

Shell Model interpretation of seniority states in Yttrium isotope around N= 50 shell gap

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Abstract. The yrast states of ^{89}Y have been investigated using large basis shell model calculation with two different effective interactions defined in different model spaces. The calculated excitation energies have been compared with available experimental data. A satisfactory agreement is observed with the *jun45pn* interaction in the low-energy region. Whereas the inclusion of neutron-core excitation becomes essential to describe high-energy, high-spin states. Calculation using the *snt* interaction shows improved agreement in describing these states. The wavefunction and seniority of a few states are discussed.

1 Introduction

Nuclei in the mass region $A\sim 80$ have drawn significant theoretical and experimental interest due to diverse interesting nuclear structure phenomena predicted as well as observed in this region [1-3]. In this region, the shell structure effect also plays a significant role in determining different nuclear properties. For Yttrium isotopes near $N=50$, the structure of nuclei is strongly governed by sub-shell and shell closure at $Z=38, 40$, and $N=50$ [4]. In many early shell model calculations, ^{88}Sr has been used as the closed shell because of the $Z=38$ subshell closure [5]. Yttrium isotopes can be described as one proton particle (with a few neutron particle (s) or hole (s)) with respect to this core. However, only very few low spin states can be described using the model space. In recent works, $\text{fpg}_{9/2}$ model space is widely employed for shell model calculations in this mass region. The presence of neutron core excitation across the $N=50$ shell gap in this mass region is also observed. In case of low spin states, the excitations are primarily generated through the excitation of protons and neutrons within Z or $N=28, 38$, and 50 shell gaps. However, excitation of nucleons across $Z=38$ or $N=50$ shell closure is necessary to describe intermediate to high spin states. Hence, a detailed investigation of the semi-magic nucleus ^{89}Y is of particular interest to explore the nuclear structure. An additional important aspect of semi-magic nuclei, in which either protons or neutrons occupy closed shells, is the concept of seniority. The seniority quantum number provides a particularly useful framework to describe nuclear structure, as it denotes the

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number of valence nucleons not paired to total angular momentum $J=0$ [6]. Due to the dominance of pairing correlation and strong spin-orbit coupling, seniority is often a good quantum number for such systems [7].

In this present work, to analyse the structure, we have carried out Large Scale Shell Model (LSSM) calculation of ^{89}Y using different model spaces and effective interactions. The details of the model space, effective interactions, and calculations are in Section 2. In Section 3, the results of the shell model calculation, i.e., the excitation energy (energy eigenvalue) and the wavefunction (eigenfunction), and the seniority number of a few states have been inspected to describe different excited states of ^{89}Y . Finally, the results and future prospects are summarised in Section 4.

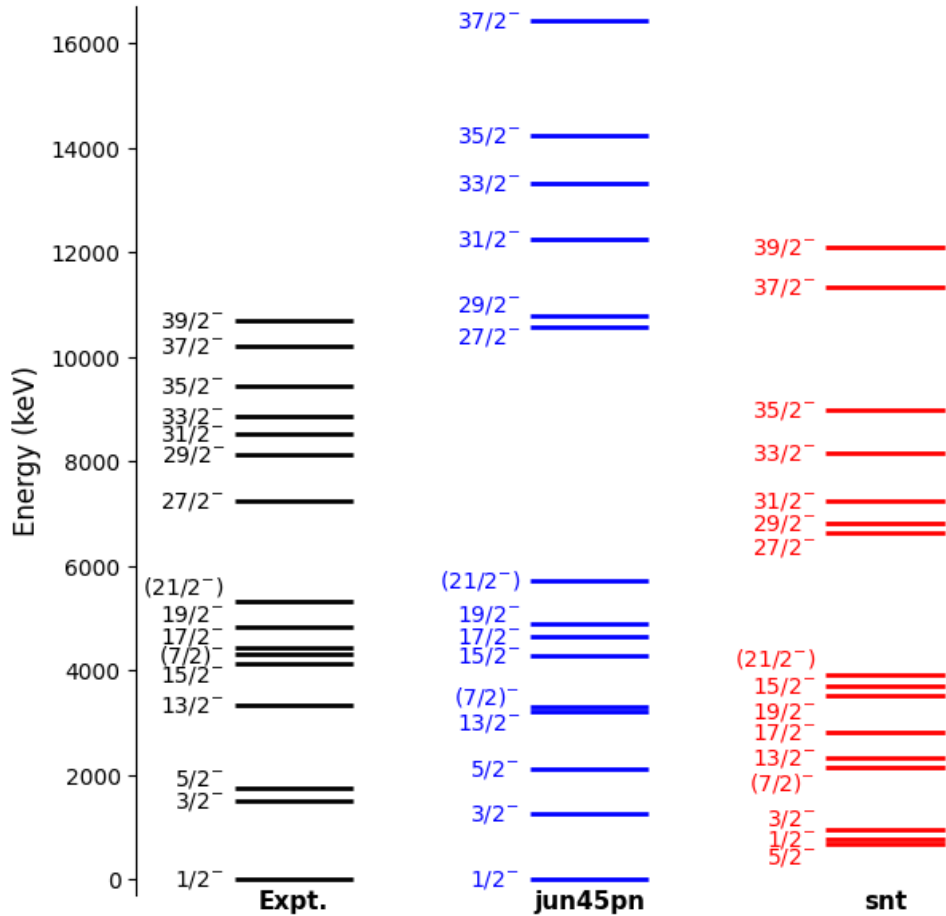
2 Details about the calculation

In this present work, large basis shell model calculation has been performed using two different interactions encompassing two different model spaces available in Nushellx@MSU [8,9]. The first effective interaction is a realistic interaction based on the Bonn-C potential, namely *jun45pn* interaction [10]. The corresponding model space includes four orbitals between ^{56}Ni and $^{100}\text{Sn} - 1f_{5/2}, 2p_{3/2}, 2p_{1/2}, 1g_{9/2}$, orbitals for both protons and neutrons, with ^{56}Ni as the core. The single particle energy of $1f_{5/2}, 2p_{3/2}, 2p_{1/2}, 1g_{9/2}$ orbitals are -8.7087, -9.8280, -7.8388, -6.2617 MeV, respectively, for both nucleons. These SPEs and two body matrix elements (TBME) have been extracted empirically to fit experimental data of mass number $A=63\sim 96$. However, for the calculation of the semi-magic nucleus ^{89}Y with $N=50$, all neutron orbitals will be completely occupied, and no neutron excitation is possible. To include neutron excitation across the $N=50$ shell gap, another interaction with expanded model space is used, namely, the *snt* interaction [11]. The model space includes four orbitals $1f_{5/2}, 2p_{3/2}, 2p_{1/2}, 1g_{9/2}$ below Z or $N=50$ shell gap, and four orbitals $1g_{7/2}, 2d_{5/2}, 2d_{3/2}, 3s_{1/2}$ above Z or $N=50$ shell gap for both nucleons. The SPE for $1f_{5/2}, 2p_{3/2}, 2p_{1/2},$ and $1g_{9/2}$ for protons are 0.525, 1.228, 5.106, and 5.518 MeV, respectively. Whereas the corresponding neutron SPEs for these orbitals are set to be 0 MeV. The SPEs of $1g_{7/2}, 2d_{5/2}, 2d_{3/2},$ and $3s_{1/2}$ for protons are 20.656, 18.893, 20.016, and 16.895 MeV, respectively. The corresponding neutron SPEs for these orbitals are 4.352, 2.313, 3.440, and 2.772 MeV, respectively [8]. But unrestricted calculation using such an enlarged model space is not computationally feasible. To overcome this, proper restrictions are absolutely necessary. For protons, no excitation across the $Z=50$ shell gap is allowed. In contrast, neutron excitations across the $N=50$ gap to $1g_{7/2}$ and $2d_{5/2}$ are included. To start with, three truncation schemes are considered to describe one-particle-one-hole (1p1h) and two-particle-two-hole (2p2h) excitations : (a) one neutron excites to $1g_{7/2}$ orbital (1p1h- $1g_{7/2}$), (b) one neutron excites to $2d_{5/2}$ orbital (1p1h- $2d_{5/2}$), and (c) promotion of up to two neutrons across the $N=50$ shell gap, with each one occupying $1g_{7/2}$ and $2d_{5/2}$ orbitals.

3 Results and discussion

We have calculated the energy spectra of yrast states of both positive and negative-parity states of ^{89}Y arising from different truncations with different interactions. The first excited state is a $9/2^+$ state, which is a spin isomer, decaying to the ground state $1/2^-$ state by $M4+E5$ decay. This state is well reproduced by *jun45pn* interaction, whereas the *snt* interaction reverses the ordering of these states for all truncation schemes. States up to 4.5 MeV are reasonably well reproduced by the *jun45pn* interaction, while calculations considering 1p1h and 2p2h excitation of *snt* interaction deviate more from experimental data, especially in low spin states. Among all the truncation schemes of *snt* interaction, 1p1h- $2d_{5/2}$ truncation scheme

yields the smallest root-mean-squared (RMS) deviation from the experimental data. These RMS calculations have been calculated considering only the low-lying positive and negative yrast states. The experimental energy is available in NNDC ENSDF [12] or XUNDL [13] database. Accordingly, only the 1p1h-2d_{5/2} truncation scheme has been shown in Figs. 1 and 2 for *snt* interaction. The calculated level scheme of ⁸⁹Y using two different interactions has been compared with the experimental data, with the positive and negative parity states shown separately due to the complexity of the spectrum.



In contrast, the *snt* interaction yields systematically lower excitation energies for the low-lying states up to $21/2^-$. For the higher-spin states, from $27/2^-$ to $39/2^-$, the overall agreement with experiment improves, and it gives better prediction than the *jun45pn* interaction in this energy range. Nevertheless, the relative spacing between these levels is somewhat larger than observed experimentally, resulting in an expanded level structure. In addition, the sequential ordering of the higher-spin states is reproduced more reliably, while the lower-lying levels show noticeable rearrangements.

Figure 2 shows the comparison for the positive-parity states. The *jun45pn* interaction reproduces the low-lying levels up to $13/2^+$ in very good agreement with experiment. Beyond the $15/2^+$ state, the predicted excitation energies gradually increase relative to the experimental values, with the deviation reaching approximately 4 MeV for the highest observed state $37/2^+$, similar to negative-parity states. This behavior indicates the importance of the inclusion of neutron excitation in the model space.

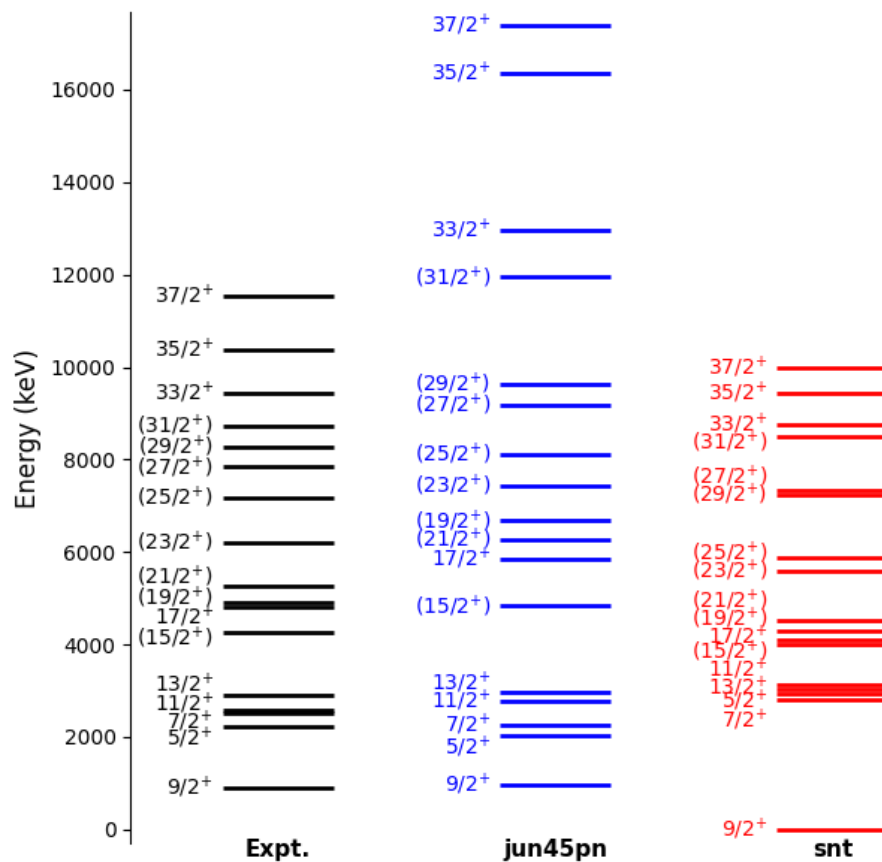


Figure 2 Comparison of the experimentally observed positive-parity states of ^{89}Y with shell-model predictions obtained with the *jun45pn* and *snt* interactions.

In case of *snt* interaction, the excitation energies of the remaining low-lying states are generally higher than the observed values, and the corresponding energy spacings do not fully reflect the experimental level scheme. For the higher-spin positive-parity states, the predicted

excitation energies tend to lie below the experimental values, with noticeable differences in the relative level spacings. Furthermore, in some states, deviations from the sequential ordering are observed for some of the low-lying states. However, the improvement is notable around the 5 MeV energy range, compared to the results obtained from the *jun45pn* interaction.

In Table 1, the wave functions of a few positive-parity yrast states (within 5 MeV) calculated with the *jun45pn* interaction are presented. Whereas Table 2 includes information extracted using the *snt* interaction for positive parity states. As mentioned earlier, for *jun45pn* interaction, all valence neutron orbitals are fully occupied; consequently, the total angular momentum is generated exclusively through proton excitation. Hence, the proton-neutron angular momentum decomposition ($J_\pi \otimes J_\nu$) is not shown in Table 1. In contrast, the *snt* interaction includes neutron orbitals above N=50 shell gap, allowing angular momentum generation by neutrons also, as clearly depicted in Table 2 for positive parity states. In the table, the seniority number of the particular state is also tabulated.

Table 1. The main proton configurations of the wavefunction and their contribution to the total wavefunction and seniority number of the particular configuration for positive parity yrast states of ^{89}Y using *jun45pn* interaction. $\pi 1$, $\pi 2$, $\pi 3$, $\pi 4$ represent the proton occupancy in $1f_{5/2}$, $2p_{3/2}$, $2p_{1/2}$, $1g_{9/2}$ orbitals, respectively. See text for details.

$2J^+$	Configurations of proton wavefunction				Contribution to total (%)	seniority number
	$\pi 1$	$\pi 2$	$\pi 3$	$\pi 4$		
9^+	6	4	0	1	60.05	1
	5	4	1	1	12.8	3
	6	2	0	3	12.44	1
11^+	6	3	1	1	58.75	3
	5	4	1	1	15.11	3
13^+	6	3	1	1	63.77	3
	6	2	2	1	6.78	3
	5	4	1	1	6.00	3
15^+	5	4	1	1	77.1	3
	5	2	1	3	12.11	3
17^+	5	3	2	1	41.1	3
	4	4	2	1	19.8	3
	6	2	0	3	16.8	3
19^+	6	2	0	3	68.8	3
	6	1	1	3	14.14	3
	5	3	0	3	6.03	3

In case of *jun45pn* interaction, the $9/2_1^+$ state is a seniority-1 state with $\pi 1g_{9/2}^{(+1)}$ (~60%) as the main configuration, as in *snt* interaction too (~65%). The yrast $11/2^+$ and $13/2^+$ has dominant configuration $\pi 2p_{3/2}^{(-1)}2p_{1/2}^{(+1)}1g_{9/2}^{(+1)}$ as seniority 3-multiplet. Furthermore, $15/2^+$ and $17/2^+$ state have main configurations as $\pi 1f_{5/2}^{(-1)}2p_{1/2}^{(-1)}1g_{9/2}^{(+1)}$ and $\pi 1f_{5/2}^{(-1)}2p_{3/2}^{(-1)}1g_{9/2}^{(+1)}$ respectively. In the case of *snt* interaction, these states are also generated through proton excitation only. Better agreement in energy is observed after $19/2_1^+$ state, which has

the dominant configuration as $\pi 1g_{9/2}^{(+1)} \nu 1g_{9/2}^{(-1)} 2d_{5/2}^{(+1)}$ in *snt* interaction as mentioned in Table 2. It indicates that promotion of neutrons above the N=50 shell gap is essential.

Table 2. The strong decomposition of angular momenta of protons and neutrons and their probability is noted. For each decomposition, the main proton and neutron configurations of the wavefunction and their contribution and seniority number of the particular configuration for positive parity yrast states of ^{89}Y using *snt* interaction ($1p1h-2d_{5/2}$). $\pi 1, \pi 2, \pi 3, \pi 4$ represent the proton occupancy in $1f_{5/2}, 2p_{3/2}, 2p_{1/2}, 1g_{9/2}$, orbitals, respectively. $\nu 1, \nu 2, \nu 3, \nu 4,$ and $\nu 5$ denote the neutron occupancy in $1f_{5/2}, 2p_{3/2}, 2p_{1/2}, 1g_{9/2},$ and $2d_{5/2}$ orbitals, respectively. See text for details.

$2J^+$	Decomposition of ang. Mom.		% probability	Configurations of the proton wavefunction				Configurations of the neutron wavefunction					Contribution to total (%)	Seniority number
	$2J_\pi$	$2J_\nu$		$\pi 1$	$\pi 2$	$\pi 3$	$\pi 4$	$\nu 1$	$\nu 2$	$\nu 3$	$\nu 4$	$\nu 5$		
9^+	9	0	91	6	4	0	1	6	4	2	10	0	64.9	1
11^+	11	0	76.1	6	3	1	1	6	4	2	10	0	34.2	3
				4	4	0	3	6	4	2	10	0	10.1	3
	9	4	14.1	6	4	0	1	6	4	2	9	1	8.65	3
13^+	13	0	85.5	4	4	0	3	6	4	2	10	0	49.6	3
				5	3	0	3	6	4	2	10	0	12.3	3
15^+	15	0	81.8	5	3	0	3	6	4	2	10	0	39.8	3
				4	4	0	3	6	4	2	10	0	14.1	3
17^+	17	0	85.7	4	4	0	3	6	4	2	10	0	59.7	3
				5	3	0	3	6	4	2	10	0	11.7	3
19^+	9	12	62.1	6	4	0	1	6	4	2	9	1	43.1	3
	9	10	26.5	6	4	0	1	6	4	2	9	1	18.2	3

4 Summary and Future Work

In this present work, two different interactions encompassing different model spaces have been used to describe the spectrum of ^{89}Y using shell model calculations. In the case of both positive and negative parity, low-lying spectra are better reproduced by the *jun45pn* interaction. While the involvement of neutron excitation across the N=50 shell gap improves the result in the high-energy region for the *snt* interaction calculation. However, a noticeable discrepancy in the relative level spacing is observed, which may arise from limitations on the number of neutrons allowed to excite across the N=50 shell gap. This issue warrants further investigation by permitting additional neutron excitations with appropriate truncation schemes.

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