Mixed-Configuration Shell-Model Calculations for Nuclei with $N = 28, 20 < Z \le 28^*$

K. LIPS AND M. T. MCELLISTREM University of Kentucky, Lexington, Kentucky 40506 (Received 4 November 1969)

Level energies, γ -ray transition rates, and proton spectroscopic factors are calculated for the nuclei with N=28 and $20 < Z \le 28$ from simple mixed-configuration shell models. First, the effective-interaction method is used to calculate wave functions in which the pure $(1_{7/2}^n)$ configuration and the $(1_{7/2}^{n-1}2p_{3/2})$ configuration are included. The results are compared with experimental values for 43 levels. The calculated and measured energies and spectroscopic factors agree well, but M1 transition rates are too slow. The model is then extended to include the configuration $(1f_{7/2}^{n-1}1f_{5/2})$. The wave functions are recalculated using additional two-body matrix elements calculated with a modified surface δ interaction (MSDI) fitted to the effective interactions of the first calculation. The expanded model provides a good fit to energies, spectroscopic factors, and transition rates. For comparison, the calculation is repeated using the reaction matrix elements of Kuo and Brown. The results are less satisfactory than those with the MSDI.

I. INTRODUCTION

N the past several years, there has been considerable L experimental investigation of the properties of nuclei with N = 28 and 20 < Z < 28. In particular, much new work has been done on ⁵¹V and ⁵³Mn.¹⁻⁹ This new information on energy levels, transfer reactions, and electromagnetic transition probabilities permits a reevaluation of shell-model-configuration assumptions used in previous calculations in this region.

There is evidence that N = 28 is a particularly stable closed shell, and thus ⁴⁸Ca forms a good closed core.^{10,11} Calculations assuming a pure $(1f_{7/2}^n)$ configuration for the protons outside that core have given satisfactory results in predicting low-lying energy levels and binding energies.^{12,13} However, these calculations are deficient in several ways. They do not predict enough levels at excitation energies $(E_x) \gtrsim 2$ MeV and do not describe some features of the nucleon-transfer-reaction data.

- Rev. C1 (to be published).
- ⁷B. J. O'Brien, W. E. Dorenbusch, T. A. Belote, and J. Rapaporte, Nucl. Phys. A104, 609 (1967).
- ⁸ J. Rapaporte, Nucl. Phys. A104, 009 (1967).
 ⁸ J. Rapaporte, T. A. Belote, and W. E. Dorenbusch, Nucl. Phys. A100, 280 (1967).
 ⁹ C. St. Pierre, P. N. Maheshwari, C. Doutriaux, and L. Lamarch, Nucl. Phys. A102, 433 (1967).
 ¹⁰ E. Kashy, A. Sperduto, H. A. Enge, and W. W. Buechner, Phys. Rev. 135, B765 (1964).
 ¹¹ T. W. Conlon, B. F. Bayman, and E. Kashy, Phys. Rev. 144 940 (1966)

- 144, 940 (1966).
- ¹² A. de Shalit, in Selected Topics in Nuclear Theory, edited by F. Janouch (International Atomic Energy Agency, Vienna, 1963), p. 209. ¹³ J. D. McCullen, B. F. Bayman, and L. Zamick, Phys. Rev
- 134, B513 (1964).

The most serious weakness of the model is that M1transitions between the states are forbidden, as are E2transitions between states of the same seniority in ⁵²Cr. These "forbidden" transitions are found to occur between the experimental levels.

The purpose of the present work is to show that calculations with relatively simple configuration mixing, allowing states with proton configurations $(1f_{7/2}^{n-1}2p_{3/2})$ and $(1f_{7/2}^{n-1}1f_{5/2})$ as well as the pure $(1f_{7/2}^{n})$ configurations, can account very well for the nucleon-transfer data and the E2 and M1 transition probabilities as well as the bound level energy spectrum.

There are two parts to this calculation. First, the method of effective interactions¹⁴ is used to construct wave functions for states which are mixtures of the configurations $(1f_{7/2}^{n})$ and $(1f_{7/2}^{n-1}2p_{3/2})$. In this method, the $f_{7/2}$ single-particle energy and the twoparticle matrix elements of the residual interaction are treated as adjustable parameters without specifying the form of the residual interaction. These parameters are varied to make the eigenvalues of the wave functions fit the corresponding experimental energies, where known. Considerable improvement over the pure configuration model is obtained, but predicted M1 transition rates are much too slow. This calculation is presented in detail because it serves as a basis for an extended model in which the states of the $(1f_{7/2}^{n-1}1f_{5/2})$ configuration are also included. The extended model uses the two-particle matrix elements determined in the effective-interaction calculation and additional matrix elements involving the $1f_{5/2}$ protons. The latter are obtained by assuming a modified surface δ residual interaction. For comparison, the entire calculation is repeated using the reaction matrix elements calculated by Kuo and Brown¹⁵ for nuclei with a ⁴⁸Ca core.

1

^{*} Work supported in part by the National Science Foundation.
¹O. F. Afonin, A. P. Grinberg, I. Kh. Lemberg, and I. N. Chugunov, Yadern. Fiz. 6, 219 (1967) [English transl.: Soviet J. Nucl. Phys. 6, 160 (1968)].
²D. D. Armstrong and A. G. Blair, Phys. Rev. 140, B1226 (1965)

^{(1965).}

⁽¹⁹⁰⁵⁾.
³ A. W. Barrows, R. C. Lamb, D. Velkley, and M. T. McEllistrem, Nucl. Phys. A107, 153 (1968).
⁴ B. Cujec and I. Szoghy, Phys. Rev. 179, 1060 (1969).
⁵ E. Newman and J. C. Hiebert, Nucl. Phys. A110, 366 (1968).
⁶ M. T. McEllistrem, K. W. Jones, and D. M. Sheppard, Phys.

¹⁴ I. Talmi, in Proceedings of Rehovoth Conference on Nuclear Structure, edited by H. J. Lipkin (North Holland Publishing Co., Amsterdam, 1958), p. 31. ¹⁵ T. T. S. Kuo and G. E. Brown, Nucl. Phys. **A114**, 241

^{(1968).}

¹⁰⁰⁹



FIG. 1. Experimental and theoretical excitation energies of ⁵⁰Ti. Several mixed-configuration shell-model calculations are shown. The states of calculation shell-model calculations are shown. The states of calculation A are mixtures of the configura-tions $f_{7/2}{}^n$ and $f_{7/2}{}^{n-1}p_{3/2}$. Calculations B and C include also the configuration $f_{7/2}{}^{n-1}f_{5/2}$. The $f_{5/2}$ two-body matrix elements used in calculation B are from a surface δ residual interaction, while the matrix elements of Kuo and Brown are used in calculation C.

II. THEORY

The normalized totally antisymmetric wave functions of n particles in the j orbit coupled to total angular momentum J will be designated by $|j^n \alpha J M\rangle$, where α represents any quantum numbers in addition to j, J, and M necessary to specify the states. For $i \leq \frac{7}{2}$ only one additional quantum number, the seniority v, is required.

The states antisymmetric in n particles form a complete subset of the states which are antisymmetric in n-1 particles; so it is possible to expand them as

$$|j^{n}vJM\rangle = \sum_{V_{1},J_{1}} [j^{n-1}(v_{1}J_{1})jJ]]j^{n}vJ] |j^{n-1}(v_{1}J_{1}),$$
$$j_{(n)};JM\rangle. \quad (1)$$

The expansion coefficients $[j^{n-1}(v_1J_1)jJ]]j^nvJ]$ are the "fractional parentage coefficients" (FPC). The wave function $|j^{n-1}(v_1J_1), j_{(n)}; JM\rangle$ designates that nparticle state coupled to total spin J which is antisymmetric to the exchange of the first n-1 particles with each other, but not with the *n*th particle.

The totally antisymmetric states can also be exdanded in linear combinations of the states antisymmetric in n-2 particles,

$$j^{n}vJM \rangle = \sum_{V_{1},J_{1},J'} \left[j^{n-2}(v_{1}J_{1})j^{2}(J')J \right] j^{n}vJ] \\ \times \left[j^{n-2}(v_{1}J_{1}), j_{(n,n-1)}^{2}(J'); JM \right].$$
(2)

The $n \rightarrow (n-2)$ FPC in the above equation can be expressed as linear sums of products of the $n \rightarrow (n-1)$ FPC and Racah coefficients.¹⁶ The FPC are real, and therefore [[]]=[]]. Using the transformations (1) and (2), the matrix elements of one- and two-body operators between *n*-particle states can be shown to be linear functions of the single-particle and two-particle matrix elements, respectively.¹⁶

In the calculations which follow, the allowed states will be $|j_1^n v J M\rangle$ and $|j_1^{n-1}(v_1 J_1) j_i J M\rangle$, both totally antisymmetric n-particle states. The single-particle angular momenta will be $j_1 = \frac{7}{2}$ and $j_i = \frac{5}{2}$ or $\frac{3}{2}$. The normalized wave function of the ath state with nprotons and total angular momentum J will be

$$\theta(nJa) = \sum_{p} A_{p} | j_{1}^{n}v_{p}JM \rangle + \sum_{q,q'} B_{q,q'} | j_{1}^{n-1}(v_{q}J_{q'})j_{2}JM \rangle + \sum_{r,r'} C_{r,r'} | j_{1}^{n-1}(v_{r}J_{r'})j_{3}JM \rangle, \quad (3)$$

with $j_2 = \frac{3}{2}$ and $j_3 = \frac{5}{2}$. The sums range over all possible values of the quantum numbers.

The matrix elements of an operator A between these states will be linear sums of terms of three types:

$$\langle j_1^n v J M \mid A \mid j_1^n v' J' M' \rangle,$$
 (4)

$$\langle j_1^n v J M \mid A \mid j_1^{n-1}(v_1 J_1) j_2 J' M' \rangle,$$
 (5)

$$\langle j_1^{n-1}(v_1J_1)j_2JM \mid A \mid j_1^{n-1}(v_1J_1)j_2JM' \rangle.$$
 (6)

When

and

$$A = \sum_{i=1}^{n} f^{(k)}(i),$$

where $f^{(k)}(i)$ is a tensor operator of order k operating on the *i*th particle, the reduced matrix elements corresponding to (4)-(6) are

$$|j_1^{n}vJ|| A || j_1^{n}v'J') = D_1(j_1 || f^{(k)} || j_1), \qquad (7)$$

 $(j_1^{n}vJ || A || j_1^{n-1}(v_1J_1)j_2J') = D_2(j_1 || f^{(k)} || j_2),$ (8)

and

$$\begin{array}{l} (j_{1}^{n-1}(v_{1}J_{1})j_{2}J \mid\mid A \mid\mid j_{1}^{n-1}(v_{1}'J_{1}')j_{2}'J') \\ = D_{3}\delta_{J_{1}J_{1}}\delta_{v_{1}v_{1}'}(j_{2}\mid\mid f^{(k)}\mid\mid j_{2}') \\ + D_{4}\delta_{j_{2}j_{2}'}(j_{1}^{n-1}v_{1}J_{1}\mid\mid \sum_{i=1}^{n-1}f_{i}^{(k)}\mid\mid j_{1}^{n-1}v_{1}'J_{1}'). \end{array}$$

The coefficients D_i are products of FPC and Racah coefficients.^{16,17} The reduced matrix elements of singleparticle tensor operators between the states (3) will then be linear functions of all possible single-particle reduced matrix elements $(j || f^{(k)} || j')$.

¹⁶ A. de Shalit and I. Talmi, *Nuclear Shell Theory* (Academic Press Inc., New York, 1963), Chap. 26. ¹⁷ A. de Shalit and I. Talmi, Ref. 16, Chap. 37.

and

When the operator A is the two-body scalar operator $\sum_{i < k} V_{ik}$, the matrix elements between states (3) become linear sums over all possible antisymmetric two-particle states.^{16,17} It can be seen, then, that the elements of the energy matrices for *n*-particle states will be linear functions of the single-particle energies and the two-particle matrix elements

$$\langle j_a j_b J^{\prime\prime} \mid V_{12} \mid j_c j_d J^{\prime\prime} \rangle.$$

If the number of these is sufficiently less than the number of known experimental energy levels in a region, then they can be treated as adjustable parameters without specifying the form of the interaction V_{12} . The eigenstates are determined by adjusting the parameters until the eigenvalues of the diagonalized energy matrices fit as well as possible the experimental energies. The diagonalization determines the coefficients A_p , $B_{qq'}$, and $C_{rr'}$ in Eq. (3).

III. CALCULATION AND RESULTS WITH $2p_{3/2}$ ADMIXTURES

A. Energies and Wave Functions

As has been explained, the calculation allowing only $(1f_{7/2}^n)$ configurations cannot successfully predict some of the properties of the nuclei with 20 < Z < 28. The simplest extension of the model is to include configurations of the type $(1f_{7/2}^{n-1}2p_{3/2})$, since $2p_{3/2}$ is the next single-particle state. The energy matrices will depend upon the $1f_{7/2}$ and $2p_{3/2}$ single-particle energies and on the two-particle matrix elements:

$$\langle f_{7/2}{}^2J \mid V_{12} \mid f_{7/2}{}^2J \rangle, \qquad J = 0, 2, 4, 6$$

$$\langle f_{7/2}p_{3/2}J \mid V_{12} \mid f_{7/2}p_{3/2}J \rangle, \qquad J = 2, 3, 4, 5$$

$$\langle f_{7/2}{}^2J \mid V_{12} \mid f_{7/2}p_{3/2}J \rangle, \qquad J = 2, 4.$$

For this calculation the single-particle energy of the $2p_{3/2}$ proton with respect to the $1f_{7/2}$ single-particle energy was considered fixed. The value 3.5 MeV was taken from the work of Erskine, Marinov, and Schiffer¹⁸ on ⁴⁹Sc. The energy of the $1f_{7/2}$ proton with respect to ⁴⁸Ca was considered a parameter. This latter singleparticle energy and the ten two-particle matrix elements were varied until the best least-squares fit to 25 well-known experimental levels was obtained. The effective-interaction two-particle matrix elements thus determined are given in Table I. The $1f_{7/2}$ single-particle energy determined by the fit is 9.62 MeV, in good agreement with the experimental value of 9.72 MeV.¹⁵

The resulting calculated energy levels are given in Table II and in Figs. 1-6, where they are designated calculation A. Calculations B and C include $1f_{5/2}$ admixtures and will be discussed later. The values given in Table II are the total energies of the levels minus the binding energy of ⁴⁸Ca. For convenience,

TABLE I. Values of effective-interaction two-particle matrix elements from least-squares fit of nuclear energies.

Matrix element	J	Value (MeV)
$\langle f_{7/2}^2 J \mid V \mid f_{7/2}^2 J \rangle$	0	2.290
	2	0.465
	4	-0.420
	6	-0.815
$\langle f_{7/2}p_{3/2}J V f_{7/2}p_{3/2}J \rangle$	2	2.675
	3	-0.875
	4	-0.100
	5	-2.200
$\langle f_{7/2}^2 J \mid V \mid f_{7/2} p_{3/2} J \rangle$	2	0.655
	4	0.400

binding energies are taken to be positive. All calculated levels within 4.0 MeV of the ground state are given except for ⁴⁹Sc and ⁵⁶Ni, where only the ground states are given. The experimental levels in Table II are those which were used in the least-squares fit. All additional known experimental levels below 3.75 MeV, some with only tentative spin assignments, are included in Figs. 1-6.

The results of the energy fitting are very good, as indicated by the rms deviation of 0.08 MeV. A similar calculation with pure $(1f_{7/2}^n)$ configuration states gives an rms deviation of 0.16 MeV.

The calculated energy spectrum predicts well the energies of several levels which were not certain when this work was begun and so were not included in the fitting. In ⁵³Mn the first $\frac{9}{2}$ and $\frac{11}{2}$ levels have been established⁶ to be at 45.29 and 45.47 MeV, respectively. The predicted values are 45.37 and 45.26 MeV. Although the order of these two levels is inverted in the calculation, they are so close together that small changes in the parameters could exchange them. In ⁵⁴Fe it has been shown¹⁹ that there is a 0^+ level at 53.20 MeV, a 4^+ level at 53.22 MeV, and a 6⁺ level at 52.81 MeV. The predicted values are 52.94, 53.14, and 52.75 MeV, respectively. The agreement between these experimental and calculated values is not as good as for those levels which were included in the fitting, but it is still reasonably close. One established level for which the agreement is not good is the 0⁺ level in ⁵²Cr at 2.56 MeV. The lowest excited 0^+ level predicted by the calculation is at 4.17 MeV. Low-lying 0+ excited states are a systematic feature of even-even nuclei in the $1f_{7/2}$ shell.²⁰ The pure $(1f_{7/2}^n)$ configuration wave functions predict only the ground-state 0^+ levels. The present calculation gives excited 0⁺ levels and predicts well the energy of the excited 0⁺ level in ⁵⁴Fe. The fact that the predicted second 0⁺ level in ⁵²Cr is too high suggests that the configuration mixing does not quite compensate for the

¹⁸ J. R. Erskine, A. Marinov, and J. O. Schiffer, Phys. Rev. 142, 633 (1966).

¹⁹ J. M. Moss, D. L. Hendrie, C. Glashausser, and J. Thirion,

Bull. Am. Phys. Soc. 14, 603 (1969).
 ²⁰ D. J. Church, R. N. Horoshko, and G. E. Mitchell, Phys. Rev. 160, 894 (1967).



FIG. 2. Experimental and theoretical excitation energies of ⁵¹V. For description and notation see caption, Fig. 1.

neglected core deformation, which will be most severe in the middle of the shell and most noticeable in its effect on the zero-spin excited states.

The level structure of 55Co has not been as well explored as that of other nuclei under consideration here. The levels and tentative spin assignments given in Fig. 6 are from (³He, d) reactions, $^{2,21}(p,\gamma)$ reactions,²² and (d, n) reactions.²³ Thus, higher spin states

²¹ B. Rosner and C. H. Holbrow, Phys. Rev. 154, 1080 (1967).
 ²² B. Erlandsson, Arkiv Fysik 34, 263 (1967).
 ²³ V. V. Okorokov and Tolchenkov, Yadern. Fiz. 1, 448 (1965)
 [English transl.: Soviet J. Nucl. Phys. 1, 320 (1965)]; D. S. Gemmell, L. L. Lee, Jr., J. P. Schiffer, and A. B. Smith, Argonne National Laboratory Report No. ANL-6848, 1964 (unpublished).

have not been seen. Further, these studies have some contradictions, so that the experimental summary of Fig. 6 is uncertain, especially above 2.6-MeV excitation energy. For the lower spin states, where comparison is possible, the agreement is good except for the first $\frac{3}{2}$ state, where the theoretical value is too low. Since only the ground state of 55Co was included in the leastsquares fit and since the $(1f_{7/2}^n)$ configuration permits no states but one $\frac{7}{2}$, the agreement obtained for ⁵⁵Co is excellent support for the validity of the configuration mixing.

The calculated wave functions will not be reproduced here in detail, but are available upon request. It was

1012

TABLE II. Experimental and calculated energy levels of the nuclei. The energy given is the total energy of the state minus the binding energy of 48 Ca. Calculated energies are given for A, the model with $2p_{5/2}$ admixtures; B, the model with $2p_{8/2}$ and $1f_{5/2}$ admixtures and MSDI matrix elements; and C, the model with $2p_{8/2}$ and $1f_{5/2}$ admixtures and the Kuo and Brown matrix elements.

	_	_	~	Energy (MeV)			_			Energy (MeV)	~ . ~
Nucleus	<i>J</i> π	Expt	Calc A	Calc B	Calc C	Nucleus	J^{π}	Expt	Calc A	Calc B	Calc C
⁴⁹ Sc	7/2~	9.62	9.720	9.720	9.720		11/2-		45.257	45.301	45.665 43.584
$^{50}\mathrm{Ti}$	0+	21.79	21.730	21.730	21.730		13/2-		43.617	43.692	43.786
	2^{+}	20.23	20.179	20.202	20.184						43.607
	4+	10.04	18.341	18.370	18.341		$15/2^{-1}$		44.009	44.134	44.599
	4 · 6+	19.04	19.070	19.085	19.118		$17/2^{-}$				43.490
	Ū	10.07	10.025	10.000	10.701	⁵⁴ Fe	0+	55.76	55.770	55.770	55.884
⁵¹ V	3/2-	28.92	28.994	29.002	29.012	10	Ū	00170	52.936	52.976	52.983
			27.172	27.233	27.184		1+			51.826	51.811
	= 10		26.166	26.173	26.171		2+	54.35	54.337	54.339	54.505
	5/2-	29.53	29.553	29.563	29.645				53.098	53.129	53.163
			26.716	26.884	27.203						52.285
	7/2-	20.05	20,002	26.202	26.594		3+		52.127	52.179	52.603
	1/2	29.05	29.902	29.912	29.993						52.147
	0/2~	28 04	20.003	20.731	20.071		4^{+}		53.135	53.179	53.457
	9/2	20.01	20.073	20.122	27 856				52.250	52.273	52.602
	11/2-	28.24	28, 155	28 202	28.324						52.250
	$15/2^{-1}$		26.990	27.039	27.340					F A 040	52.207
							0		52.749	52.842	53.219
⁵² Cr	0+	40.35	40.325	40.325	40.396		r +				52.947
	1+	00.00	36.325	36.410	36.340		31				52.815
	2+	38.92	38.862	38.872	38.954	55Co	1/2-		57.425	57.777	59.892
		37.39	37.374	37.427	37.394					57.277	57.423
	4+	37.19	37.137	37.142	37.195		$3/2^{-}$		59.159	59.191	59.628
	4	37.98	37.653	37.601	37 785				58.241	58.518	59.167
		57.53	36 736	36 783	36 757					57.460	58.507
	5+	36.73	36.701	36 738	36 933						58.107
	6+	37.24	37.246	37.294	37.575		5/2-		58.291	59.607	61.593
										58.388	59.299
$^{53}\mathrm{Mn}$	$1/2^{-}$		44.642	44.701	44.661					57.903	58.340
	0.10-	15 60	45 605	45 540	43.977		7/2-	60.82	60 816	50.905 60.858	57.925 61.057
	3/2-	45.62	45.085	45.710	45.777		1/2	00.82	58 806	58 846	50 706
			44.828	44.8/4	44.830				00.000	57 801	58 812
			43.700	43.905	43.940					57.267	58.234
	5/2-	46 53	46 640	46 673	45.500		9/2-		59.000	59.055	60.055
	0/2	10.00	44.651	44,849	45 958		,			57.467	59.041
			43.592	44.497	44.667					57.012	58.705
				43.528	43.800						57.479
					43.459		$11/2^{-}$		57.416	57.421	59.112
	$7/2^{-1}$	46.91	46.950	46.972	47.155						58.178
			44.972	45.013	44.999						57.408
			43.979	44.051	44.250		13/2-				59.240
					43.998		15/0-				58.652
	9/2-		45.374	45.392	45.524	56NT:	$\frac{15}{2^{-1}}$	60 00	60 000	60 000	58.833
			44.856	44.904	45.005	**IN1	0	08.00	08.000	08.000	08.000
					44.373				0.0045	0.0077	0 0000
					43.295	rms devi	ation		0.0815	0.0866	0.2032

found that the ground states of all the nuclei were more than 98% $(1f_{7/2}^n)$. Furthermore, the lowest excited state for each (n, J) value is more than 80% $(1f_{7/2}^n)$, with two exceptions. The exceptions are the first $\frac{9}{2}^{-1}$ states of ⁵¹V and ⁵³Mn, which are both about 40%

 $(1f_{7/2}^{n})$. The dominant strength in the $\frac{9}{2}$ state of 51 V is $|f_{7/2}^{2}(2, 6) p_{3/2}; J = \frac{9}{2} \rangle$, which has an amplitude of 57%. In 53 Mn the state $|f_{7/2}^{4}(2, 6) p_{3/2}; J = \frac{9}{2} \rangle$ is 50% of the $J = \frac{9}{2}$ state.

The dominance of the pure $(1f_{7/2}^n)$ configuration,

and





FIG. 3. Experimental and theoretical excitation energies of ⁵²Cr. For description and notation see caption, Fig. 1.

especially in the ground states, explains the success of the pure configuration calculations in predicting binding energies, low-lying levels and transfer reactions between the ground states.

The positions of the energy levels are, as expected, much more sensitive to the two-particle effective interaction between $(1f_{7/2}^2)$ states than to the matrix elements involving the $(1f_{7/2}2p_{3/2})$ states. The latter can be shifted considerably with relatively little effect on the energy spectrum. The wave functions are more sensitive to shifts of the parameters, but they are not appreciably changed by small variations in the twoparticle effective interactions involving the $(1f_{7/2}2p_{3/2})$ states. In a prior calculation of this type,²⁴ the $(1f_{7/2}^2)$ two-particle effective interactions obtained are almost the same as those obtained here, but the mixed interactions are somewhat different. The energy levels of the nuclei are much the same as those obtained here, although a somewhat better fit to the experimental data is obtained in the present work.

B. Transfer Reactions

The measured differential cross section for pickup reactions is

$$d\sigma/d\Omega = NC^2 S\sigma, \tag{10}$$

where σ is the DWBA calculated cross section, N is a

normalization factor, C is the isobaric spin Clebsch-Gordan coefficient, and S is the spectroscopic factor which gives the effect of the nuclear overlap of the target and final nuclear states. For stripping reactions

$$d\sigma/d\Omega = \left[(2J_f + 1)/(2J_0 + 1) \right] NC^2 S\sigma, \qquad (11)$$

where J_f and J_0 are the total angular momenta of the final and initial states, respectively.

For pure shell-model states,

$$|A\rangle = |j_1^{n_1} j_2^{n_2} j_3^{n_3} \cdots abc \cdots J\rangle$$

$$|A-1\rangle = |j_1^{n_1\prime}j_2^{n_2\prime}j_3^{n_3\prime}\cdots a'b'c'\cdots J'\rangle$$
 where

$$\sum n$$

$$\sum_{i} n_i = A$$
 and $\sum_{i} n_i' = A - 1$,

the spectroscopic factor for single nucleon transfer reactions $(A) \rightleftharpoons (A-1)$ is²⁵

$$S(j_k) = A[I(j_k)]^2, \qquad (12)$$

where $I(j_k)$ is the projection

$$\langle AJ \mid A-1, J'; j_{kA}J \rangle.$$
 (13)

The wave function on the right above has the last particle (the transferred nucleon) coupled with the (A-1) state to total spin J but it is not antisymmetric to the exchange of this last particle with the others.

When A and A-1 are pure j^n configurations, Eq. (1) gives

$$S(j) = n \mid [j^n v J[[j^{n-1}(v_1 J_1)jJ]] \mid^2,$$
(14)

where $|A\rangle = |j^n v J\rangle$ and $|A-1\rangle = |j^{n-1} v_1 J_1\rangle$. For mixed configurations

$$|A\rangle = |j_1^{n-1}(v_2J_2)j_2J\rangle \text{ and } |A-1\rangle = |j_1^{n-2}(v_3J_3)j_2J'\rangle_{2}$$

$$S(j_1) = (n-1)F |[j_1^{n-1}v_2J_2[[j_1^{n-2}(v_3J_3)j_1J_2]]|^2, \quad (15)$$

where F is a function of the angular momenta which arises from the recoupling necessary in evaluating the projection (13). For these same states $S(j_2) = 0$ since there is only one j_2 particle in each of the states. For transfers between a mixed and a pure state $S(j_1) = 0$. When A is a pure state and A-1 is a mixed state, $S(j_2)$ is also zero. For A-1 a pure state and A a mixed state $S(j_2) = \delta_{v_1v_2} \delta_{J_1J_2}$.

For states which are sums of the shell-model states, i.e.,

$$\theta(nJa) = \sum_{i} B_i \mid nJ\rangle_i,$$

the spectroscopic factor is

$$S(j_{l}) = \big| \sum_{i,k} B_{i} B_{k} [S_{ik}(j_{l})]^{1/2} \big|^{2},$$
(16)

where $S_{ik}(j_l)$ is the spectroscopic factor for transfer of a j_l particle between the *i*th and *k*th states

The calculated spectroscopic factors for the stripping reaction (${}^{3}\text{He}$, d) are given in column 4 of Table III.

²⁴ N. Auerbach, Phys. Letters 24B, 260 (1967).

²⁵ M. H. Macfarlane and J. B. French, Rev. Mod. Phys. 32, 567 (1960).

53 Mn MeV 13/2 5/2-5/2⁻ 13/2 13/2 5/2 13/27 3/2 3/2-1/2 7/2 3/2-3.0 7/2-7/2-15/2 7/2-15/2 9/2- $(5/2^{-})$ 15/2 1/2 5/2 5/2-3/2-3/2- $(7/2^{-})$ 1/2. 7/2 5/2 9/2-12 3/2 2.0 9/2-7/2 712 11/2-11/2~ 9/2 9/2-9/2-9/2-11/27 11/2 3/2-3/2 3/2-3/2-5/2-1.0 5/2 5/2-5/2 5/2 0.0 7/2 7/2 7/2-С Exper А В





this factor does not become important except for higher energy levels near the end of the shell, and in any case it is less than the experimental range of error, which is about 20%. The experimental values differ from each other due to uncertainties in the analyses and to the differing choices of a normalization factor $\lceil N \rangle$ in Eq. (10)]. The latter is usually chosen to best satisfy the theoretical sum rules²⁵ for the spectroscopic factors.

Because of these uncertainties, the relative strengths of transfers to different levels are of more interest than the magnitudes of the individual spectroscopic factors. More important, though, in testing a model is the presence or absence of predicted strengths in the

 ²⁶ M. A. Moinster, Nucl. Phys. A94, 81 (1967).
 ²⁷ F. Hinterberger, G. Mairle, U. Schmidt-Rohr, P. Turek, and G. J. Wagner, Z. Physik 202, 236 (1967).



Fig. 5. Experimental and theoretical excitation energies of ⁵⁴Fe. For description and notation see caption, Fig. 1.

experimental results. The pure configuration model predicts no transfers to excited states of odd-A nuclei. Experimentally, the L=1 transfer to the second $\frac{3}{2}$ level in ⁵¹V is about 60-70% of the ground-state L=3spectroscopic factor for the $({}^{3}\text{He}, d)$ reaction. The ratio for the corresponding transfers in ⁵³Mn is about 1. The lowest $\frac{3}{2}$ level in ⁵⁵Co has a spectroscopic factor 1.5 that for the transfer to the ground state. The configuration mixing calculation (calculation A) correctly predicts these strengths. It also predicts the reduction in strength of the L=3 transfer to the first 2^+ state in ⁵²Cr. The strength of this transfer predicted by the pure $(1f_{7/2}^n)$ model is one-third the ground-state strength, while the experimental value and that predicted by calculation A are about one-fourth the ground-state transfer strength.

Finally, there are the L=3 transfers to the first and second 4⁺ states in ⁵²Cr. The pure $(1f_{7/2}^n)$ model predicts zero transfer strength to the first 4⁺ level. For the second 4⁺ level it predicts S to be one-third the groundstate value. Experimentally the relative strengths are $\frac{1}{8}$ and $\frac{1}{5}$, respectively. This splitting has been taken as evidence of seniority mixing in the two 4⁺ states.^{28,29} The present calculation correctly predicts the sharing of strengths between the two levels although S for the lower state is less than the experimental value and for the higher state S is greater than the experimental value. The wave functions for these 4⁺ states are dominated by the $(1f_{7/2}^n)$ configuration states, but do show the expected seniority mixing.

The present calculation fails to predict spectroscopic factors for the $\frac{5}{2}$ and $\frac{1}{2}$ levels in ⁵¹V and ⁵³Mn. This is because no $1f_{5/2}$ or $2p_{1/2}$ protons are included in the allowed configurations. There are also relatively large transfer strengths predicted for the third $\frac{3}{2}$ states of ⁵¹V and ⁵³Mn that do not appear experimentally. It appears that experimentally the $\frac{3}{2}$ transfer strength, except for that to the 2.4-MeV level, is spread over a number of higher-lying $\frac{3}{2}$ levels. Similarly, the experimental $\frac{3}{2}$ transfer strength to levels above 2.5 MeV in ⁵⁵Co is spread over a number of states, while the calculation predicts that S=0.597 for the 2.56-MeV level and <0.002 for higher $\frac{3}{2}$ levels.



FIG. 6. Experimental and theoretical excitation energies of ⁵⁵Co. For description and notation see caption, Fig. 1. Calculation C is not included here because the level scheme it gives is not in good agreement with the others.

²⁸ T. Komada, Nucl. Phys. 51, 234 (1964).

²⁹ I. Talmi, Phys. Rev. 126, 1096 (1962).

1017

TABLE III. Calculated and experimental values of spectroscopic factors for (${}^{3}\text{He}$, d) reactions. Experimental energies are given where known. Otherwise the energies from calculation B are given in parenthesis. Calculations A and B are described in the text.

Final nucleus and level	Energy (MeV)	Transfer J^{π}	Calc A	Spe Calc B	ctroscopic stre Ex	ngth S perimental C ²	S a	
 50Ti								
0^{+}	0.00	$\frac{7}{2}$	2.000	2.000				
2+	1.56	7 7	1.702	1.678				
		5		0.004				
		<u>3</u> -	0.149	0.157				
4+	2 75	2 <u>7</u> -	1 970	1 960				
т	2.15	2 5-	1.970	0.002				
		2	0.015	0.003				
7	2 00	ž 7	0.015	0.010				
0'	3.20	2	2.000	1.994				
- 1	()	3-		0.003				
2+	(3.36)	2	0.298	0.321				
		5-		0.008				
		$\frac{3}{2}$	0.851	0.832				
^{51}V								
$\frac{7}{2}$	0.00	$\frac{7}{2}$	0.746	0.745	0.750 ^b	0.750°	0.700 ^d	
$\frac{5}{2}$	0.32	$\frac{5}{2}$		0.002				
3-	0.93	3-	0.001	0.001			0.012	
- <u>3</u>	2.41	3-	0.662	0.657	0.45	0.57	0.42	
5	3.08	5-		0.233	0.24		0.13	
4	0100	2		0.1200			0.10	
⁵² Cr								
0+	0.00	<u>7</u>	3 949	3 942	4 000			
2+	1 43	2 <u>7</u> →	1 001	1 085	1.00			
2	1.40	2 5	1.071	0.002	1.00			
		23-	0.140	0.002				
4+	0.27	27	0.149	0.130	0 510			
4'	2.37	2	0.239	0.184	0.51			
		2	0.003	0.002	0.04			
4+	2.76	1-2-	0.989	1.059	0.81			
		3- 2	0.007	0.008				
2+	2.96	$\frac{7}{2}$	0.101	0.096				
6+	3.11	$\frac{7}{2}$	1.306	1.282	1.31			
		<u>5</u>		0.004				
2+	3.16	$\frac{7}{2}$	0.061	0.068				
		<u>3</u> 2	0.091	0.103				
4+	3.46	$\frac{7}{2}$	0.052	0.043				
		$\frac{3}{2}$	0.026	0.028				
⁵³ Mn								
$\frac{7}{2}$	0.00	$\frac{7}{2}$	0.483	0.481	0.47°	0.42 ^b	0.51 ^d	
5-2	0.38	$\frac{5}{2}$		0.004				
3-	1.29	3-	0.003	0.003	0.07	0.05	0.06	
<u>7</u> -	(1.96)	<u>7</u> -	0.006	0.006				
<u>3</u> -	2.41	² <u>3</u> →	0.491	0.503	0.45	0.44	0 43	
2 5-	(2, 12)	2 <u>5</u>	0.171	0.328	0,10	0.11	0.10	
2 <u>5</u>	(2.12) (2.47)	2 <u>5</u>		0.554				
2 7	2.47)	27	0.007	0.004	0.02	0.01	0.02	
2	(2.07)	2	0.007	0.000	0.03	0.01	0.02	
2	(3.07)	Ž	0.501	0.422	0.20	0.44	0.00	
<u>5</u> 2	3.68	$\frac{3}{2}^{-}$		0.077	0.39	0.44	0.22	
5413								
°*re ∽±	0.00	7	E (02	5 640				
0-	0.00	2	5.083	5.000				
2+	1.41	$\frac{1}{2}$	0.546	0.542				
		<u>3</u> 2	0.134	0.134				
4+	2.54	<u>7</u> -	0.597	0.589				
		<u>5</u> 2		0.002				
0+	2.56	$\frac{7}{2}$	0.241	0.242				
6+	2.95	$\frac{7}{2}$	0.597	0.576				
		<u>5</u> -		0.008				

Final nucleus and level	Energy (MeV)	Transfer J^{π}	Calc A	Sp Calc B	ectroscopic	strength S Experimental C ² S ^a	
 ⁵⁴ Fe							
2+	2.96	7-	0.055	0.056			
		5-		0.002			
		$\frac{3}{2}$	0.744	0.741			
4+	3.30	7-	0.043	0.034			
		$\frac{5}{2}$		0.001			
		$\frac{3}{2}$	0.099	0.094			
3+	3.35	$\frac{7}{2}$	0.008	0.007			
		$\frac{5}{2}$		0.019			
		$\frac{3}{2}$	0.009	0.005			
⁵⁵ Co							
$\frac{7}{2}$	0.00	$\frac{7}{2}$	0.234	0.232	0.22e	0.21 ^f	
$\frac{5}{2}$	(1.25)	$\frac{5}{2}$		0.915			
3-	2.16	$\frac{3}{2}$	0.389	0.340	0.35	0.42	
$\frac{7}{2}$	(2.01)	$\frac{7}{2}$	0.014	0.013			
3-	2.56	$\frac{3}{2}$	0.597	0.541	0.21	0.26	
5	(2.47)	$\frac{5}{2}$		0.019			

^d Reference 7.

^e Reference 2. ^f Reference 21.

TABLE III. (Continued).

^a Experimental values include the factor C^2 , where C is the isobaric spin Clebsch-Gordan coefficient.

^b Reference 4.

^e Reference 9.

Experimental information on the pickup reaction $(d, {}^{3}\text{He})$ is not as extensive as that for the stripping reaction. For the transfers which have been measured, given in Table IV, the experimental strengths are found to be generally slightly less than the predictions of the $(1f_{7/2}^n)$ model. Although the individual differences are all well within the experimental uncertainties, the general trend to smaller experimental values than predicted is significant. The mixed configuration calculation gives predicted transfer strengths which are closer to the experimental values. Further, transfers to excited states of ⁵¹V, ⁵³Mn, and ⁵⁵Co are found with the mixed-configuration model, although the calculated and measured spectroscopic factors are not in good agreement. These transfers are forbidden completely for the pure configuration model.

C. Electromagnetic Transitions

Since M1 transitions are forbidden between $(1f_{7/2}^n)$ configuration states,¹² the presence of such transitions experimentally is an indication of configuration mixing. There are no low-lying M1 transitions in the even-A nuclei, so we will consider here only the transition probabilities in ⁵¹V and ⁵³Mn. These nuclei are the three-particle and three-hole states, respectively, for the $(1f_{7/2}^n)$ configuration and so are expected to closely resemble each other. The experimental and calculated energy level schemes for these nuclei are given in Figs. 2 and 4 and the similarity can be seen. The transition probabilities and mixing ratios, where known, are also much alike. They are given in Table VI.

It has been felt in the past that little success could be obtained in predicting transition probabilities from effective-interaction calculations in the $1f_{7/2}$ shell. This was partly because the transition probabilities, unlike the energies, are sensitive to small admixtures in the wave functions. Another difficulty, though, has been the quality of the available experimental information. Recent work has much improved this situation. Talmi³⁰ has shown that the $(1f_{7/2}^n)$ model can account well for the E2 reduced transition probabilities in ⁵¹V found by Afonin *et al.*,¹ if an "effective charge" is used in the single-particle E2 operator. This effective charge compensates for the neglected effects of core polarization much as the effective two-particle interactions are supposed to "absorb" the effects of neglected configurations.

The E2 transition rates in ⁵¹V and ⁵³Mn were calculated here for the mixed-configuration states using the same effective charge, e'=1.6e, used by Talmi.³⁰ The M1 strengths were calculated with the real M1operator, which successfully reproduces the measured value for the ground-state magnetic moment of ⁵³Mn. The results for the B(E2)'s in ⁵¹V are quite good, differing from the experimental values by no more than 0.07. The M1, E2 mixing ratios and the branching ratios are not as successful, though there is considerable improvement over the $(1f_{7/2}^n)$ model. The mixing ratios are too large by factors ranging from 3 to 5, with the worst disagreement that for the $\frac{9}{2} \rightarrow \frac{7}{2}$ transition in ⁵³Mn. The success with the B(E2)'s suggests that the problem with the mixing and branching ratios is due to M1transition rates which are too small. This conclusion is supported by the fact that the most difficulty is encountered with the transitions from the $\frac{9}{2}$ levels. As

³⁰ I. Talmi, Phys. Letters 25B, 313 (1967).

Final nucleus and level	Energy (MeV)	Transfer J^{π}	Spectroscopic strength S Calc A Calc B Experimental C ² S a					
 ⁴⁹ Sc							<u></u>	
$\frac{7}{2}$	0.00	$\frac{7}{2}$	2.00	2.00	1.93 ^b			
⁵⁰ Ti								
0+	0.00	$\frac{7}{2}$	0.746	0.745	0.74 ^b	0.88°	0.73 ^d	
2+	1.56	<u>7</u> -	0.344	0.338	0.37	0.42	0.39	
		<u>3</u>	0.004	0.004				
4+	2.75	$\frac{7}{2}$	0.723	0.716	0.75	0.88	0.64	
		<u>5</u> -		0.001				
6+	3.20	$\frac{7}{2}$	1.078	1.071	0.14	1.32	1.05	
		<u>5</u> -		0.003				
2+	(3.36)	<u>7</u>	0.071	0.076				
		<u>3</u> 2	0.001	0.001				
$^{51}\mathrm{V}$								
$\frac{7}{2}$	0.00	$\frac{7}{2}$	3.949	3.942	3.70 ^b			
3-	0.93	$\frac{3}{2}$	0.003	0.003				
<u>3</u>	2.41	$\frac{3}{2}$	0.0004	0.0004				
<u>7</u> -	(3.18)	$\frac{7}{2}$	0.017	0.017				
⁵² Cr								
0+	0.00	$\frac{7}{2}$	0.483	0.481				
2+	1.43	$\frac{7}{2}$	0.637	0.631				
		$\frac{3}{2}$	0.007	0.006				
4+	2.37	$\frac{7}{2}$	0.265	0.189				
		$\frac{3}{2}$	0.002	0.002				
4+	2.76	$\frac{7}{2}$	1.050	1.117				
		5-		0.001				
2+	2.96	$\frac{7}{2}$	0.072	0.067				
6+	3.11	$\frac{7}{2}$	2.093	2.040				
		$\frac{5}{2}$		0.002				
2+	3.16	$\frac{7}{2}$	0.051	0.056				
		$\frac{3}{2}$	0.003	0.003				
4+	3.46	$\frac{7}{2}$	0.130	0.112				
⁵³ Mn								
$\frac{7}{2}$	0.00	$\frac{7}{2}$	5.683	5.660	5.93 ^b			
<u>5</u> 2	0.38	<u>5</u> -		0.0004	0.18			
3-	1.29	$\frac{3}{2}^{-}$	0.012	0.012	0.10 ^b			
$\frac{7}{2}$	(1.96)	$\frac{7}{2}$	0.204	0.199				

TABLE IV. Calculated and experimental values of spectroscopic factors for $(d, {}^{3}\text{He})$ reactions. Experimental energies are given where known. Otherwise the energies from calculation B are given in parenthesis. Calculations A and B are described in the text.

 Final nucleus	Energy	Transfer		attraction attraction of the		
and level	(MeV)	J^{π}	Calc A	Calc B	Experimental C^2S°	
 ⁵³ Mn						~
<u>3</u> -	2.39	<u>3</u> - 2	0.001	0.001	0.16	
$\frac{7}{2}$	(2.92)	$\frac{7}{2}$	0.016	0.010		
<u>3</u> 2	(3.07)	$\frac{3}{2}$	0.001	0.001		
ĕ⁴Fe						
0+	0.00	<u>7</u> -	0.235	0.232		
2+	1.41	$\frac{7}{2}$	0.911	0.905		
		<u>5</u> - 2		0.003		
		3 -	0.005	0.004		
4+	2.54	$\frac{7}{2}$	2.051	1.990		
		5 <u>-</u>		0.004		
		$\frac{3}{2}$	0.017	0.015		
0+	2.56	7-2-	0.012	0.012		
6+	2.95	7-	2.942	2.763		
2+	2.96	$\frac{7}{2}$	0.181	0.176		
		3	0.001	0.001		
4+	3.30	7-	0.057	0.041		
3+	3.35	7-	0.009	0.007		
⁵⁵ Co						
<u>7</u> -	0.00	7-	7.809	7.303		
$\frac{7}{2}$	(2.01)	$\frac{7}{2}$	0.069	0.575		

TABLE IV. (Continued).

^a Experimental values include the factor C^2 , where C is the isobaric spin Clebsch-Gordan coefficient.

^b Reference 5.

^c Reference 26.

^d Reference 27.

pointed out previously, these states have large $(1f_{7/2}^{n-1}2p_{3/2})$ amplitudes. Since the M1 transition strength comes entirely from the $(1f_{7/2}^{n-1}2p_{3/2})$ components of the wave functions, it would seem that the admixtures are too small. No adjustment of the parameters of the fit can correct this without distortion of the level schemes.

There are several ways to extend the model space. Since the required modification is slight we wish to choose the simplest extension. This would be to include configurations of the type $(1f_{7/2}^{n-2}2p_{3/2}^2)$ or $(1f_{7/2}^{n-1}1f_{5/2})$ For several reasons, the latter is the better choice. The most important reason is that the single-particle energy of the $1f_{5/2}$ proton relative to the $1f_{7/2}$ is 4.7 MeV, while the $2p_{3/2}$ energy is 3.5 MeV.¹⁸ Thus, $(1f_{7/2}^{n-2}2p_{3/2}^2)$ configurations would be at higher energies than $(1f_{7/2}^{n-1}1f_{5/2})$ configurations. Furthermore, the latter will better increase the M1 transition strengths since there will be contributions from terms such as (8) as

well as (9). This is because $(\frac{7}{2} || f^{(1)} || \frac{5}{2})$ is nonzero while $(\frac{7}{2} || f^{(1)} || \frac{3}{2}) = 0$.

In Sec. IV, energies, spectroscopic factors, and transition probabilities are recalculated for a model which permits configurations $(1f_{7/2}^{n})$, $(1f_{7/2}^{n-1}2p_{3/2})$, and $(1f_{7/2}^{n-1}1f_{5/2})$.

IV. CALCULATION AND RESULTS WITH $1f_{5/2}$ ADMIXTURES

A. Effective Interactions

Extending the model space to include configurations with an $f_{5/2}$ proton requires the two-particle matrix elements:

$$\langle f_{7/2}^2 J \mid V_{12} \mid f_{7/2} f_{5/2} J \rangle, \qquad J = 2, 4, 6$$

 $\langle f_{7/2} f_{5/2} J \mid V_{12} \mid f_{7/2} f_{5/2} J \rangle, \qquad J = 1, 2, 3, 4, 5, 6 \qquad (17)$

and

$\langle f_{7/2} f_{5/2} J | V_{12} | f_{7/2} p_{3/2} J \rangle$, J = 2, 3, 4, 5.

This brings the number of parameters in the energy matrices to 24. The number of well-identified experimental levels is 32. A least-squares-fitting calculation would then be a lengthy procedure with questionable reliability. In any case, the calculation is beyond the storage capacity of the computer used (an IBM 360/50). It is necessary to determine the additional two-particle effective interactions by another method.

We decided to choose a residual interaction fitted to best reproduce the matrix elements in Table I and then use this interaction to calculate the additional twoparticle matrix elements required. We used a modification of the surface delta interaction (SDI) introduced by Green and Moszkowski.³¹ The SDI has been shown to be successful in some shell-model calculations.^{32,33} Glaudemans, Wildenthal, and McGrory showed³⁴ that it gives a good approximation to the two-nucleon matrix elements determined for the $2s_{1/2}$ -1 $d_{3/2}$ subshells from effective-interaction calculations. The SDI is based on the assumptions that the residual interactions are most important at the nuclear surface and weak in the nuclear interior, and that the effect of the finite range in the interactions can be ignored as a first approximation. Green and Moszkowski make the further assumption that all radial integrals are equal. We modified the interaction by not making this last assumption and considering the "nuclear radius" as an additional parameter. The interaction used is

$$V_{ik} = 4\pi G \delta(\mathbf{r}_i - \mathbf{r}_k) \delta(\mathbf{r}_i - \mathbf{R}).$$
(18)

The interaction is attractive, but the sign here is positive since we have taken binding energies to be positive. The effective nuclear radius is R, and the coordinate of the *i*th nucleon is \mathbf{r}_i . The matrix elements of the interaction between j-j coupled antisymmetrized two particle states are³³

$$\langle j_a j_b J | V_{ik} | j_c j_d J \rangle = A (abcd) R_0(abcd) G$$

if $l_a + l_b + J$ is odd
 $= 0$ if $l_a + l_b + J$ is even. (19)

The factor A(abcd) is

$$A(abcd) = \left[(1+\delta_{ab}) (1+\delta_{cd}) \right]^{-1/2} h_J(j_a j_b) h_J(j_c j_d)$$

$$(20)$$

with

$$h_{J}(j_{a}j_{b}) = (-)^{j_{a}+J-1/2} [(2j_{a}+1)(2j_{b}+1)/(2J+1)]^{1/2} \\ \times (j_{a}j_{b}\frac{1}{2}, -\frac{1}{2} \mid J0).$$
(21)

³¹ I. M. Green and S. A. Moszkowski, Phys. Rev. 139, B790 (1965). ³² R. Arvieu and S. A. Moszkowski, Phys. Rev. 145, 830

TABLE	v.	Effective-interaction	two-particle	matrix	elements
calculated	l wi	th modified surface δ i	nteraction an	d reactio	on matrix
elements	calc	ulated by Kuo and Br	own.		

$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	Matrix el	ement	J	Values	(MeV)
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	$\langle f_{7/2}^2 J \mid V \mid f_7$	$_{_{I/2}}{}^2J angle$	0	1.676ª	2.068 ^b
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$			2	0.399	0.755
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$			4	0.196	0.036
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$			6	0.098	-0.287
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\langle f_{7/2}p_{3/2}J \mid V$	$ f_{7/2}p_{3/2}J\rangle$	2	2.060	0.918
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$			3	0.0	-0.086
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$			4	0.636	0.083
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$			5	0.0	-0.379
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	$\langle f_{7/2}p_{3/2}J \mid V$	$ f_{7/2}^2 J angle$	2	-0.907	0.609
$\begin{array}{c ccccc} \langle f_{7/2}f_{5/2}J \mid V \mid f_{7/2}f_{5/2}J \rangle & 1 & 0.0 & -0.134 \\ 2 & -0.096 & -0.121 \\ 3 & 0.0 & -0.122 \\ 4 & -0.218 & -0.132 \\ 5 & 0.0 & -0.200 \\ 6 & -0.586 & 0.852 \\ \langle f_{7/2}f_{5/2}j \mid V \mid f_{7/2}p_{3/2}J \rangle & 2 & -0.444 & 0.104 \\ 3 & 0.0 & 0.107 \\ 4 & -0.353 & 0.182 \\ 5 & 0.0 & -0.031 \\ \langle f_{7/2}f_{5/2}J \mid V \mid f_{7/2}^2J \rangle & 2 & -0.195 & 0.127 \\ 4 & -0.206 & 0.450 \\ 6 & -0.239 & 0.705 \end{array}$			4	-0.353	0.356
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\langle f_{7/2}f_{5/2}J \mid V \mid$	$f_{7/2}f_{5/2}J\rangle$	1	0.0	-0.134
$\begin{array}{cccccccccccccccccccccccccccccccccccc$			2	-0.096	-0.121
$\begin{array}{c cccccc} 4 & -0.218 & -0.132 \\ 5 & 0.0 & -0.200 \\ 6 & -0.586 & 0.852 \\ \hline \langle f_{7/2} f_{5/2} j \mid V \mid f_{7/2} p_{3/2} J \rangle & 2 & -0.444 & 0.104 \\ 3 & 0.0 & 0.107 \\ 4 & -0.353 & 0.182 \\ 5 & 0.0 & -0.031 \\ \hline \langle f_{7/2} f_{5/2} J \mid V \mid f_{7/2}^2 J \rangle & 2 & -0.195 & 0.127 \\ 4 & -0.206 & 0.450 \\ 6 & -0.239 & 0.705 \end{array}$			3	0.0	-0.122
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$			4	-0.218	-0.132
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$			5	0.0	-0.200
$\begin{array}{c ccccc} \langle f_{7/2}f_{5/2}j \mid V \mid f_{7/2}p_{3/2}J \rangle & 2 & -0.444 & 0.104 \\ & 3 & 0.0 & 0.107 \\ & 4 & -0.353 & 0.182 \\ & 5 & 0.0 & -0.031 \\ \langle f_{7/2}f_{5/2}J \mid V \mid f_{7/2}^2J \rangle & 2 & -0.195 & 0.127 \\ & 4 & -0.206 & 0.450 \\ & 6 & -0.239 & 0.705 \end{array}$			6	-0.586	0.852
$\begin{array}{cccccccc} 3 & 0.0 & 0.107 \\ 4 & -0.353 & 0.182 \\ 5 & 0.0 & -0.031 \\ \langle f_{7/2}f_{5/2}J \mid V \mid f_{7/2}{}^2J \rangle & 2 & -0.195 & 0.127 \\ 4 & -0.206 & 0.450 \\ 6 & -0.239 & 0.705 \end{array}$	$\langle f_{7/2}f_{5/2}j \mid V \mid$	$f_{7/2}p_{3/2}J$ >	2	-0.444	0.104
$\begin{array}{ccccccc} 4 & -0.353 & 0.182 \\ 5 & 0.0 & -0.031 \\ \hline \langle f_{7/2}f_{5/2}J \mid V \mid f_{7/2}{}^2J \rangle & 2 & -0.195 & 0.127 \\ 4 & -0.206 & 0.450 \\ 6 & -0.239 & 0.705 \end{array}$			3	0.0	0.107
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$			4	-0.353	0.182
$\begin{array}{c cccc} \langle f_{7/2}f_{5/2}J \mid V \mid f_{7/2}{}^2J \rangle & 2 & -0.195 & 0.127 \\ & 4 & -0.206 & 0.450 \\ & 6 & -0.239 & 0.705 \end{array}$			5	0.0	-0.031
$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	$\langle f_{7/2}f_{5/2}J \mid V \mid$	$f_{7/2}{}^2J angle$	2	-0.195	0.127
6 -0.239 0.705			4	-0.206	0.450
			6	-0.239	0.705

^a Calculated from modified surface δ interaction with G' = 0.783 MeV and x = 1.17. ^b Reference 15.

The factor $R_0(abcd)$ in Eq. (19) is the product of the four radial wave functions at the effective nuclear radius R. For the single-particle states under consideration in this work, there are only three different R_0 's. Therefore, Eq. (19) was rewritten, for convenience, so that the factors common to the three R_0 's are absorbed into the interaction strength. For l_a+l_b+J even,

$$\langle j_a j_b J | V_{ik} | j_c j_d J \rangle = A (abcd) R_1(abcd) G', \quad (22)$$

where

$$G' = \left[(128/1575\pi^2) \left(R^{10}/\beta^{14} \right) \exp\left(-\frac{2R^2}{\beta^2} \right) \right] G.$$
(23)

In (23), β is the harmonic-oscillator constant $(\hbar/M\omega)^{1/2}$. The three radial factors are

$$R_{1}(1f, 1f, 1f, 1f) = 0.2857x^{4},$$
$$R_{1}(1f, 1f, 2p, 2p) = (\frac{5}{2} - x^{2})^{2},$$

$$R_1(1f, 1f, 1f, 2p) = 0.5245x^2(\frac{5}{2} - x^2),$$

where $x = R/\beta$.

Using Eq. (22), the two-particle matrices can be calculated as functions of the two parameters x and G'. The best values for the parameters were determined by a least-squares fit to the matrix elements of Table I.

^{(1966).} ³³ A. Plastino, R. Arvieu, and S. A. Moszkowski, Phys. Rev.

 <sup>145, 837 (1966).
 &</sup>lt;sup>34</sup> P. W. M. Glaudemans, B. H. Wildenthal, and J. B. McGrory, Phys. Letters 21, 427 (1966).

			$^{51}\mathrm{V}$			⁵³ Mn		
Transition ^a		Expt	Calc B	Calc C	Calc C Expt		Calc C	
7/2→5/2	B(E2)	0.92 ^b	0.993	0.959				
$7/2 \rightarrow 3/2$	B(E2)	0.27	0.225	0.210				
$7/2 \rightarrow 11/2$	B(E2)	0.90	0.960	0.916				
7/2→9/2	B(E2)	0.22	0.322	0.347				
5/2→7/2	$t_{1/2}$	2.9°	0.885	3.758	1.26 ^d	0.917	0.750	
	δ	0.45e	0.282	0.657	0.54^{f}	0.203	0.269	
$9/2 \rightarrow 7/2$	δ		1.256	14.8	3.2	1.96	3.95	
3/2→5/2	δ	0.18 ^g	0.267	0.532	0.18	0.502	0.566	
Branching ratio	s							
$3/2 \rightarrow 7/2$		$16\%^{h}$	27%	28%	57%	82%	64%	
5/2		84%	73%	72%	43%	18%	36%	
$0/2 \rightarrow 7/2$		7807	0807	0007	8007	8507	0207	
 5/2		22%	2%	<1%	11%	15%	8%	

TABLE VI. Experimental and theoretical E2 and M1 transition probabilities in ⁵¹V and ⁵³Mn. An effective charge of 1.6*e* is used in calculating the E2 transition strengths. The B(E2) values have units of $e^{2}10^{-50}$ cm⁴. Lifetimes are in 10^{-10} sec.

^a Transitions are between the lowest levels of the indicated angular momenta.

^b Reference 1.

^e Reference 36.

^d Reference 37.

The resulting calculated two-particle matrix elements for x=1.17 and G'=0.783 MeV are given in the third column of Table V. The rms deviation for the fit is 1.0 MeV. While not especially good, this is about the same as Glaudemans *et al.*³⁴ obtained. Close precision is not required since, as discussed in Sec. III A, the energies and wave functions are not too sensitive to the twoparticle matrix elements except for those between $f_{7/2}^2$ states.

The two-particle reaction matrix elements calculated by Kuo and Brown¹⁵ are given in the last column of Table V. These were calculated with a Hamada-Johnston nucleon-nucleon potential and include the effects of core polarization. The average deviation of the Kuo and Brown matrix elements from the effective matrix elements of Table I is about 0.7 MeV, a somewhat better fit than the MSDI matrix elements, but not significantly so.

B. Discussion of Results

The energy levels and wave functions for the nuclei with N=28, $20 < Z \le 28$ were calculated using both the MSDI and Kuo and Brown matrix elements for the two-particle interactions involving an $f_{5/2}$ proton. For the remaining matrix elements, the effective interactions of Table I were used. The predicted binding energies for these states with both $p_{3/2}$ and $f_{5/2}$ admixtures are given in the last two columns of Table II. The calculation using the MSDI two-particle matrix elements in calculation B, while that using the Kuo and Brown matrix elements is calculation C. ^e Reference 38.

f Reference 6.

^g Reference 39. ^h Reference 3.

Reference 5.

The energies of calculation B are very little changed from those of calculation A. The rms deviation increases only to 0.0866 MeV. The shifts in the levels are greater at higher energies, but even these are quite small. The difference between the two calculations is greatest in ⁵³Mn and ⁵⁵Co where the $\frac{3}{2}$ and $\frac{5}{2}$ states are brought down in energy in calculation B. For ⁵³Mn the first two $\frac{3}{2}$ levels are somewhat lower than the experimental values. The other $\frac{3}{2}$ levels are not known experimentally. Neither are the $\frac{5}{2}$ levels above the first, but there is evidence³⁵ that there may be three $\frac{5}{2}$ levels below 2.5 MeV, which supports the predictions of calculation B. Further, the energies of the $\frac{11}{2}$ level in ⁵³Mn and of the second 0⁺, first 4⁺, and first 6⁺ states in ⁵⁴Fe are all improved in this calculation. In ⁵⁵Co the first $\frac{5}{2}$ level is at 1.251 MeV and is the first excited state. Experimentally, no state has been seen this low. The calculation also predicts more levels between 3.0 and 4.0 MeV than does calculation A, but most are high spin states for which there is no experimental information. The results of calculation C, using the Kuo and Brown matrix elements, are much worse. The disagreement becomes severe high in the shell. For ⁵⁵Co agreement with experiment is such that the predicted levels were not included in Fig. 6. They are given, however, in Table II. There are too many levels below 4.0 MeV and the first $\frac{5}{2}$ state is brought down in energy below the $\frac{7}{2}$ ground state.

³⁵ C. Robertson, K. C. Chung, A. Mittler, K. Swartz, J. D. Brandenberger, and M. T. McEllistrem, Bull. Am. Phys. Soc. 14, 603 (1969).

Nucleus and transition	E (MeV)		Experimental	Calc B	Calc C	
 ⁵⁰ Ti			· · · · · · · · · · · · · · · · · · ·			
$0^+ \rightarrow 2^+$	1.55	<i>B</i> (<i>E</i> 2)	1.73 ^a 2.40 ^b	2.85	2.80	
⁵⁴ Fe						
0+→2+	1.43	B(E2)	5.33° 5.1 ^b	3.49	2.90	
52Cr			0.14			
0 ⁺ →2 ⁺	1.45	B(E2)	4.3^{a} 4.8^{b} $(4.55\pm1.4)^{d}$	4.05	3.78	
$5^+ \rightarrow 4^+$ (1st)	1.13	δ	$(0.17 - 0.55)^{e}$	0.377	0.599	
Branching ratios in	⁵² Cr					
$6^+ \rightarrow 4^+$ (1st)	0.573		99/1 ^f	96/4	99/1	
4 ⁺ (2nd)	0.397		,	,		
$5^+ \rightarrow 4^+$ (1st)	1.13		$2.2/1.0^{e}$ $1.7/1.0^{f}$	0.69/1.0	2.9/1.0	
4 ⁺ (2nd)	0.953		-			

TABLE VII. Experimental and theoretical E2 and M1 transition probabilities in 5°Ti, 52Cr, and 54Fe. An effective charge of 1.6e is used in calculating the E2 transition strengths. The B(E2) values have units $e^{2}10^{-50}$ cm⁴.

Reference 1.

^b Reference 41. ^e Reference 42.

Reference 43.

Reference 44. ^f Reference 45.

The wave functions from calculations B and C still show dominance by the $(f_{7/2}^n)$ states, as do those of calculation A. The strengths of the $f_{5/2}$ admixtures in the lower-energy states are generally quite small and in most cases these components are added at the expense of the $(f_{7/2}^n)$ amplitudes rather than the mixed state amplitudes. The only low-lying states dominated by the $f_{5/2}$ admixtures are the second $\frac{5}{2}$ states in ⁵¹V and ⁵³Mn and the excited states of ⁵⁵Co. It is for these levels that the discrepancies between experimental and theoretical energies is largest.

The spectroscopic factors from calculation B are given in the fifth columns of Tables III and IV. Those from calculation C are not given because they differ very little from the values of calculation B except for the second and third $\frac{5}{2}$ levels in ⁵¹V and ⁵³Mn, where somewhat larger values of S are obtained in calculation C. The spectroscopic factors obtained for the states with $f_{5/2}$ admixtures are very close to those obtained in calculation A except that the $f_{5/2}$ strengths to the $\frac{5}{2}$ levels of ⁵¹V and ⁵³Mn, missing in calculation A, are obtained in calculation B. Calculation B predicts spectroscopic factors for $({}^{3}\text{He}, d)$ reactions to the second and third $\frac{5}{2}$ levels of ⁵³Mn that are comparable to the groundstate strength. These transfers are found experimentally, but at an excitation energy of 3.68 MeV, almost an MeV higher than the theoretical predictions. It would seem that the wave functions for these higherenergy states require some adjustments in the strengths

of the $f_{5/2}$ components. The same situation occurs for the first $\frac{5}{2}$ state in ⁵⁵Co, where a spectroscopic factor S=0.915 is predicted. This state is not found experimentally, but Armstrong and Blair² do find L=3transfers to states at 3.34 and 4.18 MeV with strengths S = 0.54 and 0.20, respectively.

The significant improvement of calculations B and C over calculation A is in the transition probabilities, as expected. The experimental and calculated transition rates, mixing ratios, and branching ratios are given in Table VI.³⁶⁻³⁹ (Note: The signs of the mixing ratio, though known experimentally, are not given since this calculation cannot determine them.)

All quantities given in Table VI are improved over the predictions of calculation A except for the mixing ratio for the $\frac{3}{2} \rightarrow \frac{5}{2}$ transition in ⁵³Mn. The agreement between theory and experiment is good for all quantities in Table VI. The differences present suggest that for calculation C the M1 transition strengths are slightly too small, while for calculation B they are slightly too large.

 ³⁶ N. Delyagin and M. Preisa, Zh. Eksperim. i Teor. Fiz.
 36, 1586 (1959) [English transl.: Soviet Phys.—JETP 9, 1127 (1959)]; T. D. Nainan, Phys. Rev. **123**, 1751 (1961); E. N. Shipley, R. E. Holland, and F. J. Lynch, *ibid*. **182**, 1105 (1969).
 ³⁷ S. Gorodetzky, N. Schulz, E. Bozek, and A. Knipper, Nucl. Phys. **85**, 519 (1966).
 ³⁸ R. C. Ritter, P. H. Stelson, F. K. McGowan, and R. L. Robinson, Phys. Rev. **128**, 2320 (1962); I. Y. Krause, *ibid*. **129**, 1330 (1963).

^{1330 (1963).}

³⁹ J. Vervier, Phys. Letters 5, 79 (1963).

Another nuclear property for which there is recently improved experimental data is the ground-state static quadrupole moment. Childs⁴⁰ has found that for ⁵¹V it is $(-0.052\pm0.010)e \times 10^{-24}$ cm². The calculated value, using an effective charge of 1.6e, is $(-0.0557)e \times$ 10^{-24} cm² for calculation B. Since the ground states are more than 98% pure $f_{7/2}^n$ states, the values from calculation A and from the $f_{7/2}^n$ configuration model are very little different. The predicted ground-state static quadrupole moment for 53 Mn is $(0.0637)e \times 10^{-24}$ cm², close in magnitude but opposite in sign to that of ⁵¹V. There is no experimental measurement of this quantity.

Transition rates, mixing ratios, and branching ratios were calculated for all possible transitions in the six nuclei being studied, but the results are given here only for those quantities which have been experimentally determined. Table VII summarizes experimental information⁴¹⁻⁴⁵ not given in Table VI. An effective charge of 1.6e has been used in all calculations given in Tables VI and VII.

The agreement between theory and experiment for the quantities in Table VII is good, where the available data permit meaningful comparisons.

V. SUMMARY AND CONCLUSIONS

The model permitting configurations $(1f_{7/2}^n)$ and $(1f_{7/2}^{n-1}2p_{3/2})$ gives a good fit to level energies and single-proton spectroscopic factors throughout the test region. For each J^{π} the lowest level is $\geq 80\%$ pure $(1f_{7/2}^n)$, and this explains the additional success of fitting the relative E2 transition rates among the lowlying levels. Such subtle effects as the observed seniority mixing in ⁵²Cr and the excitation energies at which the $2p_{3/2}$ single-proton strength is found are fairly well represented by the model. The M1 transition rates, on the other hand, are not well represented. They are calculated to be too slow. Moreover, the failure is such that no "effective moment" assumption would permit successful calculations.

The expanded model, with configurations $(1f_{7/2}^n) + (1f_{7/2}^{n-1}2p_{3/2}) + (1f_{7/2}^{n-1}1f_{5/2})$, gives improved results. The first method, using the $1f_{5/2}$ two-body matrix elements calculated from the modified surface δ interaction is very successful. This model-space expansion, achieved with no free parameters other than the ten original matrix elements, provides a good fit to M1 transitions without altering the successes of the first calculation. This results from the fact that the admixed $1f_{5/2}$ amplitudes were quite small, and at the expense of the $(1f_{7/2}^n)$ amplitudes, so that the $2p_{3/2}$ admixtures were not altered by the expansion.

The second method of expanding the model space, using the Kuo and Brown calculations for the two-body matrix elements involving $1f_{5/2}$ protons, is not as successful. The results give a seriously distorted level scheme for the nuclei with $25 \le Z \le 27$. Many levels appear below 2-MeV excitation which are not found experimentally.

The conclusions seem to be that if $1f_{5/2}$ configurations are included, fits to most of the observed properties in this part of the f-p shell are readily obtained; that the MSDI does a good job of representing the effective residual interaction; and the Kuo and Brown matrix elements are not as effective in this mass region as the MSDI.

Note added in proof. Measured lifetimes of the first $\frac{9}{2}$ and first $\frac{11}{2}$ levels of ⁵¹V are 6.8×10^{-13} and $6.1 \times$ 10⁻¹³ sec, respectively. Calculation B predicts these values to be 10.6×10^{-13} and 8.7×10^{-13} sec, respectively, in good agreement. The authors are indebted to Professor D. J. Donahue, University of Arizona, who communicated the measurements.

ACKNOWLEDGMENTS

The authors are indebted to H. P. Kennedy for helping to define the method of analysis and procedure used in this work. We thank Alexander Lande for giving us his computer code for the calculation of fractional-parentage coefficients. We are also grateful to the University of Kentucky Computing Center for the use of its facilities and the invaluable assistance of its staff.

⁴⁰ W. J. Childs, Phys. Rev. 156, 71 (1967).

 ⁴⁰ W. J. Childs, Phys. Rev. 156, 71 (1967).
 ⁴¹ J. J. Simpson, J. A. Cookson, D. Eccleshall, and M. J. L. Yates, Nucl. Phys. 62, 385 (1965).
 ⁴² J. Bellicard and P. Barreau, Nucl. Phys. 36, 476 (1962).
 ⁴³ R. A. Ricci, J. C. Jacmart, M. Liu, M. Riou, and C. Ruhla, Nucl. Phys. A91, 609 (1967).
 ⁴⁴ M. Kaplan and D. A. Shirley, Nucl. Phys. 37, 522 (1962).
 ⁴⁵ M. S. Freedman, F. Wagner, Jr., F. T. Porter, and H. H. Bolotin, Phys. Rev. 146, 791 (1966).