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Two particle-one hole states in ^{41}Ca and ^{41}Sc

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Abstract. A prescription has been given to calculate the two particle-one hole states, to explain the occurrence of non-normal parity states in nuclei having doubly closed shell and one extra particle. This prescription has been applied to calculate the even-parity states in ^{41}Ca and ^{41}Sc nuclei. The transition probabilities for the electro-magnetic decays of these states have also been calculated.

Keywords. Two particle-one hole states; non-normal parity states; spectra of mass-41 nuclei.

1. Introduction

It is well known that the picture of a single particle outside doubly closed ^{40}Ca core is too naive to describe the energy spectra of ^{41}Ca and ^{41}Sc. To account for the large number of excited states of these nuclei, one has to consider the excitations of ^{40}Ca core. As the low-lying single-particle orbits outside ^{40}Ca are $1f$ and $2p$, the states in ^{41}Ca and ^{41}Sc are normally expected to have odd parity. However, there are quite a large number of even parity states in the energy spectra of these nuclei. The most plausible explanation for the occurrence of these is the excitation of an odd number of particles from the *s-d* shell to the *f-p* shell. Among such excitations, the excitation of one particle is expected to require minimum energy; thus the low-lying even parity states in ^{41}Ca and ^{41}Sc should arise mainly from two particle-one hole configurations.

Bansal and French (1964) studied the systematics of even parity states in odd-mass $1f_{7/2}$ shell nuclei. They attributed the origin of an even parity state, in an odd-mass nucleus, to the weak-coupling of a hole in the *s-d* shell to the ground state (0^+) of the next higher even-even nucleus. In this simple model, they could obtain the energies of the hole-states in terms of only two parameters representing average particle-hole interactions in the iso-singlet and iso-triplet states. However, this simple model is insufficient to explain the occurrence of even-parity states with large spins (7/2 and higher); also it cannot account for the fine structure of the even parity states. There have been attempts at extending the simple hole-particle coupling model of Bansal and French (1964) to explain the detailed fine structure of the even-parity states in ^{41}Ca and ^{41}Sc, by several workers, notably, Sartoris and Zamick (1967a), Armigliato *et al* (1967) and Chen Tsai *et al* (1971). These works include only the calculation of the two particle-one hole energy spectrum without explicitly going into the charge-independent, though simple, theoretical detail of the problem.

In the present paper, we present an outline of the necessary theoretical detail, in the charge-independent formalism, giving an explicit analytical expression for the typical two particle-one hole matrix element needed to set up the energy matrix. We have also calculated the transition probabilities (not calculated so far) of the various possible electromagnetic transitions among the even-parity states of the concerned nuclei.

2. Theoretical outlines

Let us denote the orbits above the closed shell by $p_1, p_2 \ldots$, and those below it by $h_1, h_2, \ldots$ Then a typical $2p$-$1h$ state looks like

$$[h_i^{-1}(p_j\,p_k)_{\Gamma_p}]_{\Gamma}. \tag{1}$$

We are using a compact notation where, in the isospin formalism, Γ stands for both the angular momentum and isospin of the state, i.e. $\Gamma \equiv JT$; similarly Γ_p $(\equiv J_pT_p)$ specifies both the angular momentum and isospin to which the two particles are coupled. An orbit label (h, p, etc.) stands for the spin (j_h, j_p, etc.) and isospin (1/2) of a single particle in that orbit. The hamiltonian, as usual, is taken to be a one-body plus two-body scalar operator, viz.

$$H = H_1 + H_2$$

$$= \sum_r \varepsilon_r [r]^{\frac{1}{2}} (A^r \times B^r)^0 - \sum_{\substack{rstu;\,\gamma \\ r<s \\ t<u}} \frac{1}{\sqrt{(1+\delta_{rs})(1+\delta_{tu})}} [\gamma]^{\frac{1}{2}} W^{\gamma}{}_{rstu}$$

$$\{(A^r \times A^s)^{\gamma} \times (B^t \times B^u)^{\gamma}\}^0.$$

Here the orbits are labelled by r, s, t, u and they are understood to be ordered in some definite fashion, ε_r is the single-particle energy of orbit r, $W^{\gamma}{}_{rstu}$ is the anti-symmetrized two-body matrix element $\langle (rs)_{\gamma}\,|H_2|\,(tu)_{\gamma}\rangle$ with γ specifying the angular momentum and isospin of the two-particle states; A^r and B^r are the operators which create and destroy a particle in the orbit r, respectively. As mentioned earlier, r stands for both the angular momentum j_r and isospin 1/2 of the single particle in orbit r. Also $[r] = (2j_r + 1)(2 \times 1/2 + 1)$, etc.

In terms of the creation and destruction operators, we can write the two particle-one hole states (1) as

$$[h_i^{-1}(p_jp_k)_{\Gamma_p}]_{\Gamma} \equiv -\frac{1}{\sqrt{1+\delta p_jp_k}} \{B^{h_i} \times (A^{p_j} \times A^{p_k})^{\Gamma_p}\}^{\Gamma}\,|\,\text{c.s.}\rangle. \tag{3}$$

These states are not directly the eigenstates of the hamiltonian. In order to find the eigenstates, we proceed in the usual manner of setting up separate hamiltonian matrices for each Γ, and then diagonalize these matrices. Using the second-quantization formalism, discussed in detail by French (1966), treating the states and operators on the same footing, and employing the standard Racah algebraic techniques, we have derived an analytic expression for the matrix element of the hamiltonian (2) between any two states of the type (3). A typical matrix element is given by the following equation:

$$\langle [h_1^{-1}(p_1p_2)_{\Gamma_p}]_\Gamma | H | [h_2^{-1}(p_3p_4)_{\Gamma'_p}]_\Gamma \rangle$$

$$= \delta_{h_1h_2}\delta_{\Gamma_p\Gamma'_p}(E_{\text{c.s.}} - \varepsilon_{h_1} + \varepsilon_{p_3} + \varepsilon_{p_4}) \frac{\delta_{p_1p_3}\delta_{p_2p_4} - (-1)^{p_1+p_2-\Gamma_p}\delta_{p_1p_4}\delta_{p_2p_3}}{\sqrt{(1+\delta_{p_1p_2})(1+\delta_{p_3p_4})}}$$

$$+ \delta_{h_1h_2}\,\delta_{\Gamma_p\Gamma_{p'}}\, W^{\Gamma_p}{}_{p_1p_2p_3p_4}$$

$$+ (-1)^{h_1+h_2}[\Gamma_p\Gamma'_p]^{\frac{1}{2}}\,[(1+\delta_{p_1p_2})(1+\delta_{p_3p_4})]^{-\frac{1}{2}} \times$$

$$\times [\delta_{p_1p_4}(-1)^{p_3-p_4+\Gamma_p}\sum_\gamma[\gamma] \begin{Bmatrix} \gamma & p_3 & h_1 \\ p_2 & p_1 & \Gamma_p \\ h_2 & \Gamma'_p & \Gamma \end{Bmatrix} W^\gamma{}_{h_1p_3h_2p_2} - \delta_{p_2p_3}(-1)^{p_1+p_3}\sum_\gamma[\gamma]$$

$$\begin{Bmatrix} \gamma & p_3 & h_1 \\ p_1 & p_2 & \Gamma_p \\ h_2 & \Gamma'_p & \Gamma \end{Bmatrix} W^\gamma{}_{h_1p_3h_2p_1} - \delta_{p_1p_3}(-1)^{\Gamma_p+\Gamma'_p+2\Gamma}\sum_\gamma[\gamma] \begin{Bmatrix} \gamma & p_4 & h_1 \\ p_2 & p_1 & \Gamma_p \\ h_2 & \Gamma'_p & \Gamma \end{Bmatrix}$$

$$W^\gamma{}_{h_1p_4h_3p_2} + \delta_{p_2p_3}(-1)^{p_1-p_2+\Gamma'_p}\sum_\gamma[\gamma] \begin{Bmatrix} \gamma & p_4 & h_1 \\ p_1 & p_2 & \Gamma_p \\ h_2 & \Gamma'_p & \Gamma \end{Bmatrix} W^\gamma{}_{h_1p_4h_2p_1}]. \quad (4)$$

In this equation $E_{\text{c.s.}}$ is the energy of the closed shell and the curly brackets are $9j$ symbols. The meaning of the rest of the symbols has already been explained. We would like to add that in the *JT* formalism, the $9j$ symbol in the above expression actually stands for a product of two $9j$ symbols, one in the angular momentum space and the other in the isospin space. It should also be noted that all the *W*'s are particle-particle interaction matrix elements.

3. Results

3.1. *Energy levels*

With the help of the prescription described in section 2, we have calculated the energies and wave-functions of the $2p$-$1h$ states in ^{41}Ca and ^{41}Sc. Our model space included $1d_{3/2}$ and $2s_{1/2}$ hole-orbits and $1f_{7/2}$ particle-orbit. A look at the result shows that this space is sufficient to produce the desired fine structure of the even-parity states. The single-particle energies of the $1d_{3/2}$ and $2s_{1/2}$ orbits with respect to that of the $1f_{7/2}$ orbit were taken as −7·24 and −9·74 MeV, respectively; these values roughly agree with the relevant observed single-particle levels of mass-39 nuclei (Endt and Van der Leun 1973). The $f^2_{7/2}$ interaction, that we used, has been derived

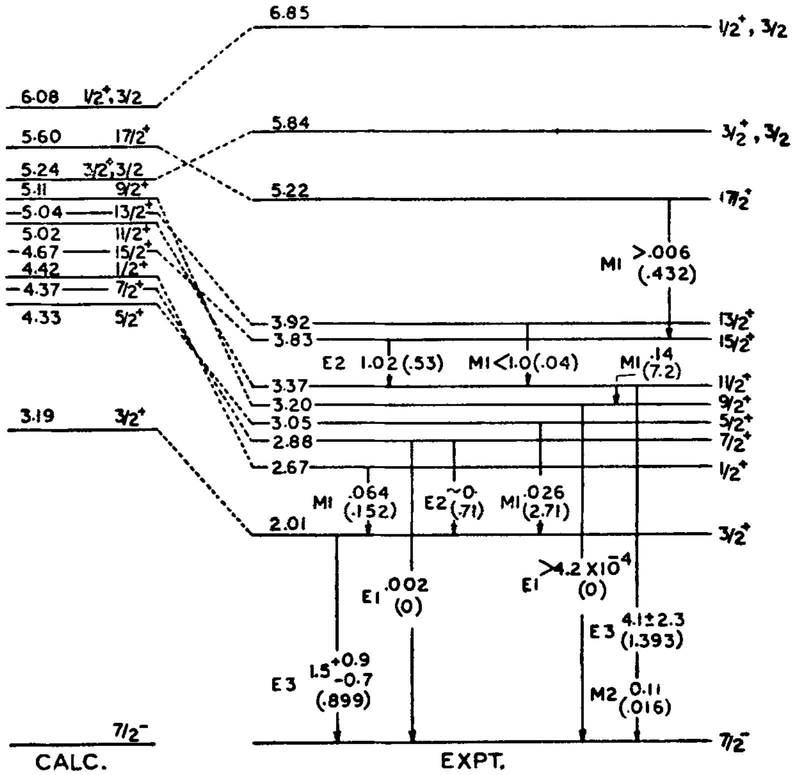

Figure 1. The even-parity states and e.m. transitions in ^{41}Ca. The diagram shows the lowest state belonging to each spin. Only those transitions are presented for which the experimental strengths are known. The transition strengths in Weisskopf units, are written in between the transition lines, the numbers in parenthesis being the calculated values. Energies of the levels are in MeV.

from the ^{42}Sc spectrum (Schiffer and True 1976). For the remaining two-body matrix elements, involving $f_{7/2}$, $d_{3/2}$ and $s_{1/2}$ orbit, we used the re-normalized reaction matrix elements given by Kuo and Brown (1968).

The calculated energies of the even-parity states in ^{41}Ca and ^{41}Sc are compared with the experimental values in tables 1 and 2, respectively. The level scheme of ^{41}Ca is shown in figure 1 also. To make the comparison easier, we have shifted the calculated spectrum (in both the tables) downwards by about 1 MeV so that the excitation energy of the lowest even-parity state, that is, the first $3/2^+$ state agrees with the corresponding experimental result. It is seen that the present calculation reproduces the relative spacings in the fine structure of the even-parity states, but the absolute energies of individual levels are not given correctly.

Table 1. Energies of the even-parity states in ^{41}Ca with respect to its ground state. The calculated and experimental energies for the lowest $3/2^+$ level are made to agree by sliding down the calculated spectrum through 1·2 MeV.

$J^\pi; T$	Excitation energy (MeV)		$J^\pi; T$	Excitation energy (MeV)	
	Calc.	Expt.[a]		Calc.	Expt.[a]
$1/2^+;1/2$	3·24	2·67	$1/2^+; 3/2$	4·90	6·85
	3·70	3·40		6·85	8·54
	4·31	3·85			
$3/2^+;1/2$	2·01	2·01	$3/2^+; 3/2$	4·06	5·84
	3·85	3·53		6·32	
	4·25	3·74	$5/2^+; 3/2$	5·97	
				7·16	
$5/2^+;1/2$	3·15	3·05			
	4·22	3·73			
	5·03	3·98			
$7/2^+;1/2$	3·19	2·88			
	4·41				
$9/2^+;1/2$	3·93	3·20			
	5·07	4·97			
	5·52				
$11/2^+;1/2$	3·84	3·37			
	4·43				
$13/2^+;1/2$	3·86	3·92			
	4·31				
$15/2^+;1/2$	3·50	3·83			
	4·80				
$17/2^+;1/2$	4·42	5·22			

(a) The experimental energies are from (i) Endt and Van der Leun 1973; (ii) Gorodetzky *et al* 1973, and (iii) Lieb *et al* 1974.

Table 2. Energies of the even-parity states in ^{41}Sc with respect to its ground state. The calculated and experimental energies for the lowest $3/2^+$ states are made to agree by sliding down the calculated spectrum through 1·1 MeV.

$J^\pi; T$	Excitation energy (MeV)		$J^\pi; T$	Excitation energy (MeV)	
	Calc.	Expt.[a]		Calc.	Expt.[a]
$1/2^+;1/2$	3·34	2·72	$13/2^+;1/2$	3·95	
	3·80	3·41		4·40	
	4·41	3·97	$15/2^+;1/2$	3·58	
		5·02		4·88	
$3/2^+;1/2$	2·10	2·10	$17/2^+;1/2$	4·51	
	3·95	(3·57)			
	4·35	(4·50)			
	4·94	(4·78)			
$5/2^+;1/2$	3·25	2·97	$1/2^+;3/2$	5·00	
	4·32	3·78		6·94	
	5·12	4.25			
	6·17	4·87	$3/2^+;3/2$	4·16	(5·94)
	6·33	5·37		6·42	
		5·57	$5/2^+;3/2$	6·06	
		6·15		7·25	
$7/2^+;1/2$	3·28				
	4·50				
	5·42				
$9/2^+;1/2$	4·02	5·03			
	5·17				
	5·61				
$11/2^+;1/2$	3·93				
	4·53				

(a) From Endt and Van der Leun (1973). Parenthesis enclosing an energy value indicate uncertainty in the spin assignment for that level.

3.2. *Electromagnetic transition strengths*

Using the wavefunctions obtained in section 3.1, we have calculated the transition strengths for the γ-decay of various even-parity states in ^{41}Ca to the ground state and other low-lying states. The ground state ($7/2^-$) is assumed to be a pure $1f_{7/2}$ single-particle state. The magnetic multipole transitions were computed using the free gyromagnetic ratios for the proton and neutron, whereas for the electric multipole transitions, we assumed effective charges of proton and neutron to be 1·5e and 0·5e, respectively. The radial integrals were evaluated using harmonic oscillator wave-functions with the oscillator parameter given by $\hbar\omega = 41\ A^{-1/3}$ MeV.

Table 3. Electromagnetic transitions in ^{41}Ca.

J_iT_i	J_fT_f	$E_i \rightarrow E_f$ (MeV) Expt.	$E_i \rightarrow E_f$ (MeV) Calc.	Type of transition	Transition strength (W.U.) Calc.	Transition strength (W.U.) Expt.	Reference for experimental value
$3/2^+1/2$	$7/2^-1/2$	2·01→0	3·19→0	E3	0·899	$1{\cdot}5\pm^{0{\cdot}9}_{0{\cdot}7}$	Tabor *et al* 1975
				M2	4·641		
$1/2^+1/2$	$7/2^-1/2$	2·67→0	4·42→0	E3	12·682	—	
	$3/2^+1/2$	2·01	3·19	E2	0·267	—	
				M1	0·152	0·064	Endt and Van der Leun 1973
$7/2^+1/2$	$7/2^-1/2$	2·88→0	4·36→0	E1	0	0·002	-do-
	$3/2^+1/2$	2·01	3·19	E2	0·707	$\simeq 0$	-do-
$5/2^+1/2$	$7/2^-1/2$	3·05→0	4·33→0	E1	0	—	
		2·01	3·19	E2	0·786	—	
				M1	2·706	0·026	-do-
$9/2^+1/2$	$7/2^-1/2$	3·20→0	5·11→0	E1	0	$>4{\cdot}2\times10^{-4}$	Gorodetzky *et al* 1973
$11/2^+1/2$	$7/2^-1/2$	3·37→0	5·02→0	E3	1·393	$4{\cdot}1\pm2{\cdot}3$	-do-
				M2	0·016	$0{\cdot}109\pm0{\cdot}008$	-do-
	$7/2^+1/2$	2·88	4·36	E2	0·646	—	
	$9/2^+1/2$	3·20	5·11	E2	0·226	—	
				M1	7·225	$0{\cdot}14\pm0{\cdot}01$	-do-
$5/2^+1/2$	$7/2^-112$	3·73→0	5·40→0	E1	0	$7{\cdot}7\times10^{-4}$	Endt and Van der Leun 1973
$15/2^+1/2$	$11/2^+1/2$	3·83→3·37	4·68→5·02	E2	0·530	$1{\cdot}02\pm0{\cdot}11$	Gorodetzky *et al* 1973
$13/2^+1/2$	$7/2^-1/2$	3·92→0	5·04→0	E3	2·847	—	
	$9/2^+1/2$	3·20	5·11	E2	0·023	—	
	$11/2^+1/2$	3·37	5·02	E2	0·095	—	
				M1	0·037	$<1{\cdot}0$	-do-

Table 3 (*contd.*)

J_iT_i	J_fT_f	$E_i \to E_f$ (MeV) Expt.	$E_i \to E_f$ (MeV) Calc.	Type of transition	Transition strength (W.U.) Calc.	Transition strength (W.U.) Expt.	Reference for experimental value
17/2+1/2	15/2+1/2	5·22→3·83	5·60→4·68	E2	1·794	—	
				M1	0·432	>0·006	Gorodetzky *et al* 1973
3/2+3/2	7/2−1/2	5·84→0	5·25→0	E3	0·300		
				M2	2·684		
	3/2+1/2	2·01	3·19	E2	0·138		
				M1	0·287		
	1/2+1/2	2·67	4·42	E2	0·268		
				M1	0·192		
	7/2+1/2	2·88	4·36	E2	1·536		
	5/2+1/2	3·05	4·33	E2	0·526		
				M1	6·603		
	5/2+1/2	3·73	5·40	E2	0·021		
				M1	15·180		
1/2+3/2	7/2−1/2	6·85→0	6·08→0	E3	0·183		
	3/2+1/2	2·01	3·19	E2	0·805		
				M1	0·150		
	1/2+1/2	2·67	4·42	M1	3·176		
	5/2+1/2	3·05	4·33	E2	0·131		
	5/2+1/2	3·73	5·40	E2	0·799		
	3/2+3/2	5·84	5·25	E2	7·081		
				M1	0·306		

Table 3 and figure 1 show a comparison between the calculated transition strengths and the experimentally determined values. Except for the 3·05 ($5/2^+$)→2·01 ($3/2^+$) and 3·37 ($11/2^+$)→3·20 ($9/2^+$) M1 transitions, and the 3·37 ($11/2^+$)→g.s. ($7/2^-$) M2 transition, the calculated strengths are in reasonable agreement with the experimental numbers. In the model space we have chosen, E1 transitions are not allowed which is not unreasonable in view of the fact that even experimentally the E1 transitions are found to be very weak.

4. Conclusions

The results presented in the last section show that the relative energy spacings of the calculated spectra and the electromagnetic transitions are (considering the large experimental errors in them) in reasonable agreement with their experimental counterparts; however, there is a discrepancy in the agreement between absolute energy values. Such a discrepancy need not worry us too much because the Kuo-Brown interaction (used by us) which is known to be weaker (i.e. less attractive) in the $T=0$ case and less repulsive in the $T=1$ case (Sartoris and Zamick 1967b; Bansal 1968; Osnes and Kuo 1973) is expected to push up the calculated spectra, as is seen in the present calculation.

Enlarging the model space does not help in obtaining better agreement with the observed level scheme; this conclusion is borne out by a calculation done by Sartoris and Zamick (1967a) with the two-particles in the whole of $1f$-$2p$ shell and the hole either in $1d_{3/2}$ or in $2s_{1/2}$ orbit.

Another calculation of the spectra and e.m. transitions, in the present problem, using a slightly different two-body interaction (bare reaction matrix elements of Kuo and Brown 1968) for the $f_{7/2}$-$d_{3/2}$ and $f_{7/2}$-$s_{1/2}$ configurations shows that the level spacings and the wave functions of the states do not change to any significant extent.

An alternative approach to the problem may lie in using an empirical sort of particle-hole interaction extracted by fitting the relevant available experimental data in this mass-region; this type of investigations are under study.

In view of the availability of many calculated results (table 3) we would like to suggest the advisability of making more measurements on the various transition probabilities between the even parity states in ^{41}Ca and other such type of nuclei.

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