)					
9	3.55	(2.25)					
9	4.66						
11	1.81	(1.68)					
11	4.43						
13	4.81						
15	3.00	(2.76)					
15	5.26						
17	8.27						
		2.10	1		0.1		
		2.62	3		0.1		
		3.29	1		0.2		
		3.31	1		0.1		
		3.57	1		0.2		
		3.81	(3)		0.2		
		3.86	1		0.1		

[a] Reference 17. [b] Reference 18. [c] Reference 14.

ping. We also show in Table III the calculated and measured single-particle strengths for neutron stripping and pickup to states below 4.0 MeV in ^{43}Ca. With the exception of the $\frac{3}{2}^-$ state at 1.69 MeV, all the states below 3 MeV in the calculated spectrum are essentially $f_{7/2}{}^3$ states. For all of these states there are reasonable possible partners in the experimental spectrum. There are many extra states in the observed ^{43}Ca spectrum for which there are no good theoretical analogs. The lowest extra negative-parity state is probably the $\frac{3}{2}^-$ state at 2.04 MeV. There are at least six nonnormal parity states below 3 MeV. There has been little theoretical effort made to understand the structure of these levels, and it is difficult to give a simple picture.

In Table III, the calculated strengths for neutron pickup and stripping are tabulated, as are the available experimentally determined strengths.[18] The lengths of the lines in Fig. 2 are proportional to the stripping strengths. There are no discrepancies of consequence for these numbers, except for the strength to $\frac{1}{2}^-$ states. The calculation yields considerable $l=1$ strength to two $\frac{1}{2}^-$ states, at 3.05 and 4.06 MeV, while there are no strong transitions to $\frac{1}{2}^-$ states known. There are a number of $l=1$ transitions observed with small strengths, implying that the $p_{1/2}$

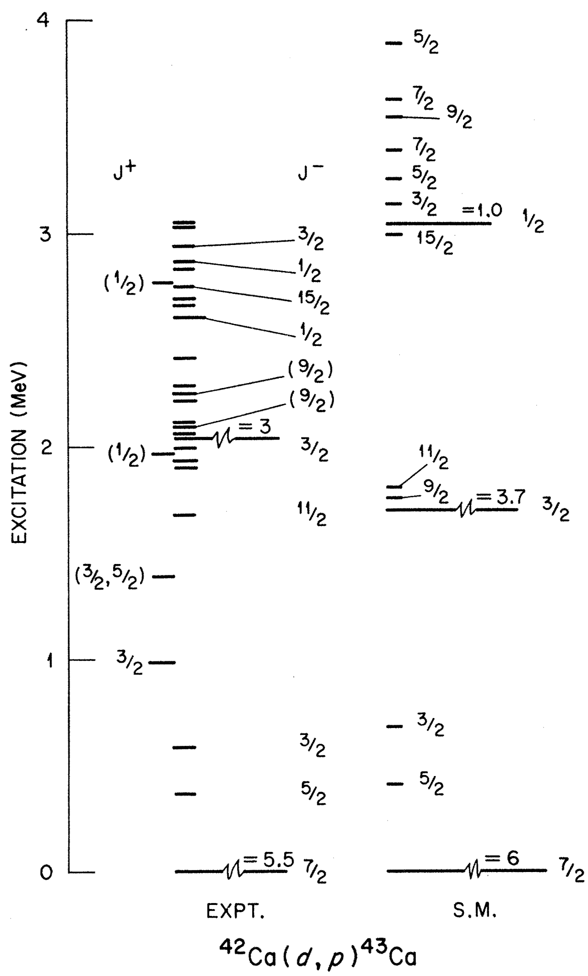

FIG. 2. Observed experimental and calculated shell-model excitation energies of ^{43}Ca. Levels seen with significant strength in the ^{42}Ca$(d,p)^{43}$Ca reaction are shown with longer lines, and the numbers above the line are $(2J+1)S$ values. All known levels below 3.0 MeV are included in experimental spectrum and all levels below 4.0 MeV are included in the calculated spectrum. In the observed spectrum, positive-parity levels are drawn to the left and negative-parity levels are drawn to the right.

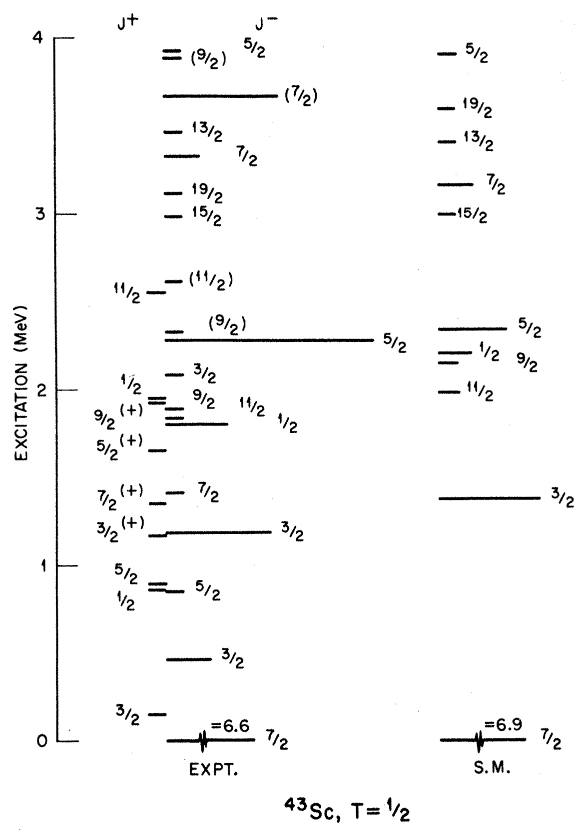

FIG. 3. Observed experimental and calculated shell-model excitation energies in ^{43}Sc. Some observed levels of indefinite spin and parity are omitted from the experimental spectrum above 3.0 MeV. The lengths of the lines are proportional to the strengths $(2J+1)S$, in the ^{42}Ca$(^3$He$,d)^{43}$Sc reaction. For a normalization, the calculated strength to the lowest $\frac{3}{2}^-$ state is 1.2. For the many short lines of equal length, no strength is to be implied. In the observed spectrum, positive-parity levels are drawn to the left, and negative-parity levels are drawn to the right.

strength is highly fractionated. The calculations for the pickup strengths are quite consistent with experiment. As pointed out above, the pure $f_{7/2}{}^3$ model[1,2] accounts for all calculated levels below 3 MeV except for the $\frac{3}{2}^-$ state at 1.69 MeV. The results here are very similar to the results for ^{43}Ca in the $f_{7/2}$-$p_{3/2}$ space.[3,4]

C. $A=43$, $T=\frac{1}{2}$

The calculated and observed[19] excitation energies for the $A=43$, $T=\frac{1}{2}$ system, ^{43}Sc, are listed in Table IV, and are shown in Fig. 3. (The energy level calculation is essentially the same as the one reported by Zamick and Ripka.[7]) The calculated and measured[20] strengths for the proton stripping reaction to states in this system are given in Table IV. In Fig. 3, the lengths of the lines are proportional to the stripping strengths. There are 11 negative-parity states below 4.0 MeV in the calculated spectrum and there are good experimental analogs now known for all these states. There are at least eight other negative-parity states below 4.0 MeV in the observed spectrum of ^{43}Sc. We have also shown nine nonnormal parity states in Fig. 3 below 5.0 MeV. There is a curious similarity between a set of states in the observed spectrum of ^{43}Sc and a set of low-lying states observed in ^{19}F. If we assume that the state observed at 1.89 MeV in ^{43}Sc is a $\frac{9}{2}^-$ state, then we see that there is a well-defined negative-parity $K=\frac{3}{2}^-$ band consisting of states as follows: $\frac{3}{2}^-$ at 0.47 MeV; $\frac{5}{2}^-$ at 0.85 MeV; $\frac{7}{2}^-$ at 1.41 MeV; $\frac{9}{2}^-$ at 1.89 MeV; and $\frac{11}{2}^-$ at 2.67 MeV. In the positive-parity spectrum, there also exists a series of states which might be identified as a $K=\frac{3}{2}^+$ band. We see that for the same J's the various members of these two $K=\frac{3}{2}$ bands of opposite parity are almost degenerate with each other. In ^{19}F, where there is a one-proton–two-neutron system as in ^{43}Sc, there is a ground-state $K=\frac{1}{2}^+$ band, and a $K=\frac{1}{2}^-$ band almost degenerate with it. In ^{19}F, these two bands are 3-p– and 4-p–1-h bands, while in ^{43}Sc, the bands have been interpreted by Johnstone[21] as 5p-2h and 4p-1h states. If this interpretation is correct, we then would say that the states observed at 1.83 and 2.33 MeV are the experimental partners to

TABLE IV. Calculated and observed excitation energies in the $A=43$, $T=\frac{1}{2}$ system, and calculated and measured strengths for proton stripping reactions to ^{43}Sc. All calculated and observed levels with known negative parity below 4.0 MeV are shown, plus the first state for each J above 4.0 MeV in the calculated spectrum. (See also last lines of caption to Table II.)

$2J$	Excitation (MeV) Calculated	Observed [a,b]	Δl	$(2J+1)S$ (^{42}Ca → ^{43}Sc) Calculated	Observed [c]
1	2.21	(1.81)	1	0.4	0.7
1	5.47		1	0.3	
3	1.37	0.47	1	1.2	0.5
3	4.80	1.18	1	1.1	1.2
3		2.09	1		0.1
5	2.34	0.85	3	0.8	0.1
5	3.90	2.29	3	0	2.4
5	5.13	3.93	3	0	0.2
7	0	0.0	3	6.9	6.6
7	3.16	1.41	3	0.4	
7	4.26	(3.33)	3	0	0.4
7	4.64	3.67	3	1.3	1.3
9	2.15	(1.89)			
9	4.14	(2.33)			
9		(3.89)			
11	1.98	1.83			
11	4.46	(2.62)			
13	3.41	3.46			
13	4.93				
15	2.99	2.98			
15	5.79				
17	4.58				
19	3.59	3.12			
19	8.87				

[a] Reference 19.
[b] J. C. Manthuruthil, C. P. Poirier, and J. Walenga, Phys. Rev. C 1, 507 (1970).
[c] Reference 20.

the $\frac{11}{2}^-$ and $\frac{9}{2}^-$ states in the $(fp)^3$ model. The calculated strengths for proton stripping to ^{43}Sc states are in only qualitative agreement with experiment. The observed strengths for transitions to the first $\frac{1}{2}^-$ and second $\frac{3}{2}^-$ states are in fair agreement with the calculated strenghts. If we consider the second observed $\frac{5}{2}^-$ state to be the partner to the first calculated $\frac{5}{2}^-$ state, then the calculated strength for the transition to this state is only one third of the observed strength. The MBZ and GF calculations account for all the levels below 4.0 MeV in the calculated spectrum in Fig. 3 except for the lowest $\frac{1}{2}^-$, $\frac{3}{2}^-$, and $\frac{5}{2}^-$ states.

D. $A=44$, $T=2$

The calculated and observed[22] excitation energies for the $A=44$, $T=2$ (^{44}Ca) system are given in Table V, as are the strengths for the neutron stripping reaction. These data are presented graphically in Fig. 4. The 0^+ and 2^+ states observed at 1.90 and 2.66 MeV are generally assumed to be core-excited states.[3,6,23,24] If we ignore these two levels, there is fairly good agreement between theory and experiment for the excitation energies of the low-lying states. For this nucleus, there is generally good agreement between theory and experiment[25] for the strengths in the neutron stripping reaction to states in ^{44}Ca. Experiment shows there is some single-particle strengths to the ground state and the deformed 0^+ state at 1.90 MeV, as well as to the first 2^+ state and to the deformed 2^+ state at 2.66. The strengths for the first 0^+ and first 2^+ calculated states are in agreement with the summed strength to the two 0^+ and two 2^+ states. There is a discrepancy here for the two 4^+ states. In nature almost all the strength goes into the second 4^+ state, while in the calculation two thirds of the strength is to the first 4^+. These states are predominantly $f_{7/2}{}^4$ states. In the $f_{7/2}{}^4$ configuration there are two 4^+ states, one with seniority 4 and one with seniority 2. Only the seniority-2 state can be strongly populated from the ground state of ^{43}Ca, which is primarily an $f_{7/2}{}^3$, $J=\frac{7}{2}$ state with seniority one. The experiment suggests there is not much seniority mixing, while the calculation implies significant mixing. In previous calculations,[5] we found that this seniority mixing was somewhat sensitive to the center of gravity of the $p_{3/2}$ strength, and that the distribution of strength in the ^{43}Ca$(d,p)^{44}$Ca reaction could be reproduced by effectively raising this centroid by about 0.5 MeV. We suggested that the center of gravity of the $f_{7/2}$-$p_{3/2}$ $T=1$ interaction in the Kuo-Brown interaction was too strong, and that raising this center of gravity by 200 keV corrected this defect in ^{44}Ca, as well as some more obvious problems for heavier calcium isotopes. Thus, this discrepancy here is not considered

TABLE V. Calculated and observed excitation energies of states in $A=44$, $T=2$ system, and strengths for neutron stripping to these states. All calculated and observed positive-parity states below 4.0 MeV are listed, plus the first state of each J above 4.0 in the calculated spectrum. (See also last lines of caption to Table II.)

J	Excitation energy (MeV) Calculated	Observed[a]	Δl	$(2J_f+1)/(2J_i+1)S$ (^{43}Ca$\to^{44}$Ca) Calculated	Observed[b]
0	0	0	3	0.5	0.4
0	4.63	1.90	3	0.0	0.1
		3.59			
1	4.45				
2	1.51	1.16	3	0.8	0.4
2	2.85	2.66	3	0	0.5
2	3.71	3.30			
2	4.71				
3	4.43				
4	2.43	2.29	3	1.0	0.2
4	2.71	3.04	3	0.5	1.5
4	4.36				
5	3.59	3.66			
5	4.79				
6	3.23	3.30	3	2.2	2.5
6	5.91				
7	6.66				
8	5.20				
...		3.93	1		0.0

[a] Reference 22. [b] Reference 25.

as a serious one. (All the energy-level calculations reported here were also done with the same interaction as we have used here, but with the $f_{7/2}$-$p_{3/2}$ interaction center of gravity raised. This change had no effect on the calculated energies of the nuclei with $A \leq 44$. There are not enough data in this energy region which are useful in determining the $f_{7/2}$-$p_{3/2}$ matrix elements, so we omitted this change.) The MBZ and GF calculations account for all the states below 4 MeV in the calculated spectrum except for the third 2^+. The complete f-p-shell results are also similar to the results obtained in the $f_{7/2}$-$p_{3/2}$ calculations,[3,4] except for some differences with regard to the first excited 0^+ state.

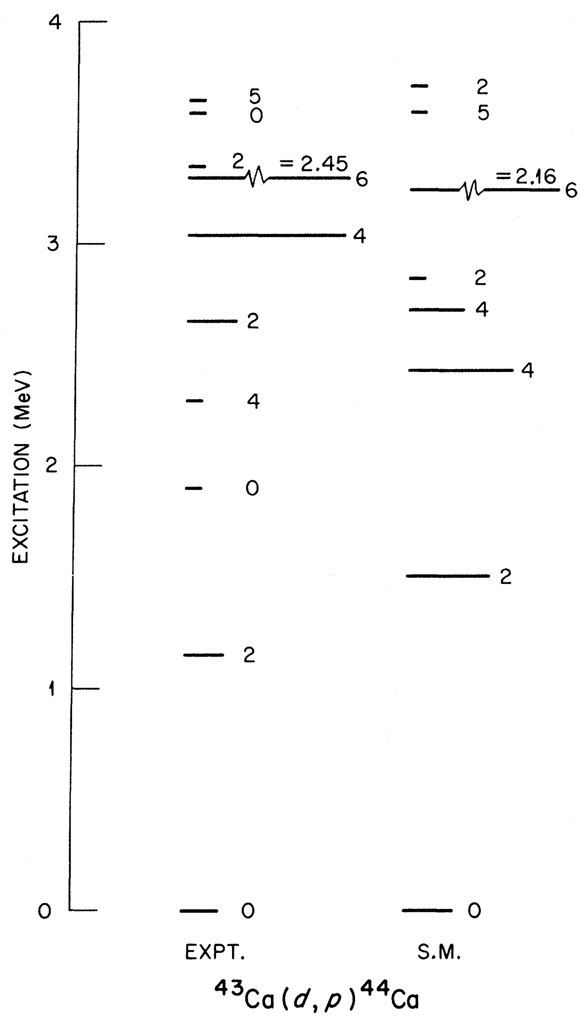

FIG. 4. Observed experimental and calculated shell-model excitation energies of states in ^{44}Ca. The lengths of the lines are proportional to the strength, $(2J+1)S$, for the ^{43}Ca$(d,p)^{44}$Ca reaction. For a normalization, the strength to the first 2^+ in the calculation is 0.8.

E. $A=44$, $T=1$

The calculated and observed[26] excitation energies of states in the $A=44$, $T=1$ (^{44}Sc) system are listed in Table VI, as are the calculated and measured strengths for the proton stripping reaction to these states. There are 11 states in the calculated spectrum up to about 2 MeV excitation. In the same energy region in the observed spectrum, there are at least 18 states with positive parity. For 10 of the 11 calculated states there are good experimental partners. This still leaves a large number of observed low-lying positive-parity states with no partner in the calculated spectrum. Johnstone[27] has studied the negative-parity states of ^{44}Sc in terms of a 5p-1h model, and suggests there is a low-lying $K=0^-$ band with states of spin 0^-, 1^-, 2^-, etc. This could account for many of the low-lying negative-parity states.

The calculated strengths are in good agreement with the experimentally determined[28] strengths. There is very little $l=1$ strength predicted or observed to the low-lying states in ^{44}Sc, and the absolute $l=3$ strengths are in better agreement with experiment than would have been reasonably expected.

In the calculation, the lowest state of each J from 1 to 7 is predominantly an $(f_{7/2})^4$ state. For this set of eight states, the calculated spectrum as shown in Fig. 5 is very similar to the MBZ and GF calculated spectra. For these same states, the calculated strengths for the ^{43}Ca$\rightarrow$^{44}Sc stripping reaction as calculated in the $(fp)^4$ space are very similar to the strengths to the same states as calculated[28] in the $f_{7/2}{}^4$ space. The main effect on the calculated spectra of low-lying states in ^{44}Sc due to increasing the space from $f_{7/2}{}^4$ to $(fp)^4$ is the introduction of a second 3^+ and 5^+ state at a rather low excitation.

F. ^{44}Ti

The calculated and observed[29] excitation energies for ^{44}Ti are shown in Fig. 6. There are only five $(fp)^4$ states below 4 MeV in the calculated spectrum. There are at least 10 states below 4.0 MeV in the observed spectrum. The first obvious "nonspherical" states in the observed are the 0^+ and 2^+ states at 1.90 and 2.54 MeV. These are again states analogous to states at a similar energy in ^{42}Sc, and most likely are 6p-2h states. As noted previously, one of the most interesting aspects of the calculated spectrum here is the fact that the levels in the "ground-state band" are almost evenly spaced, instead of the $J(J+1)$ dependence seen for the s-d shell analog of ^{44}Ti, ^{20}Ne. This point has been discussed at length.[30]

TABLE VI. Calculated and observed excitation energies of states in the $A=44$, $T=1$ system, and calculated and measured strengths for the ^{43}Ca-^{44}Sc reaction. All known calculated and observed positive-parity levels below 3.0 MeV are shown. (See also last lines of caption to Table II.)

J	Excitation energies (MeV) Calculated	Observed [a]	$(2J_f+1)/(2J_i+1)C^2S$ Calculated $l=3$	$l=1$	Observed [b] $l=3$	$l=1$
1	0.77	0.67	0.2		0.2	
1	2.70		0.1			
2	0.0	0	0.3	0.0	0.3	
2	2.23		0.0	0.1		
2	2.82		0.0	0.0		
3	0.80	0.77	0.2	0.0	0.2	0.1
3	1.35	0.98	0.4	0.0		
3	2.71	1.19	0.0	0.0	0.5	0.0
3	2.97		0.1	0.0		
4	0.43	0.35	0.5	0.0	0.5	0.0
4	1.95		0.1	0.0		
4	2.76		0.0	0.2		
5	1.23	1.06	0.4	0.1	0.3	0.2
5	1.63	1.53	0.5	0.0	0.8	0.0
5	2.79		0.1	0.0		
6	0.61	0.27	0.7		0.7	
6	2.63		0.2			
7	1.33	0.97	1.6		1.6	

[a] Reference 26.

[b] Reference 28.

It is not possible to populate states in ^{44}Ti with any single-particle transfers from stable targets.

IV. ELECTROMAGNETIC PROPERTIES

In this section we will discuss the calculated and observed $M1$ and $E2$ transition rates and the magnetic dipole and electric quadrupole moments. We first discuss the operators which we use to calculate these observables, and then compare the calculated numbers with the available experimental data.

A. Effective Magnetic Dipole Operator

The conventional starting point in the construction of the effective magnetic dipole operator for a shell-model calculation is the operator for the free nucleon. In shell-model calculations of nuclei in the s-d shell,[31] it was found that this "bare" operator led to very good agreement between calculated and observed magnetic moments. There were too few data on $M1$ transitions at the beginning of the s-d shell to assess the accuracy of the bare operator in calculating $B(M1)$ values. In the f-p shell, the measured[32] magnetic moment for the ground state of ^{41}Ca is $-1.59\mu N$. The bare operator gives a value of $-1.91\mu N$. This indicates that the bare operator is not adequate in this region. This has been discussed in some detail recently by Arima[33] and by Nomura and Yamazaki.[34]

The $M1$ operator for a free nucleon is assumed to have the form

$$O^{M1}=\sum_{i=1}^{A}\left[\tfrac{1}{2}+t_z(i)\right]\left[\bar{l}(i)+\mu_p\bar{\sigma}(i)\right]+\left[\tfrac{1}{2}-t_z(i)\right]\mu_n\bar{\sigma}(i),$$

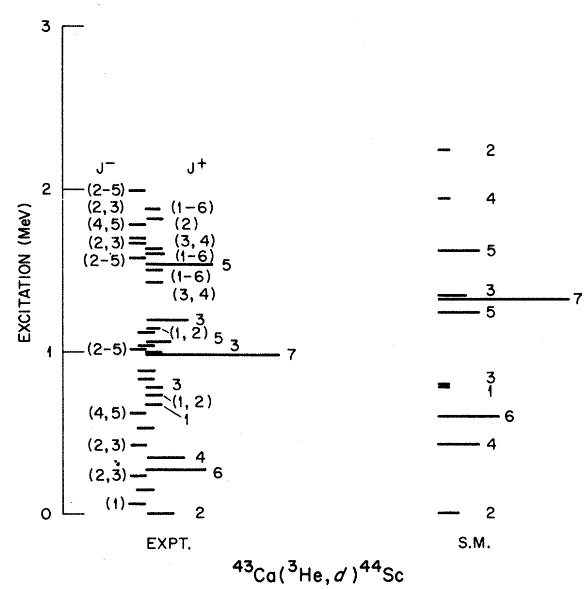

FIG. 5. Observed experimental and calculated shell-model excitation energies in ^{44}Sc. All levels below 2.0 MeV in calculated and observed spectra are shown. The lengths of the longer lines are proportional to the strengths $(2J+1)S$ in the ^{43}Ca(^{3}He,d)^{44}Sc reaction.

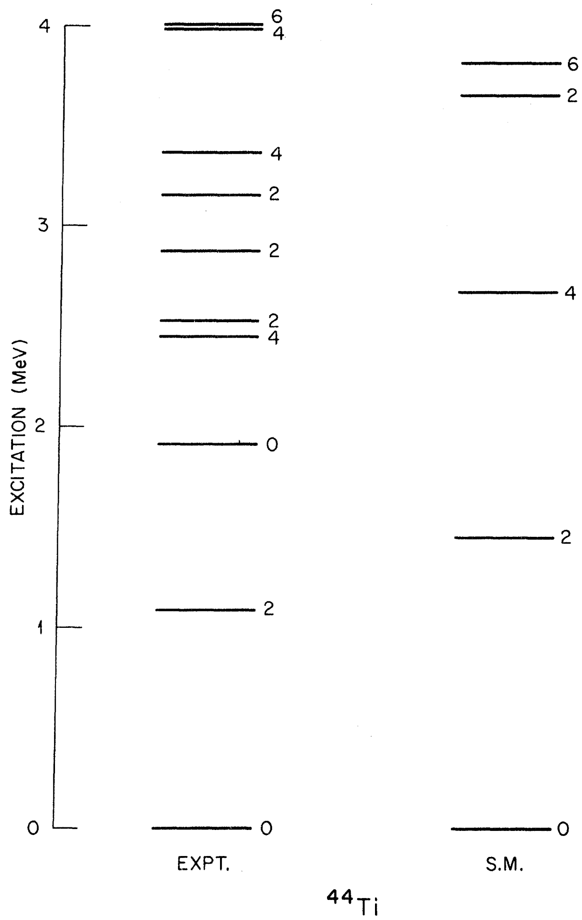

FIG. 6. Observed experimental and calculated shell-model excitation energies in ^{44}Ti. All known levels below 4.0 MeV are shown. All levels shown in this figure have positive parity.

where $t_z = +\frac{1}{2}$ for a proton.

Three types of corrections to this "bare" magnetic dipole operator have been considered:
(1) Corrections due to 1p-1h excitations of the core. For nuclei with one particle outside a closed shell, this is the only first-order correction for any one-body operator. Because of the structure of the bare $M1$ operator, there is no correction to first order for the magnetic moment of a single particle moving outside a core which is doubly closed in jj coupling. Thus, effects due to these "core-polarization" terms enter for the first time at second order in ^{41}Ca and ^{41}Sc.
(2) Corrections due to admixtures of 2p-2h deformed states in the low-lying states of these light f-p-shell nuclei, which enter first at second order.
(3) So-called meson-exchange corrections. These occur because the mesons which are exchanged by nucleons in a many-nucleon system can interact with the electromagnetic field as do the nucleons. Theoretical estimates[35] of the vector part of this effect lead to a correction to the orbital g factor

$$g = 0.2 l t_z .$$

All three types of correction should affect the $M1$ operator in both the s-d shell and the f-p shell. Apparently, a fortuitous cancellation of the contributions for light s-d-shell nuclei lead to the fact that the bare operator is the "effective" operator for that region, but such a cancellation does not occur around ^{40}Ca. Nagamiza and Yamazaki[36] have made an analysis of observed magnetic moments throughout the Periodic Table which offers

TABLE VII. Observed magnetic moments in $A = 41$–44 nuclei, and magnetic moments calculated with various $M1$ operators. Numbers in the column headed Bare were calculated with the "bare" $M1$ operator. Numbers in the second column were calculated with the operator in which an approximate meson-exchange term was added to bare operator. Numbers in third and fourth columns were calculated with these same two operators, but in both cases the isovector matrix element $\langle f_{7/2} \| M1^{T=1} \| f_{7/2} \rangle$ was modified so that the ^{41}Ca magnetic moment was reproduced in calculation.

		Magnetic moment (μ_N)				
Nucleus	J^π	Bare	Bare $+0.2lt_z$	Bare $+f_{7/2}$ effective	Bare $+0.2lt_z + f_{7/2}$ effective	Expt.
^{41}Ca	$\frac{7}{2}^-$	−1.91	−2.21	−1.59	−1.59	−1.59 [a]
^{42}Ca	6^+	−2.88	−3.41	−2.34	−2.34	−3.0 [b]; −2.52 [c]
^{43}Ca	$\frac{7}{2}^-$	−1.67	−1.99	−1.36	−1.36	−1.32 [a]
^{43}Sc	$\frac{7}{2}^-$	4.80	4.96	4.61	4.59	4.61 [a]
^{43}Sc	$\frac{19}{2}^-$	3.18	2.95	3.40	3.38	3.15 [a]
^{44}Sc	2^+	2.60	2.66	2.53	2.52	2.56 [a]
^{44}Sc	6^+	3.64		3.69	3.66	3.88 [a]

[a] Reference 32.
[b] M. Marmor, S. Cochavi, and D. B. Fossan, Phys. Rev. Lett. 25, 1033 (1970).
[c] Reference 50.

strong evidence that the approximation for the meson-exchange correction shown above is relatively accurate.

In our calculation we need an effective operator for all four orbits in our model space. The question of the state dependence of the effective operators is still unresolved. Because of various ambiguities in the effective $M1$ operator, we have calculated the $M1$ observables with four different operators so as to illustrate the sensitivity of the calculations to the various types of corrections discussed here:

(1) The bare operator.

(2) The bare operator $+0.2 l t_z$.

(3) The bare operator, but with the $\frac{7}{2} \to \frac{7}{2}$ matrix element of the isovector part of the operator modified to reproduce the observed moment of the ground state of ^{41}Ca.

(4) The bare operator $+0.2 l t_z$, but with the $\frac{7}{2} \to \frac{7}{2}$ matrix element of the isovector part of the operator modified to reproduce the observed moment of the ground state of ^{41}Ca. For all four of these operators, we assume state independence except for the indicated modification of the $\frac{7}{2} \to \frac{7}{2}$ matrix element. For the $f_{7/2} \to f_{7/2}$ matrix elements, we have assumed that the correction is completely isovector in nature. For an amplified discussion of this point, see Refs. 33 and 34. The observed value[37] of the ^{41}Sc magnetic moment is consistent with this pure isovector assumption. Most of the experimentally determined information on magnetic dipole observables in these light f-p-shell nuclei is on magnetic moments. This information is summarized in Table VII. We also show there the magnetic moments calculated with the four operators described above. For all the ground-state moments except ^{44}Sc, the calculations with the bare operator lead to significant discrepancies between theory and experiment. There are two measured values for the moment of the 6^+ states in ^{42}Ca. If the value -3.0 is correct, then the values calculated for the high-spin states in ^{42}Ca and ^{43}Sc with the bare operator are in good agreement with experiment. When the bare operator is renormalized to fit the moment in ^{41}Ca, all the ground-state moments are in satisfactory agreement with experiment, but there are significant discrepancies for the high-spin states. There are rather large effects introduced by the addition of the meson-exchange correction. The worst operator of the four used here for the magnetic-moment calculations is the bare operator with the meson-exchange corrections. When we use an $M1$ operator which includes meson-exchange contributions, but with the $f_{7/2}$-$f_{7/2}$ isovector matrix element renormalized to fit the observed ^{41}Ca moment, the calculated moments shown in Table VII are essentially identical to the moments calculated with the bare $M1$ operator which is renormalized to fit the ^{41}Ca moment. This presumably reflects the fact that these low-lying states are dominated by $f_{7/2}{}^n$ configurations.

As discussed by Arima[33] and by Nomura and Yamazaki,[34] a general interpretation of these results depends on a resolution in the discrepancy between the two measured values of the moment of the 6^+ state in ^{42}Ca. If the value of -3.0 is the correct one, then one could say that all the ground-state moments are accounted for with the bare operator renormalized to fit the observed moment of ^{41}Ca, and that the high-spin excited states are best described by the bare operator. The main exception to this is the moment of the 6^+ state in ^{44}Sc. The observed value is significantly larger than any of the calculated values. These calculated results do hint that the meson-exchange effects are significant here.

B. Effective Electric Quadrupole Operator

In these calculations, we determine electric quadrupole observables from the operator

$$Q_M{}^2 = e \sum_{i=1}^{A} r_i{}^2 Y_M{}^2(\theta_i)[\tfrac{1}{2} + t_z(i)] .$$

It is well known that this operator is inadequate for the description of observed electric quadrupole observables in terms of the conventional shell models. The primary piece of evidence for this is the observation of $E2$ transitions and electric quadrupole moments for single-neutron nuclei such as ^{17}O and ^{41}Ca. The renormalizations for this operator are generally broken up into two categories:

(1) Core-polarization effects; i.e., 1p-1h excitations of the core, where the particles and holes are in orbits omitted from the shell-model space. Since these excitations are to and from orbits outside the model space, they should not be strongly inhibited by Pauli-effect blocking when particles are added to form new nuclei. One can thus reasonably expect that these contributions should be similar for all nuclei in a given major shell.

(2) Deformation effects due to multiple-particle excitation from core states into the space of active orbits. These effects might be expected to be most important at the beginning of the shell and to be diminished in importance with increasing A due to Pauli-blocking effects. There have been numerous attempts to calculate effects due to core polarization,[38] but the calculations are still beset with problems of convergence and of what type of residual interaction to use. In some of the nuclei we discuss here, effects on electric quadrupole transitions due to deformation effects

have been studied[15, 16] with some qualitative success.

In shell-model calculations, the standard approach is to mock up the renormalization effects by introducing effective charges for the neutron and the proton. In the s-d shell, it has been found[31] that adding effective charges of 0.5 to the proton and neutron operators leads to fair agreement between shell-model calculations and experiment for many $E2$ observables in a wide range of nuclei. This effective charge is in fair agreement with the calculated[38] effective charge due to core-polarization effects. There is considerable experimental information for $E2$ transitions in f-p-shell nuclei which is especially relevant to the neutron-effective charge for these nuclei. Some of this information is summarized in Table VIII. There all known $B(E2)$'s for the isotopes $^{42,43,44}Ca$ are shown, as are the $B(E2)$ values calculated in the shell model with an effective charge 1.0. If we assume one state-independent neutron-effective charge for all the active neutron single-particle orbits, then the square root of the ratio of the measured $B(E2)$ to the calculated $B(E2)$ gives the neutron-effective charge directly. (In all these $E2$ calculations, we determine the oscillator parameter from the relation $\hbar\omega = 41A^{-1/3}$ MeV.) The effective charge calculated in this way is shown in the last column. (Some results similar to these for $^{42,43}Ca$ are discussed elsewhere.[39, 40]) The first obvious fact is that the effective charge calculated this way is very large. As we discuss briefly below, there is reason to believe that the core-polarization effective charge is about $0.5e$. To the extent that ^{18}O is two neutrons outside an inert ^{16}O core, ^{18}O is the s-d-shell analog of ^{42}Ca. If we determine this total effective charge for ^{18}O as we have done here for ^{42}Ca, it is 0.71.[31] The calculated[38] core-polarization effective charge in the s-d shell is about 0.5. This is the basis for the statement that deformation effects on $E2$ observables in the s-d shell are relatively small. They are much larger in the f-p shell. We know of no obvious reason for this difference. It is generally found[15, 16, 41, 42] that admixtures of deformed components with shell-model ground states are roughly comparable in ^{16}O and ^{40}Ca. If we arbitrarily assume the low-lying states of ^{18}O and ^{42}Ca are 50% shell model and 50% 4p-2h deformed state, then the $2 \to 0$ transition rates imply that the transition rates between deformed states in ^{42}Ca are at least an order of magnitude stronger then in ^{18}O. The calculations of Brown-Green[41] and Gerace-Green[15] suggest the transitions between deformed components in ^{42}Ca is more likely 2 to 3 times stronger than in ^{18}O.

TABLE VIII. Calculated and measured $B(E2)$ values in the calcium isotopes with $A = 42-44$. Numbers in column headed Shell Model are for a neutron effective charge of $1.0e$. Numbers in column headed ϵ_n are from the square root of the ratio of the experimental value to the calculated value.

A	J_i	J_f	Shell model (e^2 fm^4)	Experiment (e^2 fm^4)	ϵ_n
42	2	0	26	81 ± 24 [a]	1.8
	4	2	27	93 ± 28 [a]	1.9
	6	4	14	6 [a]	0.7
43	$\frac{5}{2}$	$\frac{7}{2}$	63	87 ± 7 [b]	1.2
	$\frac{3}{2}$	$\frac{7}{2}$	27	71 ± 3 [b]	1.6
	$\frac{11}{2}$	$\frac{7}{2}$	30	77 ± 19 [b]	1.6
44	2	0	42	72^{+18}_{-12} [c]; 136^{+43}_{-38} [d]	1.3; 1.8

[a] Reference 40.
[b] Reference 39.
[c] Reference 51.
[d] Reference 22.

In ^{42}Ca, the $6^+ \to 4^+$ transition implies a much smaller total effective charge than do the $4^+ \to 2^+$ and $2^+ \to 0^+$ transitions. This could be interpreted to mean that the deformation effects decrease significantly as one goes to higher-spin states. Because of the discrepancies in the experimental data, it is difficult to draw any conclusions as to the systematics of the neutron effective charge in $^{42,43,44}Ca$. The results suggest that the effective charge is not significantly decreased for transitions between low-lying states in going from ^{42}Ca to ^{44}Ca.

There is less direct evidence on the effective proton charge. The lifetime[43] of the $2^+ \to 0^+$ transition in ^{42}Ti implies a total effective charge similar to the neutron charge ($\epsilon_n = 1.6$).

Since the calcium isotopes are pure neutron states in the model used here, and states in ^{42}Ti are pure proton states, it is possible to draw inferences on the neutron and proton effective charges directly from the experimental data. It is possible to draw similar inferences on the isoscalar effective charge ($\epsilon_p + \epsilon_n$) from $T = 0 \to T = 0$ transitions. There are two $T = 0 \to T = 0$ transitions known[44] in ^{42}Sc. The $B(E2)$'s for these transitions are shown in Table IV, as are the values calculated with an isoscalar effective charge of $0.7e$. This value gives good agreement with $5^+ \to 7^+$ transition, and it gives a somewhat too small $B(E2)$ value for the $3^+ \to 1^+$ transition. Again, this could be interpreted as indicating that the deformation effects are smaller for the high-spin states. This isoscalar effective charge also suggests that the deformation effects are far less important for the $T = 0$ states.

The $2^+ \to 0^+$ transition in ^{42}Sc involves both the isovector and isoscalar parts of the effective operator, so the analyses becomes more complicated. The same is true for all the other nuclei we tried here.

C. Discussion of Electromagnetic Transitions in Individual Nuclei

In Secs. IV A and IV B, we have attempted to present a summary of the empirical information from which one can draw some direct inferences as to the effective electromagnetic operators for this region. Now we briefly discuss below the results of calculations for other transitions in these $A = 42-44$ nuclei. The discussion in the previous section gave evidence that there is considerable ambiguity as to what effective operators should be used. We have made somewhat arbitrary choices for the effective operators to be used in the following calculations. For the electric quadrupole operator we use the following state-independent effective charges

$$\epsilon_p = 0.2\,, \quad \epsilon_n = 0.5\,.$$

There are the core-polarization effective charges suggested by Arima, Brown, and McGrory[45] for the f-p shell. They assumed the core-polarization contribution is constant throughout the shell, and they treated the neutron and proton effective charges as parameters. The parameters were chosen to give a best fit to selected data on $E2$ observables in $A = 42$, 43, 50, and 54 nuclei. The data were chosen for which deformation effects were believed to be minimal, or for which it was possible to estimate deformation effects and correct the data for these effects. Thus, these effective charges are chosen to give a reasonable representation of these "constant" core-polarization contributions. If the core-polarization effects are roughly accounted for by these effective charges, then any large discrepancies between observed $B(E2)$ values and the values calculated are indicative of deformation effects. Previous experience has shown that the relative $B(E2)$ values are not very sensitive to small variations in the relative size of the neutron and proton effective charges. [In fact, we repeated the calculations reported here with effective charges $\epsilon_p = 0.5$ and $\epsilon_n = 0.5$, and the results for relative $B(E2)$ values were not significantly changed.]

For the effective $M1$ operator we present results for two operators:

(1) The bare operator.

(2) The bare operator with the meson-exchange approximation $0.2 l t_z$ added, and with the isovector part of the $\frac{7}{2} \rightarrow \frac{7}{2}$ matrix element altered to fit the observed ^{41}Ca magnetic moment.

These two operators are chosen to illustrate the sensitivity of the $M1$ calculation to the operator.

D. Calculated and Observed Electromagnetic Observables in $A = 42$ Nuclei

The calculated $E2$ transition rates for the low-lying state in ^{42}Ca are already essentially summarized in Table VIII. Those numbers are for $\epsilon_n = 1.0$. If we use $\epsilon_n = 0.5$, then the experimental values[39] for the $2 \rightarrow 0$ and $4 \rightarrow 2$ transitions are at least 10 times the calculated value, while the $6 \rightarrow 4$ transition is observed[39] to be 2 times the calculated value.

TABLE IX. Calculated and measured $B(M1)$ and $B(E2)$ values in ^{42}Sc between "$f_{7/2}{}^2$" states. Effective charges $e_p = 1.2$, $e_n = 0.5$ were used to calculated the $B(E2)$ values. The calculated $B(M1)$ values headed Bare were calculated with free $M1$ operator. The numbers headed effective were calculated with the operator including the approximate meson-exchange term and which was adjusted to fit the ^{41}Ca ground-state magnetic moment.

		$B(E2)$ (e^2 fm^4)		$B(M1)(\mu_N{}^2)$		
		Calculated	Observed	Calculated		
J_i, T_i	J_f, T_f			Bare	Effective	Expt.[a]
1, 0	0, 1			7.4	6.4	0.6 ± 0.1
3, 0	1, 0	23	35 ± 6[a]; 34.4 ± 6.3[b]			
5, 0	7, 0	21	20 ± 3[a]; $25.1^{+5.4}_{-38}$[b]			
2, 1	0, 1	19	72 ± 27[a]			
	1, 0	0.6		3.5	4.8	5.9 ± 2.4
	3, 0	2		9.7	8.3	
4, 1	3, 0	2		3.7	3.0	
	5, 0	4		6.2	5.4	
	2, 1	19				
6, 1	7, 0	3		3.2	2.7	
	5, 0	2		2.0	1.7	
	4, 1	10				

[a] Reference 44.
[b] Reference 46.

The calculated and observed transitions for low-lying states in ^{42}Sc are summarized in Table IX. There are three $B(E2)$ values measured[44,46] between the low-lying states. Two of them were discussed above. The third transition is between two $T=1$ states, and a comparison of the calculated and observed $B(E2)$'s implies a much larger deformation effect for this transition than for the $T=0\rightarrow T=0$ transitions. The qualitative features of these transitions are reproduced by the Flowers-Skouras calculations[16] for ^{42}Sc, in which calculation deformation effects are explicitly introduced.

$B(M1)$ values for two transitions in ^{42}Sc have been measured. These transitions are necessarily $\Delta T=1$ transitions, and are hence quite strong. The 2^+, $T=1\rightarrow 1^+$, $T=0$ transition is calculated to be of the right order of magnitude, but is too weak by about a factor of 2. For the 1^+, $T=0\rightarrow 0^+$, $T=1$ transition, the calculated value is too strong by an order of magnitude. This is the only case in the nuclei discussed here that the calculated $B(M1)$ value exceeds the measured one. The calculations for these two transitions do not show that one of the two effective $M1$ operators used here is better than the other. There are a number of strong $M1$ transitions calculated between the various excited states here. The measurement of these transitions would be of considerable interest.

E. Calculated and Observed Transitions in $A=43$ Nuclei

Calculated and observed $B(E2)$'s and $B(M1)$'s in ^{43}Ca are summarized in Table X. We have already discussed briefly the ^{43}Ca $E2$ calculations above, and commented on the strong effects due to deformation. For the calcium isotopes, the wave functions for the low-lying states are predominantly pure $f_{7/2}$ configurations. $M1$ transitions between identical particle states of pure j^n configurations are forbidden,[47] so $M1$ transitions in ^{43}Ca go only through admixtures of $p_{3/2}$ and $f_{5/2}$ states. Because these admixtures are small, the calculated $M1$ transitions strengths are very weak. (As pointed out by Zamick and Ripka,[48] the $p_{3/2}$ and $f_{5/2}$ contributions interfere destructively with each other to further suppress the $M1$ transitions.) There is a serious discrepancy between calculation and experiment[39] here, for the two known $M1$ transitions. They are observed to be 1 to 2 orders of magnitude stronger than the calculated rates. We see that there is considerable sensitivity both to changes in the effective two-body interaction, and to changes in the effective $M1$ operator. One might suspect that deformation effects are important here, since they are so strong for the $E2$ observables. Zamick and Ripka[48] have attempted to estimate such effects in perturbation theory, and find that they are small. Noting the sensitivity of the calculation to the two-body interaction, the uncertainty of the two-body interaction matrix elements for states involving the higher orbits, and even the uncertainty in the single-particle energies for the $p_{1/2}$ and $f_{5/2}$ orbits, we think that it is certainly possible that the discrepancy here is due to inaccuracies in the Hamiltonian used.

The calculated and observed $B(E2)$ and $B(M1)$

TABLE X. Calculated and observed $B(E2)$ and $B(M1)$ values in ^{43}Ca. See Table IX for meaning of headings of first two columns of calculated $B(M1)$ values. The third column shows $B(M1)$ values with the same operator as was used in calculating numbers in column 2, but with wave functions obtained with the Kuo-Brown interaction.

		$B(E2)$ values ($e^2\,fm^4$)		$B(M1)$ values ($\mu_N{}^2$)			
J_i	J_f	Calculated	Observed[a]	Bare	Effective	Kuo-Brown	Expt.[a]
$\frac{5}{2}$	$\frac{7}{2}$	16	87 ± 7	2×10^{-3}	1×10^{-4}	6×10^{-5}	2×10^{-2}
$\frac{3}{2}$	$\frac{7}{2}$	7	71 ± 3				
	$\frac{5}{2}$	14		7×10^{-4}	3×10^{-4}	2×10^{-3}	1×10^{-2}
$\frac{3}{2}$	$\frac{7}{2}$	6					
	$\frac{5}{2}$	0.8		7×10^{-3}	6×10^{-3}	4×10^{-3}	
	$\frac{3}{2}$	0.4		1×10^{-3}	8×10^{-4}	3×10^{-3}	
$\frac{9}{2}$	$\frac{7}{2}$	2		2×10^{-4}	2×10^{-5}	1×10^{-6}	
	$\frac{5}{2}$	2					
$\frac{11}{2}$	$\frac{7}{2}$	8	77 ± 19				
	$\frac{9}{2}$	2		2×10^{-4}	3×10^{-4}	5×10^{-4}	

[a] Reference 39.

values in ^{43}Sc are summarized in Table XI. There are four $B(E2)$ values measured.[46, 49, 50] For one case, the $\frac{3}{2}\to\frac{7}{2}$ transition, the calculation and experiment are in agreement, while for the other three transitions, the calculated numbers are too small by factors of from 2 to 6. These results further imply the great importance of deformed-state admixtures in the low-lying f-p-shell states. There are a number of relatively strong $B(M1)$ values predicted.

F. Calculated and Observed $B(E2)$ Values in $A=44$ Nuclei

The calculated and observed[22, 46, 51] $B(E2)$ values in ^{44}Ca are shown in Table XII. Because of angular momentum selection rules and the pure-configuration inhibition mentioned above, there are no strong $M1$ transitions predicted.

We have already commented on the large effect of deformation on the $2^+\to 0^+$ $E2$ transition in ^{44}Ca. The other measured $B(E2)$ is for the decay of the $6^+\to 4^+$ state. There are two low-lying 4^+ states in the observed spectrum. As mentioned above, the wave functions for the calcium isotopes are dominated by $f_{7/2}{}^n$ configurations. In the $f_{7/2}{}^4$ configuration there are two 4^+ states, one seniority 2 and one seniority 4. The sole 6^+ state has seniority 2. There is a seniority selection rule[47] that $E2$ transitions between pure configuration states are allowed only if the seniority changes by two units between the initial and final states. As discussed above, the experimental stripping data imply that the second 4^+ state is predominantly seniority 2, so the lower state must be the seniority-4 state, and 6^+ should thus decay primarily to this lower 4^+ state. This is what is observed. The calculation splits the 6^+ $E2$ strength between the two 4^+ states. We have already commented above that in a previous study[5] of ^{44}Ca, it was found that the seniority mixing between these two 4^+ states was rather sensitive to the position of the center of gravity of the $p_{3/2}$ single-particle strength, and that the stripping pattern could be reproduced by a small change in this center of gravity. We presume that such a change would improve the agreement for this transition. The results do indicate that there are significant effects due to deformation for these transitions, but they are not as large as for the $2\to 0$ transition.

The $B(M1)$ and $B(E2)$ values calculated for ^{44}Sc are summarized in Table XIII. There are no reported measurements of $B(E2)$ or $B(M1)$ values for transitions between low-lying states in ^{44}Sc. The ^{43}Ca$(p,\gamma)^{44}$Sc reaction has been studied,[52] and branching ratios reported. There are no

TABLE XI. Calculated and observed $B(E2)$ and $B(M1)$ values in ^{43}Sc. See caption to Table IX for meaning of column headings.

J_i	J_f	$B(E2)$ values ($e^2\,\mathrm{fm}^4$) Calculated	Observed	$B(M1)$ values ($\mu_N{}^2$) Bare	Effective
$\frac{3}{2}$	$\frac{7}{2}$	62	67^{+40}_{-27} [a]		
$\frac{11}{2}$	$\frac{7}{2}$	20	123^{+22}_{-16} [a]		
$\frac{9}{2}$	$\frac{7}{2}$	11		0.7	0.5
	$\frac{11}{2}$	14		2	2
$\frac{1}{2}$	$\frac{3}{2}$	68		4	3
$\frac{5}{2}$	$\frac{7}{2}$	2		3	1
	$\frac{3}{2}$	9		0.2	0.3
	$\frac{9}{2}$	2			
	$\frac{1}{2}$	27			
$\frac{15}{2}$	$\frac{11}{2}$	23	49 ± 8 [b]		
$\frac{7}{2}$	$\frac{7}{2}$	0.3		7×10^{-2}	5×10^{-2}
	$\frac{3}{2}$	4			
	$\frac{11}{2}$	11			
	$\frac{9}{2}$	20		0.6	0.5
	$\frac{5}{2}$	0.5		0.4	0.3
$\frac{13}{2}$	$\frac{11}{2}$	4		0.8	0.7
	$\frac{9}{2}$	9			
	$\frac{51}{2}$	10			1.4
$\frac{19}{2}$	$\frac{15}{2}$	15	27 ± 1 [c]		

[a] Reference 49.
[b] Reference 46.
[c] Reference 50.

TABLE XII. Calculated and observed $B(E2)$ values in ^{44}Ca. The $B(E2)$ values are calculated with $\epsilon_n=0.5$.

J_i	J_f	$B(E2)$ values ($e^2\,\mathrm{fm}^4$) Calculated	Observed
2_1	0	10	72^{+18}_{-12} [a]; 136^{+43}_{-38} [b]
4_1	2_1	5	
4_2	2_1	6	
	4_1	2	
2_2	2	9	
	4_1	6	
	4_2	0.0	
6	4_1	2	41 ± 4 [c]
	4_2	6	
5	4_1	4	
	4_2	5	
	6	7	
2_3	2_1	2	
	4_1	0.3	
	4_2	3	
	2_2	0.0	

[a] Reference 51.
[b] Reference 43.
[c] Reference 46.

TABLE XIII. Calculated $B(E2)$ and $B(M1)$ values in ^{44}Sc. The $B(E2)$ values were calculated with effective charges $\epsilon_p = 1.2$ and $\epsilon_n = 0.5$. See Table IX for the meaning of the headings over the $B(M1)$ values.

J_i	J_f	$B(E2)$ values (e^2 fm^4)	$B(M1)$ values ($\mu_N{}^2$) Bare	Effective
4	2	22		
6	4	18		
1	2	35	7	6
3	2	46	2	2
	4	4	1	1
5	4	24	2	2
	6	2	0.4	0.3
	3	27		
7	6	17	1	1
	5	23		
3_2	2	2	0.7	0.6
	4	29	4	3
	1	18		
	3_1	5	0.3	0.3
	5	2		
5_2	4	0.1	0.6	0.5
	6	19	2	2
	3_1	0.0		
	5_1	2	0.1	0.1
	7	2		
	3_2	17		

contradictions between the calculated values and the measured branching ratios. There is one possible puzzle in the data on branching ratios. There is a state at 1.052 MeV identified as a 5^+ state. This state decays predominantly to the 4^+ state at 0.350 MeV, but there is an 11% branch to the 2^+ ground state. The calculation implies there is a strong $M1$ transition from this 5^+ to the lowest 4^+ state. Since this is a 0.752-MeV transition, there is no reason to expect this $M1$ transition to be weak on the grounds of a small energy or a small matrix element. The experimental data suggest that an $M3$ or $E4$ transition is competing with a rather strong $M1$ transition. An experimental determination of the $B(E4)$ value for the $6^+ \rightarrow 2^+$ transition from the 0.271-MeV state would provide interesting information on the $E4$ effective charge in this region.

G. Electric Quadrupole Moments

There are four known ground-state quadrupole moments[32] in the nuclei discussed here. These are listed in Table XIV and compared with the values calculated with the effective operator with $\epsilon_p = 0.2$ and $\epsilon_n = 0.5$. There is a major discrepancy for ^{42}Ca. The calculated moment is small and positive, and the measured value is larger and negative. This has been discussed in detail by

TABLE XIV. Observed and calculated electric quadrupole moments. Calculated values are calculated with effective charges $\epsilon_p = 0.2$ and $\epsilon_n = 0.5$.

A	J,T	Quadrupole moment (e^2 fm^4) Calculated	Observed[a]
^{42}Ca	2, 1	+1	-19 ± 8
^{43}Sc	$\frac{7}{2}, \frac{1}{2}$	−16	−26
^{44}Sc	2, 1	−6	−10
^{44}Sc	6, 1	−16	−19

[a] Reference 32.

Towsley, Cline, and Horoshko.[53] They present an argument which suggests that the first 2^+ is strongly admixed with a 2^+ state based on a strongly deformed prolate intrinsic state, and that the quadrupole moment comes primarily from this deformed component. For the ^{43}Sc ground-state moment, the sign is correct, but the magnitude is still different by about a factor of 1.5. This is consistent with the calculated results for $B(E2)$ values for transitions in ^{43}Sc as seen in Table XI. The calculated moments for ^{44}Sc are in reasonable agreement with the observed values. This is somewhat ironic, in that it is for these two states that the magnetic-moment calculations are least successful.

V. SUMMARY

In this paper, we have presented the results from one uniform conventional shell-model treatment of the light f-p-shell nuclei with $A \leq 44$. In the calculation, the model space is spanned by all Pauli-allowed states of all possible configurations with two, three, and four particles distributed among the four f-p-shell single-particle orbits included in the model space. For the one-body part of the effective Hamiltonian, we used the observed single-particle energies. The two-body effective interaction used here is very similar to the "realistic" f-p-shell interaction of Kuo and Brown. The over-all results can be summarized as follows:

(1) Insofar as excitation energies and spectroscopic factors are concerned, there are reasonable experimental partners for all the low-lying calculated states, and the calculated single-particle transfer strengths are in qualitative agreement with experiment. There are many extra levels in the observed spectrum at low excitation energies not accounted for by the present shell model.

(2) For magnetic moments, the model is only moderately successful. The renormalizations

of the magnetic-dipole observables are much more important here than was the case in s-d-shell calculations similar to these,[31] and the data suggest there is significant state dependence in this operator. This dependence is even more important for the $M1$ transitions, where there are many mechanisms leading to strong cancellations. The poor agreement between theory and experiment for $B(M1)$ values reflects this.

(3) The situation is similar for electric quadrupole observables. The effective charges are significantly larger here than in the s-d shell, and there is a suggestion of a strong state dependence for these charges.

The results in general here are not as satisfactory as they are in similar calculations for s-d-shell nuclei. The effects of deformed states seem to be much more important in the f-p shell than in the s-d shell. In the light s-d-shell nuclei a microscopic treatment of the mixing of closed-core and core-excited states was quite successful.[42] It will be of considerable interest to see if similar calculations can be equally successful in this region. An initial attempt in this direction has been reported,[6] and some quantitative success was indicated.

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[1]J. C. McCullen, B. F. Bayman, and L. Zamick, Phys. Rev. **134**, B515 (1964).

[2]J. N. Ginocchio and J. B. French, Phys. Lett. **7**, 137 (1963).

[3]P. Federman and I. Talmi, Phys. Lett. **22**, 469 (1966).

[4]T. Engeland and F. Osnes, Phys. Lett. **20**, 424 (1966).

[5]J. B. McGrory, B. H. Wildenthal, and E. C. Halbert, Phys. Rev. C **2**, 186 (1970).

[6]A. P. Zuker, in *Proceedings of Topical Conference on the Structure of $lf_{7/2}$-Nuclei, Legnaro (Padova)*, edited by R. A. Ricci (Bologna, Italy, 1971), p. 95.

[7]G. Ripka and L. Zamick, Phys. Lett. **23**, 350 (1966).

[8]J. B. French, E. C. Halbert, J. B. McGrory, and S. S. M. Wong, in *Advances in Nuclear Physics*, edited by M. Baranger and E. Vogt (Plenum, New York, 1969), Vol. 3.

[9]J. B. McGrory and E. C. Halbert, Phys. Lett. 37B, 9 (1971).

[10]T. A. Belote, A. Sperduto, and W. E. Bueckner, Phys. Rev. **139**, B80 (1965).

[11]T. T. S. Kuo and G. E. Brown, Nucl. Phys. A114, 241 (1968).

[12]P. W. M. Glaudemans, Nucl. Phys. **56**, 529 (1964); also see Appendix A in Ref. 12.

[13]R. Sherr, T. S. Bhatia, D. Cline, and J. J. Schwartz, Ann. Phys. (N.Y.) **66**, 548 (1971).

[14]J. L. Yntema, Phys. Rev. **186**, 1144 (1969).

[15]W. J. Gerace and A. M. Green, Nucl. Phys. A93, 110 (1967).

[16]B. H. Flowers and L. D. Skouras, Nucl. Phys. **A116**, 529 (1968); B. H. Flowers and L. D. Skouras, Nucl. Phys. **A136**, 353 (1969).

[17]M. Bini, P. G. Bizzeti, and A. M. Bizzeti Sona, Phys. Rev. C **6**, 784 (1972).

[18]W. E. Dorenbusch, T. A. Belote, and O. Hansen, Phys. Rev. **146**, 734 (1966).

[19]N. Schulz, W. P. Alford, and A. Jamishida, in *Proceedings of Topical Conference on the Structure of $lf_{7/2}$-Nuclei, Legnaro (Padova)*, edited by R. A. Ricci (Bologna, Italy, 1971), p. 373.

[20]J. Bommer, K. Grabisch, H. Kluge, G. Rosehert, H. Fuchs, U. Lymen, and K. K. Seth, Nucl. Phys. A160, 577 (1971).

[21]I. P. Johnstone, Nucl. Phys. **A110**, 429 (1968).

[22]D. H. White and R. E. Birkett, Phys. Rev. C **5**, 513 (1972).

[23]J. B. McGrory and B. H. Wildenthal, Phys. Lett. **28**, 237 (1968).

[24]P. Federman and S. Pittel, Nucl. Phys. A155, 161 (1970).

[25]J. H. Bjerregaard and O. Hansen, Phys. Rev. **155**, 1229 (1967).

[26]J. C. Manthuruthil and F. W. Prosser, Phys. Rev. C **6**, 851 (1972).

[27]I. P. Johnstone, Can. J. Phys. **48**, 1208 (1970).

[28]J. J. Schwartz, Phys. Rev. **175**, 1453 (1968).

[29]J. Rapaport, J. B. Ball, R. L. Auble, T. A. Belote, and W. E. Dorenbusch, Phys. Rev. C **5**, 453 (1972).

[30]K. H. Bhatt and J. B. McGrory, Phys. Rev. C **6**, 2293 (1971).

[31]E. C. Halbert, J. B. McGrory, B. H. Wildenthal, and S. P. Pandya, in *Advances in Nuclear Physics*, edited by M. Baranger and E. Vogt (Plenum, New York, 1970), Vol. 4.

[32]Nucl. Data A5, (1969).

[33]A. Arima, in *Proceedings of Topical Conference on the Structure of $lf_{7/2}$-Nuclei, Legnaro (Padova)*, edited by R. A. Ricci (Bologna, Italy, 1971), p. 385.

[34]T. Nomura and T. Yamazaki, in *Proceedings of Topical Conference on the Structure of $lf_{7/2}$-Nuclei, Legnaro (Padova)*, edited by R. A. Ricci (Bologna, Italy, 1971), p. 437.

[35]M. Chemtob, Nucl. Phys. A123, 449 (1969).

[36]S. Nagamiza and T. Yamazaki, Phys. Rev. C **4**, 1961 (1971).

[37]See contribution by A. Sugimoto *et al.*, in Proceedings of the International Conference on Nuclear Moments and Nuclear Structure, Osaka, Japan, 1972 (to be published).

[38]For discussions of theoretical estimates of the $E2$ effective charges, see Ref. 34 and references therein, and L. Zamick, lecture notes "Renormalization of One-Body Operators" (Rutgers University, New Brunswick, N. J., 1972).

[39]R. N. Horoshko, C. Towsley, and D. Cline, in *Proceedings of Topical Conference on the Structure of $lf_{7/2}$-Nuclei, Legnaro (Padova)*, edited by R. A. Ricci (Bologna, Italy, 1971), p. 419.

[40]P. G. Bizzeti, in *Proceedings of Topical Conference on the Structure of $lf_{7/2}$-Nuclei, Legnaro (Padova)*, edited by R. A. Ricci (Bologna, Italy, 1971), p. 393.

[41]G. E. Brown and A. M. Green, Nucl. Phys. **75**, 401 (1966).

[42]A. P. Zuker, B. Buck, and J. McGrory, Phys. Rev. Lett. **23**, 983 (1969).

[43]B. A. Brown, M. Marmor, and D. B. Fossan, in *Proceedings of Topical Conference on the Structure of $lf_{7/2}$-Nuclei, Legnaro (Padova)*, edited by R. A. Ricci (Bologna, Italy, 1971), p. 122.

[44]M. C. Bertin, G. J. Kumbartzki, and R. G. Hirko, Nucl. Phys. A192, 524 (1972).

[45]A. Arima, B. A. Brown, and J. B. McGrory, to be published.

[46]B. A. Brown, D. Fossan, J. McDonald, and K. Snover, to be published.

[47]A. deShalit and I. Talmi, *Nuclear Shell Theory* (Academic, New York, 1963).

[48]L. Zamick and G. Ripka, Nucl. Phys. A116, 234 (1968).

[49]Best Doppler-shift attenuation-method values obtained from C.

P. Poirier, A. Tveter, J. C. Manthuruthil, J. Walenga, V. E. Storizhko, and B. D. Kern, Phys. Rev. C **3**, 1939 (1971); G. C. Ball, J. S. Forster, and F. Ingebretsen, Nucl. Phys. **A180**, 517 (1972).

[50]T. Nomura, T. Yamazaki, S. Nagamiza, and T. Katon, Phys. Rev. Lett. **27**, 523 (1971).

[51]H. Gruppelaar and P. J. M. Smulders, Nucl. Phys. **A179**, 737 (1972).

[52]G. P. Poirier and J. C. Manthuruthil, in *Proceedings of Topical Conference on the Structure of* $lf_{7/2}$*-Nuclei, Legnaro (Padova), edited by R. A. Ricci (Bologna, Italy, 1971), p. 375.*

[53]C. W. Towsley, D. Cline, and R. N. Horoshko, Phys. Rev. Lett. **28**, 368 (1972).