HIGH-SPIN STRUCTURE OF ⁸⁷Sr AND ⁸⁷Zr NUCLEI: SHELL-MODEL INTERPRETATION

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In the present work, we report a comprehensive analysis of shell-model results for high-spin states of ⁸⁷Sr and ⁸⁷Zr for recently available experimental data within the full $f_{5/2}pg_{9/2}$ model space using JUN45 and jj44b effective interactions developed for this model space. In this work, we have compared the energy levels, electromagnetic transition probabilities, quadrupole and magnetic moments with available experimental data. We have confirmed the structure of high-spin states of these two nuclei which were tentatively assigned in the recent experimental work. In the case of 87 Sr, for positive-parity states up to ~ 7.5 MeV, both interactions predict very good agreement with experimental data, while negative-parity states are slightly suppressed in jj44b calculation. For the ⁸⁷Zr nucleus, the jj44b interaction predicts higher energies for the negative-parity states beyond $J \geq 27/2^{-}$. The configuration, which have one hole in $\nu g_{9/2}$ orbital, is responsible for generating the states in 87 Sr. In the case of 87 Zr, low-lying positive-parity states come with the configuration having three holes in the $\nu g_{9/2}$, while the odd-parity states have configuration $\nu (f_{5/2}^{-1} g_{9/2}^{-2})$.

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1. Introduction

Experimental information on low-lying single-particle excited states is available for many nuclei. Because of the advancement in experimental techniques, now it is possible to populate high-spin states of nuclei beyond Ni.

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These experimental results are stringent test for the predicting power of shell model for high-spin excited states. It is possible to test two-body matrix elements for predicting the high-spin states which are generated by aligning the angular momenta due to broken nucleon pairs. The nuclei in Sr–Zr region show many interesting features, such as spherical shell, isomeric states, candidates of double and neutrinoless double beta decay [1-12].

High-spin states of ⁸⁸Zr have been recently populated up to ~ 20 \hbar and an excitation energy of 10 MeV was measured in ⁸⁰Se(¹³C,5*n*)⁸⁸Zr fusionevaporation reaction [13]. Similarly, the high-spin states of ⁸⁹Zr were populated using the fusion-evaporation reaction ⁸⁰Se(¹³C,4*n*)⁸⁹Zr. The observed high-spin states up to 10 MeV excitation energy and spin ~ 37/2 \hbar are reported in Ref. [14]. The dominance of single-particle excitations is shown for both positive- and negative-parity states. The high-spin band structure of ⁸⁵Sr was populated in the reaction ⁷⁶Ge(¹³C,4*n*)⁸⁵Sr [15]. The spin and parity of different levels up to the spin of ~ 35/2 \hbar and an excitation energy ~ 7.5 MeV were established. Here, shell model explains various features, such as the odd–even staggering, very well. In the case of ⁸⁶Sr, the high-spin states were populated using ⁷⁶Ge(¹³C,3*n*)⁸⁶Sr reaction. The level scheme up to 10.9 MeV excitation energy and maximum spin of ~ 19 \hbar have been reported in Ref. [16].

Experimentally, the high-spin structure of ⁸⁷Sr was previously studied in [17, 18]. Recently, using the fusion-evaporation reaction ${}^{82}\text{Se}({}^{9}\text{Be},4n){}^{87}\text{Sr}$, the states were populated up to an excitation energy of 7.4 MeV at spin $31/2\hbar$ reported in Ref. [19]. The structure of high-spin states using in-beam γ -ray spectroscopic method ${}^{87}\text{Zr}$ was studied through the ${}^{59}\text{Co}({}^{32}\text{S},3pn){}^{87}\text{Zr}$ reaction [20], the level scheme was established up to spin $(37/2^+)$ and $(43/2^-)$.

Motivated by the success of our shell-model results in this region for recently measured high-spin states of 88 Zr [13], 89 Zr [14], 85 Sr [15] and 86 Sr [16], in the present work, we will be focusing on the shell-model study of recently populated high-spin states of 87 Sr and 87 Zr.

2. Shell-model calculation

In the present shell-model calculations, 56 Ni is taken as the inert core with the spherical orbits $1p_{3/2}$, $0f_{5/2}$, $1p_{1/2}$ and $0g_{9/2}$. We have performed calculation with the jj44b and JUN45 effective interactions. The jj44b interaction was fitted with 600 binding energies and excitation energies from nuclei with Z = 28-30 and N = 48-50 available in this region. Here, 30 linear combinations of JT coupled two-body matrix elements (TBME) are varied, giving the r.m.s. deviation of about 250 keV from the experiment. The single particle energies (s.p.e.) are taken to be -9.656, -9.287, -8.269 and -5.894 MeV for the $p_{3/2}$, $f_{5/2}$, $p_{1/2}$ and $g_{9/2}$ orbitals, respectively [21]. For the JUN45, the single-particle energies for the $1p_{3/2}$, $0f_{5/2}$, $1p_{1/2}$ and $0g_{9/2}$ orbitals are -9.828, -8.709, -7.839, and -6.262 MeV, respectively. The JUN45 [3] interaction is based on Bonn-C potential, the single-particle energies and two-body matrix elements were modified empirically with $A = 63 \sim 69$ mass region. We have performed calculations using the shell-model code Antoine [22]. The maximum matrix dimension in M-scheme > 30 millions for ⁸⁷Zr.

2.1. Shell-model results for ⁸⁷Sr

Experimental data are available from the earlier works [17, 18] and recent work [19], where the states are populated up to the excitation energy of 7.4 MeV with $31/2\hbar$ spin. Useful structural information can be extracted through the study of this nucleus since both number of protons and neutrons are near closed shells and in this region spherical and collective behaviors of nuclei are important. In Fig. 1, the comparison of our shell-model calculation with the experimental data are shown, where we have used two different JUN45 and jj44b interactions.

The ground state $9/2_1^+$, which comes from the $\nu(g_{9/2}^{-1})$ configuration, is predicted correctly by both calculations. In the JUN45 calculation, the values of $5/2_1^+$ and $7/2_1^+$ energy levels are only 65 keV lower and 3 keV higher than in the experiment, respectively. In the jj44b calculation, they are 86 keV lower and 351 keV higher than in the experiment, respectively. The $1/2_1^+$, $3/2_1^+$, $5/2_2^+$ and $9/2_2^+$ levels are closer to the experiment in the jj44b calculation. The $3/2_2^+$ level is far from experiment almost at the same amount in the both calculations. The $13/2_1^+$ level comes from the $\pi(f_{5/2}^{-1}p_{1/2}^1) \otimes \nu(g_{9/2}^{-1})$ configuration. It is predicted 163 keV and 178 keV lower than in the experiment in the JUN45 and jj44b calculations, respectively.

As it is seen from Fig. 1, all the $17/2_1^+-31/2_1^+$ levels are predicted lower than in the experiment in the JUN45 calculation. In the jj44b calculation, these levels are a little bit lower than even in the JUN45 calculation up to $27/2_1^+$, but $29/2_1^+$ and $31/2_1^+$ levels are well-predicted by this calculation. According to the both shell-model calculations, these states come from $\pi((p_{3/2}f_{5/2}p_{1/2})^{-2}(g_{9/2}^2)) \otimes \nu(g_{9/2}^{-1})$ configuration. Probabilities vary within 35%-60% and 24%-49% in the calculations with the JUN45 and jj44b interactions, respectively. The JUN45 calculation predicts $17/2_2^+$ and $25/2_2^+$ levels in the experiment only with 71 keV and with 279 keV differences, respectively. In the jj44b calculation, they are comparatively low.

The negative-parity $1/2^-$, $3/2^-$, $5/2^-$, $9/2^-_1$ and $11/2^-_1$ levels, which are due to the neutrons in pf shell, are better predicted by the JUN45 calculation. The $7/2^-$ level which appears in both calculations is not measured yet in the experiment, although experimentally the doublet of levels $(5/2^-, 7/2^-)$ is supposed to be at 2656 keV. The negative-parity $13/2^-_1$ ⁸⁷Sr



Fig. 1. Comparison of the theoretical and experimental energy levels of the ⁸⁷Sr.

 $23/2_1^-$ states are due to $\pi((p_{3/2}f_{5/2}p_{1/2})^{-1}(g_{9/2}^1)) \otimes \nu(g_{9/2}^{-1})$ configuration, with 35%–64% and 33%–53% probabilities, in the calculations with JUN45 and jj44b interactions, respectively. As it is seen from Fig. 1, though the distance between $13/2^-$ and $15/2^-$ is larger and those of between the pair of levels $17/2^-$ and $19/2^-$, and $21/2^-$ and $23/2^-$ are more compressed, in general, the negative-parity states are described reasonably well by JUN45 calculation. In jj44b calculation, all negative-parity levels, except $19/2_2^-$, are lower than in the JUN45 calculation.

2.2. Shell-model results for ⁸⁷Zr

The structure of high-spin states of 87 Zr was studied using in-beam γ -ray spectroscopic method through the 59 Co(32 S,3pn) 87 Zr [20]. Positive-parity level scheme was established up to spin ($37/2^+$) and the negative-parity level scheme up to ($43/2^-$).

As in the case of ⁸⁷Sr, ground-state spin of the ⁸⁷Zr is also 9/2⁺ since still neutrons in the $g_{9/2}$ orbital play major role for the ground state. Now, we see that less energy is needed to excite nuclei to $13/2_1^+$ state. This is reasonable since now neutrons are a little bit further from the filling $g_{9/2}$ orbital as compared to the ⁸⁷Sr nucleus. In the calculation with JUN45 interaction, the $9/2_1^+$, $13/2_1^+$, $11/2_1^+$, $21/2_1^+$, $25/2_1^+$, $29/2_1^+$, $31/2_1^+$, $33/2_1^+$, $35/2_1^+$ and $37/2_1^+$ states have the configuration $\pi(g_{9/2})^2 \otimes \nu(g_{9/2})^{-3}$ with probabilities 12%–31%. The $7/2_1^+$, $17/2_1^+$ and $29/2_2^+$ states have the configuration $\pi[(p_{3/2}f_{5/2}p_{1/2})^{-2}(g_{9/2})^2] \otimes \nu(g_{9/2})^{-3}$. Here, the lower proton orbitals contribute to the configuration of these states. In the calculation with jj44b interaction, the $9/2_1^+$, $7/2_1^+$, $13/2_1^+$, $11/2_1^+$, $25/2_1^+$ and $29/2_2^+$ states have $\pi[(p_{3/2}f_{5/2})^{-2}(g_{9/2})^4] \otimes \nu(g_{9/2})^{-3}$ configuration.

From Fig. 2, we can see that between the pair of levels $9/2_1^+$ and $13/2_1^+$, there are $7/2_1^+$ and $7/2_2^+$ levels and between the $13/2_1^+$ and $17/2_1^+$ levels, there are $11/2_1^+$ and $11/2_2^+$ levels in the experiment. In both calculations, the $5/2_1^+$ and $7/2_1^+$ levels appear between the $9/2_1^+$ and $13/2_1^+$ levels, and the $7/2^{+}_{2}$ level appears after the $11/2^{+}_{1}$ level. In Fig. 2, we have not shown the levels for which spins are not assigned in the experiment. But in the experiment, there exist spin not assigned levels with energies 523.7 and 589.7 keV [23] which are close to the calculated $5/2^+_1$ level. The $7/2^+_1$ is close to the experiment in jj44b, but the $7/2^+_2$ level is much higher in both calculations. In the JUN45 calculation, $11/2_1^+$ and $11/2_2^+$ levels are between $13/2^+_1$ and $17/2^+_1$ levels as in the experiment, but in jj44b calculation, $11/2^+_2$ level is located after $17/2_1^+$ level. The $1/2_1^+$, $3/2_1^+$, $9/2_2^+$, and $19/2_1^+$ levels can be spin not assigned levels observed in the experiment [23]. The levels $21/2_1^+$ and $25/2_1^+$ are only 22 and 79 keV higher than in the experiment in the jj44b calculation, respectively. Between these levels, there are $19/2_1^+$ and $23/2^+_1$ levels which also appear in the JUN45 calculation and are not measured in the experiment. In the JUN45 calculation, between the levels $25/2_1^+$ and $29/2_1^+$, which are lower than in the experiment in both calculations, there are $25/2^+_2$ and $27/2^+_1$ levels. They are not measured in the experiment. In the jj44b calculation, only the $27/2^+_1$ level appears between the levels $25/2_1^+$ and $29/2_1^+$. The sequence of levels $29/2_1^+$ and $29/2_2^+$ is the same as the experimental one in both JUN45 and jj44b calculations. Though the distance between the levels is quite similar to the experiment, in the JUN45 calculation, they are a little bit lower than in the experiment. In the jj44b calculation, the first of these levels is only 79 keV higher and the second one is 208 keV lower than in the experiment and the distance between the levels is a little bit compressed as compared to the experiment and the JUN45 calculation.



Fig. 2. Comparison of the theoretical and experimental energy levels of the ⁸⁷Zr.

For $I \geq 29/2_1^+$ states, the $\pi[(p_{3/2}f_{5/2})^{-1}(g_{9/2})^3] \otimes \nu[(f_{5/2}^{-1}g_{9/2}^{-2}]$ configuration dominates. Agreement of the calculated $31/2^+$ level with the experimental one is approximately the same in both calculations. However, the $33/2^+$ level is in better agreement with the experimental one in the jj44b calculation and is lower in the JUN45 calculation. The $35/2^+$ level is located higher than in the experiment in both calculations. In the JUN45 calculation, its value is closer to the experimental one than in the jj44b calculation. The $37/2^+$ level is predicted lower than in the experiment in the JUN45 calculation and is predicted higher in the jj44b calculation.

The arrangement of lowest negative-parity levels of 87 Zr is very similar to those of 87 Sr. As in the case of 87 Sr, we have not shown the levels for which spins are not assigned in the experiment. Therefore, $3/2^-$, $5/2^-$, $7/2^-$ and $9/2^-$ levels which appear in the calculations may be one of these spin not assigned levels. Obviously, these levels are due to the neutrons in pf shell.

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In jj44b, the $1/2^-$ level is predicted much lower than in the experiment. In the JUN45 calculation, it is predicted only 26 keV higher than in the experiment.

The $13/2_1^-$, $21/2_1^-$, $25/2_1^-$, $29/2_1^-$, $29/2_2^-$, $31/2_1^-$ and $33/2_1^-$ levels come from $\pi(g_{9/2}^2) \otimes \nu(f_{5/2}^{-1}g_{9/2}^{-2})$ configuration with 6%–18% probabilities, respectively. All these levels are lower than in the experiment in both calculations. The $13/2_1^-$, $21/2_1^-$, $25/2_1^-$ levels are better described by the JUN45 interaction. The quality of agreement of $29/2_1^-$ and $29/2_2^-$ levels is more or less the same in both calculations. The $31/2_1^-$ and $33/2_1^-$ levels are closer to the experiment in the calculation with jj44b interaction.

The $17/2_2^-$ state comes from $\pi(g_{9/2}^2) \otimes \nu(p_{1/2}^{-1})$ configuration which is close to the experiment in the JUN45 calculation and the jj44 calculation differs from the JUN45 only to 20 keV.

The states $17/2_1^-$, $19/2_1^-$, $19/2_2^-$, $27/2_1^-$, and $31/2_2^-$ levels come from $\pi(p_{1/2}^1g_{9/2}^1)\otimes\nu(g_{9/2}^{-3})$ configuration with 16%–38% probabilities, respectively. The $17/2_1^-$, $19/2_1^-$ and $27/2_1^-$ levels are in better agreement in the JUN45 calculation, while $19/2_2^-$, and $31/2_2^-$ are better in the jj44b calculation.

The 27/2², 35/2⁻₁, and 39/2⁻₁ levels come from $\pi(f_{5/2}^{-1}g_{9/2}^3) \otimes \nu(g_{9/2}^{-3})$ configuration with 24%–50% probabilities, respectively. These states are described well by the calculation with jj44b interaction.

The experimental $43/2^-$ level is measured at 10093 keV. The JUN45 and jj44b calculations predict this level at 9716 keV and at 10527 keV, respectively.

2.3. Occupancy of the orbitals

In order to look closely to the structure of the states, we show the occupancy of different protons and neutrons orbitals for ⁸⁷Sr and ⁸⁷Zr nuclei with JUN45 interaction in Figs. 3 and 4, respectively. As it is seen from Fig. 3, for the positive-parity states in ⁸⁷Sr, the occupancy of the proton orbitals are sensitive to the nuclear spin, including states up to high spins. Here, the $\pi g_{9/2}$ occupancy is increasing at the expense of $\pi f_{5/2}$ and $\pi p_{1/2}$ occupancy. For the negative-parity states, the dependence of the occupancy of the proton orbitals from the spins still remains the same, however now, the neutron occupancy at lower spins shows irregular pattern. For negativeparity states, the occupancy of $\pi g_{9/2}$ is increasing at the expense of the $\pi p_{1/2}$ orbital occupancy only.

From Fig. 4, one can see that the proton occupancy becomes more stable up to high spins in the positive-parity states of the ⁸⁷Zr nucleus as compared to the ⁸⁷Sr nucleus. The visible changes in the occupancy with respect to spins can be seen in $g_{9/2}$ orbital, the increase in the occupancy is at the expense of the $\pi p_{1/2}$ orbital occupancy only, as in the case of ⁸⁷Sr.



Fig. 3. Occupancy of different protons and neutrons orbitals with JUN45 interaction for $^{87}\mathrm{Sr.}$



Fig. 4. Occupancy of different protons and neutrons orbitals with JUN45 interaction for $^{87}\mathrm{Zr.}$

3. Electromagnetic properties

In Table I, we have reported experimental versus calculated B(E2) and B(M1) values in W.u. with different transitions. All the B(E2) values of ⁸⁷Sr are in better agreement with the experiment in both calculations and B(E2) values of ⁸⁷Zr are predicted much larger than in the experiment in both calculations. We have used the recommended $e_p = 1.5e$, $e_n = 1.1e$ values of effective charges [3] in the JUN45 interaction. Larger neutron effective charge is more reasonable in this mass region which is adopted by Honma *et al.* [3] from the least-squares fit to the 49 known experimental values of quadrupole moments. With the $(e_p, e_n) = (1.5, 1.1)$ the agreement between theory and experiment is very good. In the present work, large B(E2) values are due to many nucleons in the valence shells and the agreement may be improved by slightly reducing the effective charges. Quality of the magnetic moment agreement with the experimental data is also like quadrupole moments: the magnetic moments of ⁸⁷Sr are better described by the calculations.

TABLE I

Nucleus	Transition	Exp.	JUN45	jj44b
$^{87}\mathrm{Sr}$	$B(E2; 5/2^+_1 \to 9/2^+_1)$	7.5(23)	10.19	12.27
	$B(E2; 13/2^+_1 \to 9/2^+_1)$	5.5(17)	8.78	9.67
	$B(E2; 5/2^+_2 \to 9/2^+_1)$	0.13^{+5}_{-13}	0.34	0.60
	$B(E2;7/2_1^+ \to 9/2_1^+)$	1.9(5)	3.63	4.46
	$B\left(\text{E2}; 11/2_1^+ \to 9/2_1^+\right)$	> 2.0	4.48	7.45
⁸⁷ Zr	$B(\text{E2}; 7/2^+_1 \to 9/2^+_1)$	3.25(14)	17.68	16.48
	$B(E2; 13/2^+_1 \to 9/2^+_1)$	> 0.36	22.17	38.92
	$B\left(\text{E2}; 21/2_1^+ \to 17/2_1^+\right)$	> 2.19(22)	6.26	1.82
⁸⁷ Sr	$B\left(M1; 7/2_1^+ \to 9/2_1^+\right)$	0.013(3)	0.021	0.0173
	$B\left(\mathrm{M1}; 11/2_1^+ \to 9/2_1^+\right)$	>0.013	0.0489	0.057
	$B\left(M1; 3/2_2^+ \to 5/2_2^+\right)$	0.09(4)	0.009	0.0004
	$B\left(\mathrm{M1}; 3/2^{-}_{1} \to 1/2^{-}_{1}\right)$	0.11(5)	0.246	0.181
⁸⁷ Zr	$B(M1;7/2_1^+ \to 9/2_1^+)$	0.00095(4)	0.003	0.0275
	$B(M1; 17/2_2^- \to 17/2_1^-)$	0.4^{+8}_{-4}	0.044	0.084
	$ B(M1; 19/2^2 \to 17/2^1) $	0.0074(21)	0.166	0.141

Experimental and calculated B(E2) and B(M1) in W.u. for different transitions with $e_p = 1.5e$, $e_n = 1.1e$.

We have listed in Tables II and III, respectively, the electric quadrupole and magnetic moments. For the ⁸⁷Sr nucleus, the $Q(9/2_1^+)$ value is +0.349 eb according to the calculation with JUN45 interaction, which is closest to the experimental +0.305(2) eb value. The jj44b predicts the value larger than experimental one. In the case of ⁸⁷Zr, the $Q(9/2_1^+)$ value is lower for JUN45, while for jj44b, it is very large. Though, in general, quadrupole moments are in excellent agreement with the experimental data, the agreement still can be improved by reducing effective charges which is reasonable for these nuclei. The shape of ⁸⁷Sr is more spherical than ⁸⁷Zr in the $7/2_1^+$ state according to the quadrupole moment values calculated by both interactions for this state.

TABLE II

		$^{87}\mathrm{Sr}$	$^{87}\mathrm{Zr}$
$Q\left(9/2_1^+\right)$	Exp. JUN45 jj44b	+0.305(2) +0.349 +0.415	+0.423 (48) +0.341 +0.649
$Q\left(5/2_1^+\right)$	Exp. JUN45 jj44b	${ m N/A}\ +0.267\ +0.289$	${ m N/A} \ +0.202 \ +0.474$
$Q\left(7/2_1^+\right)$	Exp. JUN45 jj44b	$\begin{array}{c} {\rm N/A} \\ +0.0129 \\ +0.0237 \end{array}$	${ m N/A} \ +0.439 \ +0.484$
$Q\left(11/2_1^+\right)$	Exp. JUN45 jj44b		
$Q\left(13/2_1^+\right)$	Exp. JUN45 jj44b	${ m N/A}\ +0.510\ +0.549$	${ m N/A} \ +0.583 \ +0.835$

Electric quadrupole moments, Q_s (in *e*b), with the two different interactions (the effective charges $e_p = 1.5e$, $e_n = 1.1e$ are used in the calculation).

For the calculation of magnetic moments, $g_s^{\text{eff}} = 0.7 g_s^{\text{free}}$ is used as recommended in Ref. [3]. The results of JUN45 interaction is in very good agreement with experimental data. In the case of jj44b calculation, the predicted value is slightly lower. Here, $g_s^{\text{eff}} = g_s^{\text{free}}$ may improve the results.

TABLE III

		$^{87}\mathrm{Sr}$	$^{87}\mathrm{Zr}$
$\mu\left(9/2_1^+\right)$	Exp. JUN45 jj44b	$\begin{array}{c} -1.0928 \ (7) \\ -1.0298 \\ -0.9796 \end{array}$	$\begin{array}{c} -0.895 \ (9) \\ -0.9401 \\ -0.7816 \end{array}$
$\mu\left(7/2_1^+\right)$	Exp. JUN45 jj44b	${ m N/A} \ -0.9988 \ -0.4717$	${ m N/A} \ -0.7169 \ -0.5596$
$\mu\left(1/2_1^-\right)$	Exp. JUN45 jj44b	+0.624 (4) +0.498 +0.472	+0.642 (7) +0.437 +0.395

For magnetic moments μ (in μ_N), here $g_s^{\text{eff}} = 0.7 g_s^{\text{free}}$ is used in the calculation.

4. Conclusions

Motivated by recent experimental results for high-spin states in ⁸⁷Sr and ⁸⁷Zr, we performed shell-model calculations for these nuclei in $f_{5/2}pg_{9/2}$ model space using JUN45 and jj44b effective interactions. The results for energy levels and electromagnetic transitions are presented. The high-spin energy levels are described very well by the effective interactions for the full $f_{5/2}pg_{9/2}$ model space. In general, both effective interactions show very good agreement with the experimental data. For ⁸⁷Zr, the jj44b interaction predicts negative-parity states beyond $J \geq 27/2^{-1}$ higher in energy. The calculated values of quadrupole moment are in good agreement with available experimental data.

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