

Shell-model calculations of one-hole states in the nuclei of $A = 41 - 43$

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The one-hole states of $A = 41 - 43$ nuclei are calculated with a model space spanning the $(f_{7/2}p_{3/2})^n (d_{3/2}s_{1/2})^{-1}$ configurations. The two-body effective interaction is assumed to be the modified surface-delta type. Energy spectra and spectroscopic factors are calculated and compared with the observed values. Satisfactory results are obtained.

[NUCLEAR STRUCTURE $A = 41 - 43$, calculated effective interaction,]
energy spectra, spectroscopic factors.

I. INTRODUCTION

The nuclei in the $1f-2p$ shell have long been of interest to both experimental and theoretical nuclear physicists. Extensive studies have been done¹⁻³ for the normal parity states of the nuclei in this region. For the non-normal parity levels, however, the situation is less well understood. This paper will give a systematic study of the one-hole states in the mass region of $A = 41 - 43$ within the framework of the shell model. The particles are assumed to be distributed in the $1f_{7/2}$ and $2p_{3/2}$ orbitals and one hole is assumed to be in the $1d_{3/2}$ or $2s_{1/2}$ orbital.

A least-squares fit calculation on the non-normal parity states in $1f-2p$ shell nuclei has been performed by Dieperink and Brussard⁴ within the description of the $(1f_{7/2})^n(1d_{3/2})^{-1}$ configuration. In their results, only the low-lying energy levels can be reproduced and the calculated transition rates are not in agreement with the observed values. This discrepancy is due to the fact that the configuration space they used is too small. Later, Hsieh *et al.*⁵ calculated the non-normal parity states for the nuclei in the $A = 39 - 41$ region by expanding the model space to include the complete $(1f-2p)$ shell and single-hole states in the $(2s, 1d)$ shell. Some distinct improvements were obtained. The spectroscopic factors and electromagnetic (EM) transition rates obtained were in reasonably good agreement with experimental data. For the heavier mass region $A = 42$, the extended model space has not yet

been employed. Lawson and Müller-Arnke⁶ have studied the magnetic moment of the $(3/2)_1^+$ state in ^{43}Sc and found that this state does not have a pure $(f_{7/2})^4(d_{3/2})^{-1}$ configuration. The lifetime and magnetic moment can only be accounted for simultaneously by extending the model space to include about 10% of the $(f_{7/2})^4(s_{1/2})^{-1}$ admixture. The importance of the $s_{1/2}$ hole state can also be seen in the spectrum of potassium isotopes; the $l=0$ hole strength steadily decreases in energy with increasing mass. From the $l=1$ single-particle strength observed for levels around 1 MeV in ^{42}Ca , it is clear that the contribution of the $p_{3/2}$ orbital for nuclei of $A \geq 42$ is also important.⁷ Johnstone⁸ recently reported calculations for the one-hole states in potassium isotopes ($A = 40 - 46$) using a model space based on the

$$(f_{7/2}, p_{3/2})^n (d_{3/2}, s_{1/2})^{-1}$$

configuration. The matrix elements of the residual interaction are treated as free parameters which are determined by a least-squares fit to the observed energy levels; good agreement is achieved in his results. The works mentioned above encourage us to reinvestigate the one-hole states in the mass region of $A = 41 - 43$. A better systematic prediction is expected if we expand the original model space $(1f_{7/2}^n, 1d_{3/2}^{-1})$ to include the active particle orbit $2p_{3/2}$ and the active hole orbit $2s_{1/2}$. It is hoped that so doing, and considering only one-particle, instead of multiparticle, excitation from the $1d_{3/2}$ or

$2s_{1/2}$ shell, is probably good enough. The effect due to the center-of-mass spurious-state problem will not be treated in any way here. Although we did not remove the spurious states, the effect of these on the energy level calculation is expected to be small. The reason is as follows. The spurious states are distributed in the space within $1\hbar\omega$ of excitation, and our model space contains only part of them. Furthermore, the intensities of the low-lying states are rather concentrated in certain components of the basis states. Thus, the effect of spurious states is negligible except in the calculation of $E1$ transition rates, which we are not interested in.

II. THE MODEL

In this calculation, we consider the one-hole states of $A=41-43$ nuclei; the nucleus ^{40}Ca is assumed to be the core. The active nucleons are distributed in the $1f_{7/2}$ and $2p_{3/2}$ orbitals and one active hole is allowed in the $1d_{3/2}$ or $2s_{1/2}$ orbital. In order to obtain a model space of manageable size, we neglect the $2p_{1/2}$ orbital. This should not introduce significant errors since the $2p_{1/2}$ lies about 4 MeV above the $1f_{7/2}$ orbital. Also, according to the Kuo-Brown matrix elements, the $f_{7/2}$ - $p_{1/2}$ interaction is very weakly attractive. The omission of the $1d_{5/2}$ and $1f_{5/2}$ orbitals from the model space is quite reasonable because the splitting of the observed single-particle levels of $2s_{1/2}$ - $1d_{5/2}$ and $1f_{5/2}$ - $2p_{3/2}$ are much larger than those of $1d_{3/2}$ - $2s_{1/2}$ and $2p_{3/2}$ - $1f_{7/2}$. Within this model space we diagonalize an effective one-body plus two-body Hamiltonian. We identify the resulting eigenvalues with observed energy levels and use the eigenvectors as wave functions to calculate various observables.

The effective Hamiltonian in this space has the form

$$H = H_0 + H_{pp} + H_{hp} .$$

Here H_0 is the Hamiltonian of the single particle in the effective field of the core. The single-particle energies for active orbitals were chosen initially from the observed single-particle spectra of the masses 39, 40, and 41. H_{pp} represents the effective two-body interactions between the particles in the $1f_{7/2}$ and $2p_{3/2}$ orbitals, while H_{hp} represents the effective interaction between the hole in the $1d_{3/2}$ or $2s_{1/2}$ orbital and the particle in the $1f_{7/2}$ and $2p_{3/2}$ orbitals. The two-body effective interactions are assumed to be the modified surface delta form

$$V_{ij} = 4\pi A_T (\Omega_{ij}) + B_T, \quad T=0,1 ,$$

where A_0 and A_1 are the corresponding interaction strengths for the $T=0$ and $T=1$ states, and B_0 and B_1 are the correction terms to the diagonal matrix elements for the $T=0$ and $T=1$ states, respectively.

With this prescription we carry out a least-squares fit calculation on the energy spectra of $^{41,42,43}\text{Ca}$, $^{41,42,43}\text{K}$, and ^{43}Sc . For the input experimental data, we include in principle all the available low-lying levels with reliable J^π assignments up to the point that the first level with an uncertain J^π assignment appears. Forty-three energy levels are included in the calculation. The eight interaction strengths $(A_0, A_1, B_0, B_1)_{pp}$ and $(A_0, A_1, B_0, B_1)_{hp}$ and the $1d_{3/2}$ - $2s_{1/2}$, $1f_{7/2}$ - $1d_{3/2}$, and $2p_{3/2}$ - $1d_{3/2}$ single-particle energy spacings are varied until the discrepancy between the calculated and observed energy levels is minimized. The overall rms deviation is 0.26 MeV. The best-fit interaction strengths and single-particle energy spacings are listed in Table I. The center-of-mass spurious states have not been removed in the calculation.

A. Energy spectra

The calculated energy spectra produced by the best fit parameters together with the observed values are shown in Figs. 1-3. The experimental data are taken from Endt and Leun.⁷ Those levels that are included in the least-squares fits are marked with an asterisk. The excitation energies of the one hole states were made to fit the observed energies relative to the ground state energies of the nuclei with $A=41-43$. Since we are only concerned with the energy spacings relative to the ground states in our calculation, it is hoped that the adjustable single-particle energies may absorb the discrepancy due to the effect of neglecting the three-hole configuration.

TABLE I. The particle-particle and hole-particle interaction strengths and the single-particle energy spacings (in MeV).

	A_0	A_1	B_0	B_1
pp	-1.73	-0.03	2.20	-0.66
hp	-0.57	0.02	-2.02	-0.32
$1d_{3/2}$ - $2s_{1/2}$			1.68	
$1f_{7/2}$ - $1d_{3/2}$			5.71	
$2p_{3/2}$ - $1d_{3/2}$			6.66	

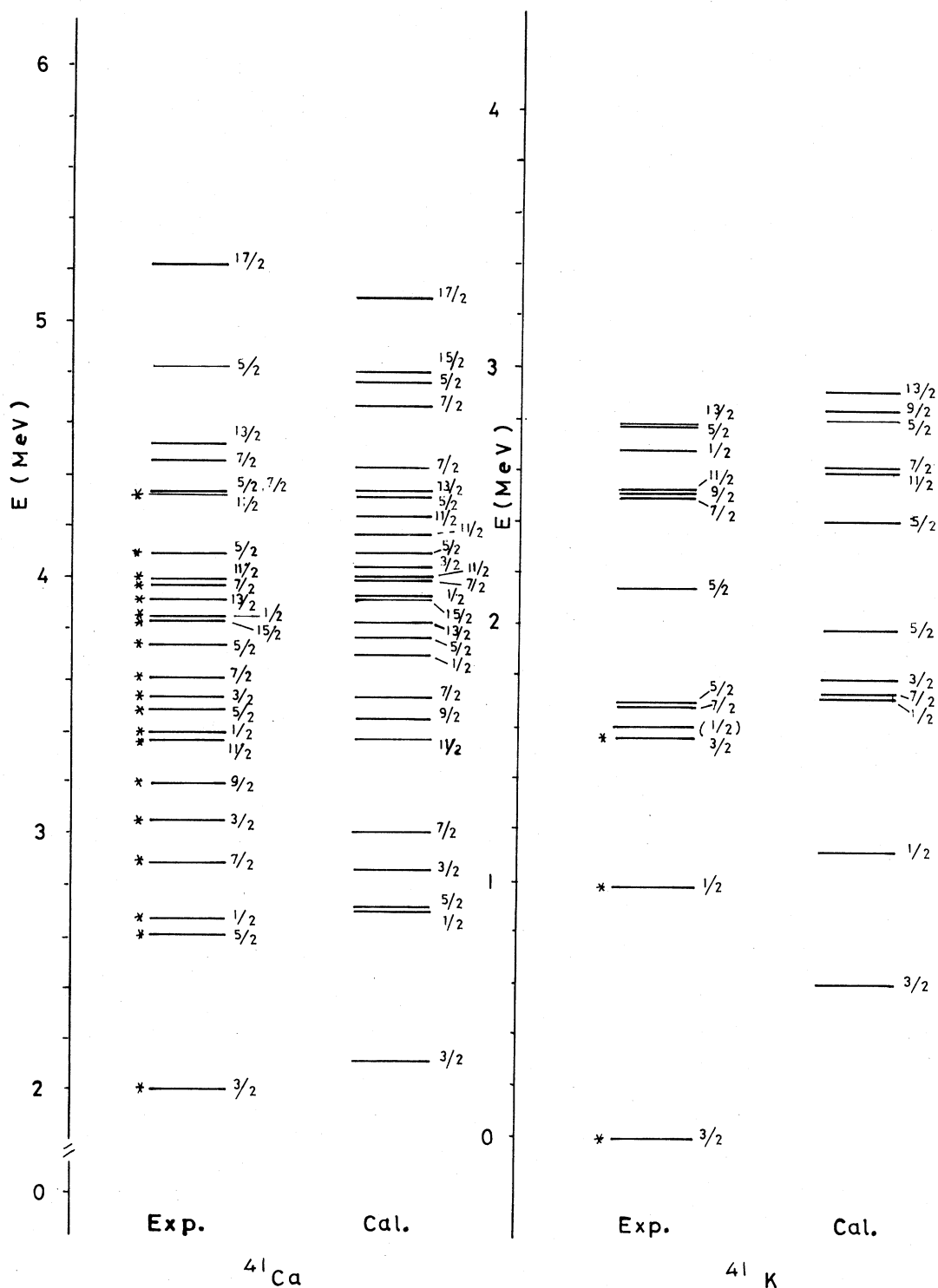


FIG. 1. Experimental and theoretical even parity energy spectra for the $A=41$ nuclei.

The energy spectra of even parity levels for $A=41$ nuclei are shown in Fig. 1. The agreement between calculated and observed energies is reasonably good for most of the levels. For ^{41}Ca our cal-

culated $K^\pi=(3/2)^+$ rotational band based on the 2.01 MeV $(3/2)^+$ level is similar to the results obtained by Hsieh *et al.*⁵ using the complete $(1f2p)^n(2s1d)^{-1}$ configuration space. This seems to

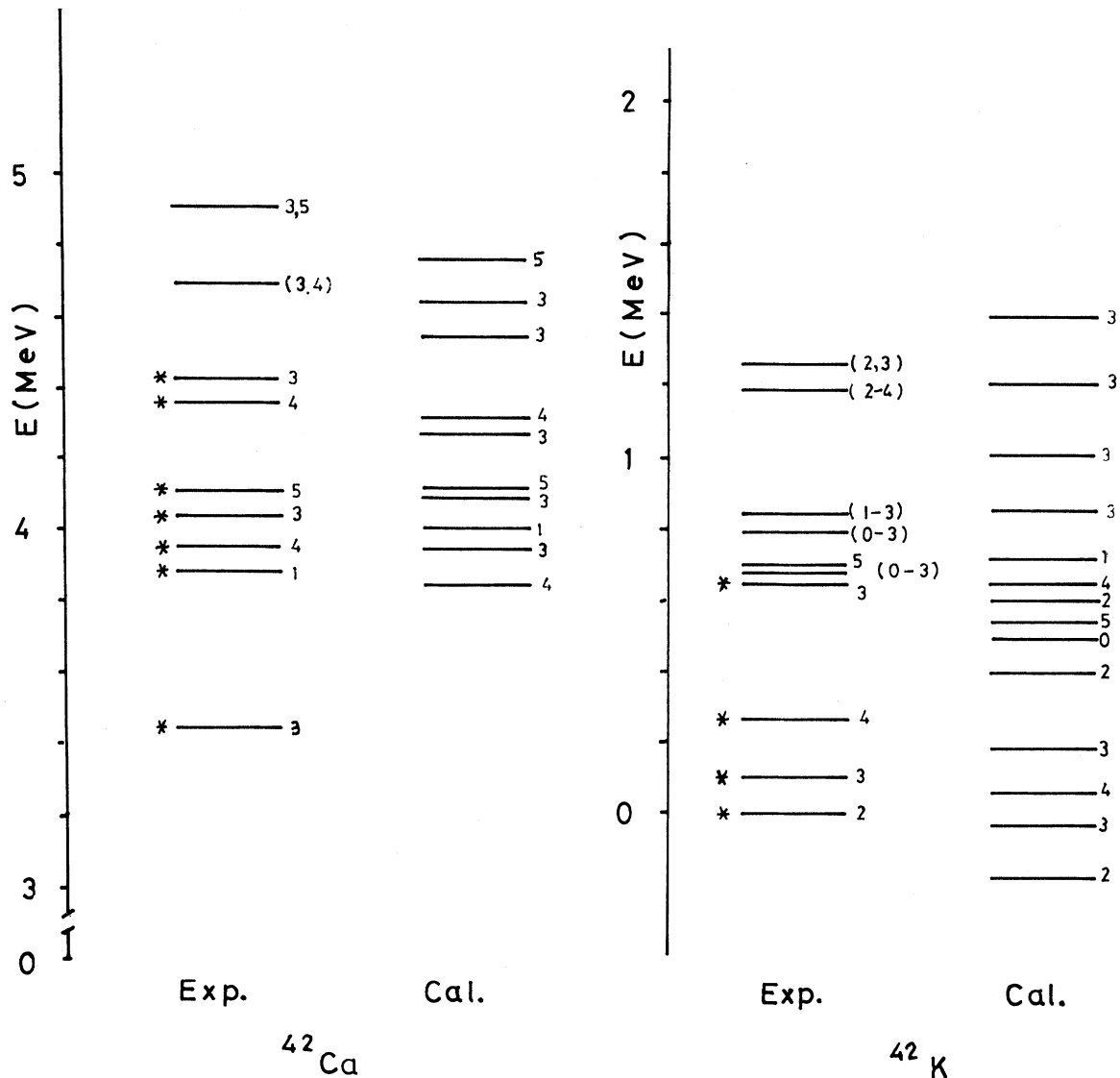


FIG. 2. Experimental and theoretical odd parity energy spectra for the $A=42$ nuclei.

indicate that the inclusion of the $d_{5/2}^{-1}$, $f_{5/2}$, and $p_{1/2}$ orbitals is not necessary. For some lower-lying levels, the intensities of $(s_{1/2}^{-1}f_{7/2})$ and $(s_{1/2}^{-1}p_{3/2})$ are rather strong. For example, the calculated $(1/2)_1^+$ ($T=3/2$) state is dominated by the $(s_{1/2}^{-1}f_{7/2}^2)$ configuration. This seems to justify the necessity of the inclusion of $s_{1/2}$ and $p_{3/2}$ configuration space at least. The four high spin states populated in the $^{39}\text{K}(\alpha,d)^{41}\text{Ca}$ experiment¹⁰ can be well reproduced in our model. The lowest $(11/2)^+$, $(13/2)^+$, $(15/2)^+$, and $(17/2)^+$ levels are given at 3.39, 3.83, 3.91, and 5.11 MeV, and are observed at 3.37, 3.92, 3.83, and 5.22 MeV, respectively. For ^{41}K , the calculated $(3/2)_1$ state gives a large

discrepancy of about 0.6 MeV compared to the observed one. In fact, this is one of the worst fittings in this mass region. The level observed at 1.56 MeV has been suggested¹¹ to be $J^\pi=(1/2)^+$. Our calculated $(1/2)_2^+$ state at 1.67 MeV supports this prediction.

Figure 2 shows the results for the odd parity states of nuclei with $A=42$. For ^{42}Ca , most of the levels are reproduced reasonably well, except the 3_1 state. The calculated energy value for this state is displaced about 0.49 MeV from the observed value. The level at 4.67 MeV is tentatively assigned as $J^\pi=(3-4)^-$. The fitted 3_4^- state at 4.56 MeV seems to favor a 3^- state at 4.67 MeV. For ^{42}K ,

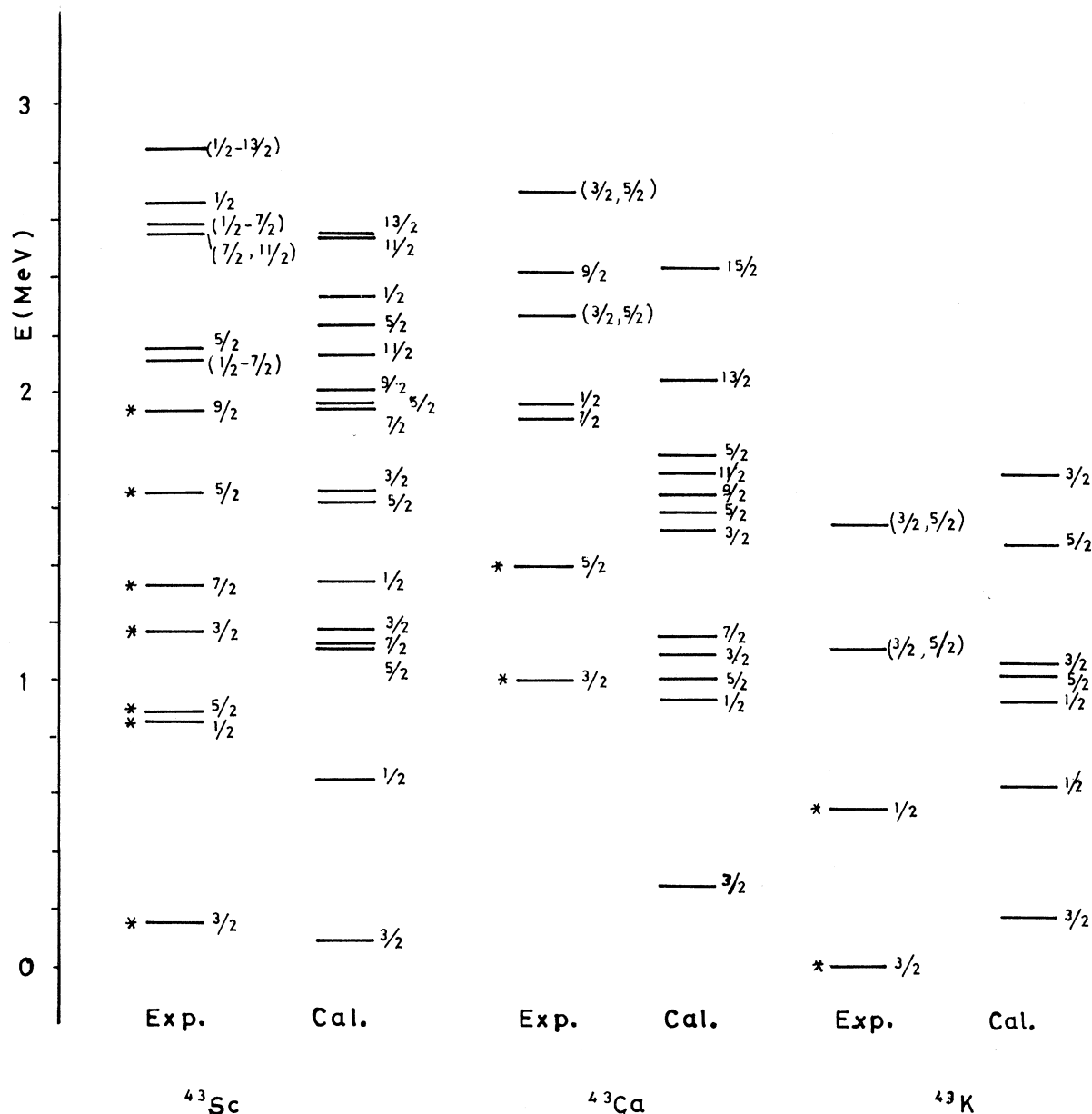


FIG. 3. Experimental and theoretical even parity energy spectra for the $A=43$ nuclei.

most of the calculated states have counterparts in the observed level scheme. The states at 0.68, 0.79, 0.84, 1.19, and 1.26 MeV are uncertainly assigned as $J^\pi=(0-3)^-$, $(0-3)^-$, $(1-3)^-$, $(2-4)^-$, and $(2-3)^-$. Our calculated states at 0.54, 0.72, 0.84, 1.01, and 1.20 MeV seem to suggest that these five levels are 0_1^- , 1_1^- , 3_3^- , 3_4^- , and 3_5^- states, respectively.

The energy spectra for the even parity states of nuclei with $A=43$ are presented in Fig. 3. The cal-

culated energy levels in ^{43}Sc are in reasonably good agreement with experimental values, especially the $(3/2)_1^+$, $(3/2)_2^+$, and $(5/2)_1^+$ states. A pickup reaction¹² leading to the $(3/2)_1^+$ state indicates that this state may be a pure $d_{3/2}$ hole state. But as mentioned above, Lawson and Müller-Arnke have shown that the observed smaller $B(M2)$ values can only be explained if some $(s_{1/2})^{-1}(f_{7/2})^4$ admixture is included. Our calculation shows that the $(3/2)_1^+$ state contains about 5% of the $s_{1/2}^{-1}$ hole com-

TABLE II. The experimental and theoretical spectroscopic factors of ^{41}K and ^{41}Ca for $l=0$ and $l=2$ pickup reactions on ^{42}Ca .

Residual nucleus	T	J_f^π	E_x^{exp} (MeV)	C^2S			
				theo.	exp.		
^{41}K	$\frac{3}{2}$	$\frac{3}{2}^+$	0.11	4.54	4.4 ^a	4.6 ^b	4.5 ^c
	$\frac{3}{2}$	$\frac{1}{2}^+$	0.98	1.06	1.2 ^a	1.0 ^b	1.3 ^c
	$\frac{3}{2}$	$\frac{3}{2}^+$	1.56	0.49		0.21 ^b	0.5 ^c
	$\frac{3}{2}$	$\frac{1}{2}^+$	2.68	1.38	0.9 ^a	0.95 ^b	0.61 ^c
^{41}Ca	$\frac{1}{2}$	$\frac{3}{2}^+$	2.01	2.54	3.0 ^d	2.9 ^e	
	$\frac{1}{2}$	$\frac{1}{2}^+$	2.67	1.04	1.0 ^d		
	$\frac{1}{2}$	$\frac{1}{2}^+$	3.40	0.18	0.18 ^d		
	$\frac{1}{2}$	$\frac{1}{2}^+$					

^aReference 15.

^bReference 13.

^cReference 14.

^dReferences 16 and 17.

^eReference 18.

ponent. For ^{43}Ca , the agreement between calculated and experimental energy levels is not as good as in the case of ^{43}Sc . The calculated excitation energy for the $(3/2)_1^+$ state lies 0.71 MeV below the observed one. In fact, the fit to this state is the worst of all the fittings. The reason for this discrepancy may be that the interaction we used is oversimplified. For ^{43}K , most of the levels came from the $^{44}\text{Ca}(d,^3\text{He})$ and $^{44}\text{Ca}(t,\alpha)$ reactions.^{13,14} Our calculated results are satisfactory.

B. Spectroscopic factors

Table II shows the spectroscopic factors of ^{41}K and ^{41}Ca for $l=0$ and $l=2$ proton and neutron pickup reactions on ^{42}Ca . Our calculated values for this mass number agree very well with the observed data. The calculated value for the $(5/2)^+$ states are zero due to the neglect of the $d_{5/2}^{-1}$ hole in the model space. For ^{41}Ca no experimental $l=2$ reaction has been found for the $(5/2)^+$ level at 2.61 MeV. Thus, the omission of the $d_{5/2}$ orbital is reasonable for low-lying levels. However, the observed strength is 0.17 for the $(3/2)^+$ level at 3.53 MeV and reaches 0.39 for the $(5/2)^+$ level at 3.74 MeV. Our calculated value of 0.01 for the $(3/2)^+$ level at 3.53 MeV is too much underestimated.

Table III shows the spectroscopic information of ^{42}K for the $l=2$ pickup reaction on ^{43}Ca . The main components of the wave functions for these four levels are

$$|d_{3/2}^{-1}, f_{7/2}^3 T_1 = \frac{3}{2}, J_1 \rangle_{T=2, J}$$

where J_1 is mainly $\frac{7}{2}$ for the $J^\pi=4^-$ and 5^- states, but is split into $\frac{5}{2}$ and $\frac{7}{2}$ for the $J^\pi=2^-$ and 3^- states. Our calculated value of 0.47 for the 3^- state at 0.11 MeV is underestimated compared to the observed value of 0.88. This is because the wave function is spread too much in this state.

The calculated and experimental spectroscopic factors of ^{43}K and ^{43}Ca for the $l=0$ and $l=2$ p or n pickup reactions on ^{44}Ca are listed in Table IV. The results for most of the states are in good agreement with the experimental results. For ^{43}Ca , the calculated value for the $(5/2)^+$ state at 1.39 MeV is zero. The experimental value for this state is also very small; however, the null result is due to the neglect of the $d_{5/2}$ orbital in our model. The level at 2.27 MeV is uncertainly assigned as $J^\pi=(3/2, 5/2)_2^+$. Our calculated strength of the $(3/2)_2^+$ state is only 0.06, while the experiment yields about 0.2. For ^{43}K the levels at 1.11, 1.55, and 2.67 MeV (not shown in Fig. 3) are all tentatively assigned to be $J^\pi=(3/2, 5/2)^+$. The good agreement of the calculated and experimental

TABLE III. The experimental and theoretical spectroscopic factors of ^{42}K for $l=2$ pickup reactions on ^{43}Ca .

Residual nucleus	T	J_f^π	E_x^{exp} (MeV)	C^2S	
				theo.	exp. ^a
^{42}K	2	2^-	0.00	0.43	0.45
	2	3^-	0.11	0.47	0.88
	2	4^-	0.26	1.18	1.1
	2	5^-	0.70	1.31	1.4

^aReference 15.

TABLE IV. The experimental and theoretical spectroscopic factors of ^{43}K and ^{43}Ca for $l=0$ and $l=2$ pickup reactions on ^{44}Ca .

Residual nucleus	T	J^π	E_x^{exp} (MeV)	C^2S			
				theo.	exp.		
^{43}K	$\frac{5}{2}$	$\frac{3}{2}^+$	0.0	4.05	2.6 ^a	3.8 ^b	3.8 ^c
	$\frac{5}{2}$	$\frac{1}{2}^+$	0.56	1.40	1.4 ^a	1.4 ^b	2.2 ^c
	$\frac{5}{2}$	$\frac{3}{2}^+$	1.11	0.29	0.27 ^a	0.60 ^b	0.35 ^c
	$\frac{5}{2}$	$\frac{3}{2}^+$	1.55	0.01			0.09 ^c
	$\frac{5}{2}$	$\frac{1}{2}^+$	2.45	0.44		0.38 ^b	
^{43}Ca	$\frac{3}{2}$	$\frac{3}{2}^+$	0.99	2.92	2.4 ^d	3.3 ^e	
	$\frac{3}{2}$	$\frac{1}{2}^+$	1.96	1.18	1.0 ^d	1.6 ^e	

^aReference 19.

^bReference 13.

^cReference 14.

^dReference 20.

^eReference 17.

strengths strongly supports the $(3/2)^+$ assignment for levels at both 1.11 and 1.55 MeV. This is consistent with the result obtained in the calculation of the energy levels. The calculated value for the $(3/2)^+$ level at the 2.67 MeV state is 0.02, which is much smaller than the observed value of 0.47.

To further test the wave functions obtained in our model, we calculated the EM transition rates using the experimental gamma energies. In general, the agreement between the calculated and observed values is satisfactory.

C. Comparison of our model space with the simple $(f_{7/2}^n, d_{3/2}^{-1}, \text{ or } s_{1/2}^{-1})$ configuration

In order to test the significance of our model space, we calculated the intensities of the components of our wave functions which are seen in the coupling of the $s_{1/2}$ or $d_{3/2}$ hole to the simple $f_{7/2}$ structure.

The calculated intensity of the $(f_{7/2}^n, d_{3/2}^{-1}, \text{ or } s_{1/2}^{-1})$ component increases, in general, as the mass number decreases. For an individual mass number, higher isospin states, in general, give a larger intensity of the component $(f_{7/2}^n, d_{3/2}^{-1}, \text{ or } s_{1/2}^{-1})$. Our results also show that the intensity of the component $(f_{7/2}^n, s_{1/2}^{-1})$ is small compared to that of the component $(f_{7/2}^n, d_{3/2}^{-1})$. One important point that has to be mentioned here is that even for certain low lying states, such as $(1/2)_1$ and $(1/2)_2$ states in ^{41}K , the $(1/2)_1$, $(5/2)_2$, and $(3/2)_3$ states in ^{41}Ca , the $(1/2)_1$ state in ^{43}Ca , and the $(1/2)_1$ and $(3/2)_3$ states in ^{43}K , the intensity of $(f_{7/2}^n, s_{1/2}^{-1})$ is larger than 32% and cannot be neglected.

The intensities of the component $(f_{7/2}^n, d_{3/2}^{-1}, \text{ or } s_{1/2}^{-1})$ contained in the wave functions for the

yrast states are larger than 77%, in general. Exceptions are the $(9/2)_1$, $(11/2)_1$, and $(13/2)_1$ states in ^{41}Ca ; the 3_1 and 1_1 states in ^{42}Ca ; and the $(3/2)_1$, $(1/2)_1$, $(5/2)_1$, $(7/2)_1$, $(9/2)_1$, and $(11/2)_1$ states in ^{43}Sc . All of them are smaller than 47%. This manifests the fact that the simple model cannot account for the lower isospin states, and the inclusion of the $p_{3/2}$ configuration space seems to be necessary in this mass region.

Figure 4 shows a typical result for the calculation of $A=42$ nuclei. For ^{42}K , the intensities of the component $(f_{7/2}^3, d_{3/2}^{-1}, \text{ or } s_{1/2}^{-1})$ for the low lying states are larger than 90%. Therefore, the simple model is suitable to account for the level structures of this nuclei. However, for ^{42}Ca , the intensities are smaller than 80%. Especially, the 1_1 , 3_1 , and 3_4 states give only 22%, 46%, and 43% intensities of the component $(f_{7/2}^3, d_{3/2}^{-1}, \text{ or } s_{1/2}^{-1})$. Furthermore, larger intensities of the component $(f_{7/2}^3, s_{1/2}^{-1})$ are also exhibited in the 2_1 and 3_1 states of ^{42}K , and the 3_2 , 3_3 , and 3_4 states in ^{42}Ca .

In conclusion, the simple model is only able to account for most of the low lying states of nuclei with a small mass number, and is only suitable for the calculation of higher isospin states for individual mass numbers. For nuclei with a large mass number, or for states with lower isospin, enlarging the model space becomes more important.

III. CONCLUSION

In this paper we have presented a systematic study on the one hole states for the nuclei of $A=41-43$. By using a modified surface delta ef-

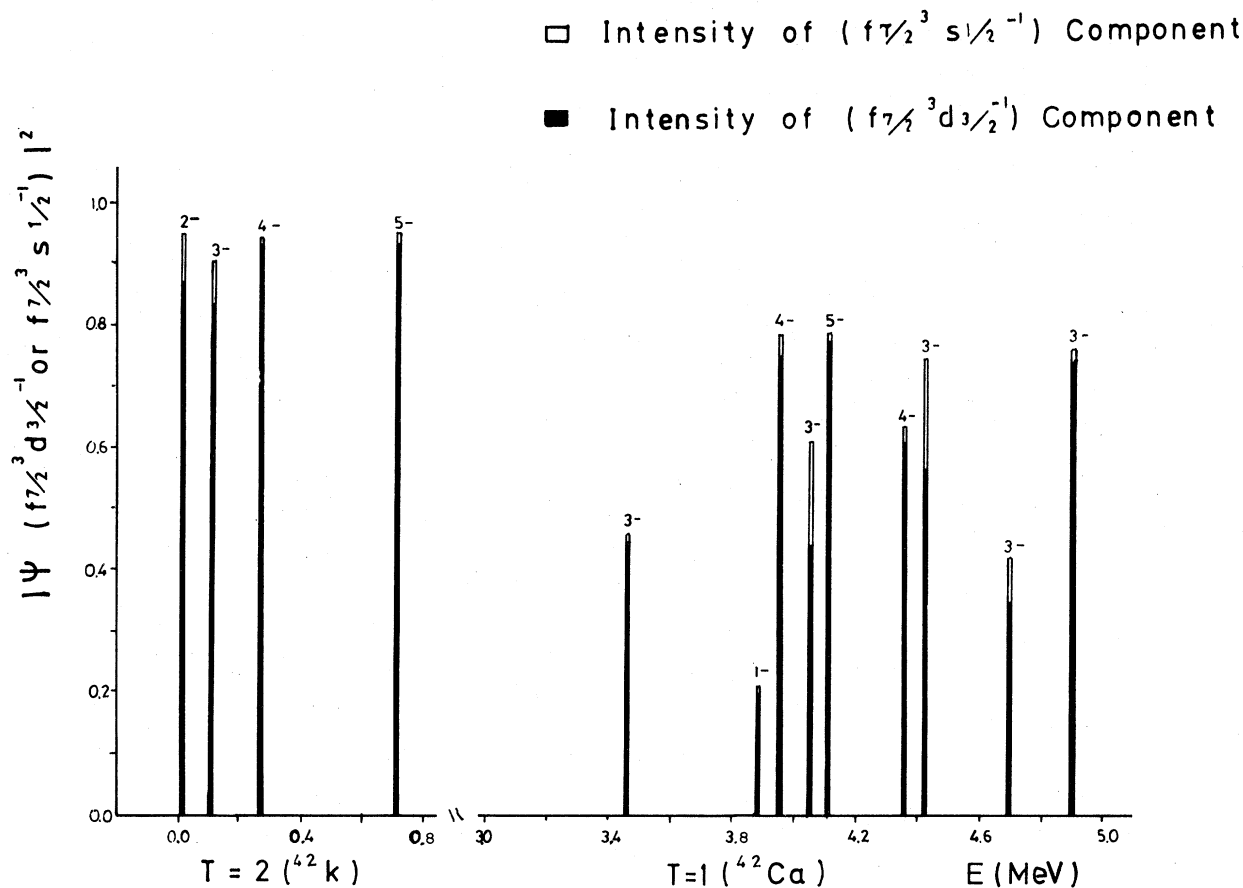


FIG. 4. The intensities of the component $(f_{7/2}^3, d_{3/2}^{-1}, \text{ or } s_{1/2}^{-1})$ for the states in ^{42}K and ^{42}Ca .

fective interaction, the calculated energy spectra are in reasonably good agreement with the experimental data, and some definite predictions are made on the spin-parity assignment for a few low-lying levels of ambiguous experimental spin-parity determination in ^{42}K , ^{42}Ca , and ^{43}K . We have assumed an inert ^{40}Ca core and allowed active $s_{1/2}$, $d_{3/2}$, $f_{7/2}$, and $p_{3/2}$ orbitals. The omission of $f_{5/2}$, $p_{1/2}$, and $d_{5/2}$ orbitals from the model space will not yield significant errors because they lie at about 4 to 6 MeV away from the $f_{7/2}$ level. The contributions of the $p_{3/2}$ and $s_{1/2}$ orbitals are, however, rather important even for some low-lying states. This clearly indicates that any shell-model calculation which attempts to successfully account for the non-normal parity levels of the range of nuclei with mass $A > 40$ will have to use a model space spanning at least the $s_{1/2}$, $d_{3/2}$, $f_{7/2}$, and $p_{3/2}$ single-particle orbitals.

We have also calculated the spectroscopic factors

to test the wave functions obtained. The calculated spectroscopic factors are in good agreement with the experiment. The $l=2$ pickup reactions on ^{43}Ca for the 3_1^- state of ^{42}K do not agree as well as the others, because the wave function of this state is spread too much. This discrepancy may be improved by enlarging the model space. The model space is tested by comparing the intensities of the picture of coupling $s_{1/2}$ and $d_{3/2}$ holes to the simple $f_{7/2}$ structure. Our results show that in this mass region, the $p_{3/2}$ and $s_{1/2}$ orbitals seem to be necessary.

In conclusion, the one-hole states for $A=41-43$ nuclei can be well explained within the conventional shell model by using a model space of $(f_{7/2}, p_{3/2})^n (d_{3/2}, s_{1/2})^{-1}$ configurations.

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