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Calculation of energy spectra in $N = 28$ nuclei †

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Abstract. Energy spectra of the nuclei for $N = 28$, $22 \leq Z \leq 26$ are calculated within the framework of the shell model by using a two-range central-plus-tensor potential proposed by Schiffer. An inert ^{48}Ca core is assumed. Calculations are made in several basic vector spaces. Good isospin is included for the case of one proton excitation.

Numerous shell-model investigations of the $1f$ - $2p$ shell nuclei have been performed in recent years. It is usual to assume ^{40}Ca or ^{48}Ca to be an inert core. The earlier calculations (McCullen *et al* 1964, de Shalit 1963, Talmi and Unna 1960) suggest that a pure $f_{7/2}$ nucleon configuration model is a reasonable first-order approximation. Later investigations by Auerbach (1967) and Lips and McEllistrem (1970) include some configurations involving $p_{3/2}$ and $f_{5/2}$ nucleons. Considerable improvement was obtained when compared with the pure configuration. Osnes (1971) has investigated further the energy spectra for $N = 28$ nuclei with a correct treatment of isospin in a mixed configuration. In the works of Lips and McEllistrem and Osnes only 17 excited levels were included in their χ^2 calculations. However, recent observations have yielded about 30 available excited levels. Furthermore, in their calculations, the two-body matrix elements were treated as parameters, so that there were a large number of parameters relative to the number of observed energy levels in their χ^2 fit. They also included the binding energies in the χ^2 fit without the correction for Coulomb interaction in their investigations. In view of this discussion, a detailed theoretical investigation of the $N = 28$ and $22 \leq Z \leq 26$ nuclei now seems worthwhile.

The calculations we shall present are all made within the framework of the conventional shell model. ^{48}Ca is assumed to have a closed neutron shell with the $Z - 20$ active protons being distributed in the $1f_{7/2}$, $2p_{3/2}$, $1f_{5/2}$ and $2p_{1/2}$ orbits. In order to investigate the importance of the model space and the effect of good isospin, we perform three calculations. First, we consider the case for where one proton jumps to higher orbits from the $1f_{7/2}$ orbit (referred to as model 1). Next we extend the model space of

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model 1 to include also the case of two protons excited from the $1f_{7/2}$ orbit (referred to as model 2). Finally we include the good isospin for the configuration $(1f_{7/2})^{n-1} (2p_{3/2}, 1f_{5/2}, 2p_{1/2})^1$ (referred to as model 3). The states with good isospin T_j for each j orbit can be constructed by applying the projection operator (Löwdin 1955)

$$P_{T_j} = \prod_{i \neq j} \frac{T^2 - T_i(T_i + 1)}{T_j(T_j + 1) - T_i(T_i + 1)}$$

to any state containing a component of isospin T_j . Osnes (1970, 1971) has applied this method successfully to the $f_{7/2}$ -shell nuclei. We use the same form of matrix elements as in his work.

The effective residual interaction is assumed to be a two-range central-plus-tensor potential as assumed in Schiffer's (1971) model. The harmonic-oscillator single-particle wavefunctions are employed in this calculation. The oscillator constant is fixed as $\nu = 0.96 \times A^{-1/3} \text{ fm}^{-2}$, where $A = 50$ (this corresponds to the oscillator energy $\hbar\omega = 10.86 \text{ MeV}$). The radial dependence of the effective residual interaction is taken to be of Yukawa type with interaction ranges $r_1 = 1.415 \text{ fm}$ and $r_2 = 2.0 \text{ fm}$, the same as those of Schiffer and True (1976). In the calculation of models 1 and 2, only one kind of nucleon (i.e. proton) is considered to be outside the inert core; thus the interaction possesses singlet-even (CSE) and triplet-odd (CTO) components for both ranges of central force, and a tensor-odd (TTO) component for short range. These five interaction strengths, treated as adjustable parameters, are determined by fitting the observed energy levels. In the calculation of model 3, there are five more interaction strengths for $T = 0$, i.e. singlet-odd (CSO) and triplet-even (CTE) components for both ranges of central force, and a tensor-even (TTE) component for short range. The binding energies of the ground states are not included in the χ^2 fit; therefore the single-particle energy of $1f_{7/2}$ is fixed to be zero. Since there are no accurate single-particle energy levels observed in experiments, the $\epsilon(2p_{3/2})$, $\epsilon(1f_{5/2})$ and $\epsilon(2p_{1/2})$ are also treated as parameters in the χ^2 calculation. It is found that the adjustment of the single-particle energies of $\epsilon(1f_{5/2})$ and $\epsilon(2p_{1/2})$ makes only a slight improvement in the least-squares fit.

Twenty-eight observed excited levels are used in the present calculation of models 1 and 3 and 29 levels in model 2. The calculated excitation energies and the corresponding experimental values for nuclei with $N = 28$, $22 \leq Z \leq 26$ are listed in table 1. We have also calculated the energies for the pure configuration $(1f_{7/2})^n$ (referred to as M0). The results are also listed in the fourth column of table 1 for comparison. The percentages of the neutron excitation based on the isospin basis are shown in parentheses in column M3. For ^{50}Ti , the result of model 3 shows that the effect of neutron excitation of these states is nearly zero. The calculated energy values of the second 2^+ state in models 1, 2 and 3 are 4.84, 4.52 and 4.60 MeV respectively. These values are in good agreement with the observed value of 4.31 MeV. For ^{51}V , Poletti *et al* (1974) have made a tentative spin assignment for the level at 2.699 MeV. Our calculated results for the level $J^\pi = \frac{1}{2}^-$ in the three models (2.708, 2.694 and 2.909 MeV respectively) give favourable support to their assignment. In the calculation of M3, 14% and 13% neutron intensities are found for $(\frac{3}{2}^-)_2$ and $(\frac{5}{2}^-)_2$ states respectively.

For ^{52}Cr , one established level for which the agreement is not good is the first excited 0^+ level at 2.65 MeV. The level is excluded in our χ^2 fit. The value we obtained is 5.17 MeV in model 1, 4.22 MeV in model 2 and 5.25 MeV in model 3. The reason for this large discrepancy is that this level has a significant component in its wavefunction due to

Table 1. The level energies (in MeV) used in the least-squares fit. The last three columns are the calculated values as defined in text. The state marked with an asterisk is not included in the least-squares fit.

Nucleus	J^π	E_{exp}	$E_{\text{cal}}(\text{M0})$	$E_{\text{cal}}(\text{M1})$	$E_{\text{cal}}(\text{M2})$	$E_{\text{cal}}(\text{M3})$	(%)
^{50}Ti	2^+	1.560	1.577	1.652	1.418	1.466	(0)
	4^+	2.680	2.450	2.362	2.208	2.308	(0)
	6^+	3.200	2.980	2.698	2.605	2.680	(1)
^{51}V	$(\frac{5}{2}^-)_1$	0.319	0.549	0.558	0.314	0.251	(2)
	$(\frac{3}{2}^-)_1$	0.926	1.065	1.173	0.950	1.013	(1)
	$\frac{1}{2}^-$	1.609	1.778	1.742	1.664	1.743	(1)
	$\frac{9}{2}^-$	1.813	1.750	1.799	1.702	1.782	(1)
	$(\frac{3}{2}^-)_2$	2.402	—	2.872	2.765	2.940	(14)
	$\frac{1}{2}^-$	2.699	2.855	2.708	2.694	2.909	(1)
	$(\frac{5}{2}^-)_2$	3.082	—	3.306	2.745	3.038	(13)
	^{52}Cr	$(2^+)_1$	1.434	1.595	1.779	1.743	1.731
$(4^+)_1$	2.370	2.452	2.528	2.476	2.504	(1)	
$(4^+)_2$	2.768	2.673	2.692	2.587	2.633	(0)	
$(2^+)_2$	2.965	3.022	3.153	3.007	3.070	(1)	
6^+	3.114	2.995	2.898	3.005	3.050	(1)	
$(2^+)_3$	3.162	—	4.560*	3.606	4.576*	(16)	
5^+	3.616	3.527	3.574	3.507	3.622	(1)	
8^+	4.751	4.898	4.665	4.704	4.969	(1)	
^{53}Mn	$(\frac{5}{2}^-)_1$	0.379	0.582	0.664	0.415	0.455	(1)
	$(\frac{3}{2}^-)_1$	1.290	1.068	1.198	1.018	1.031	(1)
	$\frac{1}{2}^-$	1.441	1.741	1.705	1.639	1.661	(1)
	$\frac{9}{2}^-$	1.621	1.753	1.782	1.669	1.736	(1)
	$(\frac{3}{2}^-)_2$	2.276	—	2.099	1.775	2.077	(20)
	$(\frac{3}{2}^-)_2$	2.407	—	2.481	2.231	2.662	(20)
	$\frac{1}{2}^-$	2.673	—	2.984	3.026	2.881	(20)
	$\frac{1}{2}^-$	2.693	2.868	2.677	2.706	2.835	(0)
^{54}Fe	2^+	1.408	1.599	1.684	1.569	1.514	(0)
	4^+	2.539	2.458	2.455	2.391	2.418	(0)
	6^+	2.948	2.995	2.878	2.887	2.953	(0)
$\epsilon(\text{p}_{3/2})$			3.22	3.05	3.11		
$\epsilon(\text{p}_{1/2})$			4.00	4.10	3.98		
$\epsilon(\text{f}_{5/2})$			4.23	4.34	4.15		
RMS			0.160	0.221	0.243	0.219	

the $(1f_{7/2}^{-2}, 2p_{2/3}^2)$ neutron configuration (Whitten 1967). Our model 3 calculation shows 16% neutron excitation for this state. For the $(2^+)_3$ level the calculated energy is too high compared with the observed energy. However, this discrepancy decreases significantly when the model space is enlarged. For ^{53}Mn , the states with $J^\pi = \frac{1}{2}^-$ and $\frac{9}{2}^-$ and excitation energies between 2 and 3 MeV are all in good agreement with the observed values. Two established levels for which the agreements are not good are the levels $(\frac{1}{2}^-)_2$ and $(\frac{3}{2}^-)_1$. The discrepancy tends to a smaller value when good isospin is considered or more configuration spaces are included. It is worthwhile to mention here that in the calculation of Benson and Johnstone (1975), the neutron excitation in the $\frac{1}{2}^-$ state at 2.67 MeV is found to be of 86.7% intensity, whereas we are able to explain this state by M3 with 20% intensity only. For ^{54}Fe , only the lowest 2^+ , 4^+ and 6^+ states of the pure $(1f_{7/2})^6$ configuration can be fitted in the present calculation. Furthermore, the theoretical number of states is much less than the experimental one. Therefore, the

present work suggests that the ^{48}Ca is no longer a good core for the calculation of ^{54}Fe . It is worthwhile to notice that the calculated value of the 0^+ state at 2.56 MeV is 4.93 MeV in model 1 and can be reduced to 4.08 MeV in model 2.

In the present calculation, neutron excitation becomes more and more important as the value of Z increases. The only exception is for the calculated first excited 0^+ state, where neutron excitations are more important in nuclei with a smaller value of Z . Furthermore, neutron excitation has a more significant effect on even nuclei than on odd nuclei. The enlargement of the model space has only a slight effect on the lowest-lying states which can be accounted for in the pure $(1f_{7/2})^n$ configuration only. For states other than the pure $(1f_{7/2})^n$ configuration, a noticeable decrease in the eigenvalues arises when enlarging the model space from model 1 to model 2 or when good isospin is taken into account.

As we mentioned before, we include only the low-lying excited states which can be accounted for in our model space. Therefore, as shown in table 2, we obtain differences between the calculated and observed binding energies which increase with the value of Z . In order to investigate which approach gives more information, we can proceed as follows.

Table 2. The binding energies (BE), Coulomb interactions and separation energies for $N = 28$, $22 \leq Z \leq 26$ as defined in the text for model 1.

Nucleus	BE				$S(n)$		
	Expt	Calc	Diff	a	Expt	Calc	HFB
^{50}Ti	-2.53	-2.50	-0.03	—	—	—	—
^{51}V	-0.96	-1.99	1.03	0.42	8.05	8.28	8.4
^{52}Cr	-1.84	-3.85	2.01	0.42	10.51	10.48	9.8
^{53}Mn	1.23	-2.44	3.67	0.42	6.56	6.54	8.6
^{54}Fe	2.00	-3.60	5.60	0.42	8.85	8.94	8.8
^{55}Co	6.58	-1.59	8.17	0.43	5.05	5.04	8.4
^{56}Ni	9.03	-2.10	11.13	0.43	7.18	7.38	—

For a pure configuration, the total Coulomb interaction energy and pairing energy of n extra-core protons can be written as

$$\begin{aligned}
 E(n) &= \frac{1}{2}n(n-1)a + [\frac{1}{2}n]b + [\frac{1}{2}n]\Delta \\
 &= \frac{1}{2}n(n-1)a + [\frac{1}{2}n]x \quad x = b + \Delta
 \end{aligned}
 \tag{1}$$

where a is the Coulomb interaction of a pair of protons. The second and third terms in the first line of equation (1) are the pairing term for the Coulomb energy and the nucleon-nucleon interaction respectively. Since the ground states of our results are almost in the pure configuration, we employ the above equation in our calculation. The third term is considered in the equation for it is not included in our calculation of the binding energies. The values of a and x are obtained from the difference between the experimental binding energies and the calculated energies. The calculated value of x is -0.25 . We obtain a negative sign for x because Δ is more attractive than the repulsion of b . The values of a are listed in the fifth column of table 2. It is found that the values of a are almost constant within an upper bound of 0.43 MeV and a lower bound of 0.42 MeV. The average value is 0.42 MeV, which is larger than the value of 0.32 MeV used by Harchol *et al* (1967) in

the calculation of the systematic trends in Coulomb displacement energies of many nuclei with mass numbers up to 145 based on the shell model.

Now let us consider the separation energy of the protons. If there are n protons in the 1f-2p shell, the separation energy can be written as

$$S(n) = S(1) - (n-1)a - \delta(n, \text{even})x - ((E_B(n) - E_B(n-1))) \quad (2)$$

where $\delta(n, \text{even}) = 0$ for n is odd and $\delta = 1$ for n is even, $S(1)$ is the experimental separation energy of protons for ^{49}Sc , i.e. 9.63 MeV. $S(n)$ can be obtained from equation (2) with $E_B(n)$ taken directly from our calculated energies. Column 7 of table 2 presents the calculated values of $S(n)$ while column 6 shows the corresponding experimental values. The last column gives the theoretical values calculated with the Hartree-Fock-Bogoliubov method by Parikh (1973). Comparison of the last three columns in table 2 shows that the calculated separation energies of protons are in good agreement with the observed values.

Table 3 gives the calculated and observed spectroscopic factors for the stripping reaction ($^3\text{He},d$). Table 4 shows the corresponding values for the pick-up reaction ($d, ^3\text{He}$). Experimental values of the spectroscopic factor C^2S , where C is the isobaric spin Clebsch-Gordan coefficient, are given in columns 8-11 of table 3. In the stripping reaction of table 3, the general results for the calculated values for the nuclei ^{51}V , ^{52}Cr , ^{53}Mn and ^{55}Co in models 2 and 3 are in better agreement with the observed values than the calculated values in model 1. For ^{52}Cr the two 4^+ excited states differ by only 0.4

Table 3. The calculated and observed spectroscopic factors for the stripping reaction ($^3\text{He},d$).

Final nucleus	Level	Energy (MeV)	Transfer J^π	Spectroscopic strength S					
				M1	M2	M3	Expt C^2S		
^{51}V	$\frac{7}{2}^-$	0.00	$\frac{7}{2}^-$	0.73	0.63	0.71	0.75 ^a	0.70 ^b	0.70 ^c
	$\frac{5}{2}^-$	0.93	$\frac{5}{2}^-$	0.00	0.01	0.00	—	—	0.01
	$\frac{3}{2}^-$	2.40	$\frac{3}{2}^-$	0.76	0.66	0.58	0.45	0.57	0.42
	$\frac{1}{2}^-$	3.08	$\frac{1}{2}^-$	0.37	0.30	0.26	0.42	—	0.13
^{52}Cr	0^+	0.00	$\frac{7}{2}^-$	3.63	3.18	3.34	3.84 ^d	4.00 ^e	—
	2^+	1.43	$\frac{5}{2}^-$	1.27	1.24	1.24	1.09	1.08	—
	4^+	2.37	$\frac{3}{2}^-$	1.21	0.44	0.27	0.47	0.51	—
	4^+	2.77	$\frac{1}{2}^-$	0.07	0.84	1.00	0.91	0.81	—
	6^+	3.11	$\frac{5}{2}^-$	1.21	1.20	1.15	1.21	1.31	—
	2^+	3.77	$\frac{3}{2}^-$	0.06	0.04	0.05	0.07	—	—
^{53}Mn	$\frac{7}{2}^-$	0.00	$\frac{7}{2}^-$	0.49	0.48	0.48	0.47 ^e	0.51 ^c	0.42 ^a 0.23 ^f
	$\frac{5}{2}^-$	1.29	$\frac{5}{2}^-$	0.01	0.02	0.01	0.07	0.06	0.05 0.04
	$\frac{3}{2}^-$	2.41	$\frac{3}{2}^-$	0.90	0.59	0.53	0.45	0.43	0.44 0.28
^{55}Co	$\frac{7}{2}^-$	0.00	$\frac{7}{2}^-$	0.25	0.26	0.25	0.21 ^g	0.22 ^e	—

^a Čujec and Szöghy (1969).

^b St-Pierre *et al* (1967).

^c O'Brien *et al* (1967).

^d Osnes (1971).

^e Armstrong and Blair (1965).

^f Gunn *et al* (1976).

^g Rosner and Holbrow (1967).

Table 4. The calculated and observed spectroscopic factors for the pick-up reaction (d, ^3He).

Final nucleus	Level	Energy (MeV)	Transfer J^π	Spectroscopic strength S					
				M1	M2	M3	Expt C^2S		
^{48}Sc	$\frac{7}{2}^-$	0.00	$\frac{7}{2}^-$	2.00	1.94	2.00	1.93 ^a		
	0^+	0.00	$\frac{7}{2}^-$	0.73	0.63	0.71	0.74 ^a	0.88 ^b	0.73 ^c
^{50}Ti	2^+	1.56	$\frac{7}{2}^-$	0.42	0.40	0.41	0.37	0.42	0.39
	4^+	2.68	$\frac{7}{2}^-$	0.71	0.69	0.69	0.75	0.88	0.64
	6^+	3.20	$\frac{7}{2}^-$	1.07	1.03	1.06	1.14	1.32	1.05
^{51}V	$\frac{7}{2}^-$	0.00	$\frac{7}{2}^-$	3.63	3.18	3.34	3.70 ^a		
	$\frac{7}{2}^-$	0.00	$\frac{7}{2}^-$	5.81	5.45	5.81	5.93 ^a		
^{53}Mn	$\frac{5}{2}^-$	0.38	$\frac{7}{2}^-$	0.01	0.04	0.01	0.18		
	$\frac{3}{2}^-$	1.29	$\frac{7}{2}^-$	0.00	0.01	0.00	0.10		
	$\frac{3}{2}^-$	2.41	$\frac{7}{2}^-$	0.00	0.05	0.00	0.16		
	$\frac{3}{2}^-$	2.41	$\frac{7}{2}^-$	0.00	0.05	0.00	0.16		

^a Newman and Hiebert (1969).^b Moenster (1967).^c Hinterberger *et al* (1967).

MeV from each other. Federman and Talmi (1965) concluded that seniority mixing exists in the 4^+ states, and the main component is $\nu = 4$ for the lower state and $\nu = 2$ for the higher state. In the present calculation with model 1, the first 4^+ state is dominated by the $\nu = 2$ state with a very small component (about 4%) of the $\nu = 4$ state. In models 2 and 3, the $\nu = 4$ state is below the $\nu = 2$ state with a large seniority mixing and the spectroscopic factors obtained are in very good agreement with the experimental values for model 2 and in reasonable agreement in model 3. This result manifests again the importance of consideration of the good isospin or the enlargement of the model space. For ^{53}Mn and ^{55}Co , the calculated values are in good agreement with the observed values, except the $\frac{3}{2}^-$ state at 2.41 MeV in ^{53}Mn . A remarkable improvement in the calculation for this state can be achieved in the extended model space or by considering the good isospin. The results of the pick-up reaction are shown in table 4. The calculated values for ^{49}Sc , ^{50}Ti and ^{51}V are all in good agreement with the experimental results. Again significant improvement can be obtained by enlarging the model space.

The interaction strengths obtained from the χ^2 fit and the results of Schiffer and True (1976) are listed in table 5. In the case of CSE, the long-range strengths are almost

Table 5. Interaction strengths (in MeV) compared with those of Schiffer and True (ST).

	Range	M1	M2	M3	ST
CSO	short	—	—	131.58	125.53
	long	—	—	- 25.32	- 44.37
CTE	short	—	—	- 89.07	- 118.09
	long	—	—	21.35	27.27
CSE	short	- 57.77	- 47.61	- 39.70	- 49.32
	long	13.53	10.19	3.72	15.47
CTO	short	- 250.92	- 279.06	- 307.24	- 155.82
	long	105.47	113.83	127.02	62.06
TTE	short	—	—	- 39.07	- 42.52
TTO	short	- 20.94	- 1.35	- 10.43	- 6.10

the same value for models 1 and 2 but less repulsive for model 3, and the short-range strengths get closer to the values obtained by Schiffer and True as more model spaces are included. For CTO, the short-range strengths of all three models are more attractive than those of Schiffer and True; this is because our results for long range are more repulsive. The five additional interaction strengths for $T = 0$ in model 3 which we obtained are very close to those of Schiffer and True. However, if only one interaction range is assumed in the calculation, an unreasonably large repulsive tensor force and larger RMS deviation are obtained. Hence, the two-range force is necessary in the least-squares calculation to fit the energy levels.

In conclusion, the general agreements of the energy levels and the spectroscopic factors of the results in the configuration of two-particle excitation or including the good isospin in the one-particle excitation are better than those of the configuration of one-particle excitation. It is found that expanding the model space beyond the $(f_{7/2})^n$ space has little effect on the low-lying levels, which consist of pure $(1f_{7/2})^n$ configuration. However, the calculations of other higher-lying states are improved by enlarging the model space.

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