

Calculation of Energy Levels and Reduced Electromagnetic Transition Probability for ^{44}Sc Isotope Using NushellX@MSU Code

Ali k. Hasan

Hadeel H.Abed

Department of Physics, College of Education for Girls, University of Kufa, Iraq.

*Corresponding Author E-mail: alikh.alsinayyid@uokufa.edu.iq

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ABSTRACT

In this article, using the NushellX@MSU shell model code, the energy levels and electromagnetic transition probabilities $B(E2)$ and $B(M1)$ were calculated for the ^{44}Sc isotope in the f7pn-shell region. The model space includes all configurations of nucleons in the f7/2 orbit, where the calculations were performed with the effective interactions F7CDPN and F742PN in full f7pn space. The low-lying states and electromagnetic transition probabilities were seen to be in reasonable agreement with the experimental data for the counterpart under study.

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حساب مستويات الطاقة واحتمالية الانتقال الكهرومغناطيسي المختزلة لنظير ^{44}Sc باستعمال كود نيوشيل

هديل حاكم عبد

علي خلف حسن

قسم الفيزياء, كلية التربية للبنات, جامعة الكوفة, العراق

الكلمات المفتاحية:

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الخلاصة

في هذه البحث، باستخدام كود نيوشيل، تم حساب مستويات الطاقة واحتمالات الانتقال الكهرومغناطيسي $B(E2)$ و $B(M1)$ لنظائر ^{44}Sc في منطقة القشرة f7pn. يتضمن فضاء النموذج جميع تكوينات النيوكليونات في المدار f7/2. حيث تم إجراء الحسابات بالتفاعلات الفعالة F7CDPN و F742PN في الفضاء f7pn الكامل وكانت الحالات المنخفضة ومعدلات احتمالات الانتقال الكهرومغناطيسي متفقة بشكل معقول مع البيانات التجريبية للنظير قيد الدراسة.

1. Introduction:

The nuclear shell model stands out as a highly effective method for providing a precise explanation of experimental observations. It relies on two fundamental components in its calculations: the nuclear-nuclear (N-N) interaction and the configuration space dedicated to valence particles. In theory, one can conduct shell model computations using either a realistic

N-N interaction within an expansive configuration space or an adjusted, effective interaction within a more confined configuration space.[1].

A shell model is a potent tool for understanding nuclear structure. The shell model can correctly predict the nuclear spectra at low energies and transition probabilities if the model space contains all physically significant degrees of freedom and the residual interaction is appropriately tuned.[2]. In reality, as is widely known, in the shell-model approach, only the particles outside a core made up of filled shells are thought to be active, and computations are carried out in a truncated Hilbert space, the so-called model space. Therefore, the shell-model Hamiltonian acting only between the valence particles should take into account the ignored degrees of freedom, namely those of the core particles as well as of the excitations of valence particles above the selected model space. To achieve this, one can turn to empirical interactions, i.e., interactions with adjustable parameters or those obtained by treating the matrix elements as free parameters. Both situations call for fitting techniques to duplicate the experimental data. Numerous shell-model calculations have used empirical interactions, which, in the majority of cases, have successfully described a range of nuclear phenomena.[3]. Light nuclei often employ well-established, effective interactions, including the Cohen-Kurath [4] and USD [5] interactions for the p and sd-shells, respectively. Similarly,

within the f7-shell, common interactions like (JJ44BPN and JUN45PN)[6, 7] are employed. In this research, we employed the NuShellX@MSU code to compute energy levels, electromagnetic transitions, and charge density distributions for the ^{44}Sc isotope. These calculations were conducted using the JJ44BPN and JUN45PN interactions within the jj44pn-shell. This isotope has been studied theoretically by[8].

2. Theory:

Bill Rae[9] has developed a suite of computer programs under the name NuShellX. It has been specifically engineered for the meticulous calculation of precise energies, eigenvectors, and spectroscopic overlaps. These calculations are performed in the context of shell model Hamiltonian matrix computations, even when dealing with exceptionally extensive basis dimensions. NuShellX relies on the utilization of the j-coupled proton-neutron basis and has the capability to handle J-scheme matrix dimensions reaching a remarkable scale of up to 100 million. Additionally, NuShellX@MSU is a set of wrapper scripts ingeniously crafted by Alex Brown[10]. These scripts have the crucial role of supplying input data to NuShellX, utilising model space and Hamiltonian data files. Furthermore, they possess the capacity to transform the output data generated by NuShellX, encompassing information regarding energy levels, gamma decay, and beta decay, into visually represented figures and organized tables.

An efficient Hamiltonian shell model can describe the many-body system as follows: [11]:

$$H = H_0 + \hat{H} \quad (1)$$

Here, H_0 and H represent the independent single-particle component and the remaining two-body interaction of H, respectively.

The non-perturbative Hamiltonian can be expressed as :

$$H_0 = \sum_{\lambda} e_{\lambda} a_{\lambda}^{\dagger} a_{\lambda} \quad (2)$$

Various theories are available for determining the permissible total angular momentum. For instance, when protons or neutrons align with nucleons in a single orbit with n greater than 2 (where n represents the number of particles outside the closed shell), the total angular momentum is equivalent to this value[12]:

$$J_M = n \left[j - \frac{(n-1)}{2} \right] \quad (3)$$

It is possible to formulate the reduced transition probability by using the reduced matrix element $\langle \psi_f || M(\sigma L) || \psi_i \rangle$ as follows [13]:

$$B(\sigma L, J_i \rightarrow J_f) = \frac{1}{2J_i+1} |\langle \psi_f || M(\sigma L) || \psi_i \rangle|^2 \quad (4)$$

$$B(M1; J_i \rightarrow J_f) = \frac{1}{2J_i+1} |\langle J_f || M1 || J_i \rangle|^2 \quad (5)$$

$$B(E2; J_i \rightarrow J_f) = \frac{1}{2J_i+1} |\langle J_f || B2 || J_i \rangle|^2 \quad (6)$$

3.Results and Discussions:

Shell model computations were conducted to study the low-energy states of the ⁴⁴Sc isotope. These calculations focused on the f7/2 space model, with three nucleons (i.e. Nn=3) and one proton (Np=1) located above the ⁴⁰Ca closed core for the mentioned isotope. The NuShellX@MSU code was utilized for these calculations. The computations were based on the (f7pn-shell) Hamiltonian, denoted as F7CDPN and F742PN. Within this framework, the energy levels ,reduced electric quadruple transition probabilities (B(E2), and magnetic quadruple transition probabilities (B(M1) were determined. These calculations were carried out using a harmonic oscillator potential (HO) with a parameter (b) that is larger than zero for the above isotope.

3-1 Energy levels

According to the nuclear shell model, the ground state of the ⁴⁴Sc is a ⁴⁰Ca nucleus closed with

twenty protons and neutrons (Np=Nn=20) together with four nucleons distributed as one proton and three neutrons in the f7pn-shell. To calculate the energy levels of this isotope, the F7CDPN and F742PN interactions were used. Tables 1 and 2 show a comparison between the theoretical values of energy levels using the two reactions and the available practical values[14].

Table 1: A comparison between the theoretical values of the energy levels relative to the ground state of the ⁴⁴Sc isotope with the experimental data [14] using the F7CDPN interaction.

Theoretical values of E(MeV)		Experimental values	
J ^π	F7CDPN results	E(MeV)	J ^π
2 ₁	0	0	2 ⁺
6 ₁	0.382	0.271	6 ⁺
1 ₁	0.456	0.667	1 ⁺
4 ₁	0.712	0.349	4 ⁺
3 ₁	0.789	0.762	3 ⁺
7 ₁	1.294	0.968	7 ⁺
5 ₁	1.299	1.197	5 ⁻
5 ₂	2.081	2.291	(2 to 5) ⁺
6 ₂	2.228	2.210	6 ⁻
3 ₂	2.241	2.584	(3,4) ⁻
1 ₂	2.369	2.333	(1 to 6)
4 ₂	2.393	2.382	-----
2 ₂	2.594	2.556	-----
0 ₁	2.99	2.779	0 ⁺
8 ₁	3.117	2.989	8 ⁻
3 ₃	3.154	3.285	(2 ⁺ to 5 ⁺)
5 ₃	3.315	3.368	(2 ⁺ to 5 ⁺)
6 ₃	3.321	3.323	-----
7 ₂	3.365	3.439	-----
9 ₁	3.408	3.829	9 ⁻
7 ₃	3.713	3.720	+
4 ₃	3.718	3.626	(2 ⁺ to 5 ⁺)
3 ₄	3.755	3.851	(2 ⁺ to 5 ⁺)
2 ₃	4.057	4.053	-----
5 ₄	4.097	4.087	(2 ⁺ to 5 ⁺)
8 ₂	4.146	4.185	-----
3 ₅	4.431	4.461	-----
1 ₃	4.516	4.560	-----
2 ₄	4.607	4.622	-----
11 ₁	4.641	4.645	-----
5 ₅	4.655	4.697	(2 ⁺ to 5 ⁺)
10 ₁	4.809	4.949	10
6 ₄	4.832	4.762	-----
4 ₄	4.848	4.820	(2 ⁺ to 5 ⁺)
9 ₂	5.457	5.336	-----
4 ₅	5.625	5.608	-----
7 ₄	5.649	5.526	(2 ⁺ to 7 ⁺)
4 ₆	5.838	5.716	-----
6 ₅	6.257	-----	-----
2 ₅	6.643	-----	-----
5 ₆	6.963	-----	-----
8 ₃	8.405	-----	-----

Through the above table and by comparing the results using the F7CDPN interaction with the practical results of this isotope, the following observations can be seen:

1. The total angular momentum and ground state parity of the 2_1^+ level were matched when compared with the available practical values.
2. When comparing our theoretical values with practical values, we found an acceptable agreement for the values of energies calculated theoretically (0.382, 0.456, 0.712, 0.789, 1.294, 2.99) MeV corresponding to the angular momentum $6_1^+, 1_1^+, 4_1^+, 3_1^+, 7_1^+, 0_1^+$.
Also, the agreement was appropriate for the values of energies calculated theoretically (1.299, 2.228, 3.117, 3.408)MeV which correspond to the angular momentum $5_1^+, 6_2^+, 8_1^+, 9_1^+$ but in different parity.
3. Total angular momentum was only confirmed for the practically uncertain energies (2.291, 2.584, 2.333) MeV corresponding to angular momentum 5, 3, 1 $^-$.
4. This study also confirmed the total angular momentum and parity for the practically uncertain energies (3.285,3.368, 3.626, 3.851, 4.087, 4.697, 4.820,5.526) MeV corresponding to angular momentum $3^+, 5^+, 4^+, 3^+, 5^+, 5^+, 4^+, 7^+$.
5. This study expected that the total angular momentum and the parity of the experimental energies (2.382, 2.556, 3.323, 3.439, 4.053, 4.185, 4.461, 4.560, 4.622, 4.645, 4.762, 5.336, 5.608, 5.716) MeV is $4_2^+, 2_2^+, 6_3^+, 7_2^+, 2_3^+, 8_2^+, 3_5^+, 1_3^+, 2_4^+, 11_1^+, 6_4^+, 9_2^+, 4_5^+, 4_6^+$,due to the convergence of practical values with our theoretical values.
6. We expected that the angular momentum of indefinite practical energy angular momentum (3.720) MeV is 7_3^+ . Additionally, we expected that the parity of the practical energy 4.949 MeV corresponding to the angular momentum 10 is positive parity.
7. In our calculations, four levels were obtained with total angular momentum and parity that have not been matched by any practical value so far. On the other hand ,we noticed that the highest calculated energy value is theoretically (8.405)MeV while the highest experimental energy value is (9.141) MeV.

Table 2: A comparison between the theoretical values of the energy levels relative to the ground state of the 44Sc isotope with the experimental data [14] using the F742PN interaction.

Theoretical values of E(MeV)		Experimental values	
J ^π	F742PN results	E(MeV)	J ^π
2 ₁	0	0	2 ⁺
6 ₁	0.379	0.271	6 ⁺
1 ₁	0.431	0.667	1 ⁺
4 ₁	0.716	0.631	4 ⁻
3 ₁	0.764	0.762	3 ⁺
7 ₁	1.271	0.968	7 ⁺
5 ₁	1.275	1.197	5 ⁻
5 ₂	2.058	2.032	-----
6 ₂	2.213	2.210	6 ⁻
3 ₂	2.217	2.584	(3,4) ⁻
1 ₂	2.346	2.333	(1 to 6) ⁻
4 ₂	2.369	2.382	-----
2 ₂	2.575	2.556	-----
0 ₁	3.041	3.035	-----
8 ₁	3.094	2.989	8 ⁻
3 ₃	3.13	3.100	(2 ⁺ to 5 ⁺)
5 ₃	3.291	3.285	(2 ⁺ to 5 ⁺)
6 ₃	3.297	3.208	-----
7 ₂	3.342	3.323	-----
9 ₁	3.385	3.829	9 ⁻
7 ₃	3.689	3.720	+
4 ₃	3.697	3.626	(2 ⁺ to 5 ⁺)
3 ₄	3.732	3.851	(2 ⁺ to 5 ⁺)
2 ₃	4.034	4.053	-----
5 ₄	4.074	4.087	(2 ⁺ to 5 ⁺)
8 ₂	4.123	4.185	-----
3 ₅	4.408	4.461	-----
1 ₃	4.492	4.560	-----
11 ₁	4.619	4.622	-----
2 ₄	4.627	4.645	-----
5 ₅	4.632	4.697	(2 ⁺ to 5 ⁺)
10 ₁	4.786	4.949	10
6 ₄	4.81	4.762	-----
4 ₄	4.825	4.820	(2 ⁺ to 5 ⁺)
9 ₂	5.435	5.336	-----
7 ₄	5.626	5.526	(2 ⁺ to 7 ⁺)
4 ₅	5.63	5.608	-----
4 ₆	5.858	5.716	-----
6 ₅	6.278	-----	-----
2 ₅	6.648	-----	-----
5 ₆	6.969	-----	-----
8 ₃	8.413	-----	-----

According to the above table and via the comparison of the theoretical results using the F742PN interaction with the practical results of this isotope, we found that :

1. The total angular momentum and ground state parity of the 2_1^+ level were matched when compared with the available practical values.
2. When comparing our theoretical values with practical values, we found an acceptable agreement for the values of energies calculated theoretically (0.379, 0.431, 0.764, 1.271) MeV corresponding to the angular momentum $6_1^+, 1_1^+, 3_1^+, 7_1^+$.

The agreement was also appropriate for theoretically calculated energies of (0.716, 1.275, 2.213, 3.094, 3.385) MeV that correspond to angular momentums of $4_1^+, 5_1^+, 6_2^+, 8_1^+$, and 8_1^+ but with different parity.

3. Total angular momentum was only confirmed for the practically uncertain energies (2.584, 2.333) MeV corresponding to angular momentum $3^-, 1^-$.

Likewise, the total angular momentum and parity were confirmed for the practically uncertain energies (3.100, 3.285, 3.626, 3.851, 4.087, 4.697, 4.820, 5.526) MeV that correspond to angular momentum $3^+, 5^+, 4^+, 3^+, 5^+, 5^+, 4^+, 7^+$.

4. Because of the convergence of practical values with our theoretical values, we also expected that the total angular momentum and the parity of the experimental energies (2.032, 2.382, 2.556, 3.035, 3.208, 3.323, 4.053, 4.185, 4.461, 4.560, 4.622, 4.645, 4.762, 5.336, 5.608, 5.716) MeV is $5_2^+, 4_2^+, 2_2^+, 0_1^+, 6_3^+, 7_2^+, 2_3^+, 8_2^+, 3_5^+, 1_3^+, 11_1^+, 2_4^+, 6_4^+, 9_2^+, 4_5^+, 4_6^+$

5. We anticipated that the angular momentum of indeterminate practical energy (3.720 MeV)

would be 7_4^+ . Additionally, we anticipated a positive parity for the practical energy 4.949 MeV, which corresponds to the angular momentum of 10.

6. In our calculations, we noticed that the highest calculated energy value is theoretically (8.413)MeV while the highest experimental energy value is (9.141) MeV .Also, three levels were obtained with total angular momentum and parity that have not been matched by any practical value so far.

3-2 Electromagnetic Transition Probability :

By using the Nushellx@MSU code and applying the nuclear shell model to calculate the electromagnetic transition probability for the ^{44}Sc nucleus, the default value of the proton and neutron charge was changed to ($e_p = 1.775$, $e_n = 0.75$) for the F7CDPN interaction and ($e_p = 1.7$, $e_n = 0.75$) for the F742PN interaction. In addition, the g factor was changed for both interactions to match the experimental values of the ground states of magnetic transitions ($g_{sp} = 1.586$, $g_{sn} = -1.826$). Tables 3 and 4 compare some of our theoretical values for the electric and magnetic transitions that we calculated using the effective interaction F7CDPN with the experimental values[14]. Tables 5 and 6 compare some of our theoretical values for electric and magnetic transitions using the effective interaction F742PN with the experimental values[14].

Table 3: Comparison of the B(E2) results by using F7CDPN interaction in unit $e^2 \text{ fm}^4$ for ^{44}Sc isotope with the experimental data [14].

Ji→Jf	Theoretical B (E2) $e^2\text{fm}^4$, F7CDPN. results $e_p = 1.775$, $e_n = 0.75$	Experimental B(E2), $e^2 \text{ fm}^4$
$4_1 \rightarrow 2_1$	34.8900	34.601
$1_1 \rightarrow 2_1$	94.1900	645.884
$3_1 \rightarrow 2_1$	45.7700	36.908

3 ₂ →2 ₁	7.7910	1.015
3 ₃ →2 ₁	0.0147	1.753
9 ₁ →7 ₁	17.2600	23.067
11 ₁ →9 ₁	13.5600	20.668
6 ₂ →5 ₁	22.4400	-----
0 ₁ →2 ₁	14.5400	-----

Table 4 : Comparison of the B(M1) results by using F7CDPN interaction in unit μ^2 for ⁴⁴Sc isotope with the experimental data [14]

Ji→Jf	Theoretical B (M1) ,F7CDPN. Results g _{sp} = 1.586, g _{sn} = -1.826 μ^2	Experimental B (M1) μ^2
1 ₁ →2 ₁	2.6890	(2.685)
3 ₁ →2 ₁	1.8030	0.381
7 ₁ →6 ₁	0.5145	> 0.034
3 ₂ →2 ₁	0.0140	(0.251)
3 ₃ →2 ₁	0.1183	0.059
6 ₂ →5 ₁	0.6658	-----
0 ₁ →1 ₁	1.6440	-----

Considering the aforementioned table and after comparing the theoretical results of the F7CDPN interaction with the experimental results, there is a good agreement for the electric transition of the ground state transition B(E2) 4₁→2₁. Also, it was found that the values of the electric transitions B(E2) 3₁→2₁, B(E2) 3₂→2₁, B(E2) 3₃→2₁, B(E2) 9₁→7₁, B(E2), B(E2) 11₁→9₁ are acceptably compatible with the experiment data. At the same time a good agreement for the magnetic transitions of the ground state transition for the transition B(M1) 1₁→2₁, as well as the magnetic compatibility for the transitions B(M1) 3₁→2₁, B(M1) 7₁→6₁, B(M1), 3₂→2₁, B(M1) 3₃→2₁, was good, according to the experimental data that was available. Through our calculations, we also found new transitions for which there are no experimental values at this time.

Table 5 : Comparison of the B(E2) results by using F742PN interaction in unit e² fm⁴ for ⁴⁴Sc isotope with the experimental data [14]

Ji→Jf	Theoretical B (E2) e ² fm ⁴ , F742PN. results e _p = 1.700, e _n = 0.750	Experimental B(E2), e ² fm ⁴
4 ₁ →2 ₁	34.5700	34.601
1 ₁ →2 ₁	92.7400	645.884
3 ₁ →2 ₁	44.7600	36.908
3 ₂ →2 ₁	7.6300	1.015
3 ₃ →2 ₁	0.0152	1.753
9 ₁ →7 ₁	17.1700	23.067
11 ₁ →9 ₁	13.5000	20.668
6 ₂ →5 ₁	22.2000	-----
0 ₁ →2 ₁	13.9800	-----

Table 6 : Comparison of the B(M1) results by using F742PN interaction in unit μ^2 for ⁴⁴Sc isotope with the experimental data [14]

Ji→Jf	Theoretical B (M1) μ^2 , F742PN. Results g _{sp} = 1.586, g _{sn} = -1.826	Experimental B (M1) μ^2
1 ₁ →2 ₁	2.6920	2.685
3 ₁ →2 ₁	1.8140	0.381
7 ₁ →6 ₁	0.5089	> 0.034
3 ₂ →2 ₁	0.0143	0.251
3 ₃ →2 ₁	0.1170	0.059
6 ₂ →5 ₁	0.6781	-----
0 ₁ →1 ₁	1.6410	-----

In the aforementioned table, a comparison was made between the theoretical findings of the F742PN interaction and the experimental data. An excellent agreement for the electric transition of the ground state transition B(E2) 4₁→2₁. Moreover, it was found that the values of the electric transitions B(E2) 3₁→2₁, B(E2) 3₂→2₁, B(E2) 3₃→2₁, B(E2) 9₁→7₁, B(E2), B(E2) 11₁→9₁ are in acceptable agreement with the experiment's results. According to the experimental data that was provided, there was also high agreement for the magnetic transition of the ground state transition 1₁→2₁. Also, the agreement was good for the magnetic transitions for the transitions B(M1) 3₁→2₁, B(M1) 7₁→6₁,

$B(M1)$, $3_2 \rightarrow 2_1$, $B(M1)$ $3_3 \rightarrow 2_1$. Our calculations also led to the discovery of new transitions for which there are currently no experimental values.

4. Conclusions:

Full-scale shell model calculations within the $f7p_n$ space were carried out using the NushellX@MSU code designed for Windows. These calculations employed the F7CDPN and F742PN effective interactions to reproduce the level levels and electromagnetic transition probability for the ^{44}Sc isotope. Comparing these calculations with recently available experimental data for the level spectra revealed a generally good agreement, demonstrating the effectiveness of the F7CDPN and F742PN interactions within the $f7p_n$ -shell region to perform shell model calculations.

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