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Shell-model calculations in the sd shell II. Mass excesses and energy spectra of exotic nuclei

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Abstract. Calculations of binding energies and energy spectra have been performed for a number of neutron- and proton-rich (exotic) nuclei in the sd shell using the K uo and Preedom and Wildenthal interactions. It is found that the Preedom–Wildenthal interaction reproduces the binding energies very well even when used for masses greater than those for which it was derived. A number of mass and spin predictions are made in cases where as yet no data are available.

1. Introduction

There has been much interest recently in the properties of neutron-rich nuclei in the sd shell, particularly in mass excesses and β decay. For some T = 2 nuclei spins and parities are established for several low-lying levels, but for most nuclei away from the line of stability the excited states have yet to be observed, and even the ground state spins have not been uniquely determined.

We present here untruncated shell-model calculations for many exotic nuclei with isospin $2 \le T \le 4$, as a first step towards explaining observed β transitions and $\log ft$ values. This work forms part of a larger study of sd shell nuclei (Whitehead and Watt 1972, Cole *et al* 1973 and to be published) in which untruncated calculations are performed throughout the shell in order to predict or explain properties of low-lying states. In this paper we report the calculation for each nucleus of the mass excess and spins and excitation energies of the first few levels, and where possible, comparison is made with experiment.

The shell-model computations were carried out using the methods of Whitehead (1972) which allow much larger calculations to be handled than with conventional techniques. For a nucleus of mass A, an inert core of 16 particles is assumed and the remaining A - 16 particles are distributed amongst $d_{5/2}$, $s_{1/2}$ and $d_{3/2}$ orbitals, restricted only by the Pauli principle. Two two-body interactions have been used. The first, due to Kuo (1967), is derived via the Hamada–Johnson potential (Hamada and Johnson 1962) from nucleon–nucleon phase shifts. The second is a modification of this due to Preedom and Wildenthal (1972). The modifications were included to improve the fit to spectra for some nuclei in the mass region A = 18-22. The single particle energies used with both interactions are taken from the ¹⁷O experimental spectrum, namely $-4.15 \text{ MeV} (d_{5/2})$, $-3.28 \text{ MeV} (s_{1/2})$ and 0.93 MeV ($d_{3/2}$).

General conclusions can be drawn from previous work (Cole et al 1974b, and to be published) about each of these interactions, and these must be borne in mind when

considering the results of the next section. The interaction of Preedom and Wildenthal (denoted PW) gives a good description of nuclei in the lower part of the shell but, particularly for energy spectra, it becomes increasingly unreliable as the effect of $d_{3/2}$ particles grows. This unreliability manifests itself as an expansion of the spectrum (with re-ordering of higher levels) which is quite marked for A = 33, but is not present in ²⁶Al or ²⁵Mg. The mass excesses (or binding energies) calculated are very accurate for $A \leq 23$ and then becomes less accurate with errors of about 2 MeV for A = 32-33.

The Kuo interaction is less successful. It was found that its main defect is to move whole bands of levels relative to one another—the moments of inertia of the bands are reasonably accurate, but the band heads may be displaced. This has been discussed in more detail elsewhere (Cole *et al* 1973, 1974a). It means that we cannot predict with any certainty ground state spins, since an excited band is sometimes shifted below the real ground state. The calculated mass excesses are not very accurate except for the lightest nuclei. The error grows as the number of particles increases, the calculated binding energy always being larger than the measured value.

Therefore, for the calculations presented here, we can expect the results obtained from the PW interaction to be reasonably reliable except where particles in the $d_{3/2}$ orbital become important. Even then we may hope that the calculation produces the correct ground state spin, and the binding energy may be accurate to a few MeV. The Kuo interaction cannot be used to predict mass excesses, but we use the results here mainly to extend the range of cases in which we can qualitatively compare this more basic interaction with PW.

2. Results

2.1. Mass excesses

In table 1 are listed all the available mass excesses for the nuclei considered here. Some are taken from the compilation of Endt and Van der Leun (1973), but data for many nuclei have been measured more recently. Klapisch *et al* (1973) have determined the masses of several sodium isotopes produced in the reaction of high energy protons on uranium with an accuracy of 150–500 keV. A group at Brookhaven have formed $T = \frac{5}{2}$ nuclei by complex transfers from heavy-ion induced reactions. The neutron-rich nucleus subsequently β decays and γ rays from the de-excitation of the daughter nucleus are observed. This not only gives the mass of the exotic nucleus (from the β end point measurement), but also enables limits to be placed on its ground state spin by employing β decay selection rules when spins for levels in the daughter nucleus are known.

The calculated values of the mass excess are listed in columns 4 and 5 of table 1. These are obtained from the calculated ground state energies by making a Coulomb correction as in Halbert *et al* (1971). The results with the PW interaction are mainly in good agreement with the experimental data (with differences less than about 1 MeV). One exception is for ³⁰Na where the calculated value is 2.7 MeV too high. The calculated masses for ²²O, ³⁰Al, and ³¹Al are too small by 2.0 MeV, 2.3 MeV and 1.8 MeV. The results are in general worse for those nuclei with large numbers of neutrons. With few exceptions the calculated masses from the Kuo interaction are inaccurate as expected. However, it should be remembered that although, for example, for ³³Si the error appears to be greater than 100%, this represents an error of only 20% in the actual calculated quantity, the binding energy relative to ¹⁶O.

Nucleus	_	Mass excess $(M - A)$ (MeV)			E_n (MeV)			$E_{\rm p}({\rm MeV})$	
	J _o PW	Experi- ment	PW	Kuo	Experi- ment	PW	Kuo	Experi- ment	PW
²⁰ O	0	3.80	3.74	2.89	7.6	7.6			
²¹ O	5	9.30	8.31	6.90	2.6	3.5	4 ·1		
²² O	õ	11.50	9.47	6.83	5.9	6.9	8.1		
²³ O	$\frac{1}{2}$		15·29			2.3			
²² F	4	2.83	3.09	1.30	5.2	4.9	5.3	13.8	12.5
²³ F	5		3.57			7.6			13.2
²⁴ F	3		8.10			3.5			14.5
²⁵ F	<u>5</u> 2		11.28			4.9			
²⁴ Ne	0	- 5.96	-6.25	- 10.60	8.9	9.2	10.7		17.1
²⁵ Ne	$\frac{1}{2}$	-2·07*	- 2.24	-8.53	4.2	4.1	6.0		17.6
²⁶ Ne	õ		-0.12			6.0			18.7
²⁷ Ne	$\frac{3}{2}$		6.86	- 6.68		1.1			
²⁶ Na	2	-6.85	- 7.83	- 15-27	5.6	5.9	7.6	12.1	12.9
²⁷ Na	$\frac{3}{2}$	-5·78⁵	- 6.97	-17.78	7.0	7.2	10.6		14.1
²⁸ Na	$\overline{2}$	- 1·26 ^d	- 2.22	<i>—</i> 16∙99	3.6	3.3	7.7		16.4
²⁹ Na	3	2.73ª	2.46	- 17-47	4.1	3.4	8.5		
³⁰ Na	ō	8·37 ^d	11.03	-15.04	2.4	-0.5	5.6		
²⁸ Mg	0	-15.02		- 29.72	8.5			16.5	
²⁹ Mg	$\frac{3}{2}$	-11.70°	-12.37		4.8			17.7	17.4
³⁰ Mg	0		-9.74	- 31.62		5.4			19-5
³¹ Mg	$\frac{3}{2}$		-1.30	- 29.04		-0.37	5.5		21.6
³⁰ Al	2	-15.89	-18.20	- 36.77	5.8			11.5	13-1
³¹ Al	52	15·06 ^f	-16.83		7.2	6.7			14.4
³² Si	ō	- 24.09		- 53-83	9.2		14.3	16.4	
³³ Si	$\frac{3}{2}$	- 20.56°	-21.44	- 53.58	4.5		7.8		

Table 1. Mass excesses and separation energies for neutron-rich nuclei.

 J_0 is the calculated ground state spin, Kuo and PW refer to calculations with the Kuo and PW interactions. Experimental data from Endt and Van der Leun (1973) and: a Wilcox *et al* (1973); b Klapisch *et al* (1973); c Goosman *et al* (1973b); d Klapisch *et al* (1973); e Scott *et al* (unpublished) and Goosman *et al* (1973c); f Goosman and Alburger (1973).

Columns 6-10 of table 1 show neutron (E_n) and proton (E_p) separation energies computed from the listed mass excesses. The masses for $T = \frac{3}{2}$ nuclei, also required to calculate some E_n , are taken from Cole *et al* (1974b, and to be published). The experimental and PW neutron separation energies agree to within 1 MeV with a single exception (³⁰Na), which the calculation erroneously predicts to be just particle unstable. ³¹Mg is also predicted to be slightly unbound, but it may be particle stable. All the nuclei considered here should be strongly bound to proton emission.

Garvey et al (1969) and Thibault and Klapisch (1972) have computed mass excesses for neutron-rich nuclei using recurrence relations connecting values for neighbouring nuclei. The accuracy of this procedure depends upon the accuracy of the input data, and indeed, the more recent work, with up-to-date data, is more successful. Thibault and Klapisch obtain a mass excess of 6.89 MeV for ³⁰Na which is slightly closer than PW to the experimental value. Their results for ³¹Al and ²²O are also more accurate. We may also compare their computed masses with PW where there are no measurements. Generally the two agree to better than $1\frac{1}{2}$ MeV, except for ³¹Mg where Thibault and Klapisch find a mass excess of -5.02 MeV, which makes this nucleus bound to neutron emission by 2.8 MeV.

2.2. Ground state spins and energy spectra

The ground state spins J_0 predicted using the PW interaction are shown in table 1, column 2. These are discussed in the following subsections, together with the energy spectra shown in the figures and in tables 2 and 3. These tables show for the PW interaction excited states only; for the Kuo calculation the excitation energies are relative to the lowest state of spin J_0 .

²¹ O				²² F			²⁶ Ne		²⁶ Na				
PW		Kuo		PW		Kuo		PW		PW		Kuo	
1.27	<u>1</u>	-0.44	+	0.11	3	-0.77	1	2.18	2	0.14	1	-0.32	0
1.66	32	0.22	3	0.29	2	-0.56	3	3.95	2	0.37	3	-0.16	1
2.78	5/2	1.06	-	1.06	1	-0.53	2	3.97	4	0.66	2	-0.09	4
3.12	$\frac{\overline{7}}{2}$	1.69	7	1.27	5	-0.17	0	4.48	0	1.63	3	0.06	1
4.33	3	3.00	3	1.37	3	0.04	3	4.78	1	1.73	1	0.11	2
439	52	3.14	57	1.56	2	0.05	2	5.62	2	1.79	4	0.35	2
4.72	32	3.19	2	2.09	1	0.58	1	6.03	4	1.97	0	0.38	3
	•		-	2.63	1	0.90	1						
	2	⁷ Na		²⁹ M	g		³⁰ N	1g				³⁰ Al	
PV	v	Ku	10	PW	V	 1	PW	Ku	10	PW	V	Ku	10
0.16	5	0.38	57	0.02	+	1.6	3 2	1.52	2	0.19	3	-0.72	0
2.50	1/2	0.71	Ĩ,	1.89	5	4.0	12	3.15	2	1.46	3	-0.07	3
2.73	2	1.73	3	2.53	7/2	4.3	94	4.33	3	1.48	1	- 0.05	1
2.84	72	2.14	$\frac{1}{2}$	3.19	32	5-1	32	4.47	4	1.58	4	0.10	0
3.45	<u>5</u> 2	2.36	$\frac{7}{2}$	3.50	$\frac{1}{2}$			4.47	2	2.07	0	0.15	1

Table 2. Excited states of some neutron-rich nuclei. For each level are shown the excitation energy in MeV and the level spin.

2.2.1. Oxygen isotopes. ²⁰O is reasonably well known experimentally (see figure 1). The PW interaction provides a good fit to the level scheme. The Kuo interaction fits the sequence 0^+ , 2^+ , 4^+ well but the other known levels, the second 2^+ and 0^+ , are over 1 MeV too low. The other calculated levels are also low compared with PW.

The computed spectra for ²¹O are shown in table 2. Compared with PW, the ground and first excited states in the Kuo calculation are inverted and all other levels are low in energy by about $1\frac{1}{2}$ MeV.

Nothing is known experimentally about the spectra of the remaining isotopes, although we may reasonably assume that the ground state of ²²O has J = 0 (as is in fact predicted by the Kuo and PW calculations, see table 3). The spin sequence from both calculations is 0, 2, 0, 3, 2, and 4, although all excited states in the Kuo spectrum appear to be about $1\frac{1}{2}$ MeV below their probable counterparts in the PW spectrum, as in ²¹O. Levels of ²³O from the PW calculation are given in table 3.

22	0	²³ O	²³ F	²⁴ F	²⁵ F	
PW Kuo		PW	PW	PW	PW	
3·22 2 4·14 0	1·74 2 2·59 0	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	0·49 2 1·59 1	$1.89 \frac{1}{2}$ $3.63 \frac{3}{2}$	
2	⁸ Na	29	'Na	30	Na	
PW Kuo		PW	Kuo	PW	Kuo	
0·32 1 0·98 3	0·41 1 1·04 3	$\begin{array}{ccc} 0.26 & \frac{5}{2} \\ 2.38 & \frac{1}{2} \end{array}$	$0.34 \frac{5}{2}$ 1-19	0·26 2 0·43 1	0.65 2 0.83 1	
²⁷ Ne 3		Мg	³¹ Al	³³ Si		
PW Kuo		PW	PW	Kuo		
1.52	$1.18 \frac{5}{2}$ $2.57 \frac{1}{2}$	$1.33 \frac{5}{2} \\ 2.25 \frac{7}{2}$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{ccc} 0.76 & \frac{1}{2} \\ 2.70 & \frac{7}{2} \end{array}$		

Table 3. Excited states of further neutron-rich nuclei. For notation see table 2.

2.2.2. Fluorine isotopes. Not much is known about any of the isotopes considered here. Several different spin assignments have been made for the ²²F ground state. Most recently Davids *et al* (to be published) found $J = (3, 4)^+$, but this disagrees with the J = 5 quoted by Endt and Van der Leun (1973). Both result from measuring the β decay to levels of ²²Ne. The PW result predicts a spin of 4⁺; however the first excited state with J = 3 is only 0.11 MeV higher. There is in fact a high density of low-lying states in the calculated spectra, particularly in that of Kuo. This appears to be quite dissimilar to the PW calculation (see table 2); however the levels with J = 1, 3, 2, 1, and 1have approximately the same relative spacings.

For predicted spins in ${}^{23}F$, ${}^{24}F$ and ${}^{25}F$ see table 3. The ground state spins are in table 1.

2.2.3. Neon isotopes. Levels in ²⁴Ne have been observed up to 6 MeV, and the spin and parity of most are known (see figure 2). The PW interaction gives good agreement with these data, suggesting that the level at 4.89 MeV has $J^{\pi} = 3^+$. In the Kuo spectrum several states are too low in energy. The PW interaction has also been used in a truncated calculation (Robertson and Wildenthal 1973): no fewer than four particles were permitted in the d_{5/2} shell, and no more than two in the d_{3/2} shell. This produced a spectrum slightly expanded compared with the untruncated one shown in figure 2, but otherwise very similar.

The calculated spectra for ²⁵Ne are shown in figure 3, compared with the known data (Wilcox *et al* 1973). The predicted ground state spin $\frac{1}{2}^+$ is consistent with the $\frac{1}{2}^+$ ($\frac{3}{2}^+$) found experimentally (Goosman and Alburger 1973). Comparison of the PW and experimental spectra suggest that the observed levels near 1.8 MeV have spins $\frac{3}{2}$ and $\frac{5}{2}$. Above 3 MeV there are more calculated states than observed ones; one explanation of this is that the existing levels at 3.25 MeV and 4.05 MeV are closely spaced doublets, as in the calculation. Or possibly, some levels were not seen in the experiment. In the Kuo spectrum many levels are much too low.



Figure 1. Spectra for ²⁰O. In the experimental spectrum brackets round a spin or parity indicate a tentative assignment. The absence of a parity assignment denotes a positive parity state, and an asterisk means that the parity is unknown. The data are from Ajzenberg-Selove (1972)

Nothing is known about the spectra of ²⁶Ne and ²⁷Ne. The PW calculations suggest that these have ground state spins 0^+ and $\frac{3}{2}^+$ respectively. Other levels are given in table 3: ²⁶Ne has a structure typical of even A, even Z nuclei.

2.2.4. Sodium isotopes. The calculated spectra for ²⁶Na and ²⁷Na are given in table 2. For the former, the Kuo interaction again leads to a much higher density of low-lying levels than PW, and also produces a different ground state spin. This is similar to the situation for other odd N, odd Z nuclei (Cole *et al* 1974b). The ground state spin can be measured from the β decay to levels in ²⁶Mg. The strong decay to the 1.81 MeV level (2⁺) limits J to 1, 2 or 3 (Endt and Van der Leun 1973), and the observed allowed decay to 3⁺ levels (Alburger *et al* 1973) rules out 1⁺ as a possibility. Recently Klotz *et al* (1973) have measured a weak decay (0.3%) to the 4⁺ level at 4.90 MeV, thus suggesting that $J^{\pi} = 3^+$ is more probable. However the shell-model calculation with the PW interaction predicts $J^{\pi} = 2^+$, the lowest 3⁺ level being the second excited state at 0.37 MeV.

The ground state of ²⁷Na is believed to be $\frac{3}{2}^+$ or $\frac{5}{2}^+$ (Alburger *et al* 1973), whereas the PW calculation produces $\frac{3}{2}^+$ with a very low-lying $\frac{5}{2}^+$ state. These are also predicted



Figure 2. Spectra for 24 Ne. Experimental data from Endt and Van der Leun (1973).

Figure 3. Spectra for ²⁵Ne. Experimental data from Wilcox *et al* (1973).

by the Kuo calculation, but here other levels fall well below the corresponding levels in the PW spectrum.

Nothing is known about the spectra of the remaining isotopes. The PW and Kuo calculations both suggest that the three lowest states of ²⁸Na have spins 2^+ , 1^+ and 3^+ but differ over higher levels. The calculations also predict that ²⁹Na has a $\frac{3}{2}^+$ ground state (with some levels given in table 3). Both calculations predict that the lowest states of ³⁰Na are 0^+ , 2^+ and 1^+ (see table 3); however, it is unusual for an odd Z nucleus to have a low-lying 0^+ state.

2.2.5. Magnesium isotopes. More is known experimentally about 28 Mg than about most of the nuclei considered here. The Kuo calculation fits the probable ground state band well, but the second 2⁺ level falls 2·3 MeV too low, as shown in figure 4.

²⁹Mg is believed to have a ground state spin of $\frac{3}{2}^+$ or $\frac{1}{2}^+$ (Goosman *et al* 1973c), whereas the PW calculation produces a ground state doublet $\frac{3}{2}^+$, $\frac{1}{2}^+$ separated by only 17 keV. This situation is obviously sensitive to minor changes in the interaction. Other levels are given in table 2.

Levels of ³⁰Mg are also shown in table 2. The two calculations agree about the spins of the first four states, although the second and third 2^+ and first 3^+ are about 1 MeV lower in the Kuo calculation. Calculated levels for ³¹Mg are given in table 3. The next level has $J = \frac{1}{2}$ (PW) or $J = \frac{7}{2}$ (Kuo), so the two calculations agree reasonably well.

2.2.6. Aluminium and silicon isotopes. Calculated levels for 30 Al are shown in table 2. The spectra are in some ways similar to those of 28 Al (Cole *et al*, to be published), where experimentally there is a ground state doublet of 3^+ , 2^+ and 0^+ and 3^+ states near 1 MeV. The PW calculation inverts the doublet and produces a 0^+ too high in energy, the 3^+ being at roughly the correct energy. In the Kuo calculation the 0^+ is much too low and becomes the ground state. The present PW calculation for 30 Al



Figure 4. Spectra for ²⁸Mg. Experimental data from Endt and Van der Leun (1973).

Figure 5. Spectra for ³²Si. Experimental data from Endt and Van der Leun (1973).

produces a ground state doublet of 2^+ , 3^+ , with a 0^+ near 2 MeV, but the Kuo ground state has J = 0. The actual ground state has been measured as $(2^+, 3^+)$ (Endt and Van der Leun 1973).

The ground state of ³¹Al, thought to be $\frac{3}{2}^+$ or $\frac{5}{2}^+$ (Goosman and Alburger 1973) is predicted to be $\frac{5}{2}^+$ using the PW interaction. Some other levels are given in table 3.

The Kuo calculation for 32 Si, shown in figure 5, agrees fairly well with the known experimental data. The second 2^+ is too high by 1 MeV (in similar nuclei it usually falls below the corresponding observed level).

The Kuo calculation for ³³Si is shown in table 3. The PW interaction would not be expected to work here (see introduction) although for other A = 33 nuclei it produces the correct ground state spin (Cole *et al* 1974b). Indeed, for ³³Si, both Kuo and PW calculations suggest that the ground and first excited states have $J^{\pi} = \frac{3}{2}^+$ and $\frac{1}{2}^+$ respectively. Goosman *et al* (1973b) have measured the former to be $(\frac{3}{2}, \frac{5}{2})^+$. Not much reliance should be placed on calculations for higher levels bearing in mind the defects of both interactions in this mass region.

3. Proton-rich nuclei

The properties of a proton-rich nucleus A_p with N neutrons and Z protons can be inferred from the properties of the corresponding neutron-rich nucleus A_n with Z neutrons and N protons. If we assume that the Coulomb term in the binding energy is given by the expression in Halbert *et al* (1971) we may relate the mass excess of A_p to that of A_n . For example, for nuclei with $T_3 = \pm 2$

$$\mathscr{E}_{p} \simeq \mathscr{E}_{n} + 13.75 + \frac{3}{2}(N-8)$$

where \mathscr{E} denotes a mass excess (and N is the number of protons in the neutron-rich nucleus). We may use these relations to predict both 'experimental' and calculated values of \mathscr{E}_n from the experimental and calculated values of \mathscr{E}_n .

Table 4 lists some mass excesses computed in this way. Also shown, in the second column, are measured values where these are known (Endt and Van der Leun 1973). The agreement between 'expt' and expt is excellent except for ²⁹S, showing that the formulae such as that above are quite accurate. The final columns in table 4 list the proton separation energies for T = 2 nuclei. PW agrees with 'expt' to within 0.4 MeV, although it predicts ²²Al to be just unbound whereas it is probably just bound, and vice versa for ²⁶P.

4. Discussion

In general the performance of both interactions is as expected from earlier work. Where the experimental spectrum is known the PW interaction gives a reasonable description of the level scheme. The Kuo calculation often fits the possible ground state band well, but other levels fall too low in energy. (This also holds for other nuclei where no experimental data are available, but where the Kuo spectrum can be compared with that from the PW interaction.) For those nuclei where limits have been placed on the ground state spin the PW calculation is usually consistent with these limits.

		Mass e	E_{p} (MeV)			
Nucleus	Expt ^e	'Expt'ª	PW	Kuo	'Expt'b	PW
¹⁹ Na	12.98	12.97	12.89	12.73	·	
²⁰ Mg		17.55	17.49	16-44	2.71	2.69
²¹ Mg	10.91	10.91	10-90	9.46		
²² Al		18.08	18.34	16.55	0.12	-0.15
²³ Al	6.77	6.75	6.76	3.89		
²⁴ Si		10.79	10.50	6.15	3.25	3.55
²⁵ Si	3.82	3.86	3.27	- 2.56		
²⁶ P		11-40	10.42	2.98	-0.25	0.14
²⁷ P		-0.43				
²⁸ S		4.73		- 9.97	2.13	
²⁹ S	- 3.16	-2.73				
30Cl		5.36	3.06	- 7.19	-0.80	
31Cl		- 7.69		- 32.33		
³² Ar		-1.34		-23.62	0.94	

Table 4. Mass excesses and proton separation energies (E_p) for some proton-rich nuclei.

Notation: a calculated from mass excess of corresponding neutron-rich nucleus, as explained in the text; b from mass excess in column 3; c from Endt and Van der Leun (1973).

However, the PW interaction is expected to give a poorer description of nuclei with many neutrons, since $d_{3/2}$ particles must become important as the sd shell fills. For this reason the predicted 0⁺ ground state for ³⁰Na should be regarded with caution.

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