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Calculation of Energy Level and B (E2) for ⁴⁴⁻⁴²Ti and ⁴⁴⁻⁴²Sc by Using Shell Model Code OXBASH

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Abstract: In this paper, shell model is applied in the f7-shell region to calculate the energy levels and B(E2) for $^{42-44}$ Ti and $^{42-44}$ Sc nuclei by employing the effective interactions, f742pn and f7cdpn and using the shell model code OXBASH for windows by applying spin-parity of valance nucleons. It is found that there is good convergence of energy level sand B(E2) values with the standard practical value.

Keywords: Energy Levels, OXBASH Code and gamma transitions.

1 Introduction

The aim of this paper is study of the energy levels and electrical transitions B (E2; \downarrow) of ⁴⁴⁻⁴²Ti and ⁴⁴⁻⁴²Sc isotopes by using OXBASH code for windows. This program is a set of codes carrying out shell-model calculations with dimensions up to about 50,000 in the J-T scheme and about 2,000,000 in the M-scheme. Oxbash comes with a library of model spaces and interactions [1, 2]. Applied the shell model and use a Modified Brown and Sherr (f7cdpn, f742pn) interaction for neutron and proton orbits in 44-42Ti and ⁴⁴⁻⁴²Sc to calculate the energy levels and B (E2) values. Various observables can be predicted accurately and systematically in terms of the nuclear shell model. For light nuclei, there are several "standard" effective interactions such as the Cohen-Kurath [3] and the USD [4] interactions for the p and sd shells, respectively. On the other hand, in the next major shell, i.e., in the f7-shell, there are also "standard" interactions such as f742pn and f7cdpn [5]. The spectroscopy of nuclei, in the f7-shell region, has been well described within the shell model framework. The best example for using several model spaces and two-body interactions is that of Brown et al. which is the most remarkable work in this field [6,7]. The starting point in all such shell-model calculations is the derivation of an effective interaction owing to the fact that the f7-shell is the most important for a variety of problems in nuclear structure such as electron capture in supernova explosions. In this work, the shell model calculations are carried out in the f7-shell region for the isotopes 44-42Ti and 44-42Sc, to test

the ability of the present effective interactions in reproducing the experiment in this mass region.

2 Shell Model Calculations

The calculations have been carried out in the nuclear shell model f7 using the code OXBASH for windows [6]. The code uses an m-scheme Slater determinant basis. With a projection technique, there are been constructed wave functions with good angular momentum J and isospin T. The f7pn model space is comprised of (1f7/2) below the closed N = Z=20 shell [8]. In addition, there have been used the harmonic oscillator potential (HO, b), b>0.In this work, one can find the calculated results of states of the odd A and even A nuclei, number of protons, i.e., 22 to the ⁴⁴⁻⁴²Ti, with neutron numbers from 20 to 22 and number of protons, 21 to the ⁴⁴⁻⁴²Sc, with neutron numbers from 21 to 23 energy levels and the B (E2) value.

2.1 Energy Levels Calculations

The calculations have been carried out using the code OXBASH for windows [9]. In the f7 model space comprised of the 0f7/2 valence orbits outside the $^{40}\mathrm{Ca}$. Two effective interactions have been employed with f7 model space for the calculations of level spectra and transition probabilities, these effective interactions are f742pn and f7cdpn [5]. It is worth mentioning that $^{42}\mathrm{Ti},\,^{43}\mathrm{Ti}$ and $^{44}\mathrm{Ti}$ have Iso spin part ($T=1,\,0.5$ and 0) respectively, while $^{42}\mathrm{Sc},^{43}\mathrm{Sc}$ and $^{44}\mathrm{Sc}$ have Iso spin part (T=0, 0.5 and 1) respectively. The energy levels values for $^{42}\mathrm{Ti}$ nucleus from f742pn and f7cdpn effective interactions are shown in table



1 and these effective interactions give good results in comparison with the experimental values.

Table1.shows a comparison of the energy levels values with respect to the ground state were calculated from f742pn and f7cdpn effective interactions with experimental excitation energies of ⁴²Ti

immini energies of 11				
Exp. Res [10]				
I^{π}	Energy	f742pn	f7cdpn	J^{π}
J	elevels			
0+	0.000	0.000	0.000	01+
2+	1.556	1.586	1.605	2+
4+	2.676	2.817	2.771	4 ₁ ⁺
6+	3.043	3.237	3.139	61+

For ⁴³Ti nucleus, the energy levels values are shown in table 2. these values are agreement with the experimental values, and new energy levels have been reached.

Table 2. Shows a comparison of the energy levels values with respect to the ground state were calculated from f742pn and f7cdpn effective interactions with experimental excitation energies of ⁴³Ti

Exp. Res [11]				
J^{π}	Energy elevels	f742pn	f7cdpn	J^{π}
7/2-	0.000	0.000	0.000	7/2-
(1/2,5/2)-	1.760	1.681	1.707	9/2-
	2.438	2.336	2.345	11/2-
	2.640	2.791	2.787	7/2-
(15/2-)	2.951	2.889	2.911	3/2-
	3.220	3.444	3.393	5/21
		3.503	3.472	13/2-
		3.512	3.471	15/2-
		3.638	3.556	19/2-
		3.937	3.916	5/2-
		4.103	4.037	9/2-
		4.136	4.057	7/2-
		4.291	4.209	17/21
		4.318	4.289	1/2-
		4.391	4.341	7/2-
		4.411	4.364	11/2-
		4.464	4.439	5/2-
		4.943	4.862	13/2-
		5.515	5.480	3/2-
		5.943	5.883	11/2-
		6.238	6.181	9/2-
		7.280	7.187	15/2-

Table 3 shows a comparison of the calculations energy levels with respect to the ground state with experimental excitation energies of 44 Ti with f742pn and f7cdpn effective interactions. The effective interactions give results reasonably consistent with experimental data. The total angular momentum and parity are $(0_1^+, 2_1^+, 4_1^+, 6_1^+, 8_2^+, 6_6^+, 2_7^+, 4_{10}^+, 2_9^+)$ respectively, confirmation of which is $(8^+, 4^+, 6^+, 10^+, 12^+, 2^+, 10^+, 4^+, 2^+, 6^+)$ respectively, as well as the confirmation of momentum only, which is $(6^-, 3^-, 3^-, 11^-)$ respectively

Table 3. Shows a comparison of the energy levels values with respect to the ground state were calculated from f742pn and f7cdpn effective interactions with experimental excitation energies of ⁴⁴Ti.

Exp. Re	s[12]			
V.T.	Energy	f742pn	f7cdpn	J^{π}
J^{π}	elevels			
0+	0.000	0.000	0.000	01+
2+	1.083	1.163	1.183	2+
4+	2.454	2.791	2.806	41+
6+	4.015	4.057	4.030	61+
	4.792	4.956	4.989	2+
		5.001	5.010	4+
(6-)	5.151	5.167	5.174	62+
		5.231	5.255	2*
(7-)	5.67	5.610	5.587	63+
		5.583	5.594	0+
		5.662	5.677	11+
3-	5.421	5.788	5.806	31+
5-	5.305	5.868	5.875	5 ₁ +
		5.947	5.942	4 + 3
		5.995	5.995	32+
		6.035	6.024	71+
(8+)	6.508	6.080	6.070	81+
(8+)	6.571	6.502	6.432	7 ₂ +
		6.506	6.464	52+
(4 ⁺)	6.959	6.707	6.713	44
(6 ⁺)	6.848	6.878	6.855	64
		7.018	7.002	5*
		7.289	7.272	54
8+	7.458	7.345	7.321	82+
(10+)	7.671	7.380	7.341	101+
		7.444	7.421	65
3-	7.34	7.448	7.434	3*
1-	7.5	7.577	7.488	1+
6+	7.670	7.551	7.529	6,
	7.634	7.600	7.598	45+



(12+)	8.039	7.689	7.624	121
(12)	0.037	7.806	7.772	2+
		7.813	7.817	2 ₄ 2 ₅
	9.067	7.979	7.941	9 ₁ ⁺
(1 2+)	8.067	7.968		
(1 – ,2+)	8.18		7.950	26
		8.143	8.120	46
		8.272	8.160	03+
		8.234	8.187	83+
	0.010	8.275	8.240	4+
	8.318	8.325	8.298	84
(2+,3-)	8.449	8.361	8.319	34
		8.369	8.330	7 ₃ +
		8.522	8.497	5 ₆ ⁺
		8.528	8.524	67
		8.573	8.530	74+
		8.616	8.556	92+
(3-)	8.534	8.688	8.652	35+
		8.782	8.750	04+
(10 ⁺)	8.984	8.891	8.827	102
		8.920	8.888	75+
		8.963	8.906	36+
(4 ⁺)	8.947	8.928	8.910	4*
	9.03	9.094	9.043	6*
2+	9.227	9.265	9.220	2+
5-	9.4	9.305	9.232	5‡
	9.478	9.354	9.312	85+
	9.632	9.639	9.601	3+
	9.668	9.723	9.690	1 ₃ +
(11-)	9.722	9.850	9.77	111+
(2 ⁺)	9.741	9.858	9.790	2*
	9.895	9.863	9.816	5*
	10.046	10.017	9.963	103+
	10.046	10.041	10.002	6+
	10.166	10.056	10.013	4+
	10.52	10.666	10.595	9*
	11.058	10.857	10.788	7 ₆ +
4+	10.7	10.861	10.810	4 ₁₀
(6 ⁺)	11.110	11.509	11.419	6+
2+	12.118	11.879	11.826	2+
	12.2	12.200	12.137	5+
	13	13.644	13.558	86
	1	l .	I	L

But for ⁴²Sc nucleus, table 4 shows a comparison of the energy levels calculations with respect to the ground state from f742pn and f7cdpn effective interactions, with experimental excitation energies. The effective interactions give results reasonably consistent with experimental data.

The total angular momentum and parity are $(0_1^+, 1_1^+, 3_1^+, 2_1^+, 4_1^+)$ respectively, confirmation of which is (5+), as well as confirmation of momentum only, which is (7, 6) respectively.

Table 4. shows a comparison of the energy levels values with respect to the ground state were calculated from f742pn and f7cdpn effective interactions with experimental excitation energies of ⁴²Sc

Exp	. Res[10]			
J^{π}	Energy elevels	f742pn	f7cdpn	J^{π}
0+	0.000	0.000	0.000	01+
1+	0.611	0.611	0.685	11+
(7)+	0.616	0.618	0.692	7 +
3+	1.490	1.491	1.565	31+
(5+)	1.510	1.511	1.585	51+
2+	1.586	1.586	1.647	21+
4+	2.815	2.817	2.877	41+
(6)+	3.242	3.237	3.295	61

The energy levels values for ^{43}Sc nucleus from f742pn and f7cdpn effective interactions are shown in table 5 and these effective interactions results reasonably consistent with experimental data. The total angular momentum and parity are ($7/2_1^-$, $5/2_1^-$, $5/2_2^-$, $7/2_4^-$, $3/2_2^+$) respectively, confirmation of which is ($17/2^-$) respectively , as well as confirmation of momentum only, which is (9/2, 11/2, 7/2, 3/2, 13/2, 19/2, 7/2, 9/2, 17/2, 11/2, 5/2, 15/2) respectively.

Table 5. Shows a comparison of the energy levels values with respect to the ground state were calculated from f742pn and f7cdpn effective interactions with experimental excitation energies of ⁴³Sc

Exp. Res [11]				
J^{π}	Energy elevels	f742pn	f7cdpn	J^{π}
7/2-	0.000	0.000	0.000	7/2-
(5/2,9/2)-	1.882	1.681	1.700	9/2-
(11/2)-	2.635	2.336	2.355	11/2-
5/2,7/2,9/2)(2.811	2.791	2.806	7/2-
(1/2,3/2,5/2)+	2.86	2.889	2.908	3/2-
5/2-	3.463	3.444	3.462	5/21
(≤ 13/2)+	3.480	3.503	3.522	13/2-
(5/2, 7/2, 9/2,)	3.631	3.512	3.531	15/2-
(5/2T019/2) ⁻	3.7	3.638	3.656	19/2-
5/2-,7/2-	3.939	3.937	3.956	5/2-



(3/2TO17/2) ⁺	4.132	4.136	4.103	7/2-3
(9/2,11/2,13/2)-	4.158	4.103	4.122	9/2-
(17/2-)	4.36	4.291	4.309	17/2-
	4.343	4.318	4.337	1/2-
5/2-,7/2-	4.383	4.391	4.409	7/2-
(11/2+,13/2-)	4.555	4.411	4.429	11/2-
(5/2:9/2)	4.455	4.464	4.461	5/2-
	4.927	4.943	4.96	13/2-
1/2-,3/2-	5.502	5.515	5.514	3/2-
	5.977	5.943	5.939	11/2-
	6.242	6.238	6.234	9/2-
5/2,17/2,19/2)(1	7.273	7.280	7.275	15/2-

For 44 Sc nucleus the energy levels calculations from f742pn and f7cdpn effective interactions are shown in table 6. The effective interactions give results reasonably consistent with experimental data. The total angular momentum and parity are $(2_1^+, 6_1^+, 1_1^+, 3_1^+, 7_1^+)$ respectively, confirmation of which is $(5^+, 5^+, 4^+, 3^+, 5^+, 3^+, 5^+, 4^+, 4^+)$ respectively, as well as confirmation of momentum only is (5, 3, 1, 4, 2) respectively

Table 6. Shows a comparison of the energy levels values with respect to the ground state were calculated from f742pn and f7cdpn effective interactions with experimental excitation energies of ⁴⁴Sc

Exp .Res[12]				
I^{π}	Energy	F742pn	F7cdpn	J^{π}
J	elevels			
2+	0.000	0.000	0.000	21+
6 ⁺	0.271	0.379	0.382	61
1+	0.667	0.431	0.456	11+
4-	0.631	0.716	0.712	41+
3+	0.762	0.764	0.789	31+
7+	0.968	1.271	1.294	7 ₁ +
5-	1.197	1.275	1.299	5+
(2TO5)+	1.957	2.058	2.081	52+
6-	2.210	2.213	2.228	62+
(2TO5)+	2.291	2.217	2.241	32+
(1706)	2.333	2.346	2.369	12+
(2TO5)+	2.424	2.369	2.393	4+
(1706)-	2.524	2.575	2.594	22+
	3.035	3.041	2.990	01+
+	3.162	3.094	3.117	81+
	3.178	3.130	3.154	33+
(2 ⁺ T05 ⁺)	3.285	3.291	3.315	5 ₃ +

	3.323	3.297	3.321	63+
	3.439	3.342	3.365	72+
	3.483	3.385	3.408	91+
+	3.72	3.689	3.713	7 ₃ +
(2 ⁺ T05 ⁺)	3.626	3.697	3.718	43+
(2 ⁺ T05 ⁺)	3.851	3.732	3.755	34
	4.053	4.034	4.057	2 ₃ +
(2 ⁺ T05 ⁺)	4.087	4.074	4.097	54+
+	4.144	4.123	4.146	82+
(2^+T05^+)	4.533	4.408	4.431	35+
	4.56	4.492	4.516	1,+
	4.595	4.627	4.607	24+
	4.622	4.619	4.641	111+
(2 ⁺ T05 ⁺)	4.697	4.632	4.655	5 +
10	4.949	4.786	4.809	101+
	4.762	4.810	4.832	64
(2 ⁺ T05 ⁺)	4.820	4.825	4.848	44
	5.500	5.435	5.457	92+
(0^+T07^+)	5.526	5.630	5.625	45+
	5.608	5.626	5.649	74+
	5.716	5.858	5.838	46+
		6.278	6.257	65
		6.648	6.643	25+
		6.969	6.963	5 ₆ +
		8.413	8.405	83+

2.2 Reduced Electric Quadrupole Transition Probability B(E2) Calculations

The transition rates represent a sensitive test for the most modern effective interactions that have been developed to describe f7-shell nuclei. The transition probability calculated in this work performed by using the harmonic oscillator potential (HO, b), where b > 0 for each in-band transition by assuming pure E2 transition. Core polarization effects have been included by choosing the effective charges for proton e_{π} = 1.7e and for neutron e_{ν} = 0.350e. Table 7 is about ⁴²Ti, which is calculated by using f742pn and f7cdpn effective interaction. In general, all of the calculated results are reasonably consistent with available experimental data.

Table 7. presents the B (E2) values in the ground-state band of 42 Ti. Their units are e^2 fm 4 . This work is assumed pure E2 transition limit.

•						
	$J_i^\pi \to J_f^\pi$	Exp [10]	F7cdpn	F742pn		
	$2_1^+ \to 0_1^+$	138.75 ± 4	138	138		
	$4_1^+ \rightarrow 2_1^+$		137.7	137.7		
	$6_1^+ \rightarrow 4_1^+$	27.58± 21	62.72	62.72		



The effective charges are taken from both proton and neutron (1.3e). For the calculations of the transition probability in Table 8, about ⁴³Ti, f742pn and f7cdpn effective Interactions are used. In general, the calculated results are reasonably consistent with available experimental data.

Table 8. presents the B (E2) values in the ground-state band of ⁴³Ti. Their units are e² fm⁴. This work is assumed pure E2 transition limit.

$J_i^{\pi} \rightarrow J_f^{\pi}$	Exp [11]	F7cdpn	F742pn
$5/2_1^- \to 1/2_1^-$		32.56	32.31
$7/2_1^- \rightarrow 3/2_1^-$		20.91	20.43
$9/2_1^- \rightarrow 5/2_1^-$		0.05065	0.01946
$11/2_1^- \to 7/2_1^-$		64.34	63.98
$13/2_1^- \rightarrow 9/2_1^-$		73.62	73.58
$15/2_1^- \rightarrow 11/2_1^-$		95.42	95.75
$17/2_1^- \rightarrow 13/2_1^-$		45.94	45.71
$19/2_1^- \rightarrow 15/2_1^-$	51±3	51.24	51.32

In Table 9, about of ⁴⁴Ti, the effective charges for proton and neutron are taken to be (0.95e and 1.1e) respectively; for the calculations of the transition forces, f742pn and f7cdpn effective Interactions are used. In general, the calculated results are reasonably consistent with available experimental data.

Table 9. presents the B (E2) values in the ground-state band of ⁴⁴Ti. Their units are e² fm⁴. This work is assumed pure E2 transition limit.

i ansinon mini.			
$J_i^{\pi} \rightarrow J_f^{\pi}$	Exp [12]	F7cdpn	F742pn
$2_1^+ \to 0_1^+$	119.94 ± 4	126.2	126.4
$4_1^+ \rightarrow 2_1^+$	276.81 ± 5	159.8	160.5
$6_1^+ \to 4_1^+$	156.86± 24	68.02	69.97
$8_1^+ \to 6_1^+$		70.03	72.52
$10_1^+ \to 8_1^+$		80.07	80.97
$12_1^+ \to 10_1^+$		43.6	43.81
$3_1^+ \to 1_1^+$		1.292	1.755
$5_1^+ \to 3_1^+$		32.5	30.99
$7_1^+ \rightarrow 5_1^+$		23.56	23.85
$9_1^+ \to 7_1^+$		27.89	29.22
$11_1^+ \to 9_1^+$		1.901	2.572

Moreover, f742pn and f7cdpn effective Interactions have been used for the calculation of the transition probability in table 10 of ⁴²Sc. The effective charges are taken from both proton and neutron (1.4e) . In general, the calculated results are reasonably consistent with available experimental data.

table 10 shows The effective charges for proton e_{π} = 1.4e and for neutron e_{ν} = 1.35e have been chosen for table 11, about ⁴³Sc, for the calculation of the transition probability, using f742pn and f7cdpn effective interactions. In general, all of the calculated results are reasonably consistent with

available experimental data.

Table10.presents the B (E2) values in the ground-state band of ⁴²Sc. Their units are e² fm⁴. This work is assumed pure E2 transition limit.

•	$J_i^{\pi} \to J_f^{\pi}$	Exp [10]	F7cdpn	F742pn
	$2_1^+ \to 0_1^+$	69.38 ±3	68.33	68.33
	$4_1^+ \rightarrow 2_1^+$		68.17	68.17
	$6_1^+ \to 4_1^+$		31.06	31.06
	$3_1^+ \rightarrow 1_1^+$	34.69±7	76.7	76.7
	$5_1^+ \to 3_1^+$		51.27	51.27
	$7_1^+ \rightarrow 5_1^+$		12.26	12.26

Table11. Presents the B (E2) values in the ground-state band of ⁴³Sc. Their units are e² fm⁴. This work is assumed pure E2 transition limit.

$J_i^{\pi} \to J_f^{\pi}$	Exp [11]	F7cdpn	F742pn
$5/2_1^- \to 1/2_1^-$		25.17	25.16
$7/2_1^- \rightarrow 3/2_1^-$		15.21	15.08
$9/2_1^- \to 5/2_1^-$		1.95	1.947
$11/2_1^- \to 7/2_1^-$	137.8 ± 24	32.86	32.69
$13/2_1^- \to 9/2_1^-$		36.22	36.22
$15/2_1^- \to 11/2_1^-$	48.32 ± 7	48.92	48.93
$17/2_1^- \to 13/2_1^-$		19.55	19.54
$19/2_1^- \to 15/2_1^-$	23.89 ± 2	26.22	26.23

For the calculations of the transition probability in table 12 of ⁴⁴Sc, the effective charges are taken for proton and neutron (0.9e, 0.8e) respectively, using f742pn and f7cdpn effective Interaction. In general, the calculated results are reasonably consistent with available experimental data.

Table 12. presents the B (E2) values in the ground-state band of ⁴⁴Sc. Their units are e² fm⁴. This work is assumed pure E2 transition limit.

$J_i^{\pi} \to J_f^z$	Exp [12]	F7cdpn	F742pn
Ji 'Jf	Exp [12]	1 /capii	1 /+2pii
$2_1^+ \rightarrow 0_1^+$		3.135	3.205
$4_1^+ \rightarrow 2_1^+$	34.6 ± 23	34.78	35
$6_1^+ \to 4_1^+$		12.42	12.34
$8_1^+ \to 6_1^+$		11.76	11.62
$10_1^+ \to 8_1^+$		4.51	14.51
$3_1^+ \rightarrow 1_1^+$		33.9	33.9
$5_1^+ \to 3_1^+$		36.72	36.74
$7_1^+ \rightarrow 5_1^+$		11.71	11.72
$9_1^+ \to 7_1^+$	23.07 ± 5	16.94	16.94
$11_1^+ \to 9_1^+$	20.66 ± 8	13.29	13.29



3 Conclusions

The present study demonstrates that interaction files used in this research give consistent results well in the calculation of the energy levels and the transition probability B (E2) when compared with modern process values. In f7-space shell model calculations were performed using the code OXBASH for windows to reproduce the level spectra and transition probability B(E2) for the nuclei ⁴⁴⁻⁴²Sc and ⁴²Ti. Good agreements were obtained by comparing these calculations with the recently available experimental data about level spectra and transition probabilities using both f742pn and f7cdpn effective interactions.

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