

Nuclear structure of  $^{45,47}\text{Sc}$ 

S. Saini

*Nuclear Physics Division, Bhabha Atomic Research Centre, Bombay 400 085, India*

M. R. Gunye

*Theoretical Reactor Physics Section, Bhabha Atomic Research Centre, Bombay 400 085, India*

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The properties of the nuclear states up to  $J = 23/2^-$  are investigated in odd- $A$  scandium isotopes  $^{45,47}\text{Sc}$ . The investigations are carried out in the framework of Hartree-Fock projection formalism by employing a realistic nucleon-nucleon interaction. An inert  $^{40}\text{Ca}$  core is assumed and all the valence nucleons are explicitly treated in the configuration space of the full  $pf$  shell. The energy levels, static electromagnetic moments and the electromagnetic transition probabilities are evaluated from the band-mixing calculations wherein the lowest four energetically close intrinsic states of the nuclei are taken into account. The theoretical results are in fair agreement with the available experimental data.

[NUCLEAR STRUCTURE Scandium isotopes: calculated energy levels, static moments,  $B(E2)$  and  $B(M1)$ . Hartree-Fock projection formalism with band mixing.]

## I. INTRODUCTION

A large amount of experimental data is now available on the  $pf$ -shell nuclei with the advent of heavy-ion induced reactions in recent years. This has revived interest in the studies of the structure of these nuclei. The early theoretical investigations on the structure of the  $pf$ -shell nuclei were carried out in the framework of the spherical shell model<sup>1</sup> and the phenomenological deformed rotator-particle coupling (RPC) model.<sup>2</sup> The restricted shell model calculations<sup>1</sup> in a pure  $(f_{7/2})^n$  configuration were able to account for a large amount of the then available experimental data on many  $pf$ -shell nuclei up to  $^{56}\text{Ni}$ . It is, however, quite obvious that the static and dynamic properties of many of the observed nuclear states cannot be described in terms of such restricted shell model calculations. The recent studies<sup>3,4</sup> with the extension of the shell model configuration space to include the full  $pf$  shell have led to a significant improvement in correlating the observed properties of calcium isotopes and the isotopes of scandium and titanium with mass number  $A \leq 44$ . Owing to the inherent complexities of the shell model calculations for heavier isotopes of scandium and other elements in the configuration space of the complete  $pf$  shell, such calculations are not so far reported for  $A > 44$ . However, in view of the substantial pile up of the experimental data, particularly on the high spin states populated in heavy-ion reactions, it is worthwhile to make a systematic study of these nuclei employing a realistic nucleon-nucleon ( $NN$ ) interaction in a large configuration space of the complete  $pf$  shell.

The high spin states have probably a simpler nature and their study may provide a significant insight into the intrinsic nuclear structure.

We are concerned here with the nuclear structure of two odd- $A$  scandium isotopes  $^{45}\text{Sc}$  and  $^{47}\text{Sc}$ . In the calculations reported here, an inert  $^{40}\text{Ca}$  core is assumed and the single particle orbitals  $0f_{7/2}$ ,  $1p_{3/2}$ ,  $0f_{5/2}$ ,  $1p_{1/2}$  are included in the active space. The calculations are performed in the framework of Hartree-Fock (HF) projection formalism,<sup>5</sup> employing the Kuo-Brown<sup>6</sup> effective  $NN$  interaction modified by McGrory *et al.*<sup>3</sup> to optimize the agreement between the experimental and the calculated energy spectra of calcium isotopes. The same effective  $NN$  interaction has been used in our previous work<sup>7</sup> on Vanadium isotopes and was found to reproduce the energy spectra and electromagnetic transition rates reasonably well. The preliminary results in  $^{47}\text{Sc}$  using the same effective interaction have been reported<sup>8</sup> earlier. This effective interaction will be referred to as KB-I interaction in this paper. We have also used a slightly different modification<sup>4</sup> of the Kuo-Brown<sup>6</sup>  $NN$  interaction wherein the matrix elements in the  $|(f_{7/2})^2JT\rangle$  states are renormalized to account for the omission of the  $q_{9/2}$  orbit included in the original model space of Kuo and Brown.<sup>6</sup> This effective  $NN$  interaction will be referred to as KB-II interaction in this paper. The HF calculations with axially symmetric deformations show that there are many energetically close intrinsic states of the two odd- $A$  nuclei under consideration. This necessitates a band-mixing calculation to determine the admixture of various close-lying intrinsic states in the computed wave functions.

The band-mixing HF projection formulation is outlined in Sec. II. The results of the calculations are discussed in Sec. III and the conclusions are presented in Sec. IV.

## II. DESCRIPTION OF THE CALCULATIONS

The calculations reported in this paper are carried out in the framework of HF projection formalism<sup>5</sup> employing the modified<sup>3,4</sup> Kuo-Brown<sup>6</sup> effective  $NN$  interactions KB-I and KB-II. All the valence nucleons outside an inert  $^{40}\text{Ca}$  core are considered to be active in the configuration space of the full  $pf$  shell. The single particle energies of the basis states  $0f_{7/2}$ ,  $1p_{3/2}$ ,  $1p_{1/2}$ , and  $0f_{5/2}$  are taken to be 0.0, 2.1, 3.9, and 6.5 MeV, respectively, as obtained from the  $^{41}\text{Ca}$  energy spectrum. The HF calculations with axially symmetric deformations yield many energetically close intrinsic states. The energy  $E_K^{\text{HF}}$  of the intrinsic HF state  $\phi_K$  is given by  $E_K^{\text{HF}} = \langle \phi_K | H | \phi_K \rangle$ , where  $H$  is the Hamiltonian of the nuclear system and  $K$  is the band quantum number. The good angular momentum states  $\psi^J$  projected from different intrinsic states may not be orthogonal. The nuclear wave function can then be expressed as

$$\Psi^J = \sum_i C_i^J \psi_i^J.$$

The band-mixing coefficients  $C_i$  and the energy  $\epsilon$  of the nuclear state  $\Psi$  can be obtained from the equation

$$\sum_j (\langle \psi_i | H | \psi_j \rangle - \epsilon \langle \psi_i | \psi_j \rangle) C_j = 0$$

for each angular momentum  $J$ . Thus energy is determined by solving the determinantal equation

$$|\langle \psi_i | H | \psi_j \rangle - \epsilon \langle \psi_i | \psi_j \rangle| = 0.$$

The static electromagnetic moments and transition probabilities are then obtained by evaluating<sup>9</sup> the matrix elements of the relevant multipole operator between the initial and final nuclear states.

## III. RESULTS AND DISCUSSION

The band-mixed wave functions obtained from the self-consistent HF projection formalism are employed in the nuclear structure calculations of the two odd- $A$  scandium isotopes  $^{45}\text{Sc}$  and  $^{47}\text{Sc}$  reported here. The magnetic moment  $\mu$  and the reduced transition probabilities  $B(M1)$  are calculated by employing the bare magnetic dipole operator corresponding to a free nucleon, whereas the electric quadrupole moment  $Q$  and the reduced transition probabilities  $B(E2)$  are evaluated by employing an effective electric quadrupole opera-

TABLE I. The band quantum number  $K$ , energy  $E_K^{\text{HF}}$  and mass quadrupole moments  $Q_K^{\text{HF}}(p)$  of proton and  $Q_K^{\text{HF}}(n)$  of neutrons are tabulated for  $^{45,47}\text{Sc}$ .

Nucleus	$K$	$E_K^{\text{HF}}$ (MeV)	$Q_K^{\text{HF}}(p)$ (fm <sup>2</sup> )	$Q_K^{\text{HF}}(n)$ (fm <sup>2</sup> )
$^{45}\text{Sc}$	$\frac{1}{2}$	-7.70	15.70	45.44
	$\frac{7}{2}$	-7.15	-12.00	-30.33
	$\frac{3}{2}$	-6.40	8.51	45.23
	$\frac{5}{2}$	-5.78	-2.43	-30.23
$^{47}\text{Sc}$	$\frac{1}{2}$	-9.87	13.10	38.07
	$\frac{3}{2}$	-9.30	7.93	37.93
	$\frac{7}{2}$	-9.20	-12.00	-24.80
	$\frac{5}{2}$	-8.35	-2.02	-24.68

tor with the effective charges assigned to the valence nucleons. The effective charges  $e_p = 1.33e$  for protons and  $e_n = 0.64e$  for neutrons employed in the present calculations were obtained<sup>10</sup> by the least squares fit to the observed  $B(E2)$  values in Ti, V, Cr, and Fe isotopes in the mass region  $44 \leq A \leq 54$ .

The band quantum number  $K$ , the energy  $E_K^{\text{HF}}$  and the mass quadrupole moments  $Q_K^{\text{HF}}(p)$  for protons and  $Q_K^{\text{HF}}(n)$  for neutrons in the intrinsic states employed in the present band-mixing calculations in  $^{45}\text{Sc}$  and  $^{47}\text{Sc}$  are shown in Table I. It should be noted that the prolate HF state is energetically the lowest for both the nuclei, though the energy difference between the lowest prolate and the lowest oblate states is rather small ( $\approx 0.5$  MeV). It is also clear from Table I that the mass quadrupole moments  $Q_K^{\text{HF}}(p)$  and  $Q_K^{\text{HF}}(n)$  in the lowest intrinsic HF states decrease slightly by  $\sim 15\%$  from  $^{45}\text{Sc}$  to  $^{47}\text{Sc}$ . This decrease of  $Q_K^{\text{HF}}(n)$  can be understood in terms of the filling of neutrons in the  $f_{7/2}$ -subshell. We find that  $Q_K^{\text{HF}}(n)$  increases from  $^{42}\text{Sc}$  to  $^{45}\text{Sc}$  where it reaches a maximum value and then decreases from  $^{45}\text{Sc}$  to  $^{49}\text{Sc}$  where it is minimum.

It should be mentioned here that the energy separation between the fourth and the fifth intrinsic HF state in  $^{45}\text{Sc}$  is 1.01 MeV. The projected energies obtained from this fifth intrinsic state are substantially higher than the corresponding energies obtained from the intrinsic states listed in Table I. Consequently, this fifth HF state does not affect the energy spectrum obtained by considering the band-mixing between the lowest four intrinsic states only. In the case of  $^{47}\text{Sc}$ , we find that the projected energies from the fourth intrinsic state itself are quite high as compared to the corresponding energies projected from the lowest three intrinsic states in Table I, and hence, the

energy spectrum is only slightly affected by including even the fourth intrinsic state. The fifth HF state in  $^{47}\text{Sc}$  is 0.10 MeV above the fourth HF state. We have, however, not considered it in the present band-mixing calculations in view of the fact that even the fourth intrinsic state is also not significant as far as the energy spectrum is concerned. Though the effect of the higher intrinsic states on the energy spectra of the two nuclei under consideration is not very significant, their effect on the  $B(E2)$  and  $B(M1)$  values may not be negligible. The electromagnetic transitions are more sensitive to even the small admixture of the intrinsic states. The band-mixing calculations with the lowest three intrinsic states show that the inclusion of the fourth intrinsic state changes the  $B(E2)$  values by less than 15% and the  $B(M1)$  values by less than 10% for various transitions in the two nuclei under consideration. The effect of the still higher intrinsic states is expected to be even smaller. We have, therefore, considered only the lowest four intrinsic states in the present calculations. The results of the nuclear structure calculations in  $^{45}\text{Sc}$  and  $^{47}\text{Sc}$  by including explicitly the band-mixing between the lowest four intrinsic states (Table I) are discussed below.

#### $^{45}\text{Sc}$

The low-lying negative parity states in this nucleus have been extensively studied through  $(p, \gamma)$ ,  $(p, p'\gamma)$ , and transfer reactions.<sup>11-18</sup> The high spin states up to  $J = \frac{15}{2}^-$  were identified and studied by Sawa *et al.*<sup>14</sup> with the  $^{42}\text{Ca}(\alpha, p)^{45}\text{Sc}$  reaction. Recently, Bizzeti *et al.*<sup>19</sup> have investigated the high spin states up to  $J = \frac{23}{2}^-$  populated by heavy-ion reactions  $^{30}\text{Si}(^{18}\text{O}, p2n)^{45}\text{Sc}$  and  $^{41}\text{K}(^7\text{Li}, p2n)^{45}\text{Sc}$ . The first structure calculations for this nucleus were performed by McCullen *et al.*<sup>1</sup> These restricted shell model calculations in  $(f_{7/2})^5$  configuration space predict the spin  $J = \frac{7}{2}^-$  for the ground state correctly and also give a good account of the yrast states from  $J = \frac{9}{2}^-$  to  $J = \frac{17}{2}^-$ . However, the excitation energies of the yrast states  $\frac{1}{2}^-$ ,  $\frac{3}{2}^-$ ,  $\frac{5}{2}^-$  and the high spin states with  $J > \frac{17}{2}^-$  obtained from these calculations are too high as compared to the experimental energies. The recent shell model calculations<sup>19</sup> in the restricted  $(f_{7/2})^5$  configuration space performed with different sets of matrix elements of effective  $NN$  interaction show that the high spin yrast states with  $J > \frac{17}{2}^-$  can be lowered, but the yrast states  $\frac{1}{2}^-$ ,  $\frac{3}{2}^-$ , and  $\frac{5}{2}^-$  are still predicted to be too high. The calculations in the framework of the rotation-particle coupling model<sup>2</sup> provide only a qualitative description of the energy spectrum of the low-lying states below 1.5 MeV; moreover, the high

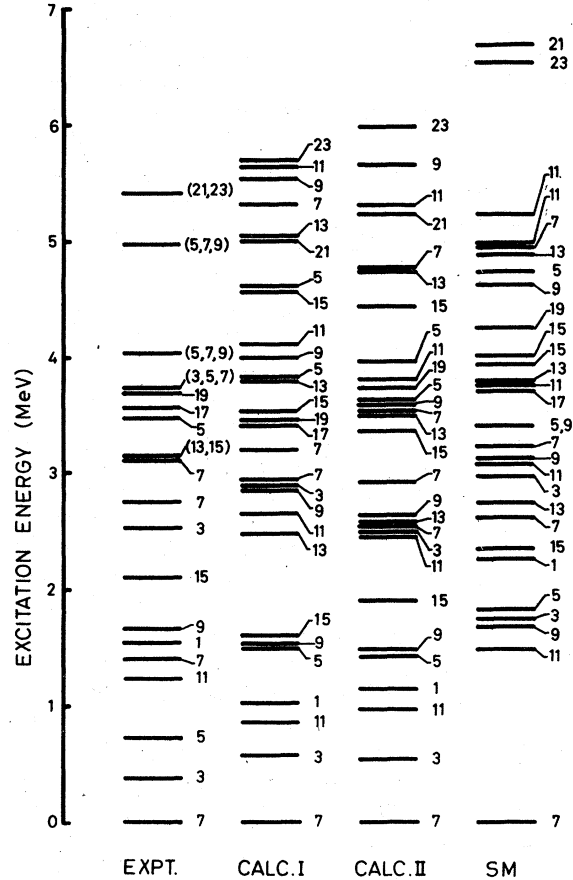


FIG. 1. The experimental and the calculated energy spectrum of negative parity states in  $^{45}\text{Sc}$ . The energy spectra computed with KB-I and KB-II effective  $NN$  interactions are shown in columns CALC I and CALC II, respectively. The shell model (SM) spectrum of Ref. 1 is also displayed. The numbers on the right of the levels indicate  $2J$  values.

spin states with  $J > \frac{15}{2}^-$  are not investigated in this RPC model.<sup>2</sup>

The energy spectra obtained in the present calculations with two slightly different versions<sup>3,4</sup> of the modified Kuo-Brown  $NN$  interaction KB-I and KB-II are displayed in Fig. 1 along with the experimental energy spectrum. The results of the shell model calculations by McCullen *et al.*<sup>1</sup> are also displayed in the same figure for comparison. The energy spectra obtained with KB-I and KB-II effective interactions are quite similar, the excitation energies in the two cases differing at the most by 200 keV for nearly all the states. The sequence of yrast states  $\frac{7}{2}^-$ ,  $\frac{9}{2}^-$ ,  $\frac{11}{2}^-$ ,  $\frac{13}{2}^-$ ,  $\frac{15}{2}^-$ ,  $\frac{17}{2}^-$ , and  $\frac{19}{2}^-$  is explained quite correctly. For any one of these yrast states, the excitation energy computed with KB-II effective  $NN$  interaction is within 250 keV of the corresponding experimental energy. The present calculations, however, do

not reproduce the first  $\frac{5}{2}^-$  state at 720 keV. The calculations predict the  $\frac{5}{2}^-$  state at 1440 keV and this excitation energy agrees well with the experimentally observed level at 1410 keV. This level was assigned<sup>13</sup> a spin  $(\frac{5}{2}^-, \frac{7}{2}^-)$  previously, but the recent experimental observations<sup>15</sup> assign a spin  $\frac{7}{2}^-$  to it. Our calculations do not predict any excited  $\frac{7}{2}^-$  state in this energy region. Our calculated  $\frac{1}{2}^-$  state is about 400 keV lower than the observed  $\frac{1}{2}^-$  level at 1550 keV. The observed level at 3.16 MeV has been assigned<sup>14</sup> a spin  $(\frac{13}{2}^-, \frac{15}{2}^-)$  tentatively, whereas the present calculations predict the yrast  $\frac{13}{2}^-$  state at 2.55 MeV and the first excited  $\frac{15}{2}^-$  state at 3.36 MeV. Our calculations thus favor a spin  $\frac{15}{2}^-$  to the experimental level at 3.16 MeV. The recently observed<sup>19</sup> level at 5.42 MeV has been assigned a spin  $(\frac{21}{2}^-, \frac{23}{2}^-)$ . Our calculations with KB-II interaction predict the yrast states  $\frac{21}{2}^-$  and  $\frac{23}{2}^-$  at 5.24 and 6.00 MeV, respectively, thus suggesting a spin  $\frac{21}{2}^-$  for the observed level at 5.42 MeV. The calculations with KB-I interaction, however, predict both the yrast states  $\frac{21}{2}^-$  and  $\frac{23}{2}^-$  close (within  $\pm 400$  keV) to the observed level at 5.42 MeV. The observed excited states  $\frac{3}{2}^-$  (2.53 MeV),  $\frac{5}{2}^-$  (3.48 MeV),  $\frac{7}{2}^-$  (2.75 and 3.14 MeV) are very well explained by the present calculations as seen from Fig. 1. The levels reported<sup>17</sup> at 4.03 and 4.97 MeV are assigned the spins  $(\frac{5}{2}^-, \frac{7}{2}^-, \frac{9}{2}^-)$  tentatively. Our calculations predict the spins  $\frac{9}{2}^-$  and  $\frac{7}{2}^-$  for these levels reported at 4.03 and 4.97 MeV, respectively. The present calculations predict a few excited states which are not experimentally identified until now. The excitation energies (in MeV) of these states obtained with the KB-II interaction are 3.96 ( $\frac{5}{2}^-$ ), 2.62 ( $\frac{9}{2}^-$ ), 2.48 ( $\frac{11}{2}^-$ ), 5.29 ( $\frac{13}{2}^-$ ), 3.52 ( $\frac{15}{2}^-$ ), 4.75 ( $\frac{17}{2}^-$ ), and 4.44 ( $\frac{19}{2}^-$ ). It is interesting to note that these

predictions agree well with those of McCullen *et al.*<sup>1</sup>

The electromagnetic properties computed with both the KB-I and KB-II interactions are similar and hence we have shown the comparison of the experimental data with the results obtained with KB-I interaction. The computed static moments for the low-lying states are shown in Table II. The experimental data is available only for the  $\frac{7}{2}^-$  ground state and as seen from Table II, the calculated magnetic dipole moment and the electric quadrupole moment of the ground state are in good agreement with the corresponding experimental values. The shell model calculations<sup>20</sup> in  $(f_{7/2})^5$  configuration space, however, predict substantially large values for both the static moments of the ground state as seen from Table II. The computed  $B(M1)$  and  $B(E2)$  values for the electromagnetic transitions are tabulated in Table III. The experimental data is available for only a few  $\gamma$  transitions and moreover, the experimental  $B(M1)$  and  $B(E2)$  values are extracted from the data with large uncertainties. The computed  $B(M1)$  values are large by a factor of 2 to 10, compared with the only available experimental measurements of Rust *et al.*<sup>15</sup> The computed  $B(E2)$  value for the  $\gamma$  transition  $\frac{3}{2}^- \rightarrow \frac{7}{2}^-$  agrees quite well with the corresponding observed value. The recent experimental  $B(E2)$  values of Rust *et al.*<sup>15</sup> for the  $\gamma$  transitions  $\frac{11}{2}^- \rightarrow \frac{7}{2}^-$  and  $\frac{9}{2}^- \rightarrow \frac{7}{2}^-$  are quite different from the average values extracted from earlier measurements.<sup>11,12,21,26-30</sup> The most recent measurements<sup>18</sup> of the  $B(E2)$  value for  $\frac{11}{2}^- \rightarrow \frac{7}{2}^-$   $\gamma$  transition is, however, in agreement with the average of earlier measurements except that of Rust *et al.*<sup>15</sup> The calculated  $B(E2)$  values (Table III) for  $\frac{11}{2}^- \rightarrow \frac{7}{2}^-$  and  $\frac{9}{2}^- \rightarrow \frac{7}{2}^-$   $\gamma$  transitions are smaller than

TABLE II. The electric quadrupole moment  $Q$  and magnetic moment  $\mu$  of the low-lying negative parity states in  $^{45,47}\text{Sc}$ . Effective charges employed are  $e_p = 1.33e$ ,  $e_n = 0.64e$ .

Nucleus	$J$	Expt <sup>a</sup>	$Q(e\text{ fm}^2)$		SM <sup>b</sup>	Expt <sup>a</sup>	$\mu(\mu_N)$	
			Calc.	SM <sup>b</sup>			Calc.	SM <sup>b</sup>
$^{45}\text{Sc}$	$\frac{7}{2}$	$-22 \pm 1$	-23.11	-38.1	4.756	4.887	5.325	
	$\frac{3}{2}$	...	-12.74		...	3.929		
	$\frac{5}{2}$	...	-12.62		...	0.898		
	$\frac{11}{2}$	...	-23.31		...	2.161		
$^{47}\text{Sc}$	$\frac{7}{2}$	$-22 \pm 3$	-22.04	-32.2	$5.34 \pm 0.02$	5.294	5.589	
	$\frac{3}{2}$	...	-10.73		...	4.720		
	$\frac{11}{2}$	...	-24.45		...	4.841		
	$\frac{5}{2}$	...	-7.11		...	3.384		

<sup>a</sup> Reference 35.

<sup>b</sup> Reference 20. The  $(f_{7/2})^n$  shell model calculations in this reference are carried out with  $e_p = 1.97e$  and  $e_n = 1.87e$ .

TABLE III. The  $B(E2)$  and  $B(M1)$  values for  $\gamma$  transitions in  $^{45}\text{Sc}$  between the negative parity states  $J_i$  and  $J_f$ . The effective charges employed are same as given in Table II.

$J_i$	$J_f$	$B(E2)$ Expt.	$e^2\text{fm}^4$ Calc.	$B(M1)$ Expt. <sup>a</sup>	$\mu_N^2$ Calc.
$\frac{3}{2}$	$\frac{7}{2}$	$150 \pm 25$ <sup>b</sup>	123.82		
$\frac{5}{2}$	$\frac{3}{2}$		26.90		2.03
$\frac{1}{2}$	$\frac{3}{2}$		128.30		2.72
$\frac{5}{2}$	$\frac{7}{2}$		3.80		2.50
$\frac{11}{2}$	$\frac{7}{2}$	$113 \pm 10$ <sup>c</sup>	55.77		
$\frac{9}{2}$	$\frac{11}{2}$		9.14	$1.0 \pm 0.3$	3.08
$\frac{9}{2}$	$\frac{5}{2}$		36.90		
$\frac{9}{2}$	$\frac{7}{2}$	$73 \pm 20$ <sup>a</sup>	32.00	$0.08 \pm 0.02$	0.70
		$55$ <sup>b</sup>			
$\frac{15}{2}$	$\frac{11}{2}$		60.35		
$\frac{13}{2}$	$\frac{15}{2}$		6.70		1.73
$\frac{13}{2}$	$\frac{9}{2}$		32.43		
$\frac{13}{2}$	$\frac{11}{2}$		10.90		0.77

<sup>a</sup> Reference 15.

<sup>b</sup> Average of  $B(E2)$  values given in Refs. 11, 12, 21, and 26–30.

<sup>c</sup> The most probable value from the recent work of Ref. 18. The average value of  $B(E2)$  for this transition from the earlier work of Refs. 11, 12, 21, 27, and 31–34 is  $125 e^2\text{fm}^4$ , while Ref. 15 gives a larger value of  $(256 \pm 47) e^2\text{fm}^4$ .

the corresponding average experimental values by almost a factor of 2. The computed  $B(E2)$  values for a few other  $\gamma$  transitions are quite small (Table III) but the experimental data for these transitions is not available for comparison. The experimental  $B(E2)$  value  $(31 \pm 10) e^2\text{fm}^4$  for the  $\gamma$  transition  $\frac{5}{2}^- \rightarrow \frac{7}{2}^-$  is very large as compared to the computed value  $3.8 e^2\text{fm}^4$ , indicating that the observed  $\frac{5}{2}^-$  yrast level at 720 keV has a much more collective nature than the computed  $\frac{5}{2}^-$  level at 1440 keV.

#### $^{47}\text{Sc}$

The negative parity states up to  $J = \frac{11}{2}^-$  in this nucleus have been extensively studied through a variety of nuclear reactions.<sup>22–25</sup> Recent experimental measurements<sup>25</sup> have assigned the spins  $\frac{13}{2}^-$  and  $\frac{15}{2}^-$  to the levels at 2.15 and 2.64 MeV, respectively. The shell model calculations<sup>1</sup> in the restricted  $(f_{7/2})^n$  configuration space provide a good account of the low-lying yrast states except the  $\frac{3}{2}^-$  state which is predicted to occur at a comparatively higher excitation energy. Recent

shell model calculations<sup>25</sup> in the same restricted configuration space predict the  $\frac{13}{2}^-$  and  $\frac{15}{2}^-$  yrast states correctly but the low-lying states  $\frac{3}{2}^-$ ,  $\frac{11}{2}^-$ , and  $\frac{5}{2}^-$  are predicted at higher excitation energies compared with the experimental data. The phenomenological RPC model also provides a good description<sup>2</sup> of the low-lying yrast states up to  $J = \frac{11}{2}^-$  in this nucleus. The intermediate coupling model calculations<sup>25</sup> carried out by coupling the odd-proton to the neighboring  $^{46}\text{Ca}$  core states also explain some of the low-lying states in  $^{47}\text{Sc}$ .

The energy spectrum up to an excitation energy of nearly 6 MeV obtained from our calculations with KB-I effective  $NN$  interaction is displayed in Fig. 2 along with the experimental spectrum. The energy spectrum obtained from the shell model calculations of McCullen *et al.* is also shown in the same figure for comparison. The sequence of yrast states up to  $J = \frac{15}{2}^-$  is well reproduced by the present calculations. The excitation energies of these states are also reproduced quite well except for the  $\frac{11}{2}^-$  and  $\frac{13}{2}^-$  states for which the computed excitation energies are lower than the corresponding experimental energies by about 400 keV. The restricted shell model calculations<sup>1</sup> predict the excitation energy of the yrast state  $\frac{3}{2}^-$  by about 600 keV higher than its observed excitation energy; the excitation energies of the yrast states  $\frac{13}{2}^-$  and  $\frac{15}{2}^-$  are also higher than the corresponding experimental energies by about 400 keV. Our calculations reproduce the excitation energies of the observed first excited states  $\frac{7}{2}^-$ ,  $\frac{3}{2}^-$ , and  $\frac{5}{2}^-$  quite correctly. The shell model calculations<sup>1</sup> predict the excitation energy of the first excited  $\frac{3}{2}^-$  state by about 500 keV higher and of the first excited  $\frac{5}{2}^-$  state by about 600 keV lower than the corresponding experimental excitation energy. Our calculations predict the first excited  $\frac{11}{2}^-$  state at 2.80 MeV, which is close to the observed level at 3.13 MeV for which a spin ( $\frac{3}{2}^-$  to  $\frac{11}{2}^-$ ) is assigned<sup>22</sup> tentatively. Our calculated second excited  $\frac{7}{2}^-$  state at 5.20 MeV agrees well with the observed  $\frac{7}{2}^-$  state at 5.38 MeV. The present calculations predict the high spin yrast states  $\frac{17}{2}^-$  and  $\frac{19}{2}^-$  at 2.90 and 3.35 MeV, respectively, and the yrast state  $\frac{1}{2}^-$  at 2.30 MeV. It should be mentioned here that McCullen *et al.*<sup>1</sup> predict these yrast states at the excitation energies which are about one MeV higher than our computed values. It is thus desirable to identify these states experimentally.

The computed static electromagnetic moments for the low-lying states in  $^{47}\text{Sc}$  are shown in Table II. The only available experimental values of the magnetic dipole moment and the electric quadrupole moment for the ground state  $\frac{7}{2}^-$  are reproduced correctly by our calculations. The

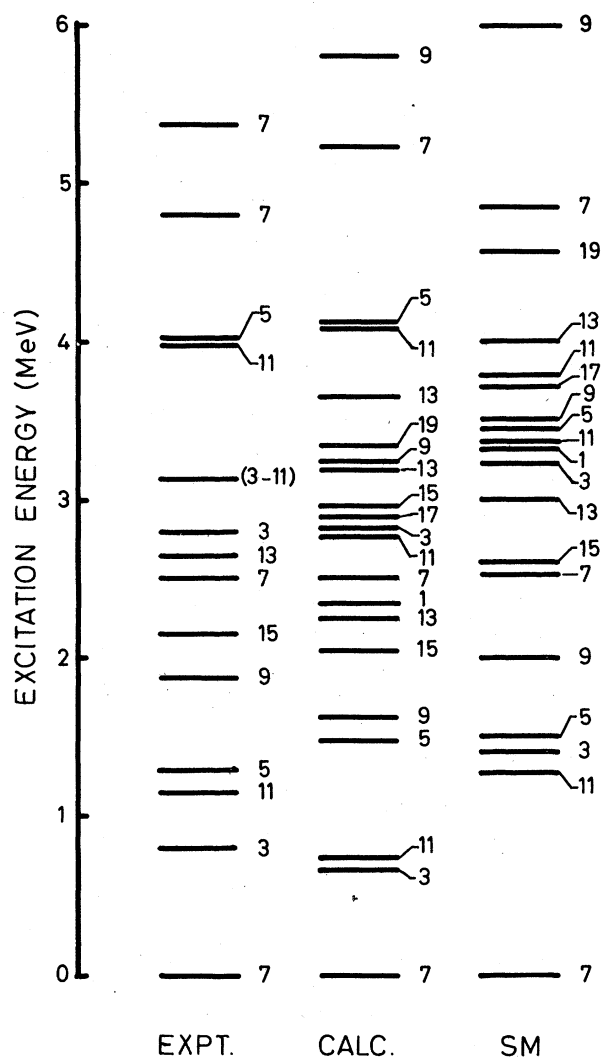


FIG. 2. The calculated (CALC) energy spectrum with KB-I effective  $NN$  interaction is shown along with the experimental energy spectrum of  $^{47}\text{Sc}$ . The shell model (SM) spectrum of Ref. 1 is also shown for comparison. The numbers on the right of the levels indicate  $2J$  values of the negative parity states in  $^{47}\text{Sc}$ .

corresponding values obtained from the restricted shell model calculations<sup>20</sup> are considerably higher than the observed values as seen from Table II. The computed  $B(M1)$  and  $B(E2)$  values are shown in Table IV along with the available experimental data. It can be seen from Table IV that the experimental data is quite uncertain due to large errors. The computed  $B(M1)$  values are large by a factor varying between 4 and 10, compared with the corresponding experimental results from the only available experimental measurements.<sup>25</sup> The computed  $B(E2)$  values are, in general, within the

TABLE IV. The  $B(E2)$  and  $B(M1)$  values for  $\gamma$  transitions in  $^{47}\text{Sc}$  between the negative parity states  $J_i$  and  $J_f$ . The effective charges employed are the same as given in Table II.

$J_i$	$J_f$	$B(E2)$ Expt. <sup>a</sup>	$e^2\text{fm}^4$ Calc.	$B(M1)$ Expt. <sup>a</sup>	$\mu_N^2$ Calc.
$\frac{3}{2}^-$	$\frac{7}{2}^-$	<292.2	91.32		
$\frac{5}{2}^-$	$\frac{3}{2}^-$	$614^{+2055.3}_{-453.4}$	41.48	$0.43 \pm 0.34$	1.78
$\frac{5}{2}^-$	$\frac{7}{2}^-$	$1.61^{+17.03}_{-1.61}$	3.33	$0.17 \pm 0.10$	1.50
$\frac{11}{2}^-$	$\frac{7}{2}^-$	$109.4 \pm 38.9$	44.34		
$\frac{3}{2}^-$	$\frac{5}{2}^-$	<23 344	38.59		
$\frac{3}{2}^-$	$\frac{11}{2}^-$	$2.02-1\ 073.0$	3.7	$0.39 \pm 0.23$	2.21
$\frac{3}{2}^-$	$\frac{7}{2}^-$	$2.62^{+11.28}_{-2.42}$	15.66	$0.043 \pm 0.025$	0.49
$\frac{15}{2}^-$	$\frac{11}{2}^-$	<272	21.76		
$\frac{13}{2}^-$	$\frac{15}{2}^-$	<2 438	33.00	$0.29- 2.92$	4.41
$\frac{13}{2}^-$	$\frac{9}{2}^-$	<2 901	17.81		
$\frac{13}{2}^-$	$\frac{11}{2}^-$	...	4.96	0.054	0.30
$\frac{1}{2}^-$	$\frac{3}{2}^-$	...	79.7	...	0.43

<sup>a</sup> Reference 25.

limits of the experimental uncertainties. The computed  $B(E2)$  values for the  $\gamma$  transitions  $\frac{11}{2}^- \rightarrow \frac{7}{2}^-$  and  $\frac{5}{2}^- \rightarrow \frac{3}{2}^-$  are, however, smaller than the corresponding experimental values.

#### IV. CONCLUSIONS

The properties of the nuclear levels in  $^{45,47}\text{Sc}$  are investigated in the framework of Hartree-Fock projection formalism by incorporating the band-mixing between the energetically close intrinsic states of these nuclei. All the nucleons outside the  $^{40}\text{Ca}$  core are explicitly treated in the configuration space of the full  $pf$  shell by employing the effective  $NN$  interactions.<sup>3,4</sup> The calculated excitation energies of the nuclear states, including those with high angular momentum, agree fairly well with the experimental data. The computed static electromagnetic moments for the low-lying states agree quite well with the experimental values wherever available. The shell model calculations<sup>20</sup> in the restricted  $(f_{7/2})^n$  configuration space, however, predict substantially large values for both the static moments in the case of both the nuclei. The computed  $B(M1)$  values in the case of  $^{45}\text{Sc}$  are large by a factor of 2 to 10 compared with the only available experimental measurements.<sup>15</sup> The calculated  $B(E2)$  values for  $^{45}\text{Sc}$  are,

in general, smaller than the corresponding experimental values except for  $\frac{3}{2}^- \rightarrow \frac{7}{2}^- \gamma$  transition where the agreement with the experimental value is quite good. In the case of  $^{47}\text{Sc}$ , there are large

uncertainties in the experimental  $B(E2)$  and  $B(M1)$  values. The computed  $B(E2)$  values are within the limits of experimental uncertainties for most of the  $\gamma$  transitions in  $^{47}\text{Sc}$ .

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