Shell-Model Study of Mn^{55}

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A shell-model calculation for Mn^{55} is carried out which includes interactions among all neutrons and protons not in closed shells. It is shown that the inclusion of the neutron-proton interactions gives good agreement with the experimental data for several sets of exchange parameters and reasonable values of the two-particle force range. The magnetic moment and quadrupole moment are also calculated and are in satisfactory agreement with experiment.

INTRODUCTION

THE jj coupling shell model has had considerable success in predicting the spins and positions of low-lying levels for nuclei which are not distorted. One such region of nuclei is in the vicinity of $A\approx 50$. An anomaly in this region is Mn^{55} which has a ground state spin of 5/2 rather than 7/2 as predicted by the shell model. This study represents an attempt to explain the anomalous ground state spin of Mn^{55} within the framework of the shell model.

The shell model says that the nucleons see primarily the central potential. With no perturbations, the energy levels of different spins to which these nucleons couple are all degenerate. Two-body interactions among the nucleons outside the closed shells are treated as a perturbation and to some extent remove this degeneracy. In particular, the odd-group model says that for odd-A nuclei with an odd number of protons (neutrons), only the interactions among the protons (neutrons) outside the closed shells determine the spins and precise energies of the ground state and low lying levels.

Using this model, Kurath,[1] whose calculations were confirmed by others,[2,3] put forth an explanation for the anomalous ground state spin of Mn^{55}. The odd group in this case is the group of five protons in the $f_{7/2}$ shell. The two neutrons outside the $f_{7/2}$ shell were assumed to couple to zero angular momentum and hence to play no role in the determining of the positions and spins of the low-lying states. Because of the equivalence of particles and holes,[4] the configurations $(1f_{7/2})^3$ and $(1f_{7/2})^5$ should give rise to similar level schemes; and because of the assumed charge independence of nuclear forces, the calculation should explain the ground state and first few excited states of Mn^{53}, Mn^{55}, V^{51}, and Ca^{43}. (Mn^{53}, V^{51}, and Ca^{43} all have a ground state spin of 7/2 and a first excited state spin of 5/2, while Mn^{55} has a ground state spin of 5/2 and a first excited state spin of 7/2.) Kurath's calculations show that while the correct level scheme for Mn^{53} (or V^{51} or Ca^{43}) can be obtained for reasonable values of the parameters, the correct level scheme for Mn^{55} requires an unusually long range for the two-body interaction.

The fact that Mn^{53}, V^{51}, and Ca^{43} all have a ground state spin of 7/2, while Mn^{55} has a ground state spin of 5/2, suggests that perhaps the neutron-proton interaction between the two neutrons outside the $f_{7/2}$ shell and the five protons in the $f_{7/2}$ shell is important enough to lower the $J=5/2$ level below the $J=7/2$ level.[5]

It is usually presumed that the single-particle level following the $1f_{7/2}$ is the $2p_{3/2}$. This is not known with certainty, however. The $1f_{5/2}$ level probably lies very close to the $2p_{3/2}$ level, and might, for some nuclei in this region, lie lower. Whether or not the $1f_{5/2}$ lies lower than the $2p_{3/2}$, it certainly lies close enough to require its inclusion in the calculation, if the results are to be meaningful. Indeed, the matrix element for the neutron-proton interaction for the neutron in the $1f_{5/2}$ will be significant since its radial wave function is the same as that for the proton in the $1f_{7/2}$ shell.

The present work is an investigation of the low-lying levels of Mn^{55} taking into account proton-proton, neutron-neutron, and proton-neutron forces. The protons are assumed to be in the configuration $(1f_{7/2})^5$ while the neutrons are assumed to be in any of the con-configurations $(2p_{3/2})^2$, $(1f_{5/2})^2$, or $(2p_{3/2}1f_{5/2})$. Various mixtures of Wigner, Majorana, Bartlett, and Heisenberg forces are used to obtain the best fit. The magnetic moment and quadrupole moment are also calculated.

The overlap between the $1f_{5/2}$ and $1f_{7/2}$ single-particle wave functions suggests that perhaps the protons are not in a pure $(1f_{7/2})^5$ configuration, but rather should be mixed with a $(1f_{7/2})^4 1f_{5/2}$ configuration. Such a calculation was carried out by Yanagawa,[6] who assumed that the neutrons were coupled to zero angular momentum, so that neutron-proton forces were neglected. The energy separation between the single-particle $1f_{7/2}$ and $1f_{5/2}$ levels is probably of the order of several MeV, so one might expect the neutron-proton interaction to be of greater importance than the $(1f_{7/2})^4 1f_{5/2}$ proton configuration.

[1] D. Kurath, Phys. Rev. **80**, 98 (1950).
[2] I. Talmi, Helv. Phys. Acta **25**, 185 (1952).
[3] A. R. Edmonds and B. H. Flowers, Proc. Roy. Soc. (London) **A215**, 120 (1952).
[4] G. Racah, Phys. Rev. **62**, 438 (1942).
[5] See discussion of this point in B. H. Flowers, Phil. Mag. **45**, 329 (1954).
[6] S. Yanagawa, J. Phys. Soc. Japan **13**, 323 (1958); **14**, 539 (1959).

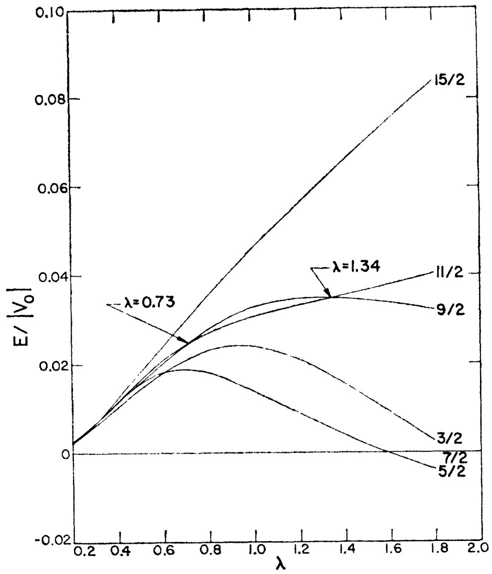

FIG. 1. Calculated energies of V^{51} as a function of the range parameter λ. Mixture of 40% Wigner, 40% Majorana, 20% Bartlett, and 0% Heisenberg forces.

PARAMETERS OF THE CALCULATION

The single-particle radial wave functions used were:

$$R_{1f_{7/2}}(r)/r = R_{1f_{5/2}}(r)/r = N_f r^3 e^{-\nu r^2}, \tag{1}$$

$$R_{2p_{3/2}}(r)/r = N_p r e^{-\nu r^2}(\tfrac{5}{2} - 2\nu r^2). \tag{2}$$

The two-body force used was

$$V(r_{12}) = V_0 e^{-(r/r_0)^2} P^x, \tag{3}$$

where P^x is the exchange operator. Different combinations of Wigner, Majorana, Bartlett, and Heisenberg exchange forces were used. It was found that the matrix elements do not depend on ν and r_0 separately, but only on the combination

$$\lambda = r_0\sqrt{\nu}, \tag{4}$$

where λ is called the range parameter. An estimate of ν can be made by equating the expectation value of r^2 to the square of the nuclear radius. From the above radial wave functions, we obtain

$$\langle r^2 \rangle = 9/4\nu. \tag{5}$$

If the nuclear radius is taken to be $R_0 A^{1/3}$, then

$$\sqrt{\nu} = (3/2R_0)A^{1/3}. \tag{6}$$

Using $R_0 = 1.25 \times 10^{-13}$ cm and $A = 55$, one gets $\sqrt{\nu} = 0.316 \times 10^{13}$ cm^{-1}. The value of r_0 for the two-body Gaussian interactions is 1.9×10^{-13} cm from Rosenfeld[7] or 1.12×10^{-13} cm from nucleon-nucleus scattering data.[8] These two values of r_0 lead to limits on λ from 0.395 to 0.600. For this range of λ Kurath's[1] results give 7/2 for the ground state. Only for $1.27 < \lambda < 1.35$ did his results give 5/2 for the ground state spin. For the above values of R_0 and A, the value of $\lambda = 1.27$ requires that $r_0 = 4.02 \times 10^{-13}$ cm. This value for the range of the nuclear force is clearly too large to be acceptable as the explanation for the spin assignments of Mn^{55}.

Schiffer, Lee, and Zeidman[9] have measured the energy separation between the $2p_{3/2}$ and $1f_{7/2}$ single-particle levels for Ti^{49} and find it to be approximately 0.9 MeV. Because of the uncertainties in this measurement the present calculations for one set of exchange parameters were carried out for three different assumed energy separations, one of which is for the $1f_{5/2}$ level lying slightly below the $2p_{3/2}$.

CALCULATIONS

The neutron-neutron and proton-proton interactions are very easily carried out using standard techniques. For the latter, the equivalence of particles and holes[4] makes the $(1f_{7/2})^5$ and $(1f_{7/2})^3$ configurations equivalent. The $(2p_{3/2}1f_{5/2})$ configuration for the neutrons was properly antisymmetrized.

The neutron-proton interaction is somewhat more complicated. The method used is that of Goldstein and Talmi,[10] in which the interaction between one neutron and the five protons is first calculated. The second neutron is then coupled in to this configuration. The details are given in the reference cited. The equivalence between particles and holes does not apply to interactions between particles in different shells, so the configuration $(1f_{7/2})^5$ must be used, not $(1f_{7/2})^3$. This im-

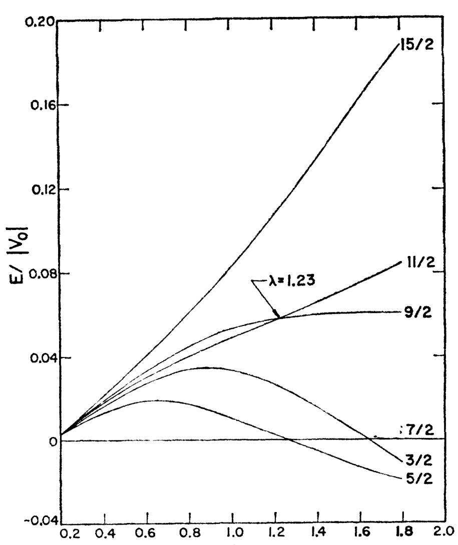

FIG. 2. Same as Fig. 1 except: 50% Wigner, 50% Majorana, 0% Bartlett, and 0% Heisenberg forces.

[7] L. Rosenfeld, *Nuclear Forces* (North-Holland Publishing Company, Amsterdam, 1948), p. 153.
[8] C. Wong, J. D. Anderson, S. D. Bloom, J. W. McClure, and B. D. Walker, Phys. Rev. **123**, 598 (1961).
[9] J. P. Schiffer, L. L. Lee, Jr., and B. Zeidman, Phys. Rev. **115**, 427 (1959).
[10] S. Goldstein and I. Talmi, Phys. Rev. **105**, 995 (1957).

poses no additional difficulties since the c.f.p.'s (coefficients of fractional parentage) $\langle(\frac{7}{2})^5J\{|(\frac{7}{2})^4J',\frac{7}{2}J\rangle$ can be readily obtained. Edmonds and Flowers[11] have obtained the orbital c.f.p. $\langle(\frac{7}{2})^4\{|(\frac{7}{2})^3\frac{7}{2}\rangle$, which can be combined with the suitable charge-spin c.f.p. of Jahn[12] to give the total c.f.p. Using a relationship for c.f.p.'s between particles and holes derived by Racah,[13] suitably modified for jj coupling, on obtains $\langle\frac{7}{2}^5\{|\frac{7}{2}^4\frac{7}{2}\rangle$.

Harmonic oscillator wave functions were used for the single-particle wave functions and a Gaussian interaction for the two-particle interaction, so that the method of Talmi[2] could be used for the evaluation of the matrix elements. Because the neutrons and protons are in different shells, the isotopic spin formalism was not used. Therefore, the calculation of the matrix elements for exchange forces was somewhat lengthy. It was most easily accomplished by expressing the two-particle matrix elements in jj coupling as a linear combination of two-particle matrix elements in LS coupling, using the LS-jj transformation tables of Kennedy and Cliff.[14]

The full energy matrix was calculated, including the interactions among the five protons in the $1f_{7/2}$ shell, the interaction between the two neutrons in any of the configurations $(2p_{3/2})^2$, $(1f_{5/2})^2$, or $2p_{3/2}1f_{5/2}$, and the interactions between the five protons in the $1f_{7/2}$ shell and the two neutrons in any of the above-mentioned configurations. The sizes of the resulting matrices for final spin states of 3/2, 5/2, and 7/2 were, respectively,

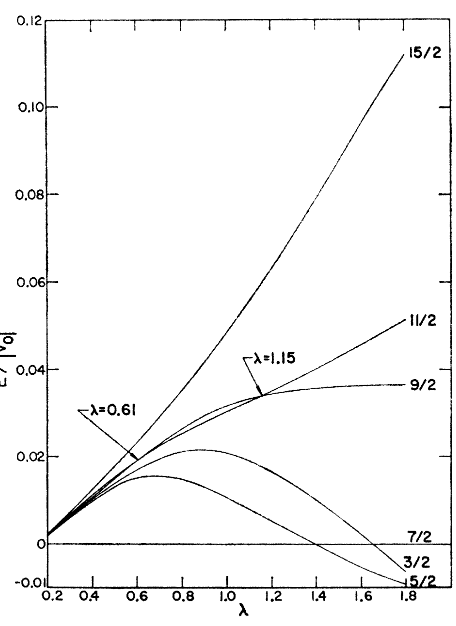

FIG. 3. Same as Fig. 1 except: 40% Wigner, 40% Majorana, 10% Bartlett, and 10% Heisenberg forces.

[11] A. R. Edmonds and B. H. Flowers, Proc Roy Soc. (London) **A214**, 515 (1952).
[12] H. A. Jahn, Proc. Roy. Soc. (London) **A205**, 192 (1951).
[13] G. Racah, Phys. Rev. **63**, 367 (1943).
[14] J. M. Kennedy and M. J. Cliff, Chalk River Report CRT-609, 1955 (unpublished).

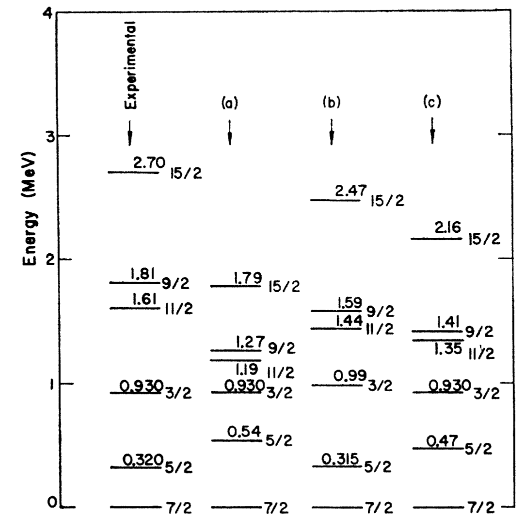

FIG. 4. Comparison of the experimental values [15] with the calculated energies of V^{51} for $\lambda=1.0$ and the following mixtures of exchange forces and potentials: (a) $V_0=38.9$ MeV, 40% Wigner, 40% Majorana, 20% Bartlett, and 0% Heisenberg forces, (b) $V_0=30.0$ MeV, 50% Wigner, 50% Majorana, 0% Bartlett, and 0% Heisenberg forces, (c) $V_0=45.0$ MeV, 40% Wigner, 40% Majorana, 10% Bartlett, and 10% Heisenberg forces.

25 by 25, 32 by 32, and 37 by 37. These were diagonalized on a digital computer to obtain the minimum eigenvalue. The procedure was repeated for various values of the range parameter and for various exchange mixtures. The diagonalization routine also computed the eigenvector, which was then used to compute the magnetic and quadrupole moments.

Coulomb effects are usually considered negligible in shell-model calculations. However, because the first excited state is at only 0.128 MeV, one calculation was carried out with Coulomb force included and it was found that they were negligible here also.

RESULTS

For all exchange parameters used the levels of V^{51} were also calculated and compared with the experimental results of Schwäger.[15] The results are given in given in Figs. 1 through 3. It is seen by comparison with Fig. 4 that the correct ordering of the levels is obtained for a range of λ on either side of $\lambda=1.0$. For some values of the exchange parameters, however, only for λ greater than about 0.6 is the level order correct. This figure is to be compared with the values of λ from 0.4 to 0.6 obtained above from experimental nucleon-nucleus scattering. The best agreement appears to be for about $\lambda=1.0$. Specific energy levels for $\lambda=1.0$ and several exchange forces are given in Fig. 4. The potential was chosen to bring the $J=3/2$ level into agreement with the experimental value for (a) and (c), but a better over-all fit for (b) was obtained for the indicated V_0.

The same set of exchange parameters were used for

[15] J. E. Schwäger, Phys. Rev. **121**, 569 (1961).

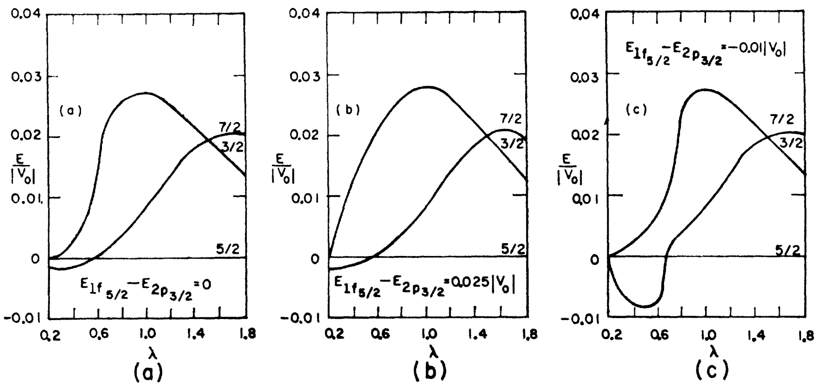

FIG. 5. Calculated energies of the first two excited states of Mn^{55} with respect to the ground state, as a function of the range parameter λ. Mixture of 40% Wigner, 40% Majorana, 20% Bartlett, and 0% Heisenberg forces.

Mn^{55}. Figures 5(a) through 5(c) show the results for different assumed $1f_{5/2}$—$2p_{3/2}$ separations for 40% Wigner, 40% Majorana, 20% Bartlett, and 0% Heisenberg. It is seen that results are qualititavely similar, the first two giving the correct level order for λ greater than about 0.6 and the third for λ greater than about 0.68.

The remaining results are for $\Delta E/|V_0|=0.025$. Figure 6 shows the results for a Serber mixture. It also gives the correct level ordering for values of λ greater than about 0.91, but gives 7/2 for the ground-state spin for lower values of λ. The lower values of λ, however, as indicated above, correspond to a more realistic two-body force range.

The above results are for the configuration mixing of the two neutrons in the $2p_{3/2}$ and $1f_{5/2}$ states. In order to see the the effects of each of these states, the neutron configurations $(2p_{3/2})^2$ and $(1f_{5/2})^2$ were considered separately. These are shown in Figs. 7 and 8, respectively. It is seen that neither configuration gives the correct level order for reasonable values of λ. However, the $(1f_{5/2})^2$ configuration gives the correct level ordering for $1.24<\lambda<1.47$.

Figure 9 gives the results for 40% Wigner, 40% Majorana, 10% Bartlett, and 10% Heisenberg. These results again give the correct level ordering for a wide range of λ.

For the parameters used in Fig. 5(b), and $\lambda=1.0$, the agreement with the experimental results of Mazari, Sperduto, and Buechner[16] is excellent. The value of $|V_0|$, chosen to give agreement with the experimental $J=3/2$ level at 0.98 MeV, is 38.0 MeV. For the case with 10% Heisenberg exchange force (Fig. 9) the correct level spacing is obtained for $\lambda=0.87$, with $|V_0|=40.6$ MeV.

It is of interest to note which neutron and proton configurations contribute most to the eigenvector for the

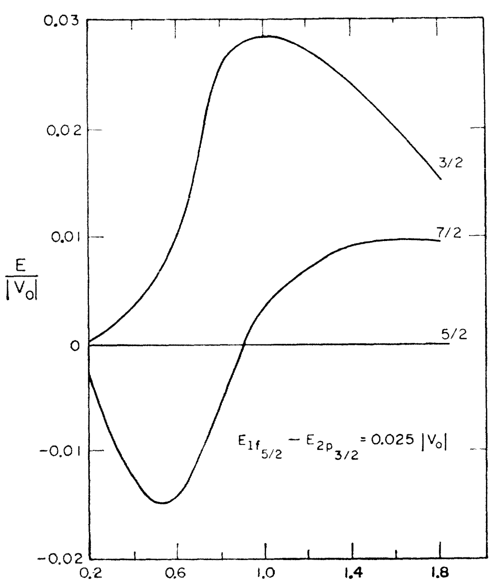

FIG. 6. Calculated energies of the first two excited states of Mn^{55} with respect to the ground state, as a function of the range parameter λ. Mixture of 50% Wigner, 50% Majorana, 0% Bartlett, and 0% Heisenberg forces.

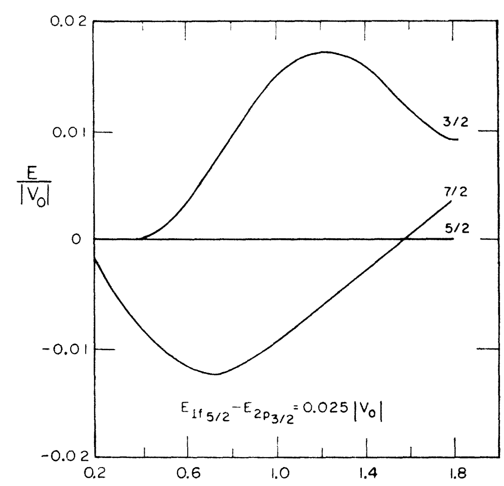

FIG. 7. Calculated energies of the first two excited states of Mn^{55} with respect to the ground state, as a function of the range parameter λ. Mixture of 40% Wigner, 40% Majorana, 20% Bartlett, and 0% Heisenberg forces. Neutron configuration assumed to be $(2p_{3/2})^2$.

[16] M. Mazari, A. Sperduto, and W. W. Buechner, Phys. Rev. **108**, 103 (1957).

TABLE I. Eigenvector components for exchange parameters corresponding to Fig. 5(b) for two values of λ.

Neutron configuration	Proton spin, J_1	Neutron spin, J_2	Eigenvector $\lambda=0.2$	$\lambda=1.0$
$(p_{3/2})^2$	5/2	0	−0.6056	−0.0017
	7/2	2	+0.7848	−0.0016
	3/2	2	−0.0593	−0.0144
	5/2	2	+0.0957	−0 0161
	9/2	2	−0.0653	−0.0040
$(f_{5/2})^2$	5/2	0	−0.0131	+0.0036
	7/2	2	+0.0041	−0.0194
	3/2	2	−0.0004	+0.0130
	5/2	2	+0.0006	+0.0132
	9/2	2	−0.0004	+0.0050
	7/2	4	0	−0.0023
	3/2	4	−0.0001	+0.0010
	5/2	4	−0.0001	+0.0041
	9/2	4	0	−0.0142
	11/2	4	−0.0001	+0.0151
$p_{3/2}f_{5/2}$	7/2	1	+0.0007	+0.8369
	3/2	1	+0.0019	+0.0866
	5/2	1	+0.0006	+0.5128
	7/2	2	−0.0078	+0.0361
	3/2	2	+0.0012	−0.0265
	5/2	2	+0.0017	−0.0157
	9/2	2	−0.0037	−0.0010
	7/2	3	−0.0023	−0.0864
	3/2	3	+0.0078	+0.0047
	5/2	3	+0.0012	−0.0372
	9/2	3	−0.0063	+0.0668
	11/2	3	+0.0074	−0.1072
	7/2	4	+0.0023	0
	3/2	4	+0.0058	−0.0009
	5/2	4	+0.0011	+0.0010
	9/2	4	0	+0.0125
	11/2	4	+0.002	−0.0162

ground state. In Table I the eigenvector components are listed for the parameters of Fig. 5(b) for two values of λ. Although one might have expected the neutron configuration $(p_{3/2})^2$ $J_2=0$ or $(f_{5/2})^2$ $J_2=0$ to be dominant, it turns out to be so only for λ less than about 0.6. For higher values of λ the $(p_{3/2}f_{5/2})$ $J_2=1$ configuration coupled to the proton configuration $(f_{7/2})^5$ $J_1=7/2$ is dominant. This observation is qualitatively similar for other exchange mixtures. In fact, the change from one component being dominant to the other takes place quite suddenly at about $\lambda=0.6$. It should be observed that several of the curves for energy levels, magnetic moment, and quadrupole moment exhibit interesting changes at about this value of λ.

A possible explanation of the cause of this effect is as follows: The matrix element of the neutron-proton interaction can be expressed as a sum over two particle neutron-proton matrix elements. Because the proton is in the $1f_{7/2}$ shell, this neutron-proton matrix element will be larger for the neutron in the $1f_{5/2}$ level than for the neutron in the $2p_{3/2}$ level. Perhaps for small values of λ, where the two particle energies are larger, the energy necessary to raise the neutron from the $2p_{3/2}$ level to the $1f_{5/2}$ is enough to leave the $(2p_{3/2})^2$ neutron configuration dominant. As λ increases, the two particle matrix elements decrease in magnitude, but not necessarily at the same rate. If the matrix element for $(p_{3/2})^2$ decreases faster than the matrix element for $(p_{3/2}f_{5/2})$, then a point might be reached where the $(p_{3/2}f_{5/2})$, even with the energy necessary to raise the neutron to the $1f_{5/2}$ level, will be dominant. This is what might be happening at about $\lambda=0.6$.

Substantiating information can be obtained by looking at the eigenvector corresponding to Fig. 5(a). Here, the separation between the $1f_{5/2}$ and $2p_{3/2}$ levels is assumed to be zero, so that the matrix element for the $(p_{3/2}f_{5/2})$ configuration should be larger than the matrix element for $(p_{3/2})^2$ even at small λ. This was indeed found to be so.

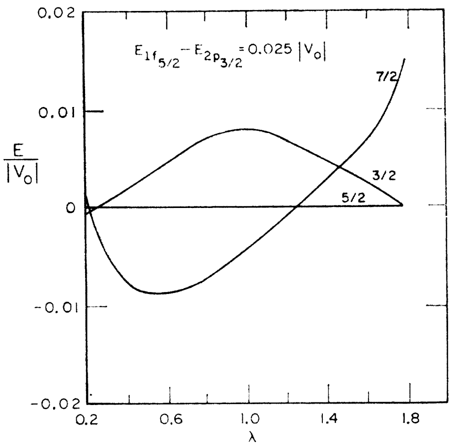

FIG. 8. Calculated energies of the first two excited states with respect to the ground state, as a function of the range parameter λ. Mixture of 40% Wigner, 40% Majorana, 20% Bartlett, and 0% Heisenberg forces. Neutron configuration assumed to be $(1f_{5/2})^2$.

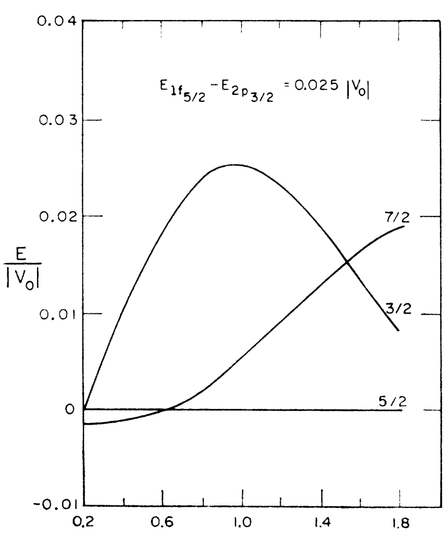

FIG. 9. Calculated energies of the first two excited states with respect to the ground state, as a function of the range parameter λ. Mixture of 40% Wigner, 40% Majorana, 10% Bartlett, and 10% Heisenberg forces.

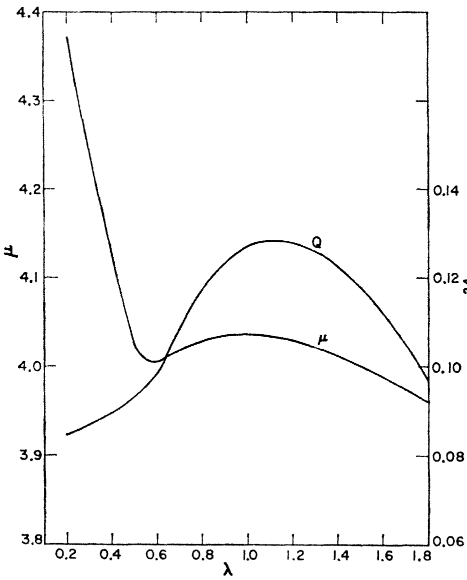

FIG. 10. Calculated magnetic and quadrupole moments as a function of range parameter λ, for mixture of 40% Wigner, 40% Majorana, 20% Bartlett, and 0% Heisenberg forces.

If the above explanation is correct, then the anomalous ground state spin of Mn^{55} would be due to a combination of two things: the two possible single-particle states for the neutrons being close enough to require configuration mixing, and one of these states having a large overlap with the proton state.

The magnetic and quadrupole moments were calculated as a function of λ for the parameters of Fig. 5(b) and are given in Fig. 10. It is seen that both are in fair agreement with the experimental values[17] of +3.46 nm for the magnetic moment and $+0.55\times10^{-24}$ cm^2 for the quadrupole moment.

CONCLUSION

The anomalous ground state spin of Mn^{55} can be explained within the framework of the shell model. Calculations for the energy levels and magnetic and quadrupole moments are in satisfactory agreement with experiment for several sets of exchange parameters, but the range parameter λ for best agreement is somewhat larger than the value one deduces from scattering data.

ACKNOWLEDGMENTS

The author is indebted to Dr. Robert Lawson of Argonne National Laboratory for calling his attention to a sign error in the tables in reference 11. The author also wishes to express his appreciation to Dr. William C. Grayson for many helpful discussions during the course of this work, and to Samuel Mendicino for computational work. The work was done under auspices of the U. S. Atomic Energy Commission.

[17] D. Strominger, J. M. Hollander, and G. T. Seaborg, Phys. Rev. **30**, 585 (1958).