

STRUCTURE CALCULATIONS FOR  $^{25}\text{Mg}$ - $^{25}\text{Al}$ 

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**Abstract:** The results of a shell model calculation for  $^{25}\text{Mg}$ - $^{25}\text{Al}$  are presented in which the Hamiltonian for the system was taken to be that of an inert  $^{16}\text{O}$  core plus nine s-d shell particles interacting through the usual one-body  $l^2$  and  $l \cdot s$  terms plus general two-body residual interactions of the Kuo-Brown type. The basis was truncated to include nine favored representations of SU(3) in each of the two leading spatial symmetries ([441]: (66), (93), (74), (82)<sup>2</sup>, (55)<sup>2</sup>, (28), (90); [432]: (10,1), (74), (82)<sup>2</sup>, (55)<sup>2</sup>, (28), (47), (90)). It is found that a ( $\lambda\mu$ )-dependent renormalization of the type proposed by Harvey but empirically modified for axially asymmetric shape distributions is required to reproduce the experimentally observed ordering of the three lowest rotational bands. The goodness of  $K_J$  as a band label for the calculated eigenstates is investigated by comparing calculated quadrupole moments with simple rotational model predictions. Calculated  $B(E2)$  and  $B(M1)$  rates are compared with the available data. Results for relative spectroscopic factors from (d, p) stripping on the ground state of  $^{24}\text{Mg}$  are also presented.

## 1. Introduction

The experimentally observed collectivity of the s-d shell nuclei continues to provide a challenge to structure theorists who have as a goal a microscopic description for these nuclei in terms of a relatively small basis <sup>1</sup>). To be sure, large machine calculations can be used to reproduce (or nearly so) experimental observations and do indeed provide a very useful guide to the chemistry of these nuclei <sup>2</sup>). However, such an approach, as useful as it is, may tend to mask underlying principles basic to the structure of these nuclei. In the present article an attempt is made to analyze results obtained from a calculation for the  $^{25}\text{Mg}$ - $^{25}\text{Al}$  nuclei in terms of concepts familiar from the single-particle Nilsson picture <sup>3</sup>).

## 2. Interaction and basis truncation

In an attempt to provide a microscopic description for the experimentally observed collectivity of the  $^{25}\text{Mg}$ - $^{25}\text{Al}$  nuclei, shell model calculations were carried out in an SU(3) truncated basis with the Hamiltonian for the system taken to be that of an inert  $^{16}\text{O}$  core plus nine s-d shell particles interacting through the usual

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$l^2$ ,  $l \cdot s$ , and residual two-body interactions. Explicitly, for the extra-core nucleons,

$$\begin{aligned} V &= V_{1\text{-body}} + V_{2\text{-body}}, \\ V_{1\text{-body}} &= \alpha \sum_i l_i^2 - \beta \sum_i l_i \cdot s_i, \\ V_{2\text{-body}} &= \sum_{i < j} V_{ij} + V_R. \end{aligned} \quad (1)$$

In the 1-body potential the constant  $\alpha$  was fixed at a value which reproduces the s-d separation in  $^{17}\text{O}$  minus 35 % [ $\alpha = \frac{1}{6}(2.03 - 0.87) - (\approx 35\%) = 0.12 \text{ MeV}$ ] while  $\beta$  was fixed at a value which reproduces the corresponding  $d_{\frac{3}{2}}-d_{\frac{5}{2}}$  splitting plus 35 % [ $\beta = \frac{2}{5} \cdot 5.08 + (\approx 35\%) = 2.8 \text{ MeV}$ ]. These values were chosen as being consistent with other independent determinations for the mass 18–24 nuclei<sup>4–5</sup>) while yielding an acceptable fit to the experimental energy spectrum. (The structure of the calculated eigenstates was observed a posteriori to be relatively insensitive to variations by  $\pm 50\%$  in  $\alpha$  and/or  $\beta$ . For comparison, results with  $\alpha$  and  $\beta$  set equal to the  $^{17}\text{O}$  values are included as part of the calculated results presented in sect. 4.)

Four sets of two-body matrix elements, the  $V_{ij}$  in eq. (1), were used: (i) a set obtained by subtracting out the 3p-1h renormalization of Kuo and Brown from the matrix elements used by the Michigan State group in their mass 18–22 work<sup>4</sup>); (ii) a set obtained by subtracting out the 3p-1h renormalization of Kuo from the matrix elements used by the group at Oak Ridge in their mass 24 work (K+12FP) [ref. <sup>5</sup>)]; (iii) the s-d shell bare  $G$ -matrix elements of Kuo and Brown<sup>6</sup>); and (iv) the pure central interaction matrix elements of Akiyama *et al.*<sup>7</sup>)

An appropriate core renormalization,  $V_R$  in eq. (1), must be added to these interactions. The form of this renormalization depends, of course, upon the way in which the basis is truncated<sup>8</sup>). (The 3p-1h renormalization of Kuo is presumably appropriate for calculations involving the full s-d shell basis.) Harvey investigated this question for axially symmetric deformations of specific SU(3) irreducible tensor character.<sup>9</sup>) The proposed renormalization,  $V_{\text{symmetric}}$ , which is to take the place of the 3p-1h core renormalization terms of Kuo, is essentially a quadrupole-quadrupole interaction appropriately weighted with a proper exchange mixture<sup>10</sup>). Explicitly,

$$V_{\text{symmetric}} = \frac{2}{3} x \hbar \omega \sum_{i < j} (3 \mathcal{A}_{ij}^{13} + \mathcal{A}_{ij}^{31} + \mathcal{A}_{ij}^{11} + 3 \mathcal{A}_{ij}^{33})(Q_i \cdot Q_j), \quad (2)$$

where the  $\mathcal{A}^{2T+1, 2J+1}$  are spin-isospin projection operators and the parameter  $x$ , a function of the distribution of oscillator quanta and hence  $\lambda$  and  $\mu$ , is defined by eq. (7) of ref. <sup>9</sup>). For nonaxially symmetric deformations (the minimum of  $\lambda$  and  $\mu$  provides a measure of asymmetry, see eq. (4) below) we empirically modified the result to obtain

$$V_{\text{asymmetric}} = [A + B \min(\lambda, \mu)] V_{\text{symmetric}}. \quad (3)$$

Reasonable results for the  $^{25}\text{Mg}$ - $^{25}\text{Al}$  nuclei were obtained with  $A \approx B \approx 0.01$ . (Calculations for  $^{18}\text{O}$  indicate that the multiplicative factor for  $V_{\text{symmetric}}$  should be on the order of one-half rather than one as predicted by Harvey. Using this normalization as a guide, we adjusted  $B$  and hence  $A$  to approximately reproduce the 2 MeV splitting of the  $K_\pi = \frac{1}{2}$  band heads in the experimental spectrum.) The dominant effect of this additional deformed field core renormalization (taken to be diagonal in the SU(3) quantum numbers) is to simply lower the average energy of an asymmetric representation of SU(3) relative to more symmetric representations. And for this reason the effect of  $V_{\text{asymmetric}}$  will be much more pronounced for nuclei whose low-lying spectrum is dominated by two competing representations of SU(3) with differing intrinsic deformations (e.g.  $^{25}\text{Mg}$  with  $(\lambda\mu) = (66)$  and  $(93)$ ) as compared to nuclei whose low-lying spectrum is dominated by a single representation of SU(3) (e.g.  $^{24}\text{Mg}$  with  $(\lambda\mu) = (84)$ ).

Of the allowed representations of SU(3),  $(\lambda\mu) = (66), (93)$  are expected to dominate the low-lying configurations<sup>1</sup>). (The importance of these representations can be anticipated from a Nilsson level scheme for the s-d shell nuclei by noting that

$$2\lambda + \mu = \varepsilon_{\text{max}} = \sum_i [2n_z(i) - n_x(i) - n_y(i)], \quad (4a)$$

$$\mu = 2A_{\text{max}} = \sum_i [n_x(i) - n_y(i)]_{\text{max}}, \quad (4b)$$

where  $n_x, n_y, n_z$  are the number of oscillator quanta associated with occupied orbitals in the limit of good asymptotic quantum numbers.) Also included were those representations of SU(3) having relatively large Casimir invariants (hence large  $Q \cdot Q$  matrix elements) and/or favored through mixing with these two by terms which dominate the residual interaction<sup>11</sup>). (A semiquantitative measure of the relative importance of normalized tensor operators can be obtained by squaring and summing amplitude factors for an irreducible tensor decomposition of the interaction. For example, from the results given in table 1 of sect. 3 one can show that  $V = V_{1\text{-body}} + V_{2\text{-body}}$  [MS-(3p-1h)] has SU(3) irreducible tensor character of the following percentages:  $(\lambda_0\mu_0) = (00) \rightarrow 75.4\%$ ,  $(22) \rightarrow 12.2\%$ ,  $(11) \rightarrow 9.2\%$ ,  $(44) \rightarrow 1.4\%$ ,  $(33) \rightarrow 1.0\%$ , and other  $(\lambda_0\mu_0) \rightarrow 0.8\%$ , where the complete scalar term with eigenvalue proportional to  $\frac{1}{2}n(n-1)$  has been removed from the analysis to get a more reliable measure of the relative importance of SU(3) symmetry breaking terms.) Only two representations of SU(6) corresponding to the highest spatial symmetries were included. Explicitly, the calculation was carried out in a truncated basis containing

$$[441] \ (66), (93), (74), (82)^2, (55)^2, (28), (90),$$

$$[432]: (10,1), (74), (82)^2, (55)^2, (28), (47), (90).$$

(The (90) representation was included to check the validity of our truncation prescription; mixing of the (90) with the other representations should be negligible.) The

dimensionality of matrices that must be diagonalized in this truncated space as compared to that of the full space is then given <sup>12)</sup> by

$J$	Truncated/full
$\frac{1}{2}$	35/1434
$\frac{3}{2}$	67/2581
$\frac{5}{2}$	94/3281
$\frac{7}{2}$	114/3444
$\frac{9}{2}$	128/3144.

### 3. Method of calculation

To avoid unnecessarily large array storage and minimize redundant numerical calculations it is convenient to introduce the techniques of second quantization and express all interactions in terms of an SU(3)-SU(4) irreducible tensor formalism <sup>13)</sup>. Starting with an interaction of SU(2) tensor character  $T_0$  in isospin space and  $J_0$  in ordinary space (for the interaction of eq. (1)  $T_0 = J_0 = 0$ ), straightforward recoupling formulae can be used to convert from the  $j$ - $j$  coupled matrix elements between antisymmetrized two-particle wave functions to the corresponding  $L$ - $S$  coupled matrix elements,

$$\begin{aligned}
 & \langle (l'_1 l'_2) L' S' J' T' || T^{T_0 \cdot J_0} || (l_1 l_2) L S J T \rangle \\
 &= \sum_{\substack{j_1 j_2 \\ j'_1 j'_2}} \sqrt{(1 + \delta_{j'_1 j'_2}) / (1 + \delta_{l'_1 l'_2})} \chi \begin{Bmatrix} l'_1 & \frac{1}{2} & j'_1 \\ l'_2 & \frac{1}{2} & j'_2 \\ L' & S' & J' \end{Bmatrix} \\
 & \times \langle (j'_1 j'_2) J' T' || T^{T_0 \cdot J_0} || (j_1 j_2) J T \rangle \chi \begin{Bmatrix} l_1 & \frac{1}{2} & j_1 \\ l_2 & \frac{1}{2} & j_2 \\ L & S & J \end{Bmatrix} \sqrt{(1 + \delta_{j_1 j_2}) / (1 + \delta_{l_1 l_2})}, \quad (5)
 \end{aligned}$$

where  $\chi\{\}$  is used to denote a unitary 9- $j$  symbol of Hope and Jahn <sup>14)</sup>. In a shell where  $\eta$  quanta are associated with each particle the conversion to SU(3) coupled two-particle states follows from

$$\begin{aligned}
 & \langle (\lambda' \mu') L' S' J' T' || T^{T_0 \cdot J_0} || (\lambda \mu) L S J T \rangle \\
 &= \sum_{\substack{l'_1 l'_2 \\ l_1 l_2}} \sqrt{\frac{1}{2}(1 + \delta_{l'_1 l'_2})} \langle (\eta 0) l'_1; (\eta 0) l'_2 || (\lambda' \mu') \kappa' L' \rangle \\
 & \times \langle (l'_1 l'_2) L' S' J' T' || T^{T_0 \cdot J_0} || (l_1 l_2) L S J T \rangle \langle (\eta 0) l_1; (\eta 0) l_2 || (\lambda \mu) \kappa L \rangle \sqrt{\frac{1}{2}(1 + \delta_{l_1 l_2})}. \quad (6)
 \end{aligned}$$

In eq. (6)  $\langle (\eta 0) l_1; (\eta 0) l_2 || (\lambda \mu) \kappa L \rangle$  is an  $SU(3) \supset R_3^1$  Wigner coefficient <sup>15)</sup>. For the s-d shell,  $\eta = 2$  and  $(\lambda \mu) = (40), (02), (21)$ . Both  $(\lambda \mu) = (40)$  and  $(02)$  are associated with a spatially symmetric coupling of the two particles ( $[f] = [2]$ ) while  $(\lambda \mu) = (21)$  corresponds to an antisymmetric spatial coupling of the two particles ( $[f] = [1^2]$ ). Antisymmetry of the total wave function under particle interchange requires conjugate spin-isospin symmetry; hence, the corresponding SU(4) symmetries are  $[\tilde{f}] = [1^2]$

and  $[\tilde{f}] = [2]$ , respectively. Note that the  $\text{SU}(4) \supset \text{SU}(2) \times \text{SU}(2)$  Wigner coefficient  $\langle [1]_{\frac{1}{2}\frac{1}{2}}; [1]_{\frac{1}{2}\frac{1}{2}} || [\tilde{f}]ST \rangle$  has the value  $+1$  for both  $[\tilde{f}] = [1^2]$  and  $[2]$ , and therefore the two-particle states on the left of eq. (6) are automatically coupled in the  $\text{SU}(4)$  quantum numbers<sup>16</sup>). Since the  $\text{SU}(4)$  labels are redundant, however, they can be suppressed in an unambiguous fashion.

If  $a^+$  and  $a$  are used to denote particle creation and annihilation operators, the irreducible tensor character of  $a^+$  is given by  $a_{(\eta 0)lmism_s m_t}^+ \equiv t(a^+)^{(\eta 0)l; \frac{1}{2}\frac{1}{2}}_{m_l m_s m_t}$ . Using the scalar nature of the number operator

$$N_{0p} = \sum_{lmism_s m_t} a_{(\eta 0)lmism_s m_t}^+ a_{(\eta 0)lmism_s m_t}$$

together with symmetries of the  $\text{SU}(2)$ ,  $\text{SU}(3)$  and  $\text{SU}(4)$  Wigner coefficients

$$\langle jm, j-m | 00 \rangle = (-1)^{j-m} \sqrt{1/(2j+1)},$$

$$\langle (\eta 0)l, (0\eta)l || (00)0 \rangle = (-1)^l \sqrt{(2l+1)/\dim(\eta 0)},$$

$$\langle [1]_{\frac{1}{2}\frac{1}{2}}; [1^3]_{\frac{1}{2}\frac{1}{2}} || [0]00 \rangle = +1,$$

to discover

$$a_{(\eta 0)lmism_s m_t} = (-1)^{\eta+l-m_l+\frac{1}{2}-m_s+\frac{1}{2}-m_t} t(a)^{(0\eta)l, [1^3]_{\frac{1}{2}\frac{1}{2}}}_{-m_l -m_s -m_t},$$

allows one to express the interaction in the form

$$\begin{aligned} T_{M_{T_0} M_{J_0}}^{T_0 J_0} &= \sum_{\substack{[(\lambda' \mu')(\mu \lambda)](\lambda_0 \mu_0) \rho_0 \kappa_0 L_0 \\ [\tilde{f}_0]}} V_{J_0} \{ [(\lambda' \mu')(\mu \lambda)](\lambda_0 \mu_0) \rho_0 \kappa_0 L_0, [\tilde{f}_0] S_0 T_0 \} \\ &\quad \times T^{[(\lambda' \mu')(\mu \lambda)](\lambda_0 \mu_0) \rho_0 \kappa_0 L_0, [\tilde{f}_0] S_0 T_0}_{M_{T_0} M_{J_0}}^{I_0}, \\ V_{J_0} \{ [(\lambda' \mu')(\mu \lambda)](\lambda_0 \mu_0) \rho_0 \kappa_0 L_0; [\tilde{f}_0] S_0 T_0 \} \\ &= -\frac{1}{2} \sum_{\substack{LL' \\ SS' \\ TT'}} (-1)^{l+\mu} \langle (\lambda' \mu') \kappa' L'; (\mu \lambda) \kappa L || (\lambda_0 \mu_0) \kappa_0 L_0 \rangle_{\rho_0} \\ &\quad \times (-1)^{\eta([\tilde{f}]ST)} \langle [\tilde{f}'] S' T'; [\tilde{f}^*] ST || [\tilde{f}_0] S_0 T_0 \rangle \\ &\quad \times \left( \sum_{JJ'} \chi \begin{pmatrix} L' & S' & J' \\ L & S & J \\ L_0 & S_0 & J_0 \end{pmatrix} 1/\sqrt{(2J_0+1)(2T_0+1)} \langle (\lambda' \mu') L' S' J' T' || T^{T_0 J_0} || (\lambda \mu) L S J T \rangle \right), \end{aligned}$$

$$T^{[(\lambda' \mu')(\mu \lambda)](\lambda_0 \mu_0) \rho_0 \kappa_0 L_0, [\tilde{f}_0] S_0 T_0}_{M_{T_0} M_{J_0}}^{J_0} = \begin{array}{c} \begin{array}{cc} [t(a)xt(a)](\lambda', \mu'), [\tilde{f}'] & [t(a)xt(a)](\lambda, \mu), [\tilde{f}^*] \\ \diagdown & \diagup \\ (\lambda_0 \mu_0) \rho_0 \kappa_0 L_0, [\tilde{f}_0] S_0 T_0 & M_{T_0} M_{J_0} \end{array} \end{array} \quad (7)$$

TABLE I  
The SU(3)-SU(4) tensor decomposition of two-body interactions

$[(\lambda'\mu')]$	$(\mu\lambda)$	$(\lambda_0\mu_0)$	$\rho_0$	$\kappa_0$	$L_0$	$[\tilde{\nu}_0]$	$V[\text{MS}]$	$V[\text{OR}]$	$V[\text{BG}]$	$V[\text{YA}]$	$V[3p-1h]$	$V[R]$	$V[l^2 + l \ s]$
<i>Scalar</i>	(40)	(04)	(00)	0		[0]	16.8475	17.2129	16.3551	17.9400	-0.1037	-1.8974	-0.7115
	(02)	(20)	(00)	0		[22]	-4.4324	-4.1533	-2.9433	-2.3149	0.1384	-0.9487	-0.4500
	(21)	(12)	(00)	0		[22]	-1.4307	-0.8225	-0.6134	-0.8459	-0.2169	1.5000	0.7500
	(40)	(04)	(22)	0		[22]	-5.5913	-4.1372	-0.9216	-4.8377	-2.5643	0.7348	-0.9186
	(40)	(04)	(22)	0		[22]	2.0931	1.9462	2.7825	-1.6126	-0.4748	-0.3674	-0.1775
	(40)	(20)	(22)	0		[0]	-3.2338	-3.1313	-2.1368	-2.7938	-0.4070	1.4199	-0.1500
	(40)	(20)	(22)	0		[22]	-0.7330	0.4250	0.4413	0.3605	-0.7389	0.7099	-0.6000
	(02)	(20)	(22)	0		[22]	3.0043	3.0149	2.0369	2.4993	0.5679	-0.3000	-0.0671
	(02)	(20)	(22)	0		[22]	-0.3261	-0.4953	-0.4829	-0.3225	-0.1462	0.1342	-0.0919
	(21)	(12)	(22)	1	0	[22]	-2.1692	-1.8517	-1.7963	-1.7359	-0.4025	0.6614	0.2430
						[22]	0.3659	0.6686	0.4309	0.2240	-1.2047	-0.3307	
						[422]	-1.4987	-1.1757	0.1963	0.8367	0.4782	0.5833	
						[422]	-0.7187	-0.2373	-0.7913	0.2790	-0.2258	-0.2916	
						[422]	-1.0184	-0.9102	0.0741	0.3162	0.0214		
						[0]	0.0214	-0.4296	-0.2991	0.1054	0.0330		
						[22]	1.4304	1.5240	0.4158	1.4171	0.3035		
<i>Vector</i>	(40)	(04)	(60)	0		[22]	-0.0832	0.5313	-0.2381	-0.1054	-0.0699	0.8333	1.7932
	(40)	(02)	(60)	0		[0]	-0.0711	0.0360	0.0074	-0.2003	-0.0865	0.5833	-1.6602
						[22]	0.0887	-0.1155	0.0006	0.0258		-0.2916	-0.6778
	(40)	(04)	(11)	1		[211]	-0.5992	0.0936	0.1512	-0.2389	-0.0239	1.7932	1.6602
	(40)	(12)	(11)	1		[211]	0.7915	-0.2048	-0.0476	0.6445	0.6445	-1.6602	-0.6778
	(02)	(20)	(11)	1		[332]	-0.0002	0.4564	0.0040	-0.0082	-0.0082	1.6602	-0.5639
	(02)	(12)	(11)	1		[211]	0.7472	-0.1472	-0.0510	0.0360	0.0360	-0.5639	-0.6778
						[211]	-0.7186	-0.2951	0.0173	0.0724	0.0724	0.0724	1.6602
						[332]	-0.2566	0.3003	-0.0050	-0.0822	0.0822	-0.0822	-0.5639
	(21)	(12)	(11)	1		[211]	1.0472	0.4135	0.9797	-0.0638	-0.0638	-0.0638	-0.5639
				2		[211]	-0.9495	-1.6410	-0.8715	-0.0095	-0.0095	-0.0095	-0.5639
	(40)	(04)	(33)	1		[211]	0.2703	0.2526	-0.0711	0.4751	0.4751	-0.0095	-0.5639
	(40)	(12)	(33)	1		[211]	-0.5073	-0.3493	0.0150	-0.1485	-0.1485	-0.0095	-0.5639
						[332]	0.0606	0.0683	-0.0044	-0.0528	-0.0528	-0.0528	-0.5639
	(21)	(12)	(33)	1		[211]	0.9082	1.1132	1.3580	0.0863	0.0863	0.0863	0.0863
	(40)	(12)	(52)	1		[211]	-0.0652	0.2176	-0.0073	-0.1229	-0.1229	-0.1229	-0.1229

(40)	(20)	(41)	1	[211]	0.1645	0.1242	0.0060	0.0210
(40)	(12)	(41)	1	[211]	0.3363	0.3475	0.0013	-0.0012
(21)	(20)	(41)	1	[332]	0.0745	-0.1858	-0.0012	0.0154
(21)	(20)	(41)	1	[211]	0.1539	0.1076	0.0108	-0.2995
(21)	(12)	(41)	1	[31]	0.0834	-0.1720	0.0020	0.0526
(21)	(12)	(41)	1	[211]	-0.0365	-0.4089	0.0000	-0.0219
(40)	(12)	(30)	1	[211]	-0.3703	-0.2142	-0.0128	-0.1172
(02)	(12)	(30)	1	[332]	0.2936	0.2832	0.0010	0.2361
(02)	(12)	(30)	1	[211]	-0.1261	-0.6486	-0.0140	-0.1388
(21)	(20)	(30)	1	[332]	0.7146	0.6213	0.0007	0.3363
(21)	(20)	(30)	1	[211]	0.1104	-0.0068	0.0035	0.0764
(21)	(12)	(30)	1	[31]	0.6078	0.0783	-0.0029	0.0309
				[211]	-0.2105	0.2373	-0.0000	-0.0135
				[22]	-0.5332	-0.8754	-0.1199	-0.3846
(40)	(04)	(11)	2	[22]	0.6248	1.0090	0.0918	0.5511
(02)	(20)	(11)	2	[22]	-1.4367	-1.6047	-1.7368	0.1489
(21)	(12)	(11)	1	[422]	1.6560	2.1195	1.7767	-0.1475
(40)	(04)	(22)	2	[422]	1.0205	0.7412	0.6621	-0.1289
		(22)	1	[22]	-2.0914	-1.5191	-1.3568	0.2637
(40)	(20)	(22)	2	[22]	-0.6351	-0.8185	-0.5917	0.0671
(02)	(04)	(22)	2	[22]	1.3603	1.4374	1.2084	-0.1201
(02)	(20)	(22)	2	[22]	-0.6814	-0.6294	-0.5883	0.0534
		(22)	2	[22]	1.3377	1.5297	1.2100	-0.1201
(02)	(20)	(22)	1	[22]	0.3901	0.4768	0.5268	-0.1322
		(22)	2	[22]	-0.7994	-0.9771	-1.0796	0.2708
(21)	(12)	(22)	1	[422]	0.1256	0.0504	-0.0586	0.2094
		(22)	1	[422]	-0.2575	-0.1034	0.1202	-0.4292
		(22)	2	[422]	-0.0537	-0.0484	-0.0222	0.0328
		(22)	2	[422]	0.1100	0.0993	0.0455	-0.0672
(40)	(04)	(33)	2	[22]	0.1079	-0.0914	-0.3667	0.1990
(21)	(12)	(33)	2	[422]	-1.4690	-1.0748	-1.3997	0.1654
(40)	(04)	(44)	1	[22]	-0.6391	-0.7595	-0.6359	0.1269
		(44)	2	[22]	1.2237	1.4543	1.2176	-0.2430
(40)	(20)	(60)	2	[22]	-0.2449	-0.1946	-0.0013	0.0207
(40)	(20)	(41)	2	[22]	-0.0964	0.0071	-0.0017	0.0880
(21)	(12)	(41)	2	[422]	0.5770	0.0774	0.0001	0.0433

Tensor

For entries which are not self-conjugate, the appropriate coefficient for the conjugate partner is simply  $(-1)^{L_0}$  times that listed. For  $L_0 = 2$  the brace is used to indicate the hermitian combination of  $\kappa_0 = 1$  and  $\kappa_0 = 2$ . All units are in MeV with  $\alpha = 0.12$  MeV and  $\beta = 2.8$  MeV for

In eq. (7)  $\rho_0$  is a label used to distinguish multiple occurrences of a given  $(\lambda_0 \mu_0)$  in the direct product  $(\lambda' \mu') \times (\mu \lambda)$  (outer multiplicity label) while  $\kappa_0$  is used to distinguish multiple occurrences of a given  $L_0$  in  $(\lambda_0 \mu_0)$  (inner multiplicity label). The tensor coupling notation follows that of Macfarlane and French<sup>17</sup>). Note that the SU(4) two-particle symmetry labels  $[\tilde{f}']$  and  $[\tilde{f}^*]$  appearing in the SU(4) Wigner coefficient are again suppressed in the tensor since they are uniquely determined by  $(\lambda' \mu')$  and  $(\mu \lambda)$ , respectively. The phase factors appear as a result of conjugation symmetry operations applied to the SU(3) and SU(4) Wigner coefficients associated with the coupling of the annihilation operators.

Table 1 gives results for the tensor decomposition,

$$V = \sum_{\text{all labels}} V\{[(\lambda' \mu')(\mu \lambda)](\lambda_0 \mu_0) \rho_0 \kappa_0 L_0; [\tilde{f}_0] S_0 T_0 = 0\} \times T^{[(\lambda' \mu')(\mu \lambda)](\lambda_0 \mu_0) \rho_0 \kappa_0 L_0, [\tilde{f}_0] S_0 T_0 = 0, J_0 = 0}, \quad (8)$$

of all interactions used in the present calculation. The results were generated using machine codes based on eqs. (5)–(7). The notation can be explained as follows: MS – the Michigan State interaction<sup>4</sup>); OR – the Oak Ridge interaction (K+12FP) [ref. <sup>5</sup>)]; BG – the s-d shell bare  $G$ -matrix elements of Kuo<sup>6</sup>); YA – the pure central interaction of Akiyama *et al.*<sup>7</sup>); 3p-1h – the three-particle-one-hole core renormalization of Kuo<sup>6</sup>). (Both MS and OR include, of course, the Kuo-Brown core renormalization. To remove this in favor of the deformed core renormalization given by eq. (3) we simply subtracted the 3p-1h terms from both MS and OR. The resultant interactions carry the labels KB(MS) and KB(OR) in the present analysis.) All units are in MeV. Also given in the table is the tensor decomposition for  $V_{\text{symmetric}}$  of eq. (2) (labelled by R for renormalization) less the factor  $\frac{1}{2} \chi \hbar \omega \times 10^2 \equiv \bar{\chi}$  which in units of MeV is on the order of  $-1$  (e.g. for  $(\lambda \mu) = (66)$ ,  $\bar{\chi} = -1.55$  whereas for  $(\lambda \mu) = (93)$   $\bar{\chi} = -1.36$ ). And finally, since  $\sum_i l_i^2$  and  $\sum_i l_i \cdot s_i$  can be expressed as two-body operators,

$$\sum_i l_i^2 = (n-1)^{-1} \sum_{i < j} (l_i^2 + l_j^2), \quad (9a)$$

$$\sum_i l_i \cdot s_i = (n-1)^{-1} \sum_{i < j} (l_i \cdot s_i + l_j \cdot s_j), \quad (9b)$$

the tensor decomposition for  $V_{1\text{-body}}$  of eq. (1) is presented in the last column of table 1 (labelled  $l^2 + l \cdot s$ )<sup>†</sup>. The strengths, as shown, correspond to an  $\alpha = 0.12$  MeV and

<sup>†</sup> A simple but powerful check on the calculation can be made by noting that

$$L \cdot S = \left( \sum_i l_i \right) \cdot \left( \sum_j s_j \right) = \sum_{i \neq j} l_i \cdot s_j + \sum_i l_i \cdot s_i = \sum_{i < j} (l_i \cdot s_j + l_j \cdot s_i) + (n-1)^{-1} \sum_{i < j} (l_i \cdot s_i + l_j \cdot s_j),$$

and hence appropriately combining the 2-body tensor decomposition for  $\sum_{i < j} l_i \cdot s_j$  with that for  $\sum_i l_i \cdot s_i$  must yield for the  $n$ -particle system the usual  $\langle L \cdot S \rangle = \frac{1}{2}[J(J+1) - L(L+1) - S(S+1)]$  diagonal matrix elements. This provides a sensitive test on phase consistency between the symmetric-antisymmetric (e.g.  $(\lambda' \mu')(\mu \lambda) = (40)(12)$ ) and antisymmetric-symmetric (e.g.  $(\lambda' \mu')(\mu \lambda) = (21)(20)$ ) cross terms in the calculation. Similar checks can be made by using the complete scalar operator, the space exchange (Majorana) operator, as well as  $L^2$ ,  $S^2$ , and the Casimir operators of SU(3) and SU(4). The latter, however, are all scalar operators and serve only to check symmetric-symmetric (e.g.  $(\lambda' \mu')(\mu \lambda) = (40)(20)$ ) and antisymmetric-antisymmetric (e.g.  $(\lambda' \mu')(\mu \lambda) = (21)(12)$ ) couplings.



Having once decomposed the interactions in terms of an SU(3)-SU(4) irreducible tensor formalism, the calculations can be carried out by making use of standard fractional parentage techniques<sup>18)</sup> for the SU(6)-SU(3) reduction<sup>19)</sup> and programs currently available for calculating SU(3) Wigner and Racah coefficients<sup>20)</sup>. The required SU(4) technology is available in ref.<sup>16)</sup>. In particular, the energy matrix can be calculated using the general expression

$$\begin{aligned} & \langle [f']\alpha'(\lambda'\mu')\kappa'L'S'T'M'_TJ'M'_J|T^{[(\lambda'_2\mu'_2)(\mu_2\lambda_2)]}[(\lambda_0\mu_0)\rho_0\kappa_0L_0;[\tilde{f}_0]S_0T_0;J_0 \\ & \quad M_{T_0}M_{J_0}] \\ & \times |[f]\alpha(\lambda\mu)\kappa LSTMT_JM_J\rangle \\ = & -n(n-1)\langle JM_JJ_0M_{J_0}|J'M'_J\rangle\langle TM_TT_0M_{T_0}|T'M'_T\rangle\chi\left\{\begin{matrix} L & S & J \\ L_0 & S_0 & J_0 \\ L' & S' & J' \end{matrix}\right\} \\ & \times \sum_{\substack{[f^{(n-2)}]_{\alpha_{n-2}} \\ (\lambda_{n-2}\mu_{n-2}) \\ \rho'\rho}} \frac{D[f^{(n-2)}]}{\sqrt{D[f]D[f']}} \langle [f^{(n-2)}]_{\alpha_{n-2}}(\lambda_{n-2}\mu_{n-2}); [f^{(2)'}](\lambda'_2\mu'_2)\rho'\rangle|[f']\alpha'(\lambda'\mu')\rangle \\ & \times \langle [f^{(n-2)}]_{\alpha_{n-2}}(\lambda_{n-2}\mu_{n-2}); [f^{(2)}](\lambda_2\mu_2)\rho\rangle|[f]\alpha(\lambda\mu)\rangle \\ & \times (-1)^{x_1} \sqrt{\frac{d(\lambda\mu)}{d(\lambda_{n-2}\mu_{n-2})}} \sum_{\rho_1} \langle (\lambda\mu)\kappa L; (\lambda_0\mu_0)\kappa_0L_0||(\lambda'\mu')\kappa'L'\rangle_{\rho_1} \\ & \times U((\lambda'\mu')(\mu'_2\lambda'_2)(\lambda\mu)(\lambda_2\mu_2), (\lambda_{n-2}\mu_{n-2})\rho'\rho(\mu_0\lambda_0)\rho_0\rho_1) \\ & \times (-1)^{x_2} \sqrt{\frac{d[\tilde{f}]}{d[f^{(n-2)}]}} \sum_{\rho_2} \langle [\tilde{f}]ST; [\tilde{f}_0]S_0T_0||[\tilde{f}']S'T'\rangle_{\rho_2} \\ & \times U([\tilde{f}'][\tilde{f}^{(2)*}][\tilde{f}][\tilde{f}^{(2)}], [\tilde{f}^{(n-2)}][\tilde{f}_0^*]\rho_2). \quad (10) \end{aligned}$$

In eq. (10),  $[f](= [441] \text{ or } [432])$  labels the irreducible representations of  $SU(6)$  while  $[\tilde{f}](= [1] \text{ or } [221])$  labels the corresponding conjugate irreducible representations of  $SU(4)$ . The  $\langle [f^{(n-2)}] \alpha_{n-2}(\lambda_{n-2} \mu_{n-2}), [f^{(2)}](\lambda_2 \mu_2) \rho \rangle [f] \alpha(\lambda \mu) \rangle$  are two-particle coefficients of fractional parentage which can be generated from the one-particle coefficients of fractional parentage of Akiyama<sup>21)</sup> by using a generalization of the techniques introduced by Elliott *et al.*<sup>18)</sup> for the p-shell  $SU(3) \supset R_3$  and  $SU(4) \supset SU(2) \times SU(2)$  reductions. The  $\rho$ -label in this coefficient is used to distinguish multiple

occurrences of a given  $(\lambda\mu)$  in the direct product  $(\lambda_{n-2}\mu_{n-2}) \times (\lambda_2\mu_2)$ . The fact that a given  $(\lambda\mu)$  may occur more than once in a specific  $[f]$  is denoted by  $\alpha = 1, 2, \dots$ . The two particle symmetries  $[f^{(2)}]$  and hence  $[\tilde{f}^{(2)}]$  are, of course, uniquely specified by the  $(\lambda_2\mu_2)$  of the operator. The appearance of a Wigner coefficient multiplying a recoupling or  $U$ -function in both SU(3)  $(\sum_{\rho_1} \langle (\lambda\mu)\kappa L; (\lambda_0\mu_0)\kappa_0 L_0 | (\lambda'\mu')\kappa' L' \rangle_{\rho_1} U((\lambda'\mu')(\mu_2'\lambda_2')(\lambda\mu)(\lambda_2\mu_2); (\lambda_{n-2})\mu_{n-2})\rho'\rho(\mu_0\lambda_0)\rho_0\rho_1))$  and SU(4)  $(\sum_{\rho_2} \langle [\tilde{f}]ST; [\tilde{f}_0]S_0T_0 | [\tilde{f}']S'T' \rangle_{\rho_2} U([\tilde{f}][\tilde{f}^{(2)'}*][\tilde{f}][\tilde{f}^{(2)}]; [f^{(n-2)}][\tilde{f}_0^*]\rho_2))$  is a result of carrying out the summation over SU(3) and SU(4) subgroup labels in the  $(n-2)$ - and  $(2)$ -particle systems. The multiplicity labels  $\rho_1$  associated with the  $(\lambda\mu) \times (\lambda_0\mu_0) \rightarrow (\lambda'\mu')$  coupling, and  $\rho_2$  associated with the  $[\tilde{f}] \times [\tilde{f}_0] \rightarrow [\tilde{f}']$  coupling, reflect the fact that although a factorization of the matrix element via a generalized Wigner-Eckart theorem is possible, care must be taken to properly account for the outer multiplicities associated with the highest symmetry groups in the factorization. The  $D[f]$  in eq. (10) are dimensionality factors for the symmetric group while  $d(\lambda\mu)$  and  $d[\tilde{f}]$  are dimensionality factors for SU(3) and SU(4), respectively. The phase factors  $\chi_1$  and  $\chi_2$  are given by

$$\chi_1 = \lambda_0 + \mu_0 - \lambda'_2 - \mu'_2 + \lambda_{n-2} + \mu_{n-2} - \lambda - \mu + \rho_{0\max} - \rho,$$

$$\chi_2 = \sigma([\tilde{f}^{(n-2)}]; [\tilde{f}^{(2)'}][\tilde{f}']) + \sigma([\tilde{f}']; [\tilde{f}_0^*][\tilde{f}]),$$

with  $\sigma$  defined by eq. (40) of ref. <sup>16</sup>†.

For the interaction of eq. (1),  $T_0 = M_{T_0} = 0$  and  $J_0 = M_{J_0} = 0$ . However, there exist two-body interactions for which this is not true [e.g. the Coulomb interaction, see ref. <sup>16</sup>]. In addition, eqs. (7) and (10) are also valid for one-body operators (and hence can be used to calculate electromagnetic transition amplitudes for which neither  $T_0$  nor  $J_0$  need be zero) if all  $(n-2)$  labels are replaced by  $(n-1)$  labels (similarly  $(2)$  labels replaced by  $(1)$  labels), the factor  $-\frac{1}{2}$  in eq. (7) is replaced by 1,

† A note of caution is in order: In forming a completely antisymmetric  $n$ -particle wave function from the product of wave functions in separate spaces,

$$\psi([1^n]) = \frac{1}{\sqrt{D[f]}} \sum_{(r)} (-1)^{P(r)} \varphi([f](r)) \chi([\hat{f}](\hat{r})),$$

the phase  $(-1)^{P(r)}$ , which is  $+1$  for  $(r)$  an even permutation or  $-1$  for  $(r)$  an odd permutation of the  $n$  particles, must be included if  $\varphi$  and  $\chi$  transform identically under particle permutation. If, on the other hand,  $\varphi$  and  $\chi$  transform contragradiently with respect to one another under particle permutation, the factor  $(-1)^{P(r)}$  need *not* be included. Compare, for example, the discussion of Hamermesh<sup>22</sup> with that of refs. <sup>18, 23</sup>. The form of eq. (10) is appropriate for the representations of SU(6) and SU(4) transforming contragradiently with respect to one another. It must be modified to include an additional phase  $(-1)^{x+x'}$  ( $\chi = \varphi([f^{(n)}][f^{(n-2)}]) + \varphi([f^{(2)}][0])$  with  $\varphi([f^{(n)}][f^{(n-2)}]) = |\sum_{t>s} f_t^{(n)} - \sum_{t>s} f_s^{(n)}$ ) when in going from the Young tableau  $[f^{(n)}]$  to  $[f^{(n-2)}]$  a box is removed from row  $r$  and  $s$ ) if under particle permutation the representations of SU(6) and SU(4) transform identically. The latter situation arises in attempting to combine the results of refs. <sup>19, 21</sup> with those of ref. <sup>16</sup>. Neglecting to include this additional phase reflects itself in non-hermitian matrices for the symmetry mixing components (e.g.  $(\lambda_2'\mu_2')(\mu_2\lambda_2) = (40)(12)$ ) in the interaction

and the factor  $-n(n-1)$  in eq. (10) is replaced by  $n$ . In this case  $(\lambda'\mu') \rightarrow (20)$  and  $(\mu\lambda) \rightarrow (02)$  are also redundant tensor labels.

Making use of eq. (10), the full matrix for each  $J$  can be generated separately for each of the 63 independent tensors listed in table 1. The resultant matrix for fixed  $J$  and a particular interaction can then be determined by first calculating the multiplicative amplitude for each matrix (e.g.  $V_{\text{total}}\{[(\lambda'\mu')(\mu\lambda)](\lambda_0\mu_0)\rho_0\kappa_0L_0; [\hat{f}_0]S_0T_0 = 0\} = V[l^2 + l \cdot s] + V[MS] - V[3p-1h] + [A + B \min(\lambda, \mu)]\bar{x}V[R]$ ) and then summing appropriately. For the current analysis all diagonalizations and subsequent analyses using the calculated eigenstates were carried out on a PDP-10 processing system.

#### 4. Calculated versus experimental results

The experimentally observed <sup>24</sup>) and calculated energy levels are shown in fig. 1. In terms of the interactions listed in table 1, the notation can be explained as follows:

$$\text{KB(MS)} + \text{R} \rightarrow V_{\text{total}} = V[l^2 + l \cdot s] + V[MS] - V[3p-1h] + [A + B \min(\lambda, \mu)]\bar{x}V[R],$$

$$\text{KB(OR)} + \text{R} \rightarrow V_{\text{total}} = V[l^2 + l \cdot s] + V[\text{OR}] - V[3p-1h] + [A + B \min(\lambda, \mu)]\bar{x}V[R],$$

$$\text{KB(BG)} + \text{R} \rightarrow V_{\text{total}} = V[l^2 + l \cdot s] + V[\text{BG}] + [A + B \min(\lambda, \mu)]\bar{x}V[R],$$

$$\text{SCALAR} + \text{R} \rightarrow V_{\text{total}} = V[l^2 + l \cdot s] + V[\text{YA}] + [A + B \min(\lambda, \mu)]\bar{x}V[R].$$

The results obtained with  $\text{KB(MS)} + \text{R}$  give the best theoretical predictions. The  $K_J$  bands appear to be well developed and compare closely to the experimental results. A percentage analysis of the calculated eigenstates for this case is given in table 2. The members of the ground state  $K_J = \frac{5}{2}$  band are predominantly  $(\lambda\mu) = (66)$ ,  $K_L = 2$  ( $\approx 70\%$ ) and  $(\lambda\mu) = (74)$ ,  $K_L = 2$  ( $\approx 10\%$ ). The first excited  $K_J = \frac{1}{2}$  band is dominated by  $(\lambda\mu) = (66)$ ,  $K_L = 0$  ( $\approx 65\%$ ) and  $(\lambda\mu) = (74)$ ,  $K_L = 0$  ( $\approx 9\%$ ) while the second excited  $K_J = \frac{1}{2}$  band is predominantly  $(\lambda\mu) = (93)$ ,  $K_L = 1$  ( $\approx 60\%$ ). For comparison the percentage analysis of the calculated eigenstates using the  $\text{SCALAR} + \text{R}$  interaction is also presented (values in parentheses). As expected for this interaction, the  $\text{SU}(3)$  and  $\text{SU}(4)$  symmetry breaking is somewhat less pronounced. However, the differences are less than one might expect, since the 2-body part of the  $\text{SCALAR} + \text{R}$  interaction includes only central ( $L_0 = 0$ ) terms. The prediction of Harvey and Sebe for preferred mixing of representations with the same  $\lambda + 2\mu$  ( $\lambda + 2\mu = 18 \rightarrow (66), (47), (28)$ ;  $\lambda + 2\mu = 15 \rightarrow (93), (74), (55)$ ;  $\lambda + 2\mu = 12 \rightarrow (10,1), (82)$ ) appears to be less well verified for  $\text{KB(MS)} + \text{R}$  than for  $\text{SCALAR} + \text{R}$ .

As can be seen from the calculated spectra, the  $\text{KB(OR)} + \text{R}$  interaction yields results similar to those for  $\text{KB(MS)} + \text{R}$  but with a larger splitting between the  $\frac{1}{2} - \frac{3}{2}$  and  $\frac{5}{2} - \frac{7}{2}$  members of the  $K_J = \frac{1}{2}_1$  band. For  $\text{KB(BG)} + \text{R}$  the predicted spectrum is simply more compressed with the  $K_J = \frac{1}{2}_2$  band head pushed up an additional



TABLE 2  
Percentage analysis of calculated eigenstates

[f] ( $\mu$ )	$\frac{1}{2}1$	$\frac{3}{2}1$	$\frac{5}{2}1$	$\frac{1}{2}2$	$\frac{3}{2}2$	$\frac{5}{2}2$	$\frac{1}{2}3$	$\frac{3}{2}3$	$\frac{5}{2}3$	$\frac{1}{2}4$	$\frac{3}{2}4$	$\frac{5}{2}4$
[441] (66)	74.8(73.6)	72.8(72.4)	67.8(74.9)	73.7(75.5)	59.1(70.4)	69.9(71.0)	30.6(59.7)	4.8 (6.0)	18.2(15.5)	8.1 (6.6)	77.5(75.3)	21.3(58.4)
(93)	1.2 (0.7)	2.3 (0.8)	6.1 (1.6)	3.8 (4.1)	15.4 (3.3)	6.2 (5.4)	39.4(16.5)	67.6(68.5)	56.9(59.3)	62.0(66.7)	0.6 (0.3)	49.0(17.8)
(74)	12.5(10.8)	11.7 (9.5)	9.6 (9.5)	9.2 (5.6)	10.4 (4.6)	7.8 (4.3)	10.0 (7.4)	0.1 (0.2)	0.9 (3.1)	1.7 (2.7)	10.4(10.3)	5.1 (2.9)
(82) <sub>1</sub>	0.0 (0.0)	0.0 (0.0)	0.1 (0.0)	0.1 (0.0)	0.4 (0.3)	0.1 (0.5)	0.9 (0.8)	3.0 (3.8)	1.6 (2.0)	2.6 (2.5)	0.0 (0.0)	1.3 (1.0)
(82) <sub>2</sub>	0.2 (0.2)	0.2 (0.2)	0.2 (0.2)	0.0 (0.2)	0.0 (0.0)	0.1 (0.2)	0.0 (0.0)	1.5 (2.0)	0.6 (0.5)	0.1 (2.3)	0.6 (0.4)	0.7 (0.3)
(55) <sub>1</sub>	0.7 (0.6)	0.7 (0.7)	0.8 (0.5)	1.0 (1.2)	1.0 (1.2)	1.2 (1.7)	1.2 (3.5)	0.0 (0.2)	0.1 (2.6)	0.0 (0.2)	0.0 (0.3)	0.6 (1.5)
(55) <sub>2</sub>	0.0 (0.1)	0.1 (0.2)	0.2 (0.2)	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)	0.0 (0.2)	0.0 (0.1)	0.0 (0.2)	0.3 (0.0)	0.1 (0.1)
(28)	0.2 (3.3)	0.6 (4.8)	0.5 (2.0)	0.1 (1.6)	0.4 (6.6)	1.0 (4.9)	0.0 (0.6)	0.0 (0.2)	0.3 (0.8)	0.1 (0.9)	0.2 (2.7)	0.2 (3.1)
(90)	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)
$\Sigma$	89.6(89.3)	88.4(88.6)	85.3(88.9)	87.9(88.7)	86.7(86.4)	86.3(88.0)	82.1(88.5)	77.0(82.9)	78.6(83.9)	74.6(83.9)	89.6(89.3)	78.3(85.1)
[432] (10,1)	0.2 (0.0)	0.3 (0.4)	1.1 (0.0)	0.5 (0.2)	2.2 (0.2)	1.0 (0.3)	6.2 (1.2)	10.6 (6.7)	8.9 (5.5)	11.4 (5.7)	0.1 (0.0)	7.7 (1.5)
(74)	2.9 (1.5)	3.2 (1.5)	3.9 (1.9)	3.6 (2.0)	3.5 (1.6)	3.3 (1.9)	3.3 (2.1)	2.5 (2.7)	2.3 (2.5)	2.8 (2.9)	2.3 (1.3)	4.2 (2.8)
(82) <sub>1</sub>	0.1 (0.0)	0.2 (0.0)	0.8 (0.0)	0.4 (0.2)	1.5 (0.2)	0.8 (0.3)	4.4 (1.0)	8.3 (6.1)	7.0 (4.8)	9.3 (5.6)	0.0 (0.0)	6.2 (1.3)
(82) <sub>2</sub>	0.1 (0.1)	0.1 (0.1)	0.2 (0.0)	0.1 (0.1)	0.2 (0.1)	0.1 (0.1)	0.4 (0.1)	0.3 (0.2)	0.4 (0.2)	0.4 (0.3)	0.0 (0.0)	0.2 (0.1)
(55) <sub>1</sub>	2.9 (1.7)	2.7 (1.7)	2.6 (1.7)	3.2 (2.0)	2.6 (1.8)	2.9 (1.9)	1.4 (1.9)	0.3 (0.2)	0.8 (0.5)	0.4 (0.2)	2.8 (1.7)	1.2 (1.8)
(55) <sub>2</sub>	0.1 (0.5)	0.5 (0.2)	0.6 (0.5)	0.4 (0.4)	0.3 (0.4)	0.4 (0.4)	0.3 (0.4)	0.1 (0.1)	0.1 (0.2)	0.1 (0.1)	0.6 (0.5)	0.2 (0.4)
(28)	0.1 (0.4)	0.1 (0.6)	0.1 (0.1)	0.1 (0.1)	0.1 (1.1)	0.1 (0.5)	0.0 (0.1)	0.1 (0.0)	0.0 (0.1)	0.1 (0.1)	0.1 (0.4)	0.1 (0.5)
(47)	3.7 (6.4)	4.4 (7.0)	5.4 (6.7)	4.0 (6.2)	2.9 (8.3)	5.0 (6.6)	1.6 (4.4)	0.5 (0.7)	1.7 (1.9)	0.7 (1.0)	4.5 (6.7)	1.6 (6.4)
(90)	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)	0.1 (0.0)	0.0 (0.0)	0.2 (0.0)	0.4 (0.4)	0.2 (0.2)	0.3 (0.2)	0.0 (0.0)	0.2 (0.1)
$\Sigma$	101(10.6)	11.5(11.5)	14.7(10.9)	12.3(11.2)	13.4(13.7)	13.6(12.0)	17.8(11.2)	23.1(17.1)	21.4(15.9)	25.5(16.1)	10.4(10.6)	21.6(14.9)

Calculated for eigenstates of the KB(MS) + R and SCALAR + R interactions; the values for SCALAR + R are enclosed in parentheses.

0.5 MeV as compared to KB(MS)+R. In this case the  $J = \frac{3}{2}$  member of the  $K_J = \frac{1}{2}_1$  band and the  $J = \frac{7}{2}$  member of the  $K_J = \frac{1}{2}_2$  band lie below 4 MeV of excitation above the ground state. The calculated spectrum using SCALAR+R interaction shows very strong decoupling effects leading to an inversion of the  $J = \frac{1}{2}$  and  $\frac{3}{2}$  members in both  $K_J = \frac{1}{2}$  bands. [This inversion of the calculated energy levels within the  $K_J = \frac{1}{2}$  bands for the pure central interaction of Akiyama *et al*<sup>7)</sup> frustrated previous attempts by Vergados<sup>26)</sup> and Yoshimi Akiyama and JPD (both unpublished) to recognize the band structure of the calculated eigenstates] Also included in fig. 1 are results for KB(MS)+R with  $\alpha$  and  $\beta$  in  $V_{1\text{-body}}$  set equal to their  $^{17}\text{O}$  values. This is labelled by \*KB(MS)+R. No significant changes are observed in either the spectrum or the structure of the calculated eigenstates. On the far right in fig. 1 is the calculated spectrum for the KB(MS) interaction, i.e., KB(MS)+R *less* the renormalization. The dominant effect of the renormalization can be explained most simply as a shifting of the  $K_J = \frac{1}{2}_2$  band (dominated by  $(\lambda\mu) = (93)$ ) through the  $K_J = \frac{5}{2}$  and  $K_J = \frac{1}{2}_1$  bands (dominated by  $(\lambda\mu) = (66)$  and  $(74)$ ). This is indicated in the figure by lines connecting to those states whose structure is similar to the band head configurations of \*KB(MS)+R. The decoupling inversion of the  $\frac{1}{2}$  and  $\frac{3}{2}$  members of the  $K_J = \frac{1}{2}_2$  band when the renormalization is not present is due to a lesser  $J(J+1)$  strength because of the quadrupole-quadrupole nature of the excluded interaction. Although not shown, results using the bare  $G$ -matrix of Kuo plus the 3p-1h renormalization differ only slightly from those for KB(BG) alone and are similar to the KB (MS) results shown on the far right of fig. 1. This means that the 3p-1h renormalization of Kuo and Brown and the Harvey renormalization as modified in eq. (3) produce quite different effects insofar as the energy spectrum is concerned. It is important to emphasize, however, that  $V_{\text{asymmetric}}$  does not change the structure of the calculated eigenstates in any dramatic fashion.

The dashed levels in fig. 1 are intruder states whose structure in each case is such that they can be clearly identified as band heads for spin-orbit partners of what should be more highly excited configurations. For example, the first dashed  $\frac{3}{2}$  level is a mixture of the  $K_J = \frac{3}{2}$  partners of  $K_J = \frac{1}{2}_2$  (built mainly from the  $K_L = 1$  member of  $(\lambda\mu) = (93)$ ) and  $K_J = \frac{5}{2}$  (built mainly from the  $K_L = 2$  member of  $(\lambda\mu) = (66)$ ). Similarly, the dashed  $\frac{9}{2}$  level is the lower member of the  $K_J$  doublet built from the  $K_L = 4$  member of the  $(66)$  representation. These tell us that the  $K_J$  splitting generated by the interaction is somewhat askew.

As a test of the goodness of  $K_J$  as a band label for the calculated eigenstates, a comparison between the calculated quadrupole moments and those predicted on the basis of a simple rotational model<sup>27)</sup> is given in table 3. The calculated result for the lowest member of each band in  $^{25}\text{Mg}$  was used to fix  $Q_0$ . The results for the  $K_J = \frac{5}{2}$  band are very well reproduced, even down to the sign change associated with the  $J = \frac{9}{2}$  member of the band (this would not be the case for the dashed  $\frac{9}{2}$  level of fig. 1). The results for the  $K_J = \frac{1}{2}$  bands are less convincing but understandable in terms of decoupling and representation mixing effects which are

TABLE 3  
Band structure (quadrupole moments)

$K_J$	$J$	Pure $K_J$ band prediction		Calculated value <sup>a)</sup>	
		$Q/Q_0 = \frac{3K_J^2 - J(J+1)}{(J+1)(2J+3)}$		$^{25}\text{Mg}$	$^{25}\text{Al}$
$\frac{5}{2}$	$\frac{5}{2}$ <sup>a)</sup>	0.232	$(Q_0 = 0.650)$	0.232	0.214
	$\frac{7}{2}$	0.043		0.051	0.061
	$\frac{9}{2}$	-0.059		-0.035	-0.012
$\frac{1}{2}_1$	$\frac{1}{2}$	0	$(Q_0 = 0.675)$	0	
	$\frac{3}{2}$	-0.135		-0.135	-0.126
	$\frac{5}{2}$	-0.193		-0.150	-0.126
	$\frac{7}{2}$	-0.225		-0.244	-0.236
$\frac{1}{2}_2$	$\frac{1}{2}$	0	$(Q_0 = 0.565)$	0	
	$\frac{3}{2}$	-0.113		-0.113	-0.111
	$\frac{5}{2}$	-0.161		-0.085	-0.102

<sup>a)</sup>  $Q_{\text{expt}} = +0.22$ ,  $Q_{\text{calc}} = +0.23$  for  $^{25}\text{Mg}$  ground state with effective charge  $\frac{1}{2}$

expected to be more important for members of the excited bands. Note that the calculated values were obtained using an effective charge of  $\frac{1}{2}$  yielding  $Q_{\text{calc}} = +0.23$  as compared to  $Q_{\text{expt}} = +0.22$  for the ground state of  $^{25}\text{Mg}$ . With an effective charge of  $\frac{1}{3}$  rather than  $\frac{1}{2}$ ,  $Q_{\text{calc}} = +0.19$ .

A more sensitive test of the goodness of  $K_J$  as a band label can be made by comparing the amplitudes for the dominant  $(\lambda\mu)$  component of the calculated eigenstates with predictions for a pure  $K_J$  band having the same SU(3) tensor character <sup>28)</sup>. The coefficients  $a_{\kappa_L K_L}[(\lambda\mu)L]$  in the pure  $K_J$  band expansion,

$$|(\lambda\mu)K_J S J M\rangle = \sum_L \langle L K_L S K_S | J K_J \rangle \sum_{\kappa_L \leq K_L} a_{\kappa_L K_L}[(\lambda\mu)L] |(\lambda\mu)\kappa_L L S J M\rangle, \quad (11)$$

can either be obtained from eqs. (3.45) and (H.12) of ref. <sup>28)</sup> together with results for overlap integrals in ref. <sup>29)</sup> or more directly from the orthonormalization matrix of ref. <sup>15)</sup> as simply

$$a_{\kappa_L K_L}[(\lambda\mu)L] = \frac{1}{N} \begin{cases} 1/O_{K_L K_L} & \kappa_L = K_L \\ O_{\kappa_L K_L} & \kappa_L \neq K_L, \end{cases}$$

$$N = \sum_L \langle L K_L S K_S | J K_J \rangle^2 \langle (\lambda\mu)K_L L | (\lambda\mu)K_L L \rangle. \quad (12)$$

The comparison for the dominant  $(\lambda\mu)$  component in each of the calculated eigenstates is made in table 4. As the quadrupole moment predictions indicate, the components with  $(\lambda\mu) = (66)$  in the ground state band (75 % of the total eigenstate for the ground state) do indeed correspond to a well developed pure  $K_J = \frac{5}{2}$  band. Note that the mixing of  $K'_J > K_J$  bands with the  $K_J$  band (e.g. the  $K'_J = \frac{9}{2}$  mixing in the

TABLE 4  
Band structure (eigenstates)

State $K_J$	Domi- $J$ Percentage of $(4\mu)$ eigenstate	Amplitudes for pure $K_J$ band prediction (Calculated amplitudes renormalized to unity)	
$\frac{1}{2}_2$			
$\frac{1}{2}_2$ (66)	75	$(\begin{smallmatrix} 0.06 \\ 0.11 \end{smallmatrix}) \kappa_L = 0, L = 2\rangle + (\begin{smallmatrix} 0.93 \\ 0.92 \end{smallmatrix}) \kappa_L = 2, L = 2\rangle + (\begin{smallmatrix} -0.36 \\ -0.39 \end{smallmatrix}) \kappa_L = 2, L = 3\rangle$	
$\frac{1}{2}_2$	73	$(\begin{smallmatrix} 0.11 \\ 0.21 \end{smallmatrix}) \kappa_L = 0, L = 4\rangle + (\begin{smallmatrix} 0.41 \\ 0.46 \end{smallmatrix}) \kappa_L = 2, L = 4\rangle + (\begin{smallmatrix} -0.91 \\ -0.86 \end{smallmatrix}) \kappa_L = 2, L = 3\rangle + (\begin{smallmatrix} 0.00 \\ -0.06 \end{smallmatrix}) \kappa_L = 4, L = 4\rangle$	
$\frac{1}{2}_2$	68	$(\begin{smallmatrix} 0.23 \\ 0.39 \end{smallmatrix}) \kappa_L = 0, L = 4\rangle + (\begin{smallmatrix} 0.87 \\ 0.75 \end{smallmatrix}) \kappa_L = 2, L = 4\rangle + (\begin{smallmatrix} -0.44 \\ -0.42 \end{smallmatrix}) \kappa_L = 2, L = 5\rangle + (\begin{smallmatrix} 0.00 \\ 0.00 \end{smallmatrix}) \kappa_L = 4, L = 4\rangle + (\begin{smallmatrix} 0.00 \\ 0.19 \end{smallmatrix}) \kappa_L = 4, L = 5\rangle$	
$\frac{1}{2}_1$			
$\frac{1}{2}_1$ (66)	74	$(\begin{smallmatrix} 1.00 \\ 1.00 \end{smallmatrix}) \kappa_L = 0, L = 0\rangle$	
$\frac{3}{2}_2$	59	$(\begin{smallmatrix} 1.00 \\ 1.00 \end{smallmatrix}) \kappa_L = 0, L = 2\rangle + (\begin{smallmatrix} 0.00 \\ 0.01 \end{smallmatrix}) \kappa_L = 2, L = 2\rangle$	
$\frac{3}{2}_2$	70	$(\begin{smallmatrix} 1.00 \\ 0.98 \end{smallmatrix}) \kappa_L = 0, L = 2\rangle + (\begin{smallmatrix} 0.00 \\ 0.00 \end{smallmatrix}) \kappa_L = 2, L = 2\rangle + (\begin{smallmatrix} 0.00 \\ 0.20 \end{smallmatrix}) \kappa_L = 2, L = 3\rangle$	
$\frac{1}{2}_2$	31	$(\begin{smallmatrix} 1.00 \\ 0.97 \end{smallmatrix}) \kappa_L = 0, L = 4\rangle + (\begin{smallmatrix} 0.00 \\ 0.22 \end{smallmatrix}) \kappa_L = 2, L = 4\rangle + (\begin{smallmatrix} 0.00 \\ 0.03 \end{smallmatrix}) \kappa_L = 4, L = 4\rangle + (\begin{smallmatrix} 0.00 \\ 0.11 \end{smallmatrix}) \kappa_L = 2, L = 3\rangle$	
$\frac{1}{2}_2$			
$\frac{1}{2}_2$ (93)	68	$(\begin{smallmatrix} 1.00 \\ 1.00 \end{smallmatrix}) \kappa_L = 1, L = 1\rangle$	
$\frac{3}{2}_2$	57	$(\begin{smallmatrix} 0.53 \\ 0.84 \end{smallmatrix}) \kappa_L = 1, L = 1\rangle + (\begin{smallmatrix} 0.85 \\ 0.54 \end{smallmatrix}) \kappa_L = 1, L = 2\rangle$	
$\frac{5}{2}_2$	62	$(\begin{smallmatrix} 0.64 \\ 0.97 \end{smallmatrix}) \kappa_L = 1, L = 2\rangle + (\begin{smallmatrix} 0.77 \\ 0.24 \end{smallmatrix}) \kappa_L = 1, L = 3\rangle + (\begin{smallmatrix} 0.00 \\ -0.03 \end{smallmatrix}) \kappa_L = 3, L = 3\rangle$	



$J = \frac{3}{2}$  state identified as a member of the  $K_J = \frac{5}{2}$  band) is readily apparent by noting the nonzero character of the corresponding amplitude factors for  $\kappa_L > K_J$ . For the  $J \geq \frac{5}{2}$  members of the  $K_J = \frac{1}{2}_1$  and for the  $J \geq \frac{3}{2}$  members of the  $K_J = \frac{1}{2}_2$  band the identification of the dominant components of the calculated eigenstates as members of a particular band is less convincing.

TABLE 5  
Reduced electromagnetic transition rates

$J_i$	$J_f$	Band in/out	$B(E2) (e^2 \cdot \text{fm}^4)$			$B(M1) (\mu_N^2)$		
			Chi <sup>a)</sup>	Expt <sup>b)</sup>	SU(3) <sup>c)</sup>	Chi	Expt	SU(3)
$\frac{1}{2}$	$\frac{5}{2}$	out	4.7	3.5	53			
$\frac{3}{2}$	$\frac{5}{2}$	out	1.6	5.2	18	0.22	0.0027	0.0084
	$\frac{3}{2}$	in	10	96	72	0.11	0.045	0.024
$\frac{7}{2}$	$\frac{5}{2}$	in	15	110	136	1.8	0.54	0.39
$\frac{5}{2}'$	$\frac{5}{2}$	out	0.003	2.8	2.2	0.014	0.0036	0.0096
	$\frac{3}{2}$	in	10	150	77			
	$\frac{3}{2}$	in	2.4	22	34	1.6	0.021	0.79
$\frac{1}{2}'$	$\frac{3}{2}$	out	4.8	2.5	4.4			
	$\frac{1}{2}$	out				0.039	0.11	0.22
	$\frac{1}{2}$	out	0.35		7.9	2.7		0.21
$\frac{7}{2}'$	$\frac{3}{2}$	out	0.31	< 1.3	0.02	0.14	< 0.0007	0.0041
	$\frac{3}{2}$	in	9.6	142	77			
	$\frac{3}{2}$	in	1.1	< 690	7.1	0.012	< 0.03	0.023
$\frac{3}{2}'$	$\frac{3}{2}$	out	0.70		0.43	0.29	< 0.02	0.020
	$\frac{1}{2}$	out	1.0		5.4	0.10	< 0.07	0.051
	$\frac{3}{2}$	out	1.6		0.0	0.14	1.2	0.70
$\frac{9}{2}$	$\frac{3}{2}$	in	8.5	2.2	24			
$\frac{7}{2}$	$\frac{3}{2}$	in	7.3	22	109	1.0	0.30	0.61

<sup>a)</sup> Asymmetric ( $\gamma = 27^\circ$ ) model, ref. <sup>30)</sup>

<sup>b)</sup> Litherland *et al*, ref. <sup>3)</sup>.

<sup>c)</sup> Effective charge  $\frac{1}{2}$ .

Table 5 makes a comparison of the calculated reduced electromagnetic transition rates ( $B(E2)$  and  $B(M1)$  values) to experiment and those predicted by Chi for an asymmetric unified model calculation <sup>30)</sup>. The *intra*-band  $B(E2)$  values for the low-lying members of the spectrum are in overall reasonable agreement with experiment. The *inter*-band  $B(E2)$  values, on the other hand, show two discrepancies in the low-lying spectrum. The transitions from the  $J = \frac{1}{2}$  and  $\frac{3}{2}$  ( $K_J = \frac{1}{2}_1$ ) levels to the  $J = \frac{5}{2}$  ( $K_J = \frac{5}{2}$ ) ground state are off by an uncomfortably large amount. This we do not fully understand. Part of the reason, however, is related to the fact that the SU(3) Wigner coefficient which governs the strength of the inter-band transition is not small compared to one ( $\langle (66)\kappa_L = 0, L = 0; (11)\kappa_L = 1, L = 2 | (66)\kappa_L = 2, L = 2 \rangle = [\frac{1}{2} \cdot 29]^{\frac{1}{2}} \approx 0.47$ ). In contrast, however, for the  $J = \frac{1}{2}$  member of the  $K_J = \frac{1}{2}_2$  band the corresponding transition to the ground state is necessarily hindered because the

SU(3) coupling between dominant amplitude factors is unallowed ( $\langle(93)\kappa_L = 1, L = 1; (11)\kappa_L = 1, L = 2|[(66)\kappa_L = 2, L = 2] = 0$ ). Hence, an improper mixing of the two  $K_J = \frac{1}{2}$  bands could, in principle, account for the observed discrepancies.

A comparison of the  $B(M1)$  rates, also given in table 5, shows favorable agreement (at least in comparison to predictions of the asymmetric model) to experiment. The ground state magnetic moment was calculated to be  $-0.68 \mu_N$  whereas experimentally it has been determined to be  $-0.86 \mu_N$ . It is interesting to note that the predictions of the asymmetric model were based on an axially asymmetric deformation of  $\gamma = 27^\circ$ . Simple arguments<sup>25)</sup> based on eq. (4) show that the dominant (66) component in the ground state band corresponds to an intrinsic state with a  $\gamma = 30^\circ$ .

TABLE 6  
Spectroscopic factors for  $^{24}\text{Mg}(d, p)^{25}\text{Mg}$

$K_J$	$J$	Nilsson <sup>a)</sup>	Expt <sup>b)</sup>	SU(3) <sup>c)</sup>
$\frac{5}{2}$	$\frac{5}{2}$	0.18	0.18	0.18
	$\frac{7}{2}$	0		0
	$\frac{9}{2}$	0		0
$\frac{1}{2}_1$	$\frac{1}{2}$	0.24	0.29	0.27
	$\frac{3}{2}$	0.10	0.13	(0.01 $\approx$ 0.03)
	$\frac{5}{2}$	0.04	0.07	(0.05 $\approx$ 0.07)
	$\frac{7}{2}$	0		0
$\frac{1}{2}_2$	$\frac{1}{2}$	0.19	0.11	(0.07 $\approx$ 0.09)
	$\frac{3}{2}$	0.17	0.17	(0.08 $\approx$ 0.10)
	$\frac{5}{2}$	0.00		(0.02 $\approx$ 0.04)
	$\frac{7}{2}$			

<sup>a)</sup>  $|C_J|^2$  for  $\eta = +3$  normalized to 0.18 for ground state SU(3) prediction <sup>3)</sup>.

<sup>b)</sup> Compilation by Endt and Van der Leun <sup>24)</sup>.

<sup>c)</sup> Prediction based on a pure (84) ground state for  $^{24}\text{Mg}$ .

A final comparison between experimental results and theoretical predictions is given in table 6 where spectroscopic factors for the  $^{24}\text{Mg}(d, p)^{25}\text{Mg}$  stripping reaction are quoted. The Nilsson predictions are for a deformation  $\eta = +3$  which is less than that required to obtain a reasonable fit to the energy spectrum <sup>3)</sup>. The calculated results in parentheses are for a range of values as calculated using the different interactions of the current analysis. The only serious discrepancy is for the  $J = \frac{3}{2}$  member of the  $K_J = \frac{1}{2}_1$  band. Again, this we do not fully understand. Note, however, that the predictions are based on the assumption of a pure  $(\lambda\mu) = (84)$  ground state for  $^{24}\text{Mg}$ . Since this is only valid to approximately 73 % amplitude squared of the wave function <sup>5)</sup>, significant discrepancies may be expected for spectroscopic factors which derive their strengths (or lack thereof) from coherent effects. Since this is the situation for those values in table 6 which are enclosed in parentheses, the results may be inconclusive.

### 5. Concluding remarks

The successes of the current calculation depend to a great extent upon the validity of using  $V_{\text{asymmetric}}$  of eq. (3) as a proper renormalization of the interaction. Empirically, insufficient examples exist (namely one) to fully justify its inclusion. This we hope to rectify. Nevertheless, the structure of the calculated eigenstates (particularly members of the  $K_J = \frac{5}{2}$  ground state band) can in no way deviate significantly from the present determination without risking serious experimental-theoretical impasses. For example, without the renormalization, the (93) representation dominates the low-lying configurations. And if this were to be a correct description, we know of no simple way to generate a  $J = \frac{5}{2}$  ground state having a positive quadrupole moment of the right order of magnitude.

As already pointed out, however, there may indeed be insufficient mixing between the (66) and (93) representations to adequately reproduce observations related to the  $K_J = \frac{1}{2}$  bands. If additional mixing is required, it can only be generated directly for the  $J = \frac{1}{2}$  states through vector ( $L_0 = 1$ ) components in the residual interaction with  $(\lambda_0 \mu_0) = (33)$  (For the (66) representation  $J = \frac{1}{2}$  implies  $L = 0$  whereas for (93) it implies  $L = 1$  and hence direct mixing can only occur for  $L_0 = 1$ ; but the strongest candidate,  $(\lambda_0 \mu_0) = (11)$ , does not couple (66) to (93).) A more plausible conclusion is that the  $K_J$  splitting, although already large, is still inadequately splitting the  $K_J = \frac{5}{2}$  and  $\frac{1}{2}_1$  bands. Increasing this splitting while decreasing  $B$  in eq. (3) could lead to more nearly degenerate  $J = \frac{1}{2}$  levels in zeroth order forcing greater mixing through relatively small off-diagonal elements in the diagonalization process. (For comparison, note from table 2 the differences in the (66) and (93) mixing for the  $J = \frac{1}{2}$  and  $J = \frac{3}{2}$  members of the  $K_J = \frac{1}{2}$  bands.) Additional  $K_J$  splitting of this type may be available by increasing the strengths of the spatially antisymmetric part  $[(\lambda' \mu')(\mu \lambda) = (40)(12) \text{ and } (02)(12)]$  of the interaction<sup>31,32</sup>.

Additional coherence may, of course, be gained by expanding the basis. In particular, the [4311]: (74), (82) and the [4211]: (82) representations should be included on the basis of the (74) and (82) mixing observed in the present calculation (15 % for (74) in the ground state and 13 % for (82) in the second excited  $\frac{1}{2}$  level). There appears, however, to be no good reason to include additional representations of  $\text{SU}(3)$ . One thing is clear; namely, that sensitive tests such as  $B(E2)$  rates and spectroscopic factors are a necessary part of any final test of the validity of calculated eigenfunctions.

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