Nuclear Moments of Sc^{43} and Sc^{47}†

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The magnetic and quadrupole moments of the radioactive isotopes Sc^{43} and Sc^{47} have been measured by atomic-beam magnetic resonance. Measurements were made of the hyperfine structure of these isotopes in the ${}^2D_{5/2}$ state of the scandium atom. The results (without diamagnetic or Sternheimer corrections) are Sc^{43}: $A=+105.7\pm0.9$ Mc/sec, $B=-44\pm10$ Mc/sec, $\mu=+4.61\pm0.04$ nm, $Q=-0.26\pm0.06$ b. Sc^{47}: $A=122.2\pm0.5$ Mc/sec, $B=-38\pm6$ Mc/sec, $\mu=+5.33\pm0.02$ nm, $Q=-0.22\pm0.03$ b. The electronic g value in both cases was close to the LS-coupling value, and consistent with previous measurements on Sc^{44}. The mean value of g_J was determined from Sc^{43}, Sc^{44}, and Sc^{47} to be $g_J=-1.20061\pm0.00013$. Using this, the Sc^{44} moments were recalculated. A discussion of the interpretation of the moments of the scandium isotopes is included.

I. INTRODUCTION

As part of a continuing study in this laboratory of the electromagnetic moments of medium-weight nuclei, we have measured the magnetic dipole and electric quadrupole moments of the radioactive nuclei Sc^{43} and Sc^{47}. The measurements were made using the atomic-beam magnetic resonance method. In this method the energy difference between atomic hyperfine levels is measured as a function of magnetic field. From the measurements one may infer the hyperfine splittings at zero field. If the atomic parameters are known from independent measurements of the nuclear moments and hyperfine structure of another isotope (in this case Sc^{45}), the nuclear moments of the unknown isotope may then be calculated from the zero-field values.

The details of the procedure, and the relevant hyperfine theory, may be found in several references[1–4] and will not be treated here. The conditions of the present experiment restricted our observations to transitions between states within a given F level. With sufficient power on the resonance loop, however, more than one dipole quantum could be absorbed by the atom, and hence to each final state (after transitions had been induced) there corresponded several transitions from different initial states, each involving different numbers of absorbed quanta. This type of transition has been studied extensively[2–4]; our use of them is described in the previous work[4] on Sc^{44}.

With these measurements, knowledge of the moments of five scandium isotopes (six nuclear states) is now available. A comparison of these with shell-model predictions will be discussed at the end of the paper.

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[1] N. Ramsey, *Molecular Beams* (Oxford University Press, New York, 1956).
[2] J. C. Walker, Phys. Rev. **127**, 1739 (1962).
[3] R. L. Christensen, D. R. Hamilton, H. G. Bennewitz, J. B. Reynolds, and H. H. Stroke, Phys. Rev. **122**, 1361 (1961).
[4] D. L. Harris and J. D. McCullen, Phys. Rev. **132**, 310 (1963).

II. EXPERIMENT

The experiments were performed on the atomic-beam apparatus of Lemonick, Pipkin, and Hamilton.[5] The beams were produced from tantalum ovens heated by electron bombardment to temperatures around 1500°C. Both the direct and the flopped parts of the beam were collected on clean copper, and counted with scintillation counters. The procedure was essentially that of Ref. 4, and further details may be found there.

The radioactive Sc^{43} was produced in the Princeton cyclotron by $Ti^{46}(p,\alpha)$ reaction on natural titanium foil. This technique did not produce sufficient Sc^{47} [by $Ti^{50}(p,\alpha)$] to either serve as a contaminant in the Sc^{43} experiments or as a separate source of Sc^{47}, because the longer half-life of the latter limited the decay rates which could be obtained. To minimize the Sc^{47} activity in the Sc^{43} experiments, however, short (2–3 h) proton bombardments were used.

Several techniques were tried to obtain sufficient Sc^{47}. The one which proved most successful, and which was used to prepare all the sources for the moment measurements, was the $Ti^{47}(n,p)$ reaction. Samples of natural titanium were irradiated in the fast-neutron flux of the ORL reactor for 4 days. This gave sufficient activity for the experiments, with negligible contamination from other scandium isotopes.

The hyperfine structure studies for both isotopes were made with the atomic electrons in the metastable ${}^2D_{5/2}$ state, rather than the ${}^2D_{3/2}$ ground state. The former is adequately populated thermally at the oven temperatures used, and was more convenient to study because the large electronic magnetic moment enhanced its transmission through the apparatus. Zeeman resonances were observed for both isotopes corresponding to spins $J=\frac{5}{2}$, $I=\frac{7}{2}$, $F=6$, 5, and 4, verifying the assumed nuclear spin of $\frac{7}{2}$ for each.

The magnetic field was then increased, and the deviation of the resonance frequency from linear field de-

[5] A. Lemonick, F. M. Pipkin, and D. R. Hamilton, Rev. Sci. Instr. **26**, 1112 (1955).

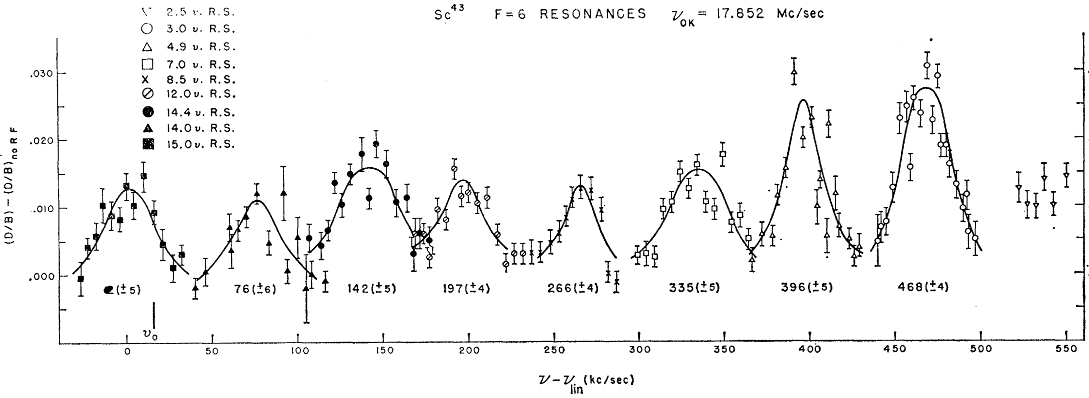

FIG. 1. The Sc^{43} resonance comb for $I=\frac{7}{2}$, $J=\frac{5}{2}$, $F=6$. Ordinate is the ratio of flopped to unflopped counting rates (D/B), normalized to zero for no rf signal. The various points are taken at different powers; most resonances are empirically close to optimally powered. The powers are listed in terms of voltage applied by the Rhode Schwarz rf oscillator (V R.S.), 0.25 V R.S. being the optimum power for K^{39}. The abscissa is the frequency deviation from a linear field dependence for Sc^{43}, ignoring the linear effect of g_I.

pendence was observed. In both isotopes, the resonant structure of the $F=6$ and $F=5$ levels was studied. At fields high enough to resolve the multiple quantum resonances, searches were made varying the rf power applied to the loop, in an effort to maximize the resonance height for the various multiple quantum transitions. Typical curves for the results for each isotope are shown in Figs. 1 through 4. The roughly equal spacing between resonances is typical of the pattern expected for a series of multiple quantum transitions in magnetic fields low enough so that a second-order expansion in the magnetic-field strength is a good approximation. The resonance frequencies in the figures correspond to those expected for as many as three different multiple quantum transitions (see Ref. 4). The power necessary to maximize the peak height for each corresponds to that which should overpower that transition with the lowest quantum multiplicity, and should underpower the highest.

Although the relative amounts of rf power necessary to see the multiple quantum resonances varied according to expectations, identification of a resonance by its power characteristics is not a sensitive test. The spacing between peaks in Figs. 1 and 2, and their analogues in the $F=5$ studies, are sufficient to obtain first-order values of the hyperfine constants A and B independent of the quantum multiplicities of the transitions. But more accurate values could be obtained from the same data if the quantum multiplicities of the resonance were known. In addition, a value of g_J for the ${}^2D_{5/2}$ state of scandium could be determined by extrapolating the resonance comb back to the resonance whose frequency

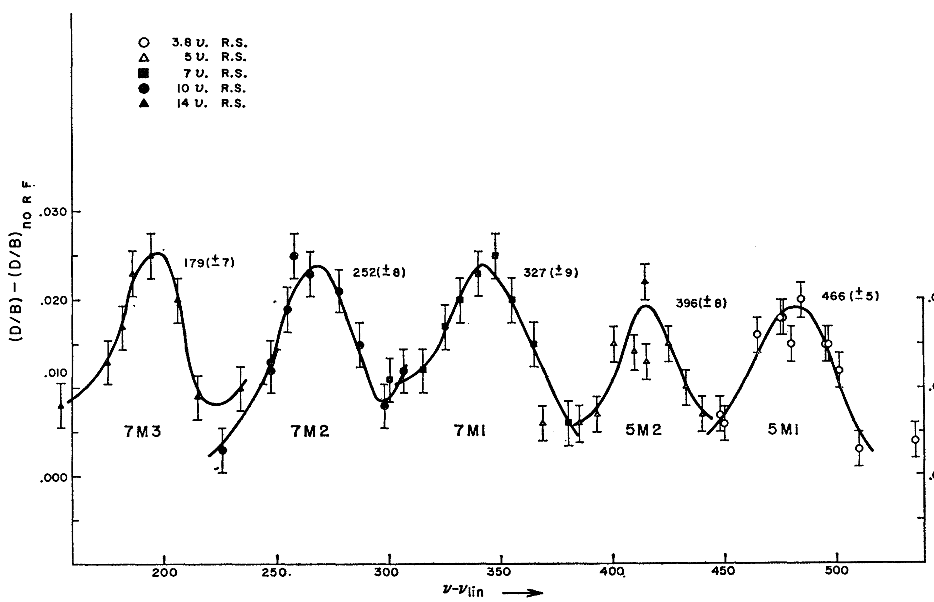

FIG. 2. The Sc^{47} resonance comb for $I=\frac{7}{2}$, $J=\frac{5}{2}$, $F=6$. Ordinate is the ratio of flopped to unflopped counting rates (D/B), normalized to zero for no rf signal. The various points are taken at different powers; most resonances are empirically close to optimally powered. The powers are listed in terms of voltage applied by the Rhode Schwarz rf oscillator (V R.S.), 0.25 V R.S. being the optimum power for K^{39}. The abscissa is the frequency deviation from a linear field dependence for Sc^{47}, ignoring the linear effect of g_I.

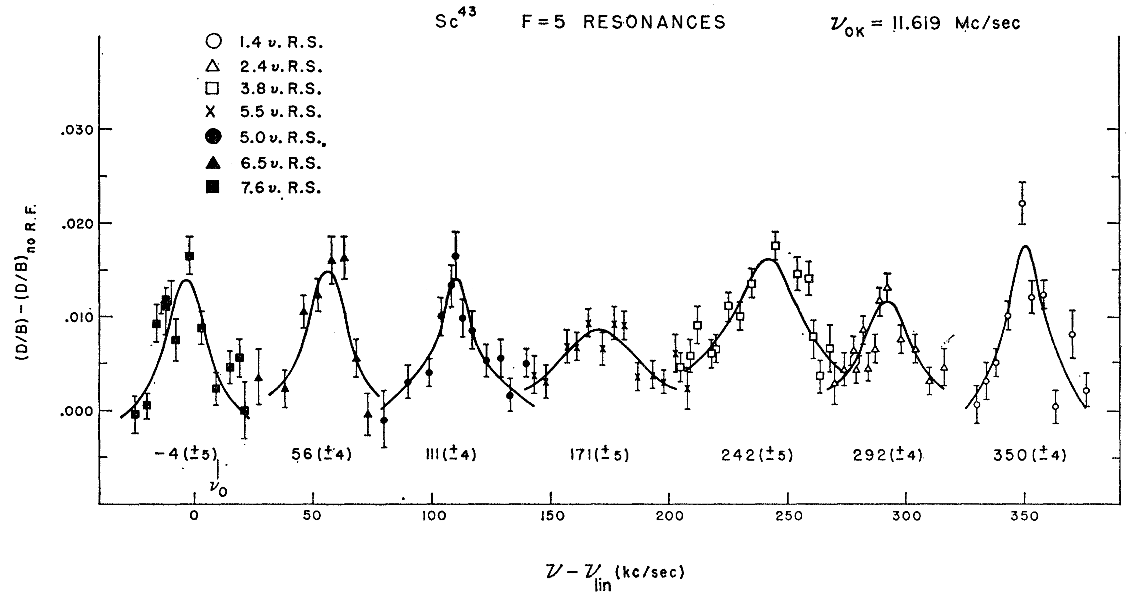

FIG. 3. The Sc^{43} resonance comb for $I=\frac{7}{2}$, $J=\frac{5}{2}$, $F=5$. Ordinate is the ratio of flopped to unflopped counting rates (D/B), normalized to zero for no rf signal. The various points are taken at different powers; most resonances are empirically close to optimally powered. The powers are listed in terms of voltage applied by the Rhode Schwarx rf oscillator (V R.S.), 0.25 V R.S. being the optimum power for K^{39}. The abscissa is the frequency deviation from a linear field dependence for Sc^{43}, ignoring the linear effect of g_I.

varied linearly with the magnetic field. By observing the field dependence of several resonances in the $F=6$ and $F=5$ states of both isotopes, unambiguous identification of the quantum multiplicities was possible. In particular, the combs for Sc^{43} (shown in Figs. 1 and 3) were experimentally followed back to the linear resonance, permitting a direct measurement of g_J. This was not possible for the Sc^{47} work, because of power restrictions.

With so many possible transitions in a relatively narrow frequency range, the possibility of spurious frequency shifts from an overpowering of the transitions was of some concern. The magnitude of such power pulling effects is in principle calculable, but is extremely

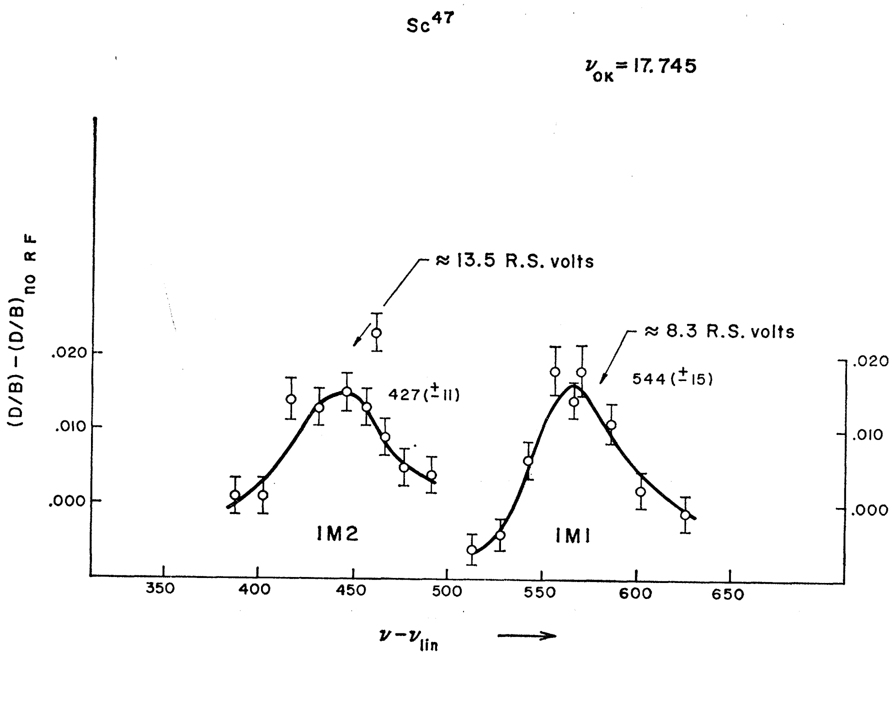

FIG. 4. Two resonances of the Sc^{47} resonance comb for $I=\frac{7}{2}$, $J=\frac{5}{2}$, $F=5$. Ordinate is the ratio of flopped to unflopped counting rates (D/B), normalized to zero for no rf signal. The various points are taken at different powers; most resonances are empirically close to optimally powered. The powers are listed in terms of voltage applied by the Rhode Schwarz rf oscillator (V R.S.), 0.25 V R.S. being the optimum power for K^{39}. The abscissa is the frequency deviation from a linear field dependence for Sc^{47}, ignoring the linear effect of g_I.

sensitive to C field inhomogeneities[6] which are imperfectly known in our apparatus. Empirically, the resonance positions observed did not shift outside the assigned errors in the power studies made, except when the power was increased by a factor of 2 over the optimal value. Operating at the experimental optimum power apparently minimized any pulling. The regularity of the observed combs indicated that any nonsystematic pulling was less than the linewidth of the resonance. Some systematic pulling may well have been present; it would not have seriously affected the values for A and B deduced from the data, but would affect the calculation of g_J.

III. RESULTS

The resonance positions in all the data were taken from the centroid of a Gaussian curve fitted to the experimental points, with errors corresponding to goodness of fit. Rough values of A and B using second-order perturbation theory were obtained in the process of the experiment; the final determinations for each isotope were obtained by an exact diagonalization of the hyperfine energy matrix, using the 7090 computer program HF 3–9.[7] In using the program, it was necessary to associate each experimental resonance with only one of the two or three possible overlapping transitions occurring at that frequency. In all cases the transition chosen was that with the best machine optics, consistent with the power applied. A listing of the resonances used in the fits, together with their transition assignments and relative weights, is shown in Tables I and II.

In initial calculations the parameters A, B, and g_J for the atomic $^2D_{5/2}$ state were calculated from the data for each isotope. The g_I in each case was related to the nuclear moment of Sc^{45} through the Fermi-Segré formula. As in the Sc^{44} cases, the data for each isotope could be fitted by either positive or negative values of A; in each case the positive assumption led to a g_J value greater in magnitude than the LS-coupling estimate, and the negative to a smaller value. On the basis of any single determination, then, a choice could not be made, and the sign of A remained ambiguous (although B/A was determined). But by combining the four independent values, a selection is clearly obvious, for the positive A assumption leads to consistent g_J measurements in each isotope, while the negative A does not (see Fig. 5). By averaging the only consistent choices from the four experiments, the g_J for the $^2D_{5/2}$ state was determined to be

$$g_J=-1.20061\pm0.00012,$$

and the magnetic moments of all four nuclear states were required to be positive.

Having fixed this value for g_J, the data for all four nuclear states (Sc^{43}, Sc^{47}, Sc^{44}, and Sc^{44m}) were reanalyzed, varying only A and B. The results are presented in Table III. The magnetic moments of the Sc^{44} states are not appreciably affected by this reanalysis, but the quadrupole moments are improved by the restriction to two variables.

TABLE I. Summary of Sc^{43} data. Headings are self-explanatory. The residual is the result of the final fit to the data; (F_1,M_1) and (F_2,M_2) label initial and final states, respectively.

Calibration frequency K^{39} (Mc/sec)	Observed frequency	Observed error	Residual from χ^2 minimization	(F_1,M_1)	(F_2,M_2)	Weight factor
20.0820	18.2910	0.0050	−0.00091	(6, −1)	(6, −6)	1557
20.0740	18.2880	0.0060	0.00276	(6, −1)	(6, −6)	1090
20.0520	18.1960	0.0050	−0.00363	(6,0)	(6, −6)	1081
20.1090	18.1750	0.0050	−0.00454	(6,1)	(6, −6)	795
20.0610	18,1390	0.0050	−0.00106	(6,1)	(6, −6)	795
20.0240	18.0450	0.0040	0.00190	(6,2)	(6, −6)	937
20.0380	17.9880	0.0040	−0.00026	(6,3)	(6, −6)	741
20.0430	17.9350	0.0060	0.00868	(6,4)	(6, −6)	259
20.0800	17.9630	0.0050	0.00690	(6,4)	(6, −6)	390
20.0750	17.8970	0.0060	0.01076	(6,5)	(6, −6)	226
20.0290	17.7900	0.0050	0.00574	(6,6)	(6, −6)	271
20.0140	17.7720	0.0070	−0.00036	(6,6)	(6, −6)	140
12.5380	11.0230	0.0040	0.00186	(5, −1)	(5, −5)	3740
12.5350	11.0260	0.0060	0.00739	(5, −1)	(5, −5)	1702
12.5340	10.9600	0.0040	0.00140	(5,0)	(5, −5)	2129
12.5260	10.8890	0.0050	−0.00424	(5,1)	(5, −5)	1002
12.5470	10.8490	0.0040	−0.00312	(5,2)	(5, −5)	1224
12.5310	10.7740	0.0040	−0.00722	(5,3)	(5, −5)	938
12.5340	10.7220	0.0040	−0.00425	(5,4)	(5, −5)	742
12.5460	10.6720	0.0050	−0.00682	(5,5)	(5, −5)	390
12.5210	10.6560	0.0050	−0.00306	(5,5)	(5, −5)	364
16.0000	13.3510	0.0080	−0.00666	(5,5)	(5, −5)	151

[6] W. Happer, Princeton University Technical Report No. PUC-1964-148 (unpublished).

[7] We thank Dr. H. Shugart for making the Berkeley programs available to us.

TABLE II. Summary of Sc^{47} data. Headings are self-explanatory. The residual is the result of the final fit to the data; (F_1,M_1) and (F_2,M_2) label initial and final states, respectively.

Calibration frequency K^{39} (Mc/sec)	Observed frequency	Observed error	Residual from χ^2 minimization	(F_1,M_1)	(F_2,M_2)	Weight factor
20.0190	18.1730	0.0100	0.00268	(6, −1)	(6, −6)	389
23.1120	20.6950	0.0150	−0.00725	(6, −1)	(6, −6)	176
31.0450	26.9300	0.0080	0.00508	(6, −1)	(6, −6)	603
20.0190	18.1130	0.0100	−0.00004	(6,0)	(6, −6)	270
23.1120	20.6250	0.0080	−0.00319	(6,0)	(6, −6)	417
31.0450	26.7980	0.0080	−0.00290	(6,0)	(6, −6)	419
19.8900	17.9490	0.0100	−0.00129	(6,1)	(6, −6)	199
23.1120	20.5560	0.0090	0.00158	(6,1)	(6, −6)	244
20.0190	17.9980	0.0100	−0.00109	(6,2)	(6, −6)	152
23.1120	20.4810	0.0080	0.00002	(6,2)	(6, −6)	235
20.0190	17.9370	0.0120	−0.00545	(6,3)	(6, −6)	84
23.1120	20.4080	0.0070	0.00014	(6,3)	(6, −6)	240
20.0190	17.8820	0.0150	−0.00404	(6,4)	(6, −6)	44
19.9500	16.8800	0.0100	−0.00538	(5,0)	(5, −5)	390
30.9450	25.1810	0.0070	−0.00176	(5,0)	(5, −5)	782
19.9500	16.7630	0.0110	−0.00298	(5,1)	(5, −5)	225
20.2480	16.9930	0.0100	−0.00282	(5,1)	(5, −5)	271
20.2510	16.8800	0.0100	0.00334	(5,2)	(5, −5)	200

The errors assigned to the A and B values for Sc^{43} and Sc^{47} in Table III are not the usual standard deviations resulting from the computer analysis. The standard random-error analysis is not germane here, because systematic effects such as power pulling may introduce errors in parts of the data which are larger than any measuring uncertainty. The general trend of the data indicates that the systematic errors are not serious; the approximately equal spacing of the resonance peaks in Figs. 1–4, for example, argues that any power distortion affected each resonance in the same way, which would be an extremely unlikely situation. However, to investigate the possible presence of systematic errors, a number of cross-checks were taken in Sc^{43}. The data were separated into several parts, an A and B value were calculated for each part, and the results were compared. Also, the assumption was relaxed that the transitions with best machine optics be assigned as the resonant states, and arbitrary assignments were made. In general the cross checks were consistent to the full set of data within the errors assigned. A systematic discrepancy, however was noted between the $F=6$ and $F=5$ data, indicating that the very high quantum multiplicity transitions in either F level might be somewhat displaced. The errors assigned in Table III are based on the range of the variations in A and B values found in these cross checks. They correspond to something like $1\frac{1}{2}$ standard deviations in the results of calculations with the full set of data. The errors in Sc^{47} and in the recalculation of the Sc^{44} parameters were correspondingly adjusted. The size of the errors precluded sensible diamagnetic and Sternheimer corrections to the moments, and no such corrections were made.

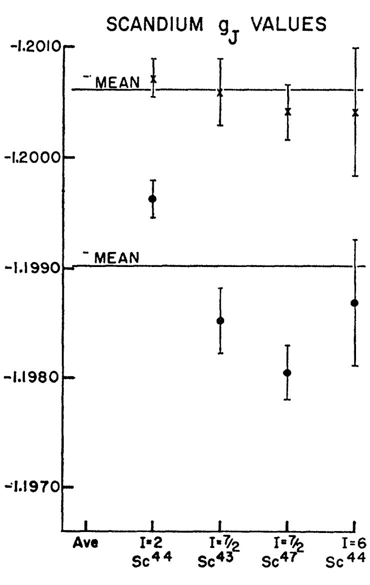

FIG. 5. Comparison of consistency of the choice for g_J in Sc^{43}, Sc^{47}, and Sc^{44}. There are two choices of g_J for each isotope; one assumes $A>0$, the other $A<0$. The choice $A>0$ in each case gives a consistent mean.

IV. DISCUSSION

The zero-order shell model, in which the nuclear moments are presumed to be due to the last odd particle (or, in odd-odd nuclei, to the last odd particle

TABLE III. Hyperfine constants and moments for radioactive scandium isotopes (no diamagnetic or Sternheimer corrections). $g_J=-1.20061\pm0.00013$.

Isotope	I	A (Mc/sec)	B (Mc/sec)	μ (nm)	Q (barns)
Sc^{43}	$\frac{7}{2}$	105.7±0.9	−44±10	+4.61±0.04	−0.26±0.06
Sc^{44}	2	102.5±1.2	+18± 8	+2.56±0.03	+0.10±0.05
Sc^{44m}	6	51.7±0.2	−33± 3	+3.87±0.01	−0.19±0.02
Sc^{47}	$\frac{7}{2}$	122.2±0.5	−38± 6	+5.33±0.02	−0.22±0.03

in each shell) is inadequate when applied to the results of these experiments. The single-particle model predicts for Sc^{43}, Sc^{45}, and Sc^{47} a common magnetic moment of $+5.79$ nm, and a quadrupole moment of -0.07 b. It is clear (see Table III) that the nuclei are somewhat more deformed than this simple model permits, and that there is a neutron number dependence for the magnetic moments. The corrections necessary to explain these effects can be separated into two types, corresponding to the failure of two separate assumptions of the zero-order model. First, the assumption that the particles outside the closed Ca^{40} core are coupled in a simple way, so that a single-particle wave function is sufficient, is not very valid. Second, the restriction that the added particles are confined to the next available orbit (here the $1f_{7/2}$ shell) is not correct, and in fact, even the excitation of particles from the closed shell to higher orbits probably contributes to the total moment.

The simple coupling approximation has been improved recently[8,9] by diagonalizing the energy matrix of an empirical residual force between the extra-core particles (assuming only $1f_{7/2}$ particles are present) and using the resulting eigenfunctions to calculate magnetic[10] and quadrupole[11] moments. The results of these calculations have significantly improved the agreement of the shell-model theory with experiment; the pertinent numbers are shown in Table IV. In order to achieve this agreement, however, the single-particle moment operators had to be modified. The protons and neutrons in the shell were allowed to have arbitrary charges and magnetic moments, and a mean value for each was determined by least-squares fitting to the 17 quadrupole moments and transition rates, and the 18 magnetic moments experimentally known. The mean values of these quantities are: $\bar{e}_p=+1.97e$; $\bar{e}_n=+1.87e$; $g_p=+1.50$ nm, and $g_n=-0.39$ nm. Here g_p and g_n are the effective bound g's in the $1f_{7/2}$ shell; the corresponding Schmidt values are $g_{ps}=+1.65$ nm and $g_{ns}=-0.545$ nm. The improvement rests partly, then, in the wave functions, and partly in this operator "renormalization."

The renormalization is an arbitrary method of taking into account the second correction to the moments,

TABLE IV. Comparison of moments of scandium isotopes with shell-model predictions.

Nucleus	μ(expt) (nm)	μ(calc)[a] (nm)	Q(expt) (b)	Q(calc)[b] (b)
Sc^{43}	$+4.61\pm0.04$	$+4.53$	-0.26 ± 0.06	-0.22
Sc^{44}	$+2.56\pm0.03$	$+2.21$	$+0.10\pm0.05$	$+0.11$
Sc^{44m}	$+3.87\pm0.01$	$+3.62$	-0.19 ± 0.02	-0.46
Sc^{45}	$+4.7563$[c]	$+4.75$	-0.22[c]±0.01	-0.37
Sc^{46}	$+3.04$[d]	$+3.23$	$+0.119$[d]±0.006	$+0.036$
Sc^{47}	$+5.33\pm0.02$	$+5.04$	-0.22 ± 0.03	-0.30

[a] See Ref. 10.
[b] See Ref. 11.
[c] G. Fricke, H. Kopfermann, S. Penselin, and K. Schüpmann, Z. Physik 156, 416 (1959).
[d] F. R. Petersen and H. A. Shugart, Phys. Rev. 128, 1740 (1962).

namely the configuration mixing. First-order configuration admixtures have been considered before,[12] but only to the zero-order wave functions of the simple shell model. The previous calculations have tended to overemphasize the importance of such contributions, partly because they started from incorrect basis states, and partly because of unrealistic estimates of the energy splittings involved. The effects of second-order perturbing effects have usually been disregarded. As has been recently shown,[13] these are not negligible. The magnitude of each contribution is smaller than the first-order term, but the number of possible perturbations is so much larger that the net effects are comparable. The quenching used in Ref. 10 is about the order of the second-order corrections calculated by Ichimura and Yasaki. At least part of these authors' corrections should be expressible in terms of a general quenching over the shell, since they consider the excitation of core particles to completely unfilled states.[14]

This is the apparent origin of the renormalization effect; the remaining second-order correction and a more realistic first-order calculation should further improve the theoretical agreement.

ACKNOWLEDGMENTS

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[8] J. D. McCullen, B. F. Bayman, and L. Zamick, Phys. Rev. 134, B515 (1964).
[9] J. Ginnochio, Nucl. Phys. 63, 449 (1965).
[10] B. F. Bayman, J. D. McCullen, and L. Zamick, Phys. Rev. Letters 11, 215 (1963).
[11] L. Zamick and J. D. McCullen, Bull. Am. Phys. Soc. 10, 485 (1965).
[12] A. Arima and H. Horie, Progr. Theoret. Phys. (Kyoto) 11, 509 (1954). R. J. Blin-Stoyle, Proc. Phys. Soc. (London) A66, 1158 (1933).
[13] M. Ichimura and K. Yazaki, Nucl. Phys. 63, 401 (1965).
[14] See, e.g., A. de-Shalit, in *Selected Topics in Nuclear Theory* (International Atomic Energy Agency, Vienna, 1963).