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NUCLEAR STRUCTURE OF ^{42,43}Sc ISOTOPES CALCULATED WITH THE F742PN INTERACTION

In this article, using the NuShellX@MSU code and the F742PN interaction in the f7pn-shell model space, the nuclear shell model is employed to calculate the energy levels and electromagnetic transition probability for the ^{42,43}Sc isotopes. The ^{42,43}Sc isotope's electromagnetic transition probability and energy level results are generally in reasonable agreement with the available experimental data. A comparison of the theoretical results and the experimental data shows that the use of the nuclear shell model utilizing the interaction F742PN is successful within the f7pn-shell.

Keywords: energy levels, f7pn-shell, shell model, NuShellX@MSU code, electromagnetic transitions.

1. Introduction

Having access to a nucleus' nuclear structure and energy levels is one necessity for improving studies of its properties. The shell model is one of the most well-known and effective nuclear models. Nuclear models can aid in understanding nuclear structure, which contains the primary physical characteristics of nuclei [1, 2]. According to the fundamental tenet of the nuclear shell model, each nucleon moves independently of the others [3]. As a result, the single-particle model, which implies that nucleons move freely inside the nucleus, served as the foundation for the development of the nuclear shell model [4]. Choosing the proper effective interaction and model space that can result in the systematic and accurate prediction of a wide range of observables from the nuclear shell model is one of the key difficulties in nuclear physics comprehending the nuclear structure [5, 6]. A set of single-particle energies and two-body interaction matrix elements, also known as two-body matrix elements, are the fundamental needs for the computations of shell-model configuration mixing. Recently, these sets have been referred to as model space Hamiltonians or effective interactions. There are two approaches to explain this Hamiltonian in model space: The "realistic" approach is the first and is built for a specific shell model space using the information on the free nucleon-nucleon force that is already known. The second, "empirical", approach is based on parameters whose values are established by agreement between the shell model eigenvalue and measured level energies [7]. The matrix elements pertain to the free nucleon-nucleon interaction, and they should be viewed as simple parameters that may be changed to gain agreement with empirical spectroscopic data [8, 9]. In this study, the electromagnetic transitions and energy levels of the ^{42}sc and ^{43}sc isotopes were determined using the NuShellX@MSU code and the interaction F742PN [10] within the f7pn-shell. The isotopes under research have already been theoretically investigated by [11, 12], these isotopes were chosen because they have not been studied previously with the same interaction mentioned above, and the f7pn-shell was chosen because the nucleus rich in neutrons is important in studying nuclear structure.

2. Theory

The force that results from the collision of two nucleons is known as the residual interaction. This interaction is caused by a perturbation of the Hamiltonian operator, which is equal to the sum of the potential energies of the two particles. The Hamiltonian oper-

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ator including the perturbation state is shown in the equation [13, 14]:

$$H = H_0 + \sum_{i<j} V_{ij}. \tag{1}$$

The residual two-body interaction is denoted by V_{ij}, and the Hamiltonian operator without perturbation is denoted by H_0. In the mean-field approximation, it is assumed that each particle moves in an effective field generated by the remaining particles, and this is included in H_0. However, there remains a portion of the interaction that cannot be included in this field, is referred to as the residual interaction [15]. The remaining interaction is responsible for correlations between nucleons and for phenomena such as nuclear pairing and $E2$ and $M1$ transitions and energy corrections that are not explained by the simple shell model [16].

It is crucial to understand that there are residual interactions between each of the particles in each situation (secondary shells), and that residual interactions manifest themselves in in the final secondary shell if it is partially filled. All filled levels of the nucleus have zero momentum and positive parity, thus the remaining interactions may be used to determine the angular momentum and parity of the ground state of the nucleus [17].

For calculating the total angular momentum allowed, there are numerous theories that can be used, such as when protons or neutrons are congruent with nucleons in a single orbit with $n > 2$, where n is the number of particles outside the closed shell, the total angular momentum is equal to [13]:

$$J_M = n\left[j - \frac{(n-1)}{2}\right]. \tag{2}$$

The equation describes the maximum possible total angular momentum J_M. for a set of n identical nucleons (protons or neutrons) occupying the same single-momentum orbital j. According to the Pauli principle, identical particles cannot occupy the same magnetic state m_j so the highest possible values of m_j are filled in successively $(j, j-1, j-2, ...)$. Summing these values yields the maximum projection $M_{\max}$ of the total momentum, which, in turn, is equal to the maximum allowed value of the total momentum J_M. This result corresponds to the fully aligned state and sets an upper bound on the total angular momentum of the nucleus [18].

The transition probability $\lambda(\sigma L)$ for a gamma-ray emission with multipolarity L and character σ is given by [19]:

$$\lambda(\sigma L, J_i \longrightarrow J_f) = \frac{8\pi\,(L+1)}{\hbar L\,[(2L+1)!!]^2}\left(\frac{E_\gamma}{\hbar c}\right)^{2L+1} \times$$
$$\times\, B(\sigma L, J_i \longrightarrow J_f), \tag{3}$$

where $B(\sigma L)$ is the reduced transition probability; $E\gamma$ is the γ ray energy.

The above equation describes the probability of a radiative transition $\lambda(\sigma L)$ for gamma-ray emission when a nucleus transitions from a state J_i to J_f. It links the nature of the transition σL and the energy of the emitted photon E_γ on the one hand, and the internal structure of the nucleus represented by the transition strength $B(\sigma L)$ on the other hand. It follows that low-order, high-energy transitions are more likely, while high-order transitions are less likely due to damping by the factor $\left(\frac{E_\gamma}{\hbar c}\right)^{2L+1}$ [20].

The reduced matrix element $\langle \psi f \parallel M(\sigma L) \parallel \psi i\rangle$ can be used to express the reduced transition probability [21]:

$$B(\sigma L, J_i \longrightarrow J_f) = \frac{1}{2J_i+1}\,|\langle \psi\, f \parallel M(\sigma L) \parallel \psi i\rangle|^2 \tag{4}$$

$B(\sigma L)$. It is the strength or probability of an electromagnetic transition (reduced transition probability). It expresses how easy or difficult it is for a nucleus to undergo a transition from an excited state $(I)J_i$ to a lower state J_f with the emission of gamma radiation. While $\langle \psi f \parallel M(\sigma L) \parallel \psi i\rangle$ represents the reduced matrix element [19].

Each of the transition operators is represented by [13]:

$$\begin{aligned} M1 &= \mu_N \sum_{i=1}^{A}\left[\hat{g}_s\,(i)\,\vec{s}_i + \hat{g}_l(i)\,\vec{l}_i\right] Y_{10}, \\ E2 &= \sum_{i=1}^{A} \hat{e}\,(i)\, r_i^2 Y_{20}. \end{aligned} \tag{5}$$

3. Results and Discussions

Shell model calculations of low-lying energy states for ^{42,43}Sc isotopes have been performed for the f7pn space model using the Windows NuShellX@MSU code [10] with the F742PN effective interaction to calculate energy levels and reduced electromagnetic transition probabilities by employing the harmonic oscillator potential (HO, b), $b > 0$ for all isotopes.

3.1. Energy levels

3.1.1. The nucleus ^{42}Sc

^{42}Sc nucleus is an odd-odd nucleus containing (N_p = = 21, N_n = 21). The closed core of this nucleus has been identified as the closed nucleus ^{40}Ca, as the expected states of nucleons are formed within the f7pn-shell. To calculate the energy levels of this isotope, the nuclear shell model was applied and the F742PN interactions were used. Table 1 shows a comparison of the theoretical values of the energy levels and the available experimental data [22]. From the table below for F742PN interaction, we conclude:

The total angular momentum and ground state parity of the 0_1^+ level are in agreement with the available experimental data.

The agreement is satisfactory for the values of energies calculated theoretically (0.611, 0.618, 1.491, 1.511, 1.586, 2.817) MeV corresponding to the angular momentum (1_1^+, $7_1^+ 3_2^+$, 5_2^+, $2_1^+ 4_1^+$) when compared with the available experimental data.

Total angular momentum is only confirmed for the experimentally uncertain energy level 3.238 MeV corresponding to angular momentum 6.

From our calculations it is observed that the highest calculated theoretical energy value is (3.237) MeV while the highest experimental energy value is (15.966) MeV.

Calculation results using the effective F742PN interaction show good agreement with experimental values for the energy levels of the ^{42}Sc nucleus, especially for the low- and intermediate-energy levels, where the differences were very small (less than 0.1 MeV in most cases). However, a relatively larger difference was observed at the energy 2.817 MeV (about 0.38 MeV) and some deviations were found at the high energy levels. These differences could be due to the limited model space used, the inaccuracy of the experimental assignment of some high levels.

Overall, the agreement between the theoretical and experimental results can be considered very good and confirms the effectiveness of the F742PN interaction in describing the energy structure of the ^{42}Sc isotope.

3.1.2. The nucleus ^{43}Sc

^{43}Sc nucleus is an odd-even nucleus containing (N_p = = 21, N_n = 22). According to the nuclear shell model, the closed core is represented by ^{40}Ca nuclei with one proton and two neutrons outside the closed shell occupying the f7pn-shell. The nuclear shell model and the F742PN interaction were used for calculating the energy levels of this isotope. The comparison of the theoretical values of the energy levels and the available experimental data [23] is shown in Table 2 below. According to a comparison of our theoretical calculation using the F742PN interaction and the experimental value for this isotope listed in the table below, we conclude:

The total angular momentum and ground state parity of the $7/2_1^-$ level are in agreement with the available practical values.

When comparing the theoretically calculated energies (3.444, 3.937, 4.136, 4.391, 5.515) MeV which corresponds to the angular momentum ($5/2_1^-$, $5/2_2^-$, $7/2_3^-$, $7/2_4^-$, 3/22), they were found to be in good agreement with the experimental data.

Total angular momentum is only confirmed for the experimentally uncertain energies (1.882, 2.635, 2.760, 2.860, 3.480, 3.700, 4.158, 4.360) MeV corresponding to angular momentum 9/2, 11/2, 7/2, $3/2^+$, $13/2^+$, 19/2, 9/2, and 17/2. Also the angular momentum was confirmed only for experimentally uncertain energies (4.301, 4.430, 7.273) MeV which corresponds to angular momentum 11/2, 5/2, 15/2, and the parity was determined as negative parity.

In our calculations, we expected that the total angular momentum and the parity of the experimental energies (3.613, 4.343, 4.927, 5.977, 6.242) MeV is $15/2_1^-$, $1/2_1^-$, $13/2_2^-$, $11/2_3^-$, $9/2_3^-$, due to the convergence of experimental values with our theoretical values.

Table 1. **Comparison of the theoretical values of the energy levels relative to the ground state of the ^{42}Sc isotope and the experimental data [22] using the F742PN interaction**

Theoretical values of E MeV		Experimental values	
J^π	E (MeV)	F742PN results	J^+
0^+	0	0	0_1
1^+	0.611	0.611	1_1
7^+	0.616	0.618	7_1
3^+	1.490	1.491	3_1
5^+	1.510	1.511	5_1
2^+	1.586	1.586	2_1
4^+	2.433	2.817	4_1
$(5, 6, 7)^+$	3.238	3.237	6_1

Our calculations show that the highest theoretically calculated excitation energy is (7.28) MeV whereas the highest experimental energy value is (19.208) MeV.

Table 2. **Comparison of the theoretical values of the energy levels relative to the ground state of the ^{43}Sc isotope and the experimental data [23] using the F742PN interaction**

Theoretical values of E, MeV		Experimental values	
J^-	F742PN results	E, MeV	J^π
$7/2_1$	0	0	$7/2^-$
$9/2_1$	1.681	1.882	$(5/2, 9/2)^-$
$11/2_1$	2.336	2.635	$(11/2)^-$
$7/2_2$	2.791	2.760	$(5/2, 7/2, 9/2)^-$
$3/2_1$	2.889	2.860	$(1/2, 3/2, 5/2)^+$
$5/2_1$	3.444	3.463	$5/2^-$
$13/2_1$	3.503	3.480	$(\leq 13/2)^+$
$15/2_1$	3.512	3.613	–
$19/2_1$	3.638	3.700	$(5/2$ to $19/2)^-$
$5/2_2$	3.937	3.939	$5/2^-$, $7/2^-$
$9/2_2$	4.103	4.158	$(9/2, 11/2, 13/2)^-$
$7/2_3$	4.136	4.236	$7/2^-$
$17/2_1$	4.291	4.360	$(17/2)^-$
$1/2_1$	4.318	4.343	–
$7/2_4$	4.391	4.383	$5/2^-$, $7/2^-$
$11/2_2$	4.411	4.301	$(9/2, 11/2, 13/2^+)$
$5/2_3$	4.464	4.430	$(1/2^+, 3/2, 5/2)$
$13/2_2$	4.943	4.927	–
$3/2_2$	5.515	5.502	$1/2^-$, $3/2^-$
$11/2_3$	5.943	5.977	–
$9/2_3$	6.238	6.242	–
$15/2_2$	7.28	7.273	$(15/2, 17/2, 19/2^+)$

Table 3. **Comparison of the $B(E2)$ results by using F742PN interaction in unit e^2 fm^4 for ^{42}Sc isotope and the experimental data [22]**

$J_i \to J_f$	Theoretical $B(E2)$, e^2 fm^4, F742PN. Results $e_p = 2.75$, $e_n = 1.12$	Experimental $B(E2)$, e^2 fm^4
$2_1 \to 0_1$	83.6400	83.251
$2_1 \to 1_1$	4.2390	<60.704
$3_1 \to 1_1$	93.8400	34.688
$5_1 \to 7_1$	20.4800	22.547
$4_1 \to 3_1$	18.8400	<667.743
$4_1 \to 5_1$	30.6200	<607.039
$6_1 \to 7_1$	22.8400	–
$6_1 \to 5_1$	26.6400	–

The results of calculations performed using the effective F742PN interaction show good agreement with experimental values for the energy levels of the ^{42}Sc nucleus, particularly for low- and intermediate-lying states, where the differences between theoretical and experimental values were very small. However, some minor differences appeared at high levels due to the limited model space used or the inaccuracy of the experimental mapping for some cases.

These differences could be due to inaccurate experimental mapping. Overall, the agreement between theoretical and experimental results is very good, demonstrating the effectiveness of the F742PN interaction in describing the energy structure of the ^{43}Sc nucleus.

3.2. The electromagnetic transition probability

3.2.1. The nucleus ^{42}Sc

Electromagnetic transition probabilities for the ^{42}Sc isotope were calculated within the nuclear shell model using F742PN interaction. The calculations were performed using the harmonic oscillator potential (HO, b), where $b > 0$ for each in-band transition. The primary polarization effect was included by selecting the effective charge for proton and neutrons ($e_p = 2.75$, $e_n = 1.12$), also, the program's default value for the g factor was used to obtain an agreement with the experimental values of the ground state of the magnetic transitions ($g_s p = 5.586$, $g_s n = -3.826$).

Tables 2 and Tables 3 show a comparison of some of our theoretical values using effective interaction F742PN and the practical values [22] for electric and magnetic transitions, respectively.

For F742PN interaction we found a good correspondence for the electric transitions $B(E2)$ $2_1 \to 0_1$, $B(E2)$ $5_1 \to 7_1$, with available experimental data. also, the magnetic transition $B(M1)$ compatibility was good for the transition $B(M1)$ $1_1 \to 0_1$ with available experimental data. At the same time, the compatibility was reasonable for the rest of the transfers, and through our calculations, we also obtained new transitions for which there have been no experimental values until now. Theoretical results for the F742PN interaction have shown reliable predictions for transitions lacking experimental data in the ^{42}Sc nucleus, such as $B(E2;\ 6_1 \to 7_1)$ and $B(M1;\ 6_1 \to 5_1)$. The calculated values reflect logical and consistent behavior with other known transitions. The likely reason for the absence of these experimental data is the difficulty of their measurement due to the weak intensity of the transition or the short lifetime of the upper levels. These theoretical values provide an important basis for guiding future experimental studies and verifying the accuracy of the used interaction.

3.2.2. The nucleus ^{43}Sc

By applying the nuclear shell model and using the NushellX@MSU code to calculate the probability of electromagnetic transition of a ^{43}Sc nucleus, the default value of the proton and neutron charge in the calculations of the electric transition was changed to (e_p = 4.3, e_n = 2.999). Additionally, the g factor was adjusted to agree with the experimental values of the magnetic transitions' ground states ($g_S p = 2.250$, $g_S n = -1.500$).

For the electric and magnetic transitions, respectively, Tables 5 and 6 compare some of our theoretical values obtained using the effective interaction F742PN with the experimental values [23].

Through the table below and after comparing the theoretical results of the F742PN interaction with the experimental results, shows agreement for the values of the electric transition $B(E2)$ $3/2^-_1 \to 7/2^-_1$. Additionally, according to the available experimental data, the magnetic transitions compatibility for the transitions $B(M1)$ $5/2^-_1 \to 7/2_1$, $B(M1)$ $3/2^-_2 \to 5/2^-_1$, $B(M1)$ $5/2^-_2 \to \to 7/2^-_1$, $B(M1)$ $5/2^-_3 \to 7/2^-_1$ was good. We also discovered new transitions through our calculations for which there are no experimental values until now.

Calculation results using the F742PN interaction show good agreement with experimental values for the $B(E2)$ and $B(M1)$ transitions in the ^{43}Sc nucleus, especially at low and intermediate levels. Some transitions, such as $3/2^-_1 \to 7/2^-_1$, were in close agreement with experimental values, demonstrating the accuracy of the interaction used.

Slight differences in some transitions can be attributed to uncertainties in the experimental measurements.

Overall, the F742PN interaction demonstrates a high degree of efficiency in describing the electric and magnetic transitions in the ^{43}Sc nucleus, and the theoretical values for the transitions not measured experimentally represent important predictions that can be utilized in the future.

Table 4. **Comparison of the $B(M1)$ results by using F742PN interaction in unit μ^2 for ^{42}Sc isotope and the experimental data [22]**

$J_i \to J_f$	Theoretical $B(M1)\mu^2$ F742PN. Results $g_S p = 5.586$, $g_S n = -3.826$	Experimental $B(M1)\mu^2$
$1_1 \to 0_1$	6.0750	6.086
$2_1 \to 1_1$	6.9430	0.716
$4_1 \to 3_1$	6.1720	<0.141
$4_1 \to 5_1$	6.2680	<0.172
$6_1 \to 7_1$	2.3370	–
$6_1 \to 5_1$	3.7390	–

Table 5. **Comparison of the $B(E2)$ results by using F742PN interaction in unit e^2 fm^4 for ^{43}Sc isotope and the experimental data [23]**

$J_i \to J_f$	Theoretical $B(E2)$, e^2 fm^4 F742PN. Results $e_p = 4.3$, $e_n = 2.999$	Experimental $B(E2)$, e^2 fm^4
$3/2^-_1 \to 7/2^-_1$	145.6000	145.859
$5/2^-_1 \to 7/2^-_1$	5.6610	187.916
$3/2^-_2 \to 3/2^-_1$	12.0300	268.451
$3/2^-_2 \to 7/2^-_1$	0.2298	134.226
$7/2^-_3 \to 3/2^-_1$	1.6720	214.761
$11/2^-_1 \to 7/2^-_1$	171.5000	137.805
$5/2^-_3 \to 7/2^-_1$	0.0251	<4.474
$15/2^-_1 \to 11/2^-_1$	256.7000	48.321
$19/2^-_1 \to 15/2^-_1$	137.7000	23.892
$7/2^-_3 \to 7/2^-_1$	6.1250	–
$17/2^-_1 \to 13/2^-_1$	107.3000	–

Table 6. **Comparison of the $B(M1)$ results by using F742PN interaction in unit μ^2 for ^{43}Sc isotope and the experimental data [23]**

$J_i \to J_f$	Theoretical $B(M1)\mu^2$ F742PN. Results $g_S p = 2.250$, $g_S n = 1.500$	Experimental $B(M1)\mu^2$
$5/2^-_1 \to 7/2^-_1$	0.4665	0.408
$3/2^-_2 \to 5/2^-_1$	0.2905	0.483
$3/2^-_2 \to 3/2^-_1$	1.0190	0.269
$7/2^-_3 \to 5/2^-_1$	1.6630	0.161
$5/2^-_2 \to 7/2^-_1$	0.0003	>0.147
$5/2^-_3 \to 7/2^-_1$	0.2975	0.107
$7/2^-_3 \to 7/2^-_1$	0.3184	–
$17/2^-_1 \to 15/2^-_1$	0.4312	–

4. Conclusions

Calculations for the full f7pn-space shell model were carried out on windows using the NushellX@MSU code. The level spectra, reduced electric quadruple transition probability B(E2) and magnetic quadrilateral transition probability $B(M1$ for the ^{42,43}Sc isotopes are reproduced using the f7pn model space and the effective interaction F742PN. Generally speaking, these calculations were compared with the most recent experimental data for the level spectra using F742PN effective interaction, and good agreement was found, where numerous energy levels were confirmed, and new energy levels were found. Additionally, the calculated $B(E2)$ and $B(M1)$ are in good agreement with the results of the experiment. These results provide new insights into the nuclear structure of intermediate-mass nuclei in the f_p shell region and highlight the effectiveness of the F742PN effective interaction in describing the properties of electromagnetic transitions. This study also opens new avenues for future research, such as improving the effective interaction parameters to achieve closer agreement with experimental results, expanding the study to include neighboring isotopes, and investigating the effects of inter-shell excitations on nuclear structure. These efforts will contribute to a deeper understanding of nuclear behavior within the framework of the nuclear shell model.

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ЯДЕРНА СТРУКТУРА ІЗОТОПІВ
^{42,43}Sc В МОДЕЛІ ІЗ ВЗАЄМОДІЄЮ F742PN

В рамках моделі ядерних оболонок було розраховано енергетичні рівні та ймовірності електромагнітних переходів для ізотопів ^{42,43}Sc із використанням коду NuShellXMSU та взаємодії F742PN у модельному просторі f7pn-оболонки. Результати щодо ймовірності електромагнітного переходу та енергетичних рівнів ізотопів ^{42,43}Sc досить добре узгоджуються з наявними експериментальними даними. Використання моделі ядерних оболонок із взаємодією F742PN є успішним в межах f7pn-оболонки, про що свідчить порівняння теоретичних висновків з експериментальними даними.

Ключові слова: енергетичні рівні, f7pn-оболонка, модель оболонок, код NuShellX@MSU, електромагнітні переходи.