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Shell-model calculations in the sd shell I. Energy spectra

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Abstract. Shell-model calculations have been performed for a number of nuclei in the sd shell to obtain binding energies and energy spectra. The realistic interactions of Kuo, and Elliott *et al*, and the empirically determined matrix elements of Preedom and Wildenthal were used in the full sd shell basis. Comparison with experiment shows that the Preedom–Wildenthal interaction works well in the lower part of the shell, whereas the other two give rise to shifts of whole rotational bands in most nuclei.

1. Introduction

This paper is the first in a series reporting results obtained from untruncated shell-model calculations in the nuclear sd shell. We present here energy spectra for a considerable number of nuclei, mainly with masses between 22 and 34. Calculations for other nuclei, especially masses 27 and 29 and the exotic nuclei, and a description of other properties, such as transition rates, will be published in subsequent papers of this series.

By 'untruncated' we mean that an inert core of 16 particles is assumed, and the remaining nucleons occupy the $d_{5/2}$, $s_{1/2}$ and $d_{3/2}$ subshells with no further restriction beyond the requirements of the Pauli principle. Untruncated calculations have previously been reported for $A \leqslant 22$ (Halbert *et al* 1971), for $A \geqslant 34$ (Wildenthal *et al* 1971a) and for a few nuclei in the middle of the shell (Whitehead and Watt 1972, Cole *et al* 1973) In other calculations in the range $23 \leqslant A \leqslant 33$ (McGrory and Wildenthal 1971, Wildenthal *et al* 1971b, Wildenthal and McGrory 1973, de Voigt and Wildenthal 1973, Robertson and Wildenthal 1973) restrictions, sometimes severe, were imposed on the subshell occupancies to reduce the matrices involved to dimensions suitable for conventional methods of calculation (French *et al* 1969). The present work uses the methods of Whitehead (1972) which can handle larger calculations.

An important reason for doing large basis calculations, despite their difficulty, is that we thus minimize the constraining effects of truncation, which tend to mask effects arising from the interaction employed. Also, it is possible to use the same interaction consistently throughout the shell, thus displaying possible systematic trends, and allowing the calculation of observables involving more than one nucleus, such as β-decay rates and spectroscopic factors, in a consistent manner.

One of the most widely used two-body interactions for sd shell calculations is that produced by Kuo (1967) which includes approximate corrections for the neglect of configurations outside the sd shell. This paper extends the untruncated calculations of energy spectra with this interaction to several more nuclei in the middle of the shell.

The more recently introduced Sussex interaction (Elliott *et al* 1968, Sanderson *et al* to be published) has also been employed to produce spectra for nuclei up to mass 24. Sanderson *et al* have modified the original Sussex matrix elements by including short-range repulsion in order to give better saturation properties. Both one- and two-body parts of this interaction are mass dependent.

An effective interaction which has been particularly successful for $A \leqslant 22$ is that derived by Preedom and Wildenthal (1972). This was obtained by modifying the Kuo interaction so as to obtain better fits to selected energy levels for $18 \leqslant A \leqslant 22$. The main changes are in matrix elements which do not involve $d_{3/2}$ particles. Untruncated calculations with this interaction are presented here for a number of nuclei in the middle of the shell.

The single-particle energies used with the two-body parts of the Kuo interaction and that of Preedom and Wildenthal (denoted by PW) are the experimental energies from ^{17}O, namely: $-4{\cdot}15$ MeV ($d_{5/2}$), $-3{\cdot}28$ MeV ($s_{1/2}$) and $0{\cdot}93$ MeV ($d_{3/2}$). For calculations with the Sussex interaction the appropriate A-dependent corrections (E A Sanderson private communication) were applied to these values. The matrix elements corresponding to an oscillator parameter value of $b = 1{\cdot}8$ were used, although the Sussex group now prefer a value closer to 2·0 (J P Elliott, private communication).

2. Results

2.1. Binding energies

Table 1 gives the experimental ground-state binding energies, relative to ^{16}O, for various sd shell nuclei of interest here. These were obtained from the mass excess tables of Endt and Van der Leun (1973), with Coulomb corrections applied as in Halbert *et al* (1971). Columns 3 to 5 show the deviations (calculated quantity − experimental value) produced by the various interactions used in our calculations. The overbinding of the Kuo interaction is seen to increase quite rapidly with the number of valence particles; on the other hand the PW interaction gives rise to relatively small errors throughout the range of nuclei investigated. The Sussex interaction underbinds consistently, but not too badly for the cases studied.

2.2. Energy spectra

Figures 1 to 19 show the energy spectra for the nuclei under consideration. Spectra calculated with the Kuo and PW interactions for $A \leqslant 22$ are included here to provide a comparison with the Sussex interaction which is here used for the first time in a large-scale investigation. In the experimental spectra all known or possible positive-parity states below the highest shown have been included. The angular momentum labels give J for even-A nuclei and $2J$ for odd-A nuclei. Brackets around a spin or parity indicate that the assignment is tentative; an assignment such as 5(3) means that the spin is probably 5, but 3 is not completely ruled out. The absence of a parity assignment indicates a positive-parity state, and an asterisk means that the parity is unknown. In the calculated spectra all levels below the highest shown are included unless otherwise stated. Two sets of identification labels against one level indicate a close pair of states. Where the lowest calculated state does not correspond to the known ground state the various spectra are arbitrarily aligned for convenience.

Results for individual nuclei are discussed in the relevant subsection.

Table 1. Binding energies for some sd shell nuclei. For details see text. Where the spin of the calculated ground state differs from the observed spin J_0 (cases marked with an asterisk) the calculated binding energy of the lowest state with $J = J_0$ has been given. All energies are in MeV

A	T	Binding energy (experiment)	Error in binding energy		
			Kuo	PW	Sussex
19	$\frac{1}{2}$	23·79	0·68	0·10	−1·72
	$\frac{3}{2}$	16·15	0·24*	0·08	−1·55*
20	0	40·71	0·90	−0·10	−3·98
	1	30·35	1·13	0·30	−1·47
21	$\frac{1}{2}$	47·46	1·79	−0·01	−2·95
	$\frac{3}{2}$	38·45	1·45*	0·01	−1·88*
22	0	58·52	1·93*	−0·07	−3·38*
	1	57·83	2·72	−0·05	−3·40
23	$\frac{1}{2}$	70·97	3·66	0·00	−3·47
	$\frac{3}{2}$	63·02	2·86*	−0·01	−2·77*
24	0	87·51	5·91	0·26	−4·06
	1	77·85	3·96*	0·05	−3·14*
25	$\frac{1}{2}$	94·84	6·85*	0·52	
	$\frac{3}{2}$	86·93	6·42*	0·59	
26	0	106·21	7·74*	0·84	
	1	105·97	9·59		
28	0	136·48	16·70		
	1	127·08	14·40*	1·78	
30	0	156·35	22·55		
	1	155·70	21·66		
31	$\frac{1}{2}$	168·74	25·83		
	$\frac{3}{2}$	162·16	24·64*		
32	0	183·95	31·25		
	1	176·80	29·64*	2·27*	
33	$\frac{1}{2}$	192·67	34·64*	2·70	
	$\frac{3}{2}$	186·70	34·71	2·39	

2.2.1. ^{19}F (*figure 1*). Some levels are missing from the Kuo and PW spectra, notably $\frac{3}{2}^+$ levels near 4·0 and 5·5 MeV. These are almost certainly 'interloper' states arising from configurations outside our sd shell space.

2.2.2. ^{19}O (*figure 2*). The PW spectrum fits the data well, at least below 4 MeV; above this the experimental level scheme is not sufficiently well known. A second $\frac{9}{2}^+$ state is predicted near 5·3 MeV (corresponding states occur in the other calculated spectra). The Kuo spectrum is generally similar except that the order of the ground and first excited states are reversed and the level spacings are in less good agreement with experiment.

2.2.3. ^{20}Ne (*figure 3*). Both PW and Kuo agree well with experiment, except that near 7 MeV there are two 0^+ and two 2^+ states experimentally but only one of each in the calculated spectra. Some higher states have been calculated, including an 8^+ state at 11·76 MeV (PW) and 12·55 MeV (Kuo) corresponding to the observed 11·95 MeV level. More extensive calculations of the spectrum of ^{20}Ne, including various degrees of

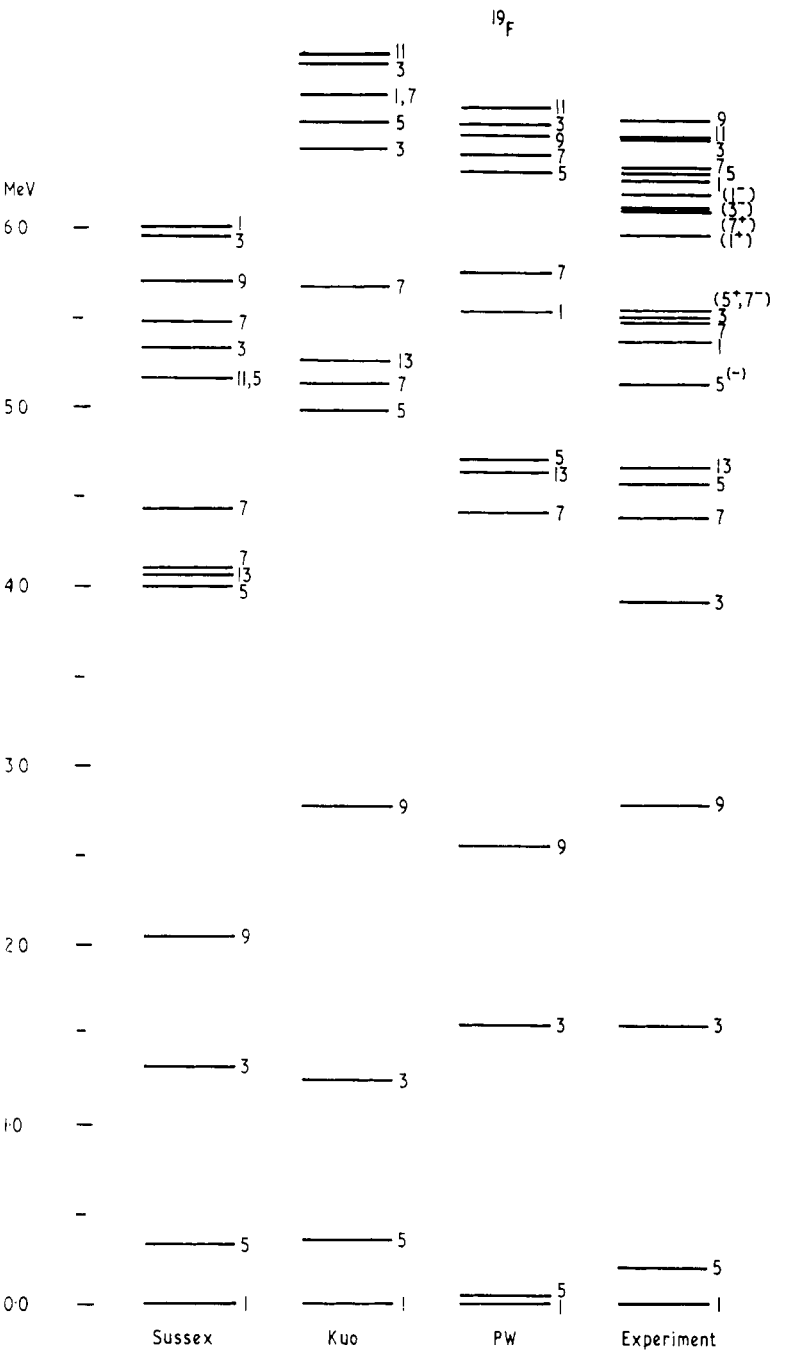

Figure 1. Spectra for ^{19}F. For the notation used in this and subsequent figures see text. The experimental data are from Ajzenberg-Selove (1972) and Bingham *et al* (1971).

core breaking, have been reported by Irvine *et al* (1973) and Engeland and Strottman (1973).

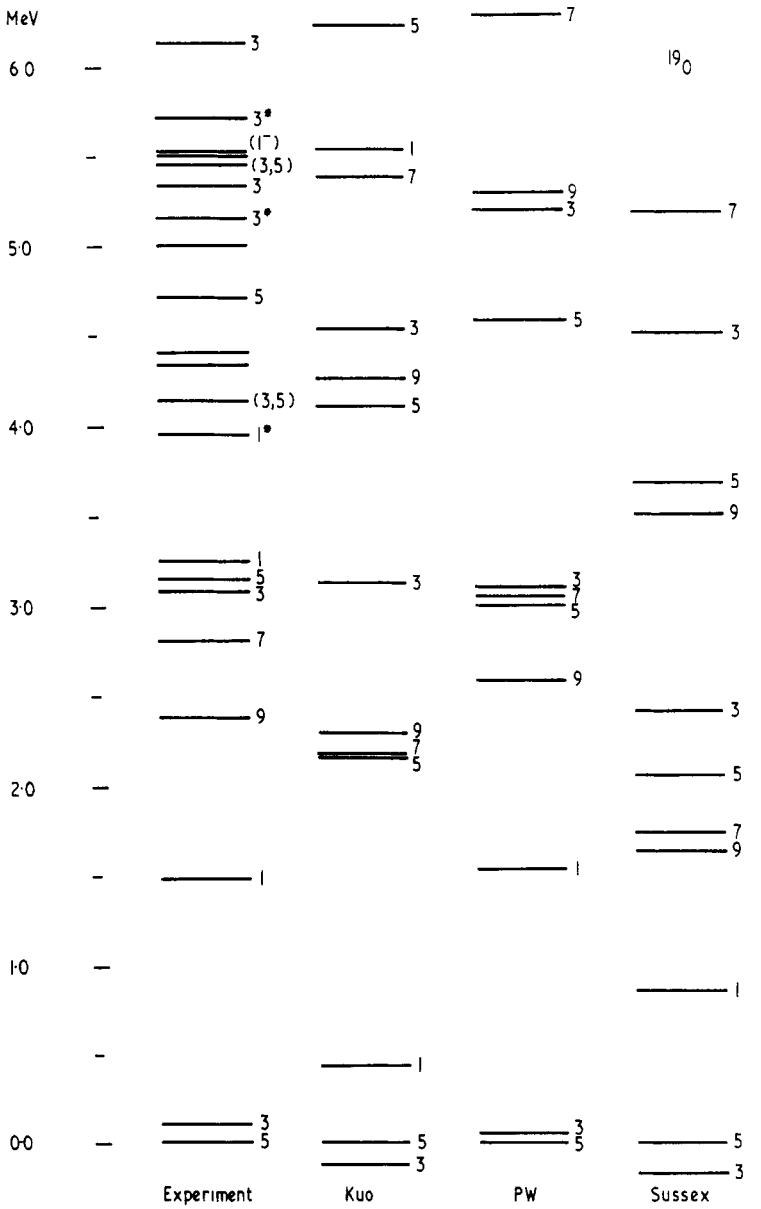

Figure 2. Spectra for ^{19}O. The experimental data are from Ajzenberg-Selove (1972), Wiza and Fortune (1973), Donoghue (1973), Crozier *et al* (1972) and Hibou *et al* (1971).

2.2.4: ^{20}F (*figure 4*). More experimental data are required before comparison can be made, although the known levels below 2·5 MeV are well described by PW. In the Kuo spectrum several states come out too low in energy, causing the order of the low-lying 4^+ and 1^+ levels to be reversed.

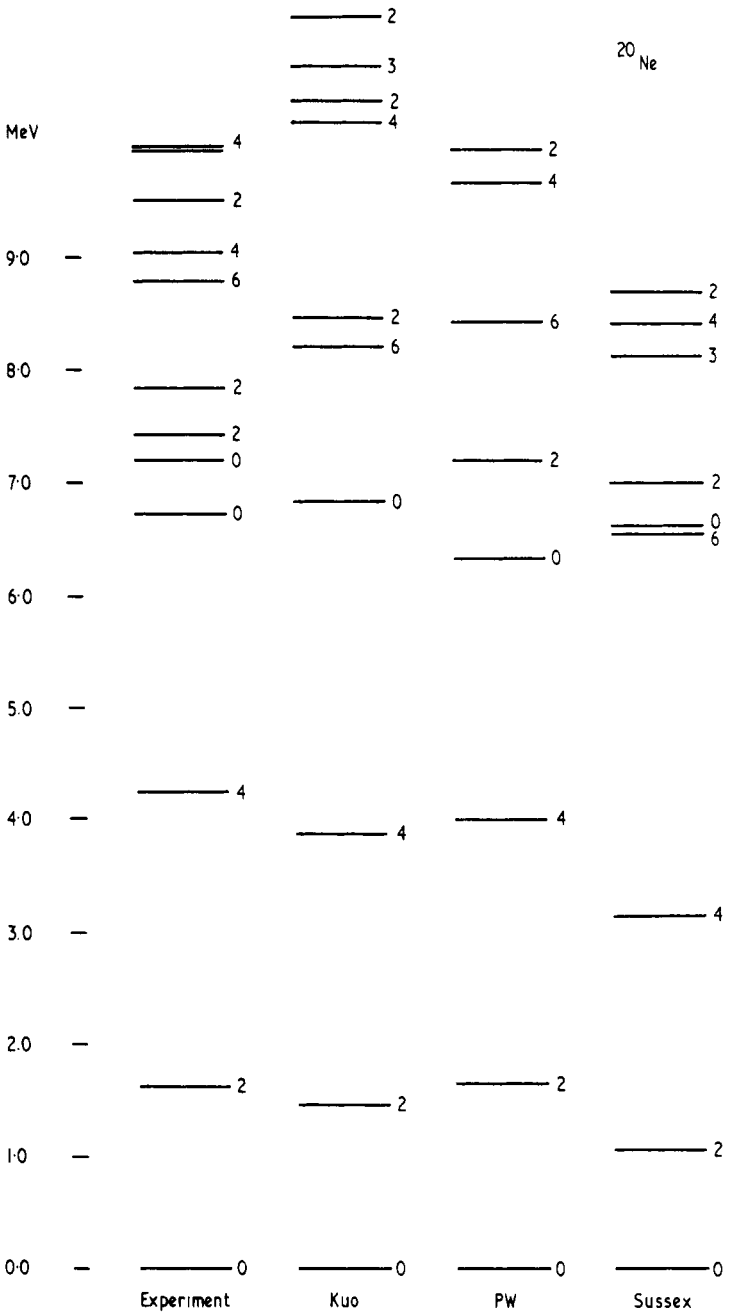

Figure 3. Spectra for ^{20}Ne. The experimental data are from Ajzenberg-Selove (1972).

2.2.5. ^{21}Na–^{21}Ne (*figure 5*). In the Kuo spectrum a $\frac{1}{2}^+$, a $\frac{3}{2}^+$ and a second $\frac{1}{2}^+$ level are depressed about 1 MeV, although the ground-state band is well described. Excellent agreement for all levels results from shifting the calculated $\frac{1}{2}^+$ bands up 0·75 MeV and the $\frac{5}{2}^+$ band (based on the level at 4·33 MeV) down 0·75 MeV, and assuming the band structure given by Rolfs *et al* (1972).

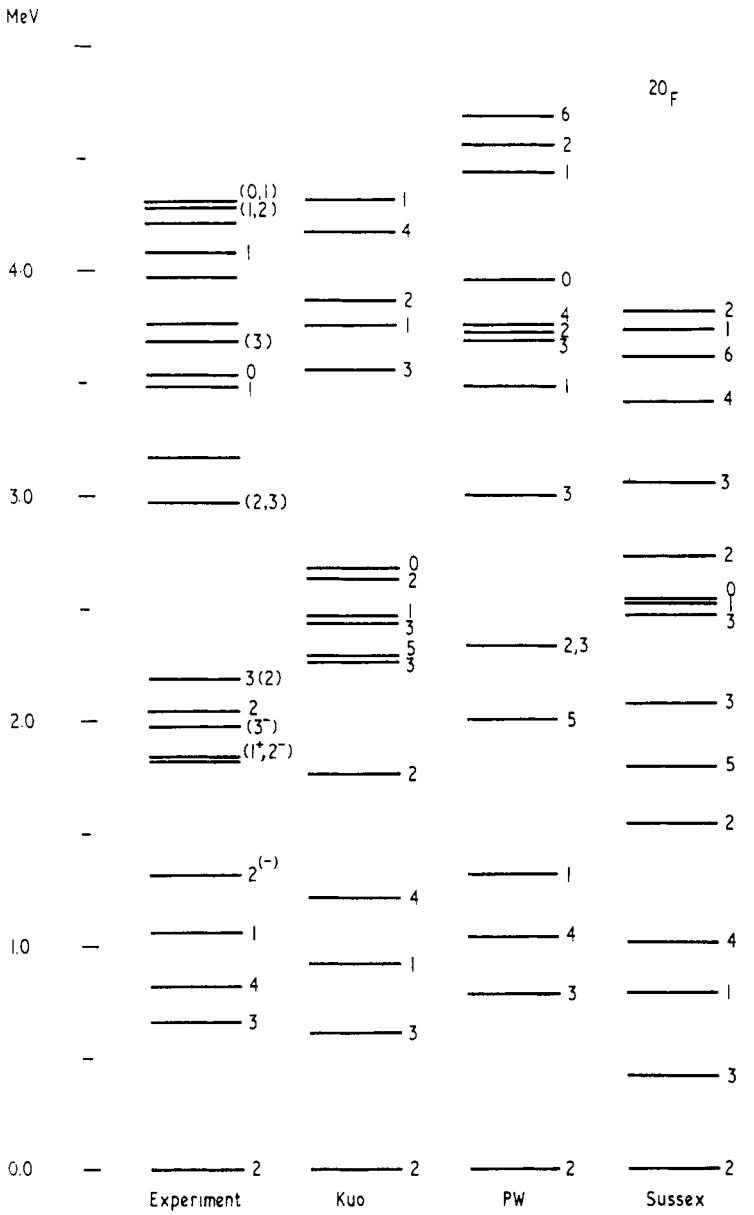

Figure 4. Spectra for ^{20}F. The experimental data are from Ajzenberg-Selove (1972), Hardy and Lee (1973) and Fortune *et al* (1972).

2.2.6. ^{21}F (*figure 6*). The spins of only two states have been uniquely determined experimentally, so no real comparison can be made with the calculations. A $\frac{9}{2}^+$ state predicted near 2 MeV has not been observed. In the Kuo spectrum the ground and first excited states are inverted and several other states are obviously too low.

2.2.7. ^{22}Na (*figure 7*). Below 4 MeV the PW calculation gives good agreement with experiment, except that an extra 2^+ level is predicted near 3 MeV. The ground-state

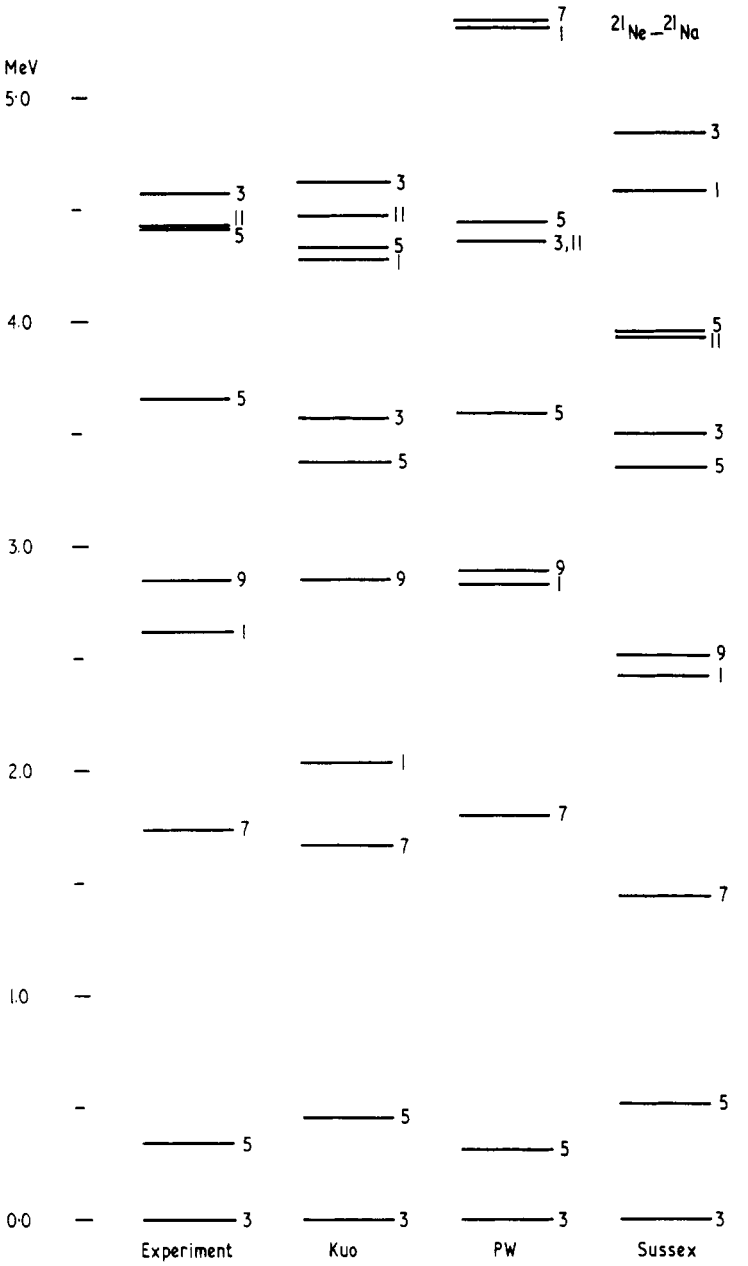

Figure 5. Spectra for the $A = 21$, $T = \frac{1}{2}$ system. The experimental spectrum is the average of data for ^{21}Na and ^{21}Ne from Endt and Van der Leun (1973).

band produced by the Kuo interaction fits the experimental band well, but most other levels are relatively too low in energy causing the counterpart of the observed first excited state to become the ground state of the calculated spectrum.

2.2.8. ^{22}Ne *(figure 8).* Again the ground-state band is well described in the Kuo spectrum, but many other levels fall approximately 1 MeV below their observed positions.

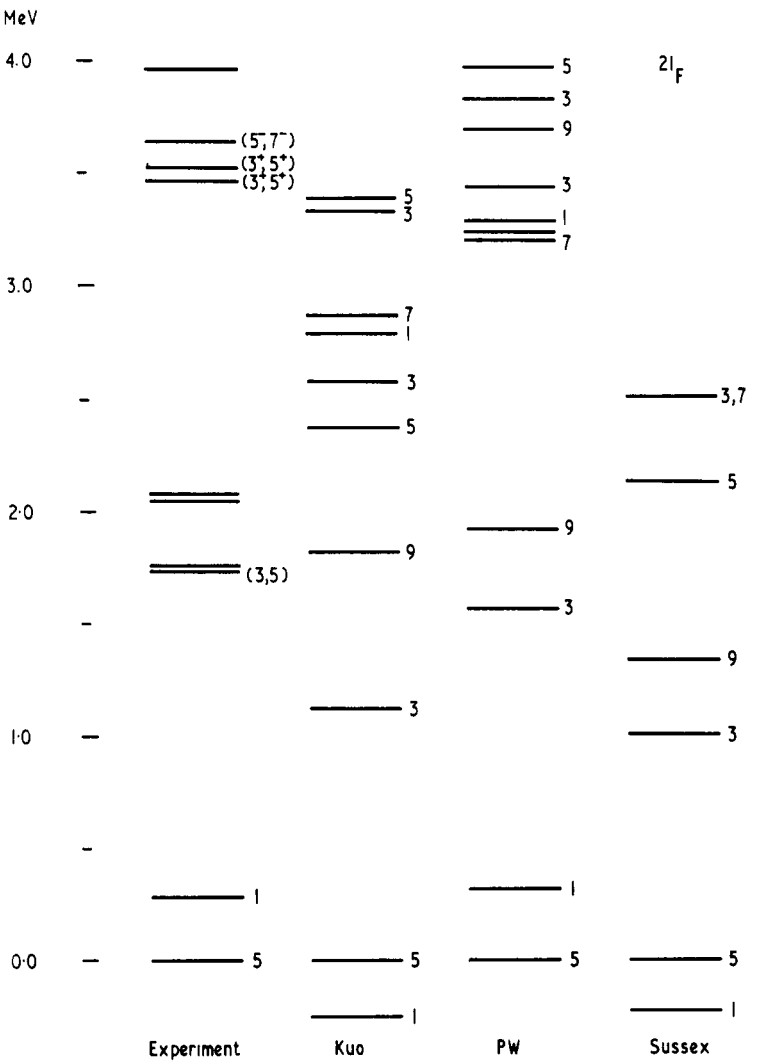

Figure 6. Spectra for ^{21}F. The experimental data are from Endt and Van der Leun (1973) and Benenson *et al* (1973).

2.2.9. ^{23}*Na* (*figure 9*). The PW interaction describes the ground-state band well, although, yet again, other levels are depressed by about 0·5 MeV. The same interaction was used for this nucleus by McGrory and Wildenthal (1971) in a truncated space in which no more than four particles were allowed outside the $d_{5/2}$ shell and no more than two could occupy the $d_{3/2}$ shell. This produced a slightly compressed but otherwise very reasonable looking spectrum, which illustrates once again the dangers of truncation. The Kuo interaction also gives a good fit to the ground-state band, but all other calculated states are 2 MeV or more lower than the observed levels. Indeed, very good agreement may be obtained by raising all but the ground-state band by 2 MeV (see figure 3 of Cole *et al* 1973).

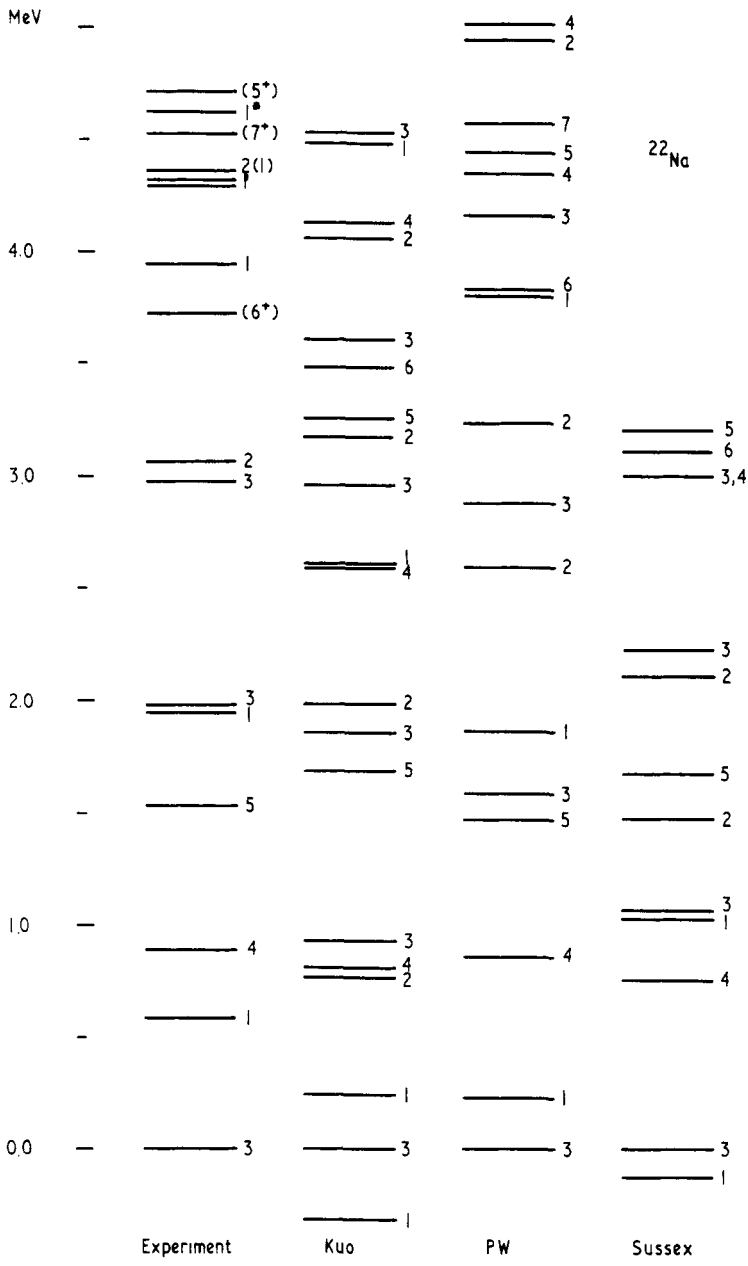

Figure 7. Spectra for ^{22}Na. The experimental data are from Endt and Van de Leun (1973) and Del Campo *et al* (1973).

2.2.10. ^{23}*Ne* (*figure 10*). The experimental spectrum for ^{23}Ne still contains many levels of undetermined spin, and more data are required. In the PW level scheme the order of the probable $\frac{3}{2}^+$ and $\frac{7}{2}^+$ states is reversed. Comparison with the data suggests that the spin of the state seen at 2·31 MeV is $\frac{5}{2}^+$, and that of the 2·52 MeV state is $\frac{9}{2}^+$. The Kuo interaction produces the wrong ground state. It is difficult to identify levels in

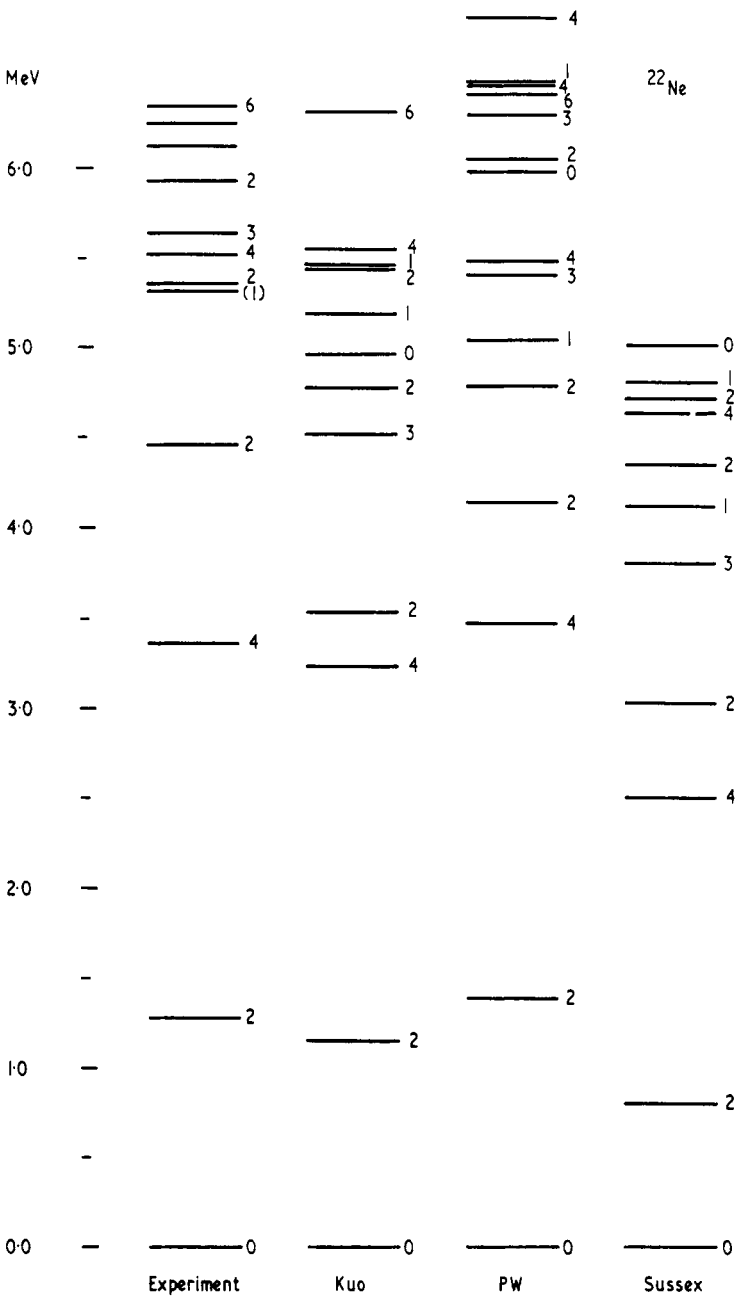

Figure 8. Spectra for ^{22}Ne. The experimental data are from Endt and Van der Leun (1973).

the Kuo spectrum with those in the PW spectrum because of the high density of states in the former. Obviously many levels are coming out too low relative to the ground state. Reasonable agreement can be obtained by lowering an assumed $K = \frac{5}{2}^+$ band by about 2 MeV relative to the remaining levels, as in the spectrum marked Kuo + shift.

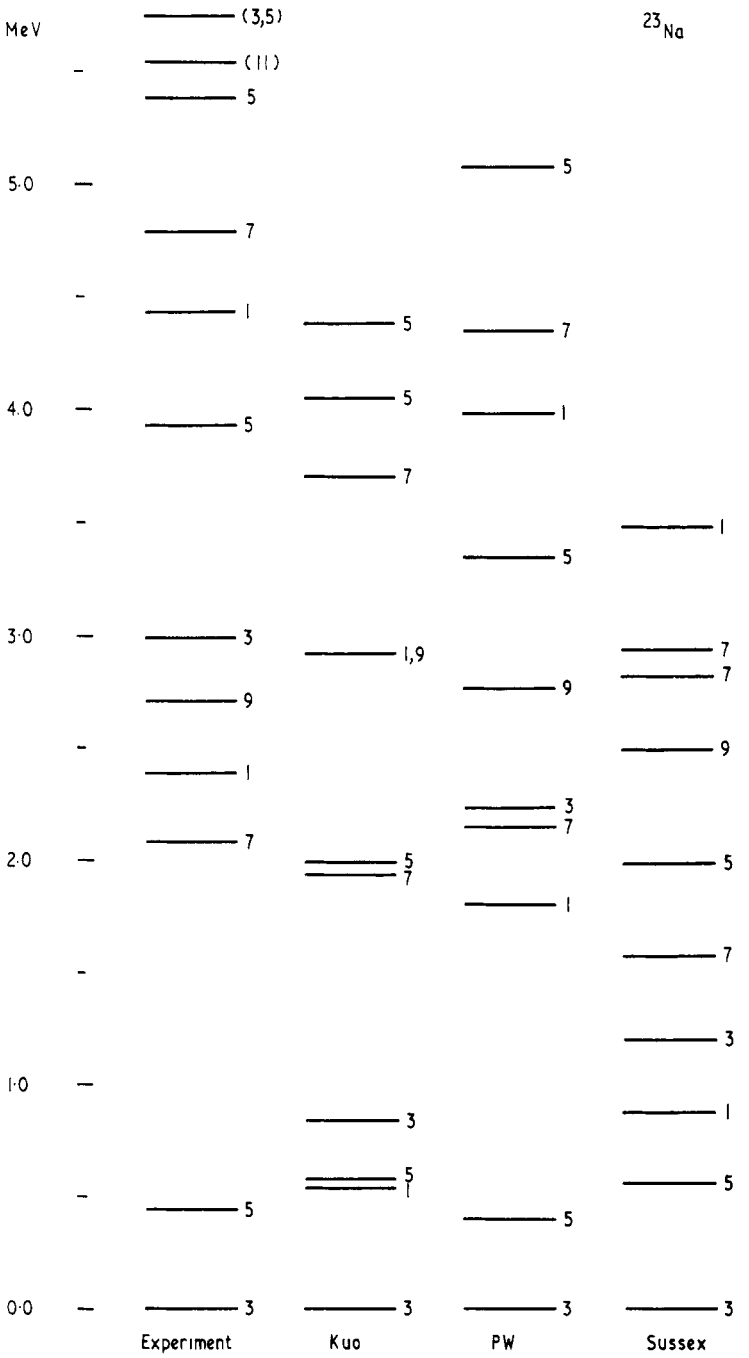

Figure 9. Spectra for ^{23}Na. The experimental data are from Endt and Van der Leun (1973), Meyer and Smit (1973) and Nelson and Roberson (1972).

2.2.11. ^{24}*Mg* (*figure 11*). In common with most interactions Kuo predicts a $K = 2$ band at about 1·5 MeV below its observed position. Also the first excited 0^+ state is found to be 1·2 MeV too high. The fit obtained with the PW interaction is better in

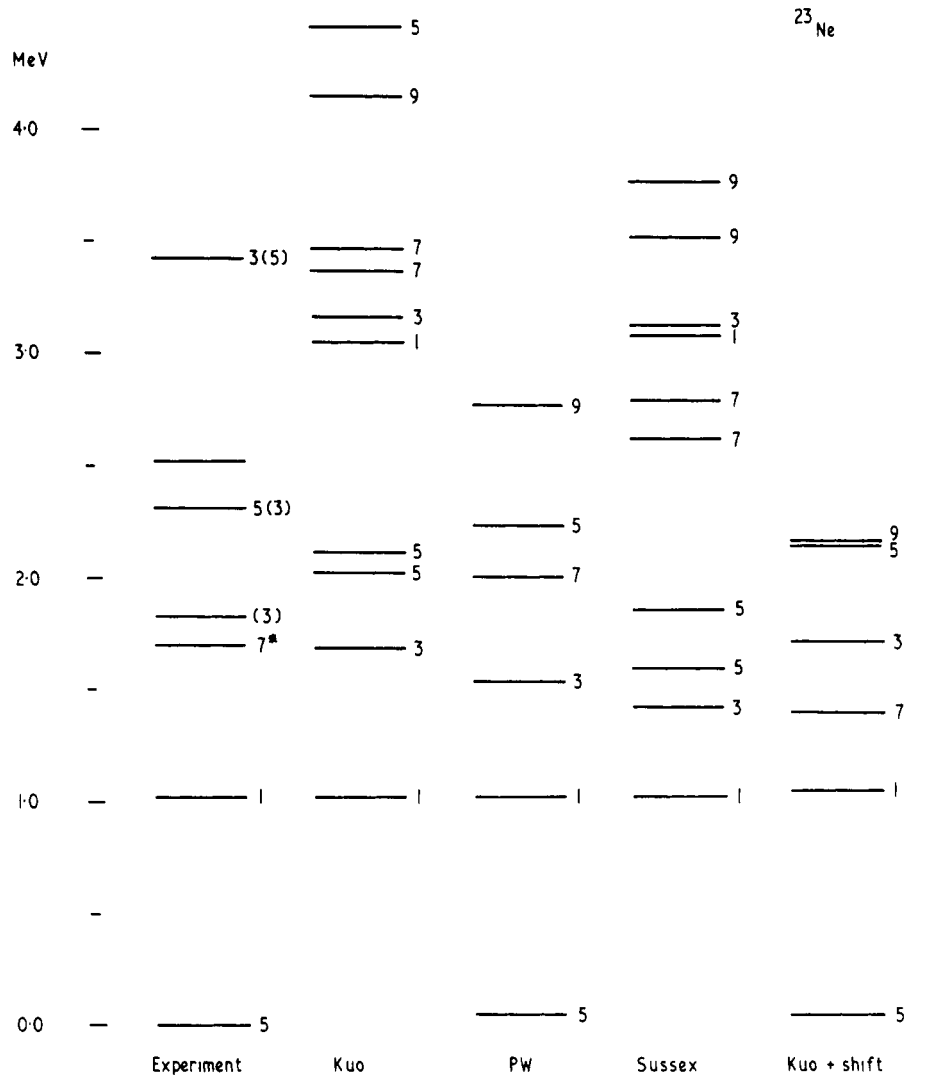

Figure 10. Spectra for ^{23}Ne. The experimental data are from Endt and Van der Leun (1973).

that the excited band is depressed by only 0·5 MeV, but the 0^+ state is still too high. In the truncated calculation of McGrory and Wildenthal (1971) the positions of the first few states of both $K = 0$ and $K = 2$ bands are accurately given, but above 6·5 MeV the agreement is poor.

2.2.12. ^{24}*Na* (*figure 12*). The Kuo calculation for this nucleus has been discussed by Cole *et al* (1973); the 4^+ ground state appears as the eighth excited state in the calculated spectrum, and there is no 5^+ state in the range of excitation investigated. The PW calculation does predict the correct ground-state spin, but all the other levels are too low relative to the 4^+ and 5^+. The overall fit to the data is worse than usual with this interaction. More experimental work is required on this nucleus.

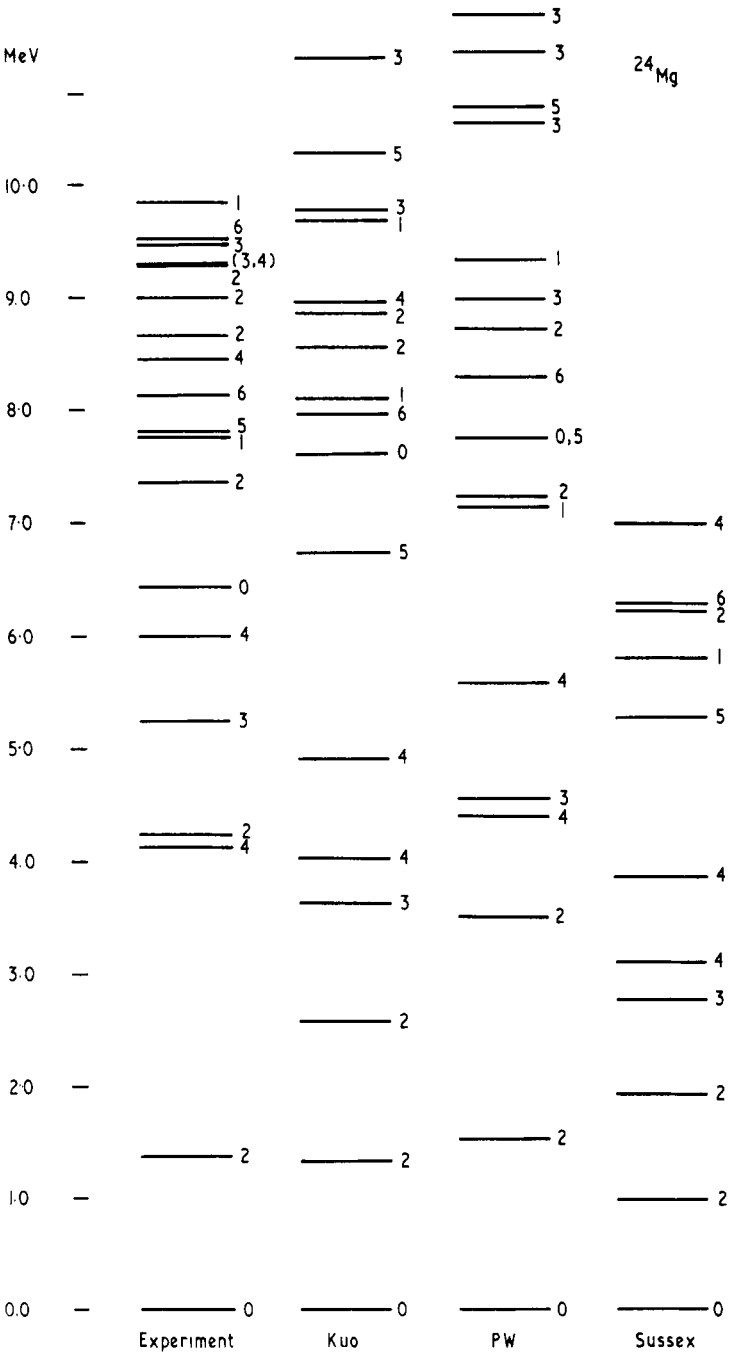

Figure 11. Spectra for ^{24}Mg. No even spin states have been shown above 8·72 and 8·96 MeV respectively in the PW and Kuo calculations. The data are from Endt and Van der Leun (1973).

2.2.13. ^{25}*Na* (*figure 13*). The PW interaction gives a reasonable fit to the known data, predicting a $\frac{9}{2}^+$ state near 2·75 MeV and confirming that the first excited state has

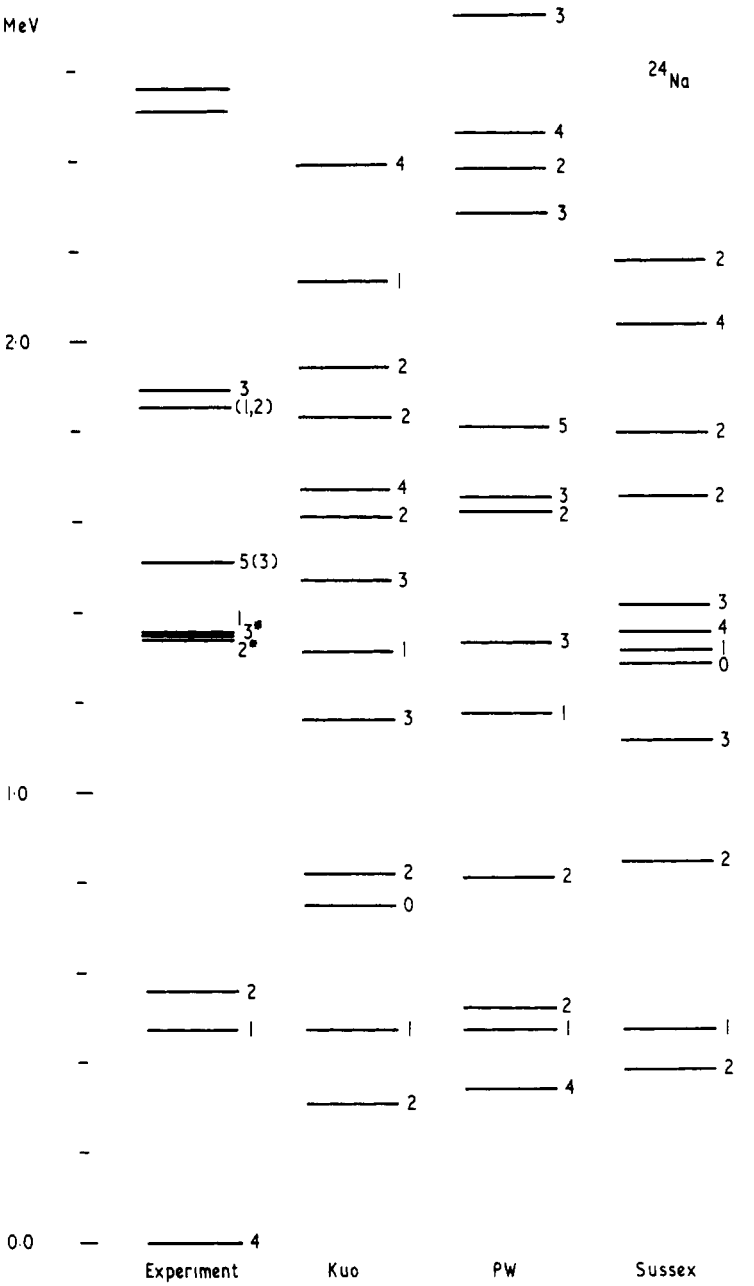

Figure 12. Spectra for ^{24}Na. The experimental data are from Endt and Van der Leun (1973) and Smulders (1973).

$J = \frac{3}{2}$. The Kuo interaction, on the other hand, gives poor agreement. In this nucleus it is difficult to identify the band structure, and there may be considerable mixing of bands (Kramer *et al* 1971).

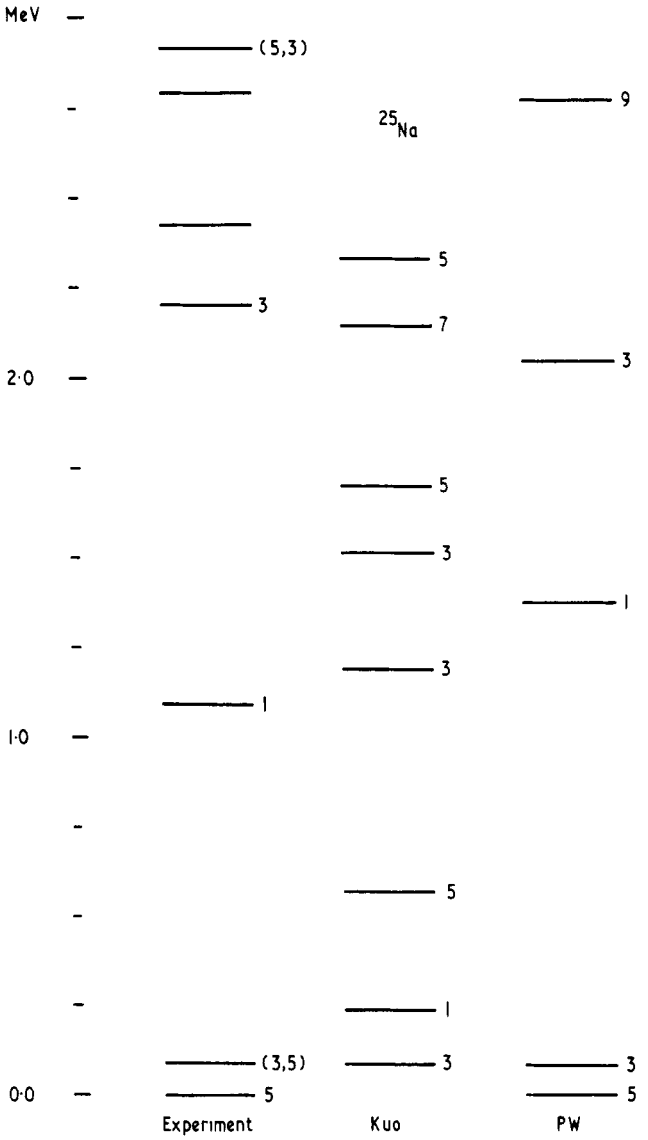

Figure 13. Spectra for ^{25}Na. The experimental data are from Endt and Van der Leun (1973). In the PW spectrum there may be a $\frac{7}{2}^+$ level below the $\frac{9}{2}^+$ level shown.

2.2.14. ^{26}*Al.* The Kuo spectrum for this nucleus is discussed in Cole *et al* (1973).

2.2.15. ^{26}*Mg* (*figure 14*). Qualitatively the spectrum of ^{26}Mg is similar to those of other nuclei with even numbers of protons and neutrons. The excited 2^+ band is again too low in the Kuo calculation, and the first excited 0^+ level is about 2 MeV below its observed counterpart.

2.2.16. ^{28}*Si.* The Kuo spectrum for ^{28}Si is given in figure 2 of Whitehead and Watt (1972). Again some levels appear too low in energy, notably the second 2^+ and 0^+ states.

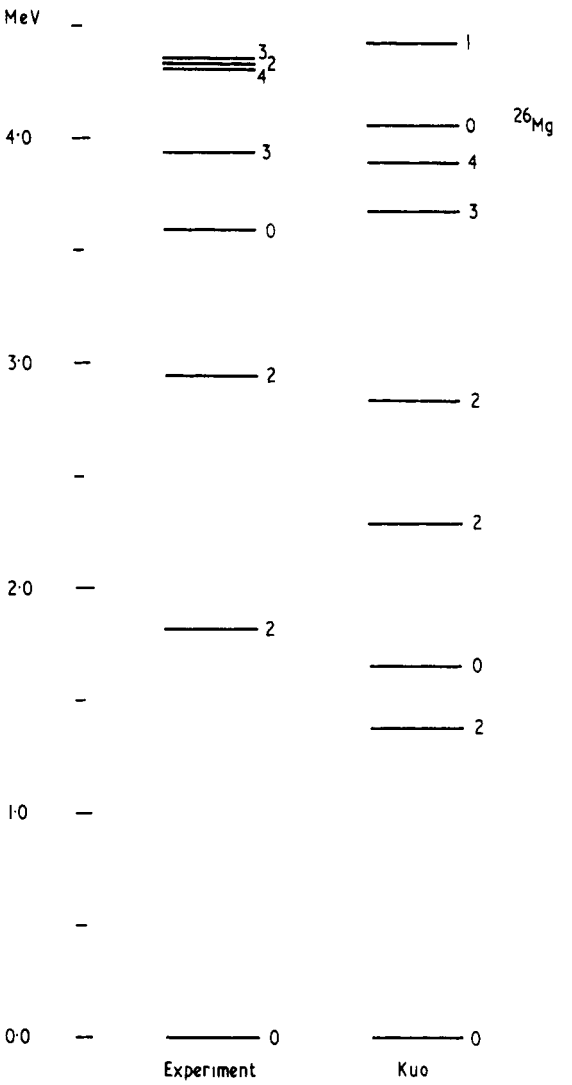

Figure 14. Spectra for ^{26}Mg. The experimental data are from Endt and Van der Leun (1973).

2.2.17. ^{30}P (*figure 15*). The Kuo interaction gives fair agreement with the experimental spectrum. Near 4 MeV 4^+ and 5^+ levels are predicted which have not been observed. Further information on levels above 3 MeV would be helpful.

2.2.18. ^{30}Si (*figure 16*). In the Kuo calculation many states fall too low in energy, resulting in too high a density of states between 3 and 5 MeV.

2.2.19. ^{31}Si (*figure 17*). The Kuo interaction apparently gives a bad fit to the experimental spectrum. However, if one assumes the ground and first excited states to be band heads most of the other states become likely candidates for the continuations of these bands. Very good agreement can then be obtained by raising the $\frac{1}{2}^+$ band by

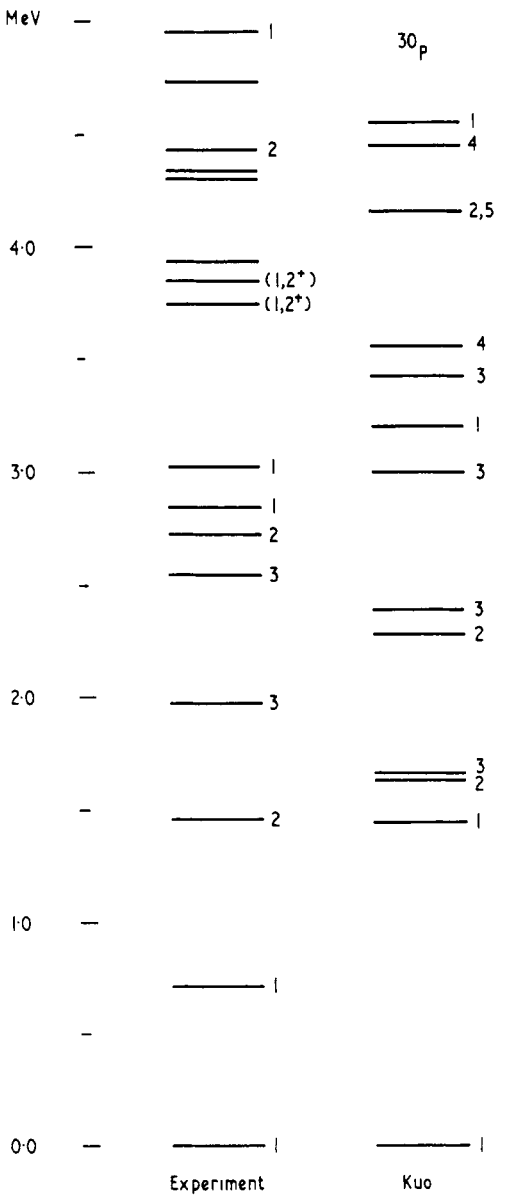

Figure 15. Spectra for ^{30}P. The experimental data are from Endt and Van der Leun (1973).

1 MeV and the $\frac{5}{2}^+$ band by 2·6 MeV (see spectrum marked Kuo+shift in figure 17). A further $\frac{7}{2}^+$ level then remains near 4·8 MeV, but different combinations of band shifts could put this state at almost any excitation. The actual band structure of ^{31}Si is as yet unknown.

2.2.20. ^{32}*S*. The Kuo calculation for this nucleus is given in figure 3 of Whitehead and Watt (1972). Several excited states come out too low whereas the first excited 0^+ is 2·5 MeV too high.

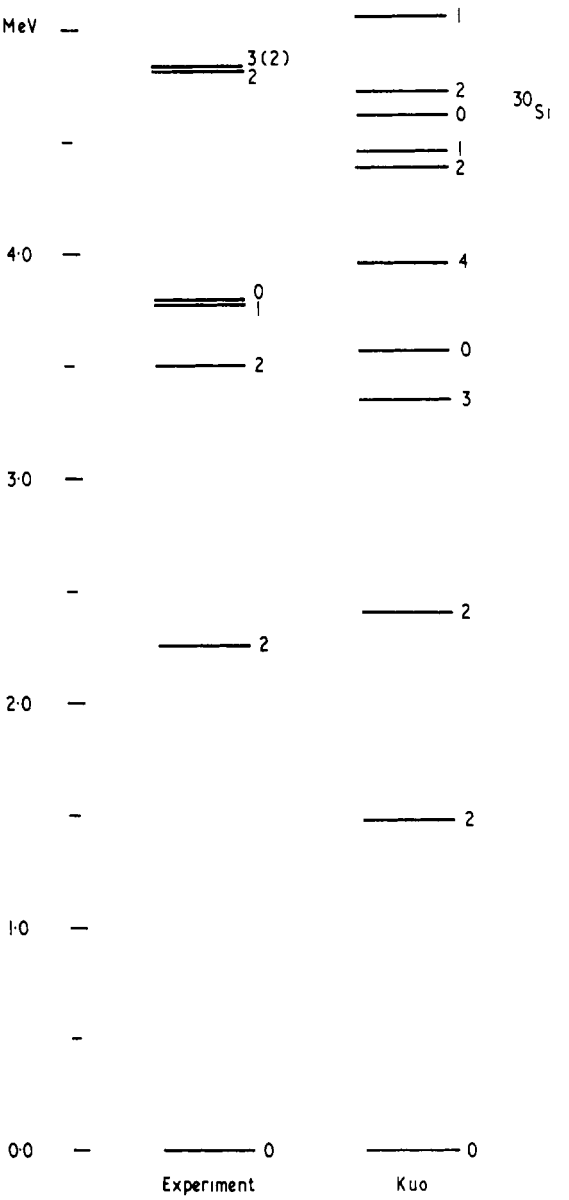

Figure 16. Spectra for ^{30}Si. The experimental data are from Endt and Van der Leun (1973).

2.2.21. ^{32}P (*figure 18*). The PW calculation gives fair agreement with the experimental spectrum. There is an overall expansion and the order of the first two states is reversed. The Kuo spectrum is in poor agreement with the data.

2.2.22. ^{33}S (*figure 19*). The results of the Kuo calculation are at first sight poor. However, as in the case of ^{31}Si much better agreement results if one shifts bands. The ground state and first and fourth excited states are again assumed to be band heads and the

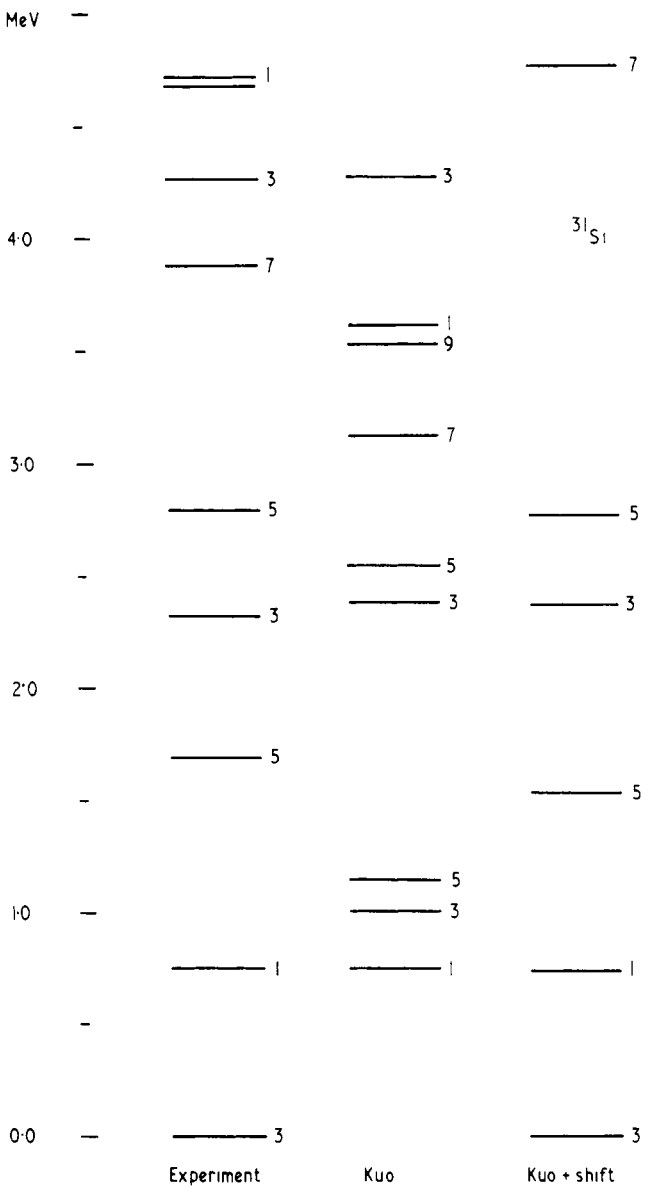

Figure 17. Spectra for ^{31}Si. The experimental data are from Endt and Van der Leun (1973).

$\frac{1}{2}^+$ and $\frac{5}{2}^+$ (hypothetical) bands are raised by 0·9 and 2·5 MeV respectively relative to the lowest $\frac{3}{2}^+$ level. The resulting spectrum is marked Kuo + shift in figure 19. The calculated $\frac{7}{2}^+$ state corresponds to the observed level at 4·07 MeV (Butler *et al* 1973). The shifts needed to give a good fit to the data are almost identical with those used in ^{31}Si. Calculations have also been done using the PW interaction, but the agreement is poor, showing considerable expansion of the spectrum. The spins of the first two states are, however, correctly reproduced.

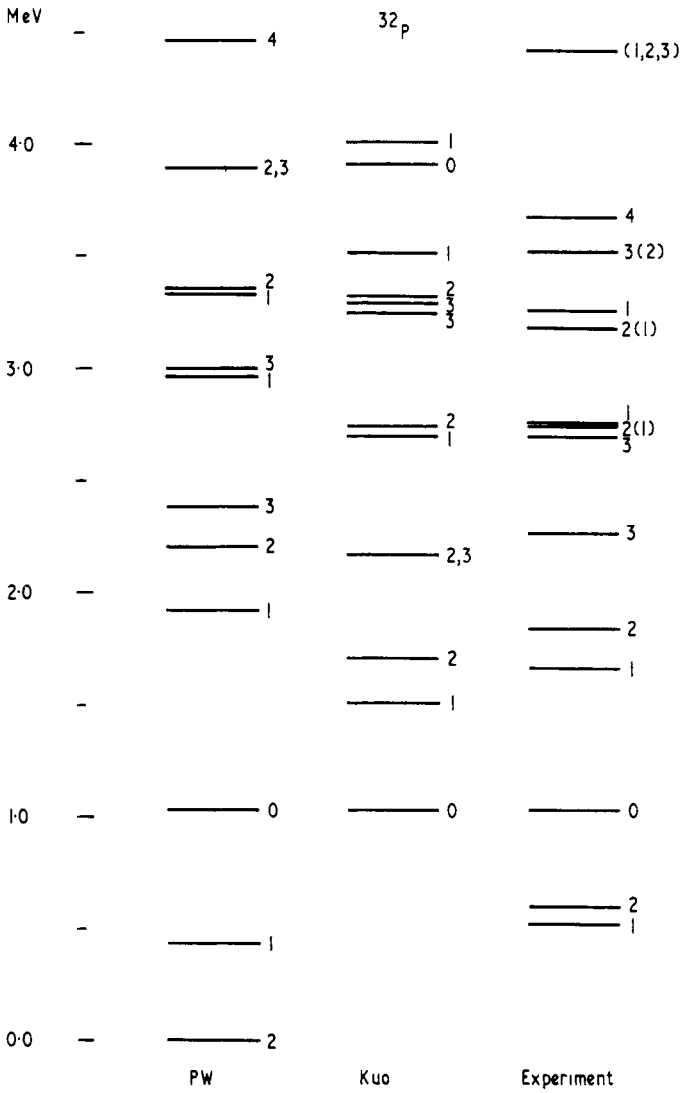

Figure 18. Spectra for ^{32}P. The experimental data are from Endt and Van der Leun (1973).

2.2.23. ^{33}P. The results of the Kuo calculation were given by Cole *et al* (1973). By raising an assumed $K = \frac{3}{2}$ band by 2 MeV reasonable agreement is achieved for the low-lying levels. Experimental spin assignments are less certain for the higher states. The PW spectrum (not shown) is again expanded compared with experiment, although the correct spin sequence is obtained for the four lowest levels.

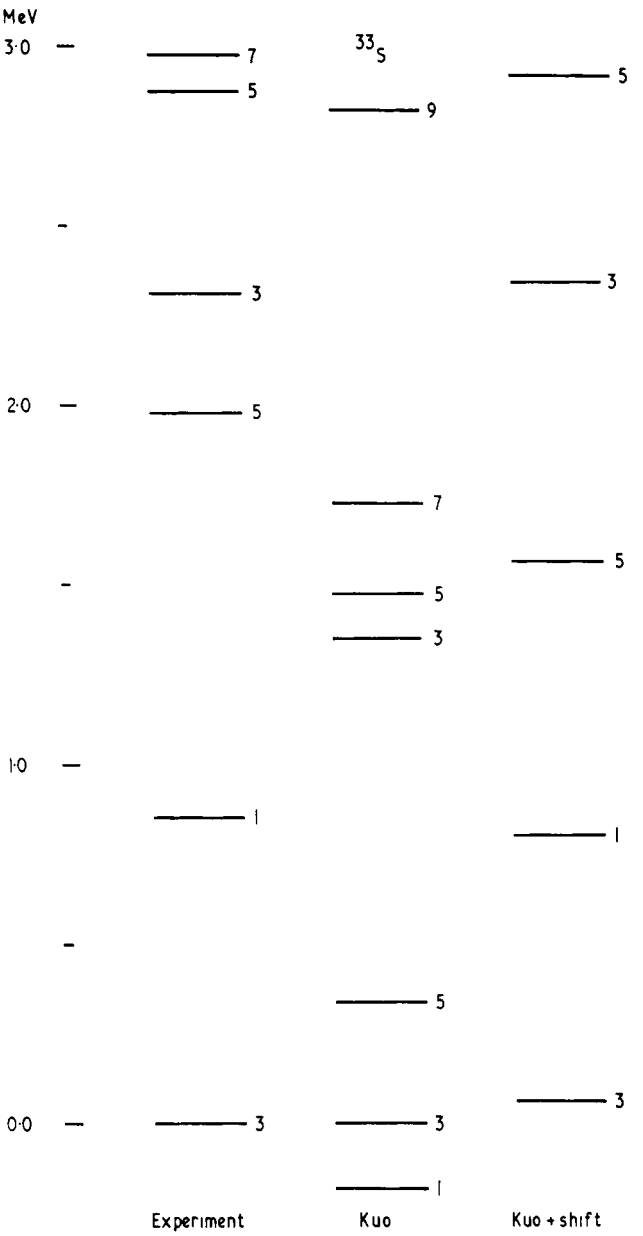

Figure 19. Spectra for ^{33}S. The experimental data are from Endt and Van der Leun (1973) and Butler *et al* (1973).

3. Discussion

In the lightest nuclei there are some levels, presumed to be interlopers, which are missing from all the calculated spectra, while in a few cases, noted in the previous section, additional states appear in the calculations. However, the main defect of the Kuo interaction, in common with most others in current use, is that it appears to move

whole bands of levels relative to each other. This has already been discussed by Cole *et al* (1973) and a number of further instances are found in the present work. By raising or lowering assumed bands good (sometimes very good) agreement can be achieved. The Kuo interaction predicts the correct inter-band spacings, and hence the correct moments of inertia for the bands, but the relative positions of the band heads are incorrect. To understand this phenomenon is one of the outstanding problems of sd-shell spectroscopy. Of course, in some of the nuclei treated here band structure is not well developed or the bands are considerably mixed and so no clear picture of band shifting emerges.

The interaction of Preedom and Wildenthal was produced by a fit to nuclei with $A \leqslant 22$, and so it must give a good description of these nuclei. However its success extends to heavier nuclei, at least as far as $A_n = 26$. The tendency to shift bands is

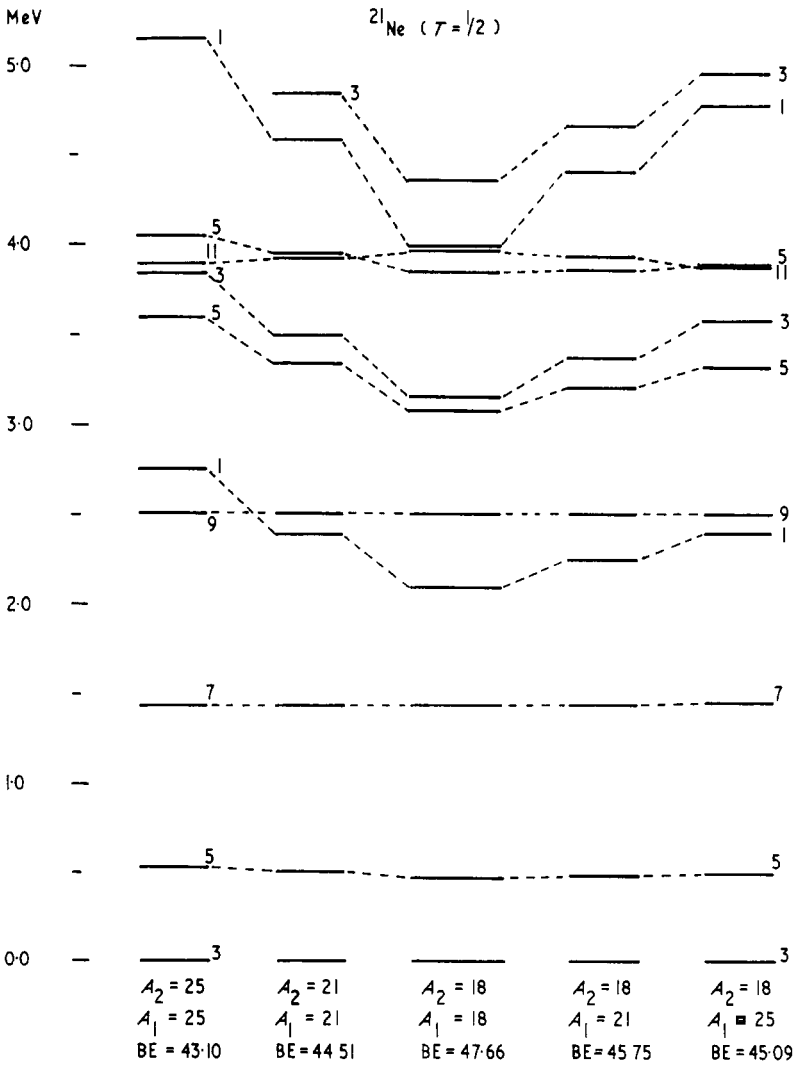

Figure 20. Mass dependence of the Sussex interaction spectra for $A = 21$, $T = \frac{1}{2}$. BE is the calculated binding energy.

present, but to a much smaller extent than in the Kuo interaction. The main difference between PW and Kuo lies in the matrix elements involving $d_{5/2}$ and $s_{1/2}$, and one would expect the PW calculations to show improvement over Kuo only where these matrix elements dominate (ie in the lower part of the shell). This is in fact what is found. In the upper part of the shell the interaction usually provides a poor fit to the data, since here $d_{3/2}$ particles are important. For $A = 32$ and 33 there is a 50% expansion of the spectrum, although the low-lying levels are still in roughly the correct order, and the ground-state binding energy is much more accurately predicted than by the Kuo interaction.

The Sussex interaction also produces band shifts, but the effect is somewhat masked by an overall compression of the spectra. However there is some evidence that the shifts are sometimes smaller than those produced by the Kuo interaction (see, for example, the spectrum of ^{24}Na, figure 12). There is also a certain amount of underbinding, evident in table 1. It is possible that the use of a larger oscillator parameter value would improve the results to some extent, but it is our impression the other two interactions used here are generally more satisfactory in the sd shell.

Both the one- and two-body parts of the Sussex interaction are mass dependent. Figure 20 shows the results of a series of calculations for ^{21}Ne done in order to try to assess the importance of this mass dependence. The figure shows spectra in which the one-body part appropriate to mass A_1 has been used together with the two-body part for mass A_2. The main effect seems to be one of band shifting in which both parts contribute about equally. It is well known that bands may be shifted by limited amounts by variation of the single-particle energies (see eg Cole *et al* 1973), but the role of the two-body part here is difficult to assess.

As noted many times in § 2 there still remain many gaps in the experimental data and it is now more important than ever that these should be filled. Of particular importance is the experimental assignment of states to rotational bands wherever this is possible.

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