Shell-Model Calculations for V^{51} and Cr^{52}

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(Received 28 October 1970)

Employing Ca^{48} as the core and the reaction matrix elements of Kuo and Brown for the residual interaction among the three valence protons, the nuclear energy levels of V^{51} are calculated within the spherical shell-model framework. All the $0f$-$1p$ configurations are included. The wave functions obtained on diagonalizing the Hamiltonian matrices are used to calculate the transition rates and spectroscopic factors for the reaction $Ti^{50}(He^3,d)V^{51}$. Good agreement with experiments is found suggesting that it is not necessary to include deformation in V^{51} as in the papers of Scholz and Malik. The consequences of mixing effective interaction matrix elements of Lips and McEllistrem and realistic Kuo-Brown matrix elements are studied and it is pointed out that such a mixture does not yield a successful effective interaction model. Our results are further supported by similar calculations on Cr^{52}.

I. INTRODUCTION

During the last several years considerable interest has been directed to nuclei in the $0f_{7/2}$ shell. Ample data exist especially on V^{51} to warrant a detailed study of this nucleus. The data on the magnetic moment of the ground state and first excited state have been available for some time.[1,2] The ground-state quadrupole moment has been measured by Nagasawa, Takeshita, and Tomono[3] and more recently by Childs.[4] The lifetime of the first excited state has been measured by Delyagin and Preisa and others[5] and of the first $\frac{9}{2}^-$ and $\frac{11}{2}^-$ levels by Goodman and Donahue[6] of the University of Arizona. The spectroscopic factors for the (He^3, d) reactions have been measured by Cujec and Szoghy,[7] O'Brien *et al.*,[8] and Pierre and collaborators.[9]

A number of theoretical papers have also appeared. Many of them treat V^{51} as a nucleus having three protons outside the closed shells with $Z = 20$ and $N = 28$. There is ample evidence that Ca^{48} forms a good closed core.[10,11] Assuming a pure $(0f_{7/2})^3$ configuration for the three valence protons, a calculation for V^{51} has been made by McCullen, Bayman, and Zamick.[12] Auerbach[13] allows the three protons to be shared between the $0f_{7/2}$ and $1p_{3/2}$ orbitals.

Recently a very elegant study of $N = 28$, $20 < Z \leq 28$ nuclei has been carried out by Lips and McEllistrem[14] employing the method of effective interactions, first suggested by Talmi. Lips and McEllistrem assume that these nuclei can be described by mixing configurations of the form $0f_{7/2}^n$, $0f_{7/2}^{n-1}1p_{3/2}$, and $0f_{7/2}^{n-1}0f_{5/2}$. Their calculations are carried out in two steps. In the first step, only the first two of the above mentioned configurations are considered and the two-particle matrix elements, treated as adjustable parameters, are determined to fit some of the chosen experimental energies. In the next step the configurations of the form $0f_{7/2}^{n-1}0f_{5/2}$ are also included. The additional matrix elements needed in the calculation were obtained from a modified surface δ residual interaction (MSDI) chosen to fit the matrix elements of the previous step. The effective matrix elements and the ones obtained by the MSDI are then compared with the Kuo-Brown matrix elements for the Hamada-Johnston potential calculated with Ca^{48} as the core. It is found that the average deviation of the Kuo-Brown matrix elements from the effective matrix elements is about 0.7 MeV, a better fit than the MSDI matrix elements. In the present calculation higher configurations not considered by Lips and McEllistrem are included and their effects studied.

Using the Coriolis-coupling model, Scholz and Malik[15] have also calculated the energy levels of V^{51}. The free parameters used in the calculation are the deformation parameter β and the rotational constant $A = \hbar^2/2I$. Their calculations for a deformation of -0.32 do not give a good fit with the observed energy level spectrum. The first $\frac{5}{2}^-$ and $\frac{3}{2}^-$ levels lie very close, though experimentally they are separated by 0.611 MeV. The order of the $\frac{11}{2}^-$ and $\frac{9}{2}^-$ levels is reversed and the large density of states between 3.0 and 5.0 MeV is not reproduced. In the other comparison which Scholz and Malik show in their paper for $\beta = 0.2$, the order of the first $\frac{5}{2}^-$ and $\frac{3}{2}^-$ levels is also reversed. These authors, however, do succeed in explaining such contradictory features as the enhanced reduced transition probability from the first excited state to the ground state and the small quadrupole moment of the ground state that are found in V^{51}.

In the present paper an extended study of V^{51} is

undertaken within the framework of the spherical shell model for nuclei and the three valence protons are allowed to be shared among the $0f_{7/2}$, $1p_{3/2}$, $0f_{5/2}$, and $1p_{1/2}$ orbitals. Three different types of calculations are carried out. In the first one, referred to as approximation A in the text, the Kuo-Brown renormalized matrix elements are used for the residual interaction, and the single-particle energies listed in their paper are employed. In the second, referred to as approximation B, the same interaction is used but some of the values of the single-particle energies are taken from the paper of Erskine, Marinov, and Schiffer.[16] In the third (approximation C) the Lips-McEllistrem effective matrix elements are used for the configurations considered by them and Kuo-Brown matrix elements for the remaining configurations. The last calculation shows that when matrix elements of both interactions are combined, one obtains results which are inferior to both of those obtained with Kuo-Brown matrix elements and to the limited space calculations of Lips and McEllistrem. The results of this entire study are reported in Sec. II. In Sec. III, a similar study for Cr^{52} is made. In Sec. IV, a brief discussion of the results is reported. It is pointed out that the Kuo-Brown interaction is not a realistic way to extend an effective interaction fit. No justification for including deformation in V^{51} is found.

A drawback of our calculation, as of all other similar ones, is that except for the case of three protons in the $f_{7/2}$ orbit, the isospin of the calculated states is generally mixed. In V^{51}, the maximum isospin violation is not expected to exceed 14%. However, it is found that all the low-lying levels in V^{51} are predominantly of the $f_{7/2}{}^3$ type, and the calculated wave functions are therefore expected to be quite realistic.

II. SHELL-MODEL CALCULATIONS FOR V^{51}

In the present calculation V^{51} is treated as a closed core of Ca^{48} with the three valence protons occupying the $0f_{7/2}$, $1p_{3/2}$, $0f_{5/2}$, and $1p_{1/2}$ single-particle orbitals. For a given total angular mo-

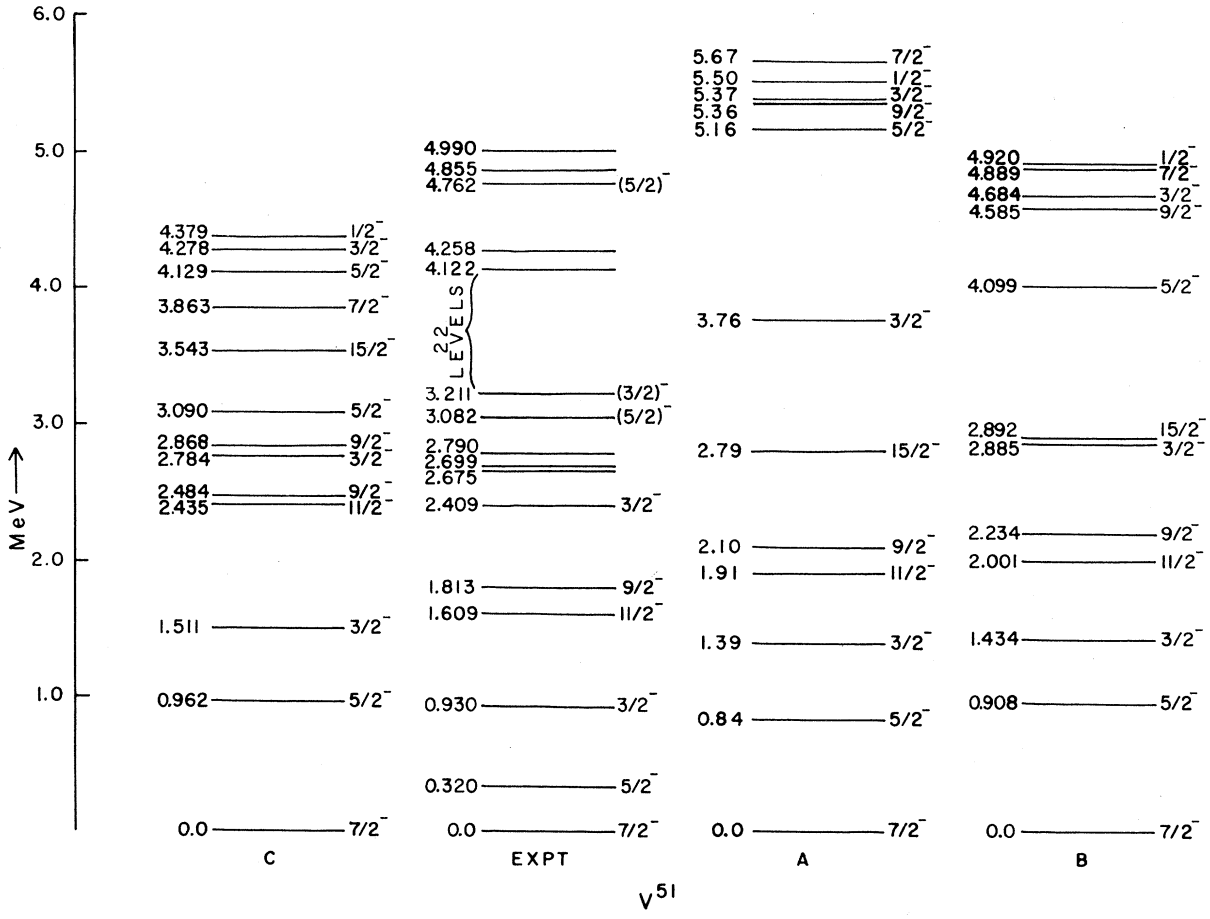

FIG. 1. Comparison of experimental (Expt) and shell-model spectrum for V^{51} in approximations A, B, C, which are explained in the text.

TABLE I. The calculated and observed magnetic dipole moments (μ) and electric quadrupole moments (Q.M.) for the ground and first few excited states of V^{51} in three approximations A, B, and C. Approximations A, B, and C are described in the text. The μ's are expressed in μ_N and quadrupole moments in units of $e\times10^{-26}$ cm^2.

	Approximation A		Approximation B		Approximation C		Expt.	
J^π	μ	Q.M.	μ	Q.M.	μ	Q.M.	μ	Q.M.
$\frac{7}{2}^-$	5.53	−3.99	5.52	−4.18	5.51	−4.44	5.148 [a]	±0.007 [b] −5.2±1.0 [c]
$\frac{5}{2}^-$	3.85	−8.04	3.80	−7.41	3.78	−5.58	4.2±0.7 [d]	
$\frac{3}{2}^-$	2.28	8.61	2.29	9.1	2.41	9.27		
$\frac{11}{2}^-$	8.32	−4.98	8.14	−6.05	7.96	−7.34		
$\frac{9}{2}^-$	6.75	5.56	6.61	5.63	6.44	−6.34		
$\frac{15}{2}^-$	11.28	−10.90	10.93	−11.71	10.56	−12.12		

[a]Reference 1. [b]Reference 3. [c]Reference 4. [d]Reference 2.

mentum, the three protons can have the following possible configurations:

$$|j^3J\nu\rangle, \quad |j_1{}^2J_1, j_3; J\rangle, \quad |j_1j_2J_{12}, j_3; J\rangle .$$

Here J is the total angular momentum, ν is the seniority, and the subscripted J's denote the intermediate-coupled angular momenta of nucleon pairs. The above configurations give rise to several possible values of the total angular momentum starting from $\frac{1}{2}^-$ and ending at $\frac{19}{2}^-$, each successive value differing from the preceding one by an integer. The highest order of the matrix encountered in the calculation is 28×28 for $J=\frac{5}{2}$. The diagonalization of the matrices was carried out on a CDC 6400 computer located at the State University of New York at Buffalo and the resulting eigenfunctions were used to calculate the various moments and transition rates.

In order to confirm the correctness of our calculations reported here, two independent programs, one incorporating the isospin formalism and the other one without it, were written. These programs generated the required three-particle configurations and then set up the energy and transition matrices for a given set of single-particle states, total spin, and parity. The output from the two programs completely agreed.

The entire calculation was carried out in three stages. In the first (approximation A) the Kuo-Brown renormalized matrix elements were used for residual interaction and the single-particle energies for the valence protons were taken from Table 5 of their paper. These are the single-particle energies used by Kuo and Brown in calculating the spectra of Ti^{50}. The results of these calculations are shown in Fig. 1. It is found that the effective matrix elements of Kuo and Brown repro-

TABLE II. Experimental and theoretical $B(E2)$ and $B(M1)$ values for V^{51} in the three approximations A, B, and C. The $B(E2)$ values are given in units of $e^2\times10^{-50}$ cm^4 and $B(M1)$ in $\mu_N{}^2$.

Transition $J^\pi{}_i\rightarrow J^\pi{}_f$		Approximation A	Approximation B	Approximation C	Expt.
$\frac{5}{2}^-\rightarrow\frac{7}{2}^-$	$B(M1)$	9.53×10^{-4}	29.0×10^{-4}	64.8×10^{-4}	$(49\pm4)\times10^{-4}$
$\frac{7}{2}^-\rightarrow\frac{5}{2}^-$	$B(E2)$	0.65	0.66	0.70	0.92
$\frac{9}{2}^-\rightarrow\frac{7}{2}^-$	$B(M1)$	2.44×10^{-4}	1.10×10^{-4}	1.18×10^{-2}	$(4.7\pm1.6)\times10^{-4}$
$\frac{7}{2}^-\rightarrow\frac{9}{2}^-$	$B(E2)$	0.10	0.11	0.30	0.22
$\frac{7}{2}^-\rightarrow\frac{3}{2}^-$	$B(E2)$	0.27	0.30	0.27	0.27
$\frac{7}{2}^-\rightarrow\frac{11}{2}^-$	$B(E2)$	0.31	0.32	0.33	0.90
$\frac{3}{2}^-\rightarrow\frac{5}{2}^-$	$B(M1)$	1.35×10^{-4}	1.45×10^{-4}	2.87×10^{-6}	$(29\pm4)\times10^{-4}$
	$B(E2)$	0.29	0.36	0.58	$(107\pm9)\times10^{-2}$
$\frac{9}{2}^-\rightarrow\frac{11}{2}^-$	$B(E2)$	0.11	0.09	0.05	
$\frac{9}{2}^-\rightarrow\frac{5}{2}^-$	$B(E2)$	0.12	0.11	0.15	$(32.7\pm5)\times10^{-2}$
$\frac{15}{2}^-\rightarrow\frac{11}{2}^-$	$B(E2)$	0.33	0.35	0.39	

duce the energy level spectrum but, in general, the calculated levels lie higher than the experimentally observed ones. The lowest $\frac{13}{2}^-$ level is found to be located at 6.71 MeV.

In the second calculation (approximation B) the single-particle energies were taken from the paper of Lips and McEllistrem and the calculations were repeated with the Kuo-Brown matrix elements. It is known that the reaction matrix elements are rather insensitive to such changes in the single-particle energies. The resulting spectrum (Fig. 1) shows no significant changes when compared with the previous calculation (approximation A) below an excitation energy of 2.7 MeV. Above 2.7 MeV, the levels are on the average suppressed by about 0.8 MeV. This, however, does not apply to the level $\frac{15}{2}^-$.

In the third calculation (approximation C) carried out with all the Lips-McEllistrem effective matrix elements and remaining Kuo-Brown matrix elements, the energy levels below 1.5 MeV are not noticeably affected. However, the levels $\frac{11}{2}^-$, $\frac{9}{2}^-$ are significantly pushed up and some others are pushed down to increase the density of states for the excitation energies between 2.40 to 4.4 MeV. None of the above calculations shows the fine agreement obtained by Lips and McEllistrem in their simple calculation. The disagreement is brought about by the mixing of effective matrix elements of two different models.

Table I reports the results of calculations for the magnetic dipole and electric quadrupole moments for the ground and excited states in all three approximations. Good agreement with experimental values is found. This is quite unexpected in view of the fact that unlike the calculation of Lips and McEllistrem, the present calculation does not reproduce the correct position of the energy levels.

Table II lists the reduced transition probabilities for $M1$ and $E2$ transitions in all three approximations. No effective charges were used. In some cases the agreement is remarkable. These results are considerably superior to those of Scholz and Malik who predicted $B(M1)$ values which are generally too large by several orders of magnitude.

The calculated spectroscopic factors are shown in Table III. These are in reasonable agreement with the calculations of Lips and McEllistrem as well as with experiments. Considerable differences, however, exist with the calculations of Lips and McEllistrem for the $(\frac{3}{2}^-)_2$ and $(\frac{5}{2}^-)_2$ states and can be understood in terms of the increased number of configurations not included by these authors (see Table IV). It is clear from this table that the low-lying states in V^{51} are predominantly of the $f_{7/2}{}^3$ type. The coefficients of the $f_{7/2}{}^3$ term for the first $\frac{11}{2}^-$, $\frac{9}{2}^-$, and $\frac{15}{2}^-$ states, which are not listed in the table, are 0.97, 0.98, and 0.98, respectively.

Goodman and Donahue[6] have measured the lifetimes of the first $\frac{9}{2}^-$ and first $\frac{11}{2}^-$ states to be 6.8×10^{-13} and 6.1×10^{-13} sec, respectively. The calculated lifetime for the $\frac{9}{2}^-$ state in approximations A, B, and C is found to be 15.5×10^{-13}, 10.8×10^{-13}, and 2.28×10^{-13} sec, respectively. For the $\frac{11}{2}^-$ state, the calculated values in the three approximations are 6.98×10^{-13}, 5.25×10^{-13}, and 1.89×10^{-13} sec. In both cases the agreement is quite satisfactory.

The calculated energy levels for Ti^{50} in all three approximations are shown in Fig. 2. Since the completion of our work and submission of our paper, we have learned of a paper by Horoshko, Cline, and Lesser[17] in which calculations on the energy levels and transition rates for V^{51} corresponding to our approximation A have been reported. Their results on the energy eigenvalues agree with our earlier[18] as well as present work. The eigenfunctions also agree when the proper phase convention for the coefficients of fractional parentage is used. However there are disagreements in the $B(E2)$ and $B(M1)$ values which may be partly

TABLE III. Calculated and experimental values of spectroscopic factors for the $Ti^{50}(He^3, d)V^{51}$ reaction in approximations A, B, and C which are explained in the text.

J^π_f	Spectroscopic strength S Approximation A	Approximation B	Approximation C	Expt. C^2S
$\frac{7}{2}^-$	0.755	0.759	0.759	0.750 [a], 0.750 [b], 0.700 [c]
$\frac{5}{2}^-$	0.003	0.005	0.008	
$\frac{3}{2}^-$	0.001	0.003	0.001	0.012 [c]
$(\frac{3}{2}^-)_2$	0.952	0.951	0.868	0.45 [a], 0.57 [b], 0.42 [c]
$(\frac{5}{2}^-)_2$	0.698	0.845	0.859	0.24 [a], 0.13 [c]

[a] Reference 7. [b] Reference 9. [c] Reference 8.

TABLE IV. Wave functions of V^{51} in approximations A, B, and C. Only amplitudes greater than 0.10 are listed.

J	Approximation	$f_{7/2}^3$	$f_{5/2}^3$	$p_{3/2}^3$	$f_{7/2}^2(0)f_{5/2}$	$p_{3/2}^2(0)f_{5/2}$	$p_{3/2}^2(0)f_{7/2}$	$f_{5/2}^2(0)f_{7/2}$	$f_{5/2}^2(0)p_{3/2}$	$f_{7/2}^2(0)p_{3/2}$
$\frac{7}{2}^-$	A	0.96					−0.11	−0.21		
	B	0.94					−0.13	−0.25		
	C	0.93					−0.13	−0.27		
$\frac{5}{2}^-$	A	0.96								
	B	0.94								
	C	0.87								
$\frac{3}{2}^-$	A	0.95								
	B	0.91								
	C	0.81								
$\frac{1}{2}^-$	A									
	B									
	C									
$\frac{5}{2}^-$	A		0.13		0.83					
	B		0.18		0.90	0.11				
	C		0.17		0.91	0.11				
$\frac{3}{2}^-$	A								0.21	0.95
	B								0.25	0.94
	C	0.17							0.25	0.89

due to the difference in the accuracies of the computers used. Horoshko *et al.* have not reported any results on the spectroscopic factors for the reaction $Ti^{50}(He^3, d)V^{51}$.

III. SHELL-MODEL CALCULATIONS FOR Cr^{52}

In Cr^{52} the four protons outside the Ca^{48} core are distributed in $0f_{7/2}$, $0f_{5/2}$, $1p_{3/2}$, and $1p_{1/2}$ orbitals in the following types of configurations:

$$|j^4 J\nu\rangle; \quad |j_1^3 J_1 \nu_1, j_2; J\rangle; \quad |j_1^2 J_1, j_2^2 J_2; J\rangle,$$
$$|j_1^2 J_1, j_2 j_3 J_2, J\rangle, \quad |j_1 j_2 J_1; j_3 j_4 J_2; J\rangle.$$

The dimensions of the complete matrices involving all the possible four-proton excitations are for $J^\pi = 0^+$, 28×28; for 1^+, 54×54; for 2^+, 94×94; for 3^+, 91×91; for 4^+, 99×99; for 5^+, 75×75; for 6^+, 59×59; for 8^+, 22×22. The numerical calculations were performed only in approximation C. The results for approximation A have already been reported.[19] In approximation C the effective matrix elements corresponding to the two-proton configurations $0f_{7/2}^2$, $0f_{7/2}1p_{3/2}$, and $0f_{7/2}\,0f_{5/2}$ are replaced by the Lips-McEllistrem matrix elements. In order to reduce the dimensions of the matrices,

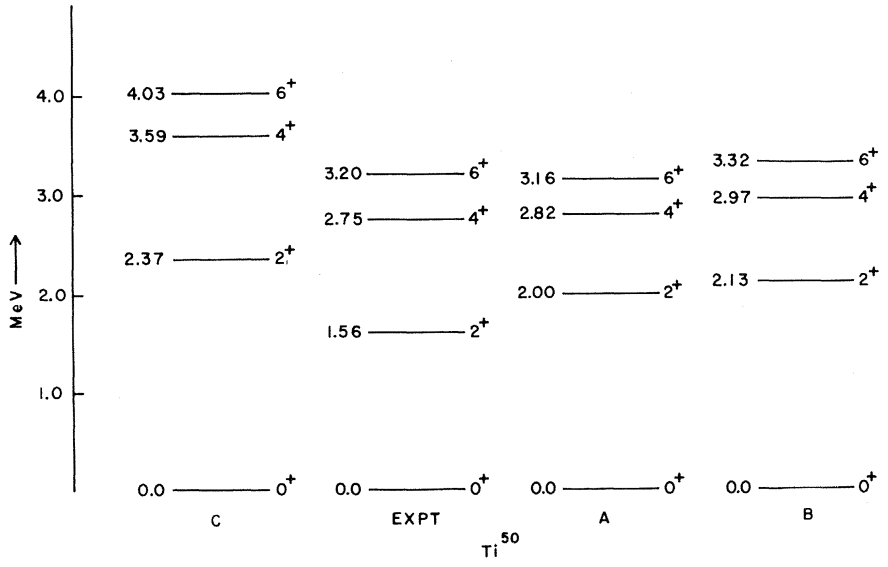

FIG. 2. Comparison of experimental (Expt) and shell-model spectrum for Ti^{50} in approximations A, B, C, which are explained in the text.

TABLE IV *(Continued)*

$f_{7/2}^2(2)p_{3/2}$	$f_{7/2}^2(4)p_{3/2}$	$f_{7/2}^2(0)p_{1/2}$	$f_{7/2}^2(2)p_{1/2}$	$f_{5/2}^2(0)p_{1/2}$	$f_{5/2}^2(2)f_{7/2}$	$f_{7/2}^2(2)f_{5/2}$	$f_{5/2}^2(4)f_{7/2}$	$p_{3/2}f_{5/2}(4)f_{7/2}$
−0.15	−0.17							
−0.18	−0.20							
−0.25	−0.32				0.11			
−0.27								
−0.34								
−0.51								−0.12
0.74		0.60		0.11		0.19		−0.17
0.84		0.39				0.26		−0.22
0.34		0.57				0.52	−0.11	−0.49
0.38	0.28					0.18		
0.23	0.16					0.17		
0.17	0.19					0.15		
0.13								
0.12								
0.22								−0.11

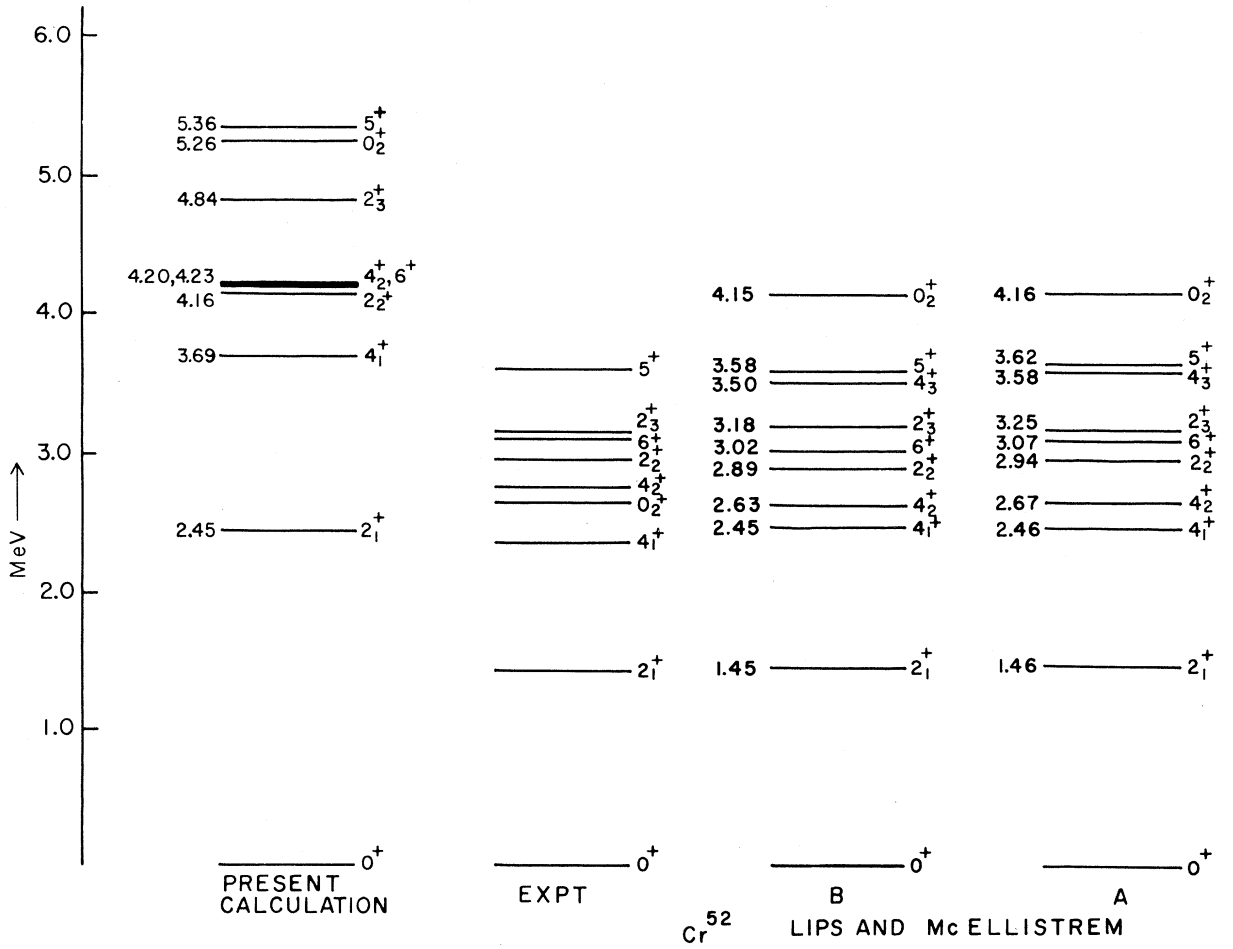

FIG. 3. Comparison of experimental (Expt) and shell-model spectrum for Cr^{52} in approximation C (present calculation). The results of calculations by Lips and McEllistrem in their notation are denoted by A and B.

a reasonable truncation of the original basis is made by choosing a maximum unperturbed energy of 16 MeV. The dimensions of the matrices were reduced to

0^+, 19×19; 2^+, 68×68; 4^+, 78×78, and 6^+, 52×52.

The results of the numerical computation are shown in Fig. 3. The results of Lips and McEllistrem in their approximations A and B are included here for the sake of completeness. When compared with the calculations of Lips and McEllistrem, it was found that most of the levels, on the average, are moved up by an MeV or more. The results for the spectroscopic factors are shown in Table V. Except for two cases, the agreement with experiment becomes considerably worse.

IV. CONCLUSIONS

It is clear from the results reported in Sec. II of this paper that the Kuo-Brown matrix elements provide a reasonably good description of V^{51}. The calculated ground-state magnetic dipole moment and electric quadrupole moment are in good agreement with the observed values. The $E2$ reduced transition probabilities are fairly well reproduced and the calculated $B(M1)$ values differ from the measured ones by at the most a factor of 5 except for the $\frac{3}{2}^- \rightarrow \frac{5}{2}^-$ transition. These results are superior to those of Scholz and Malik who employed the strong Coriolis-coupling model. Scholz and Malik not only did not succeed in reproducing the energy levels in the correct order but predicted magnetic transition strengths which were generally too large by several orders of magnitude. In view of the general success of the spherical shell model, it seems that the claim made by Scholz and Malik about deformation in V^{51} is unjustified.

It is found that models which mix effective interaction matrix elements and realistic matrix elements will not successfully give an effective-interaction model. This is clearly demonstrated in Secs. II and III for V^{51} and Cr^{52}.

ACKNOWLEDGMENTS

The authors are grateful to Professor G. Breit for his active interest in this work. Thanks are due to the staff of the Computing Center of the

TABLE V. Calculated and experimental values of the spectroscopic factors for the $V^{51}(He^3,d)Cr^{52}$ reaction in approximations A and C.

J^π_f	Transfer J^π	Approximation A	Approximation C	Lips and Mc Ellistrem A	Lips and Mc Ellistrem B	Expt.
0^+	$\frac{7}{2}^-$	2.756	2.32	3.949	3.942	4.00[a]
2^+	$\frac{7}{2}^-$	0.952	0.778	1.091	1.085	1.08
	$\frac{5}{2}^-$	0.005	0.006		0.002	
	$\frac{3}{2}^-$	0.018	0.032	0.149	0.150	
4^+	$\frac{7}{2}^-$	0.873	0.702	0.259	0.184	0.51[a]
	$\frac{5}{2}^-$	0.008	0.012			
	$\frac{3}{2}^-$	0.002	0.005	0.003	0.002	
	$\frac{1}{2}^-$	0.002	0.002			
4_2^+	$\frac{7}{2}^-$	0.093	0.114	0.989	1.059	0.81
	$\frac{5}{2}^-$	0.002	0.002			
	$\frac{3}{2}^-$	0.0004	0.001	0.007	0.008	
	$\frac{1}{2}^-$	0.000	0.000			
2_2^+	$\frac{7}{2}^-$	0.002	0.004	0.101	0.096	
	$\frac{5}{2}^-$	0.000	0.000			
	$\frac{3}{2}^-$	0.001	0.003			
6^+	$\frac{7}{2}^-$	0.987	0.842	1.306	1.282	1.31
	$\frac{5}{2}^-$	0.005	0.008		0.004	

[a] D. D. Armstrong and A. G. Blair, Phys. Rev. 140, B1226 (1965). The other experimental values are from Ref. 14.

State University of New York at Buffalo, which is partially supported by National Institute of Health Grant No. FR-00126 and NSF Grant No. GP-7318, for providing the machine time. Thanks are also due to the Research Foundation of the State University of New York for a grant-in-aid. The patient help of Miss Terri DeGeorge with the manuscript is gratefully acknowledged.

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