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Nuclear Shell Model Calculations for A=49 Isobars

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ABSTRACT

One of the common methods used to investigate the nuclear structures of the atomic nucleus is the nuclear shell model. As in the case of the shell model of the atom for electrons, the atomic nucleus is assumed to be composed of nuclear shells. Protons and neutrons (nucleons) fill the orbits in the shells according to the quantum mechanical restrictions. Each nucleon moves independently under an average potential created by the others. In the model, a very stable nucleus having nuclear magic numbers for nucleons is considered as an inert core. Only valance nucleons outside the core are active in the considered model space and taken into account in the calculations. In the present study, by using the nuclear shell model, we have investigated the nuclear structure properties of *A=49* isobars. Doubly magic ^{40}Ca nucleus was considered as an inert core and *fp* model space was taken into account for the valance nucleons. For two-body interaction Hamiltonian, different matrix element sets existing in the literature were used. The results have been compared with each other and the available experimental data.
Keywords : *Nuclear Shell Model, Nuclear Structure, Energy Level, Transition*

A=49 İzobarları için Nükleer Kabuk Modeli Hesaplamaları

ÖZET

Atom çekirdeğinin nükleer yapısını araştırmak için kullanılan yaygın yöntemlerden biri de nükleer kabuk modelidir. Elektronlar için olan atomun kabuk modelinde olduğu gibi, nükleer kabuki modelinde de, atom çekirdeğinin kabuklardan oluştuğu varsayılır. Protonlar ve nötronlar (nükleonlar) kuantum mekaniksel kısıtlamalara göre kabuklardaki yörüngeleri doldurur. Her bir nucleon, diğerleri tarafından yaratılan ortalama bir potansiyel altında bağımsız olarak hareket eder. Modelde, nükleonlar için nükleer sihirli sayılara sahip kararlı bir çekirdek, kor çekirdek olarak kabul edilir. Bu kor çekirdek dışındaki değerlik nükleonları, düşünülen model uzayında aktiftir ve hesaplamalarda dikkate alınırlar. Bu çalışmada, nükleer kabuk modelini kullanarak A = 49 izobarlarının nükleer yapı özellikleri araştırılmıştır. Çift sihirli ^{40}Ca çekirdeği, kor çekirdek olarak kabul edilmiş ve değerlik nükleonlarının fp model uzayında dağıldıkları dikkate alınmıştır. İki cisim etkileşim Hamiltonyeni için, literatürde mevcut olan farklı matris eleman setleri kullanılmıştır. Sonuçlar, birbiriyle ve mevcut deneysel verilerle karşılaştırılmıştır.
Anahtar Kelimeler : *Nükleer Kabuk Modeli, Nükleer Yapı, Enerji Seviyesi, Seviyeler Arası Geçiş*

INTRODUCTION

In the orbital model of the atom, electrons are thought to be located in the orbits. The placement of the electrons is based on the Pauli Exclusion Principle and two electrons with the same quantum number can never be in the same orbit. It is known that some atoms with a certain number of electrons (noble gases) are more stable than the others as a result of the orbits being filled with electrons. It has been observed that a model similar to this model can be applied to protons and neutrons, which are located in the nucleus of the atom and whose common names are nucleons. In this model, called nuclear shell model (Mayer, 1948, Haxel et al. 1949, Mayer, 1949, Mayer, 1950, Talmi, 2005), proton and neutrons are located separately in the orbits within the nucleus. Similar to noble gases, some nuclei having particular numbers of proton and neutron (2, 8, 20, 28, 50, 82, and 128) were observed to be more stable than others, which are called double magic nuclei (Caurier et al. 2005, Brown, 2001). The large distance between single-particle orbits with a magic number and subsequent orbits results in the orbits being grouped. These groups are called shells and the nuclear shell model name comes from here.

In the nuclear shell model calculations, an appropriate double magic nucleus is considered as inert core and the valence nucleons that are more than this are included in the calculations. It is assumed that the nucleons that give $J = 0$ total angular momentum in the core are not moving. Accordingly, it is not possible for these nucleons to be included in valence nucleons out of the core. Assuming that the valence nucleons may be distributed in the shells just above the core, these shells are considered as model space. Nucleons in the model space can be placed in all combinations in each orbit. Different combinations cause different energy levels of the nucleus. In this study, some *A=49* isobars in *fp*-shell were investigated by using the nuclear shell model with ^{40}Ca core. So, there are 9 nucleons exist in the model space. Excited energy levels, reduced quadrupole transition probabilities and reduced magnetic transition probabilities were calculated for ^{49}Fe, ^{49}Mn, ^{49}Cr, ^{49}V, ^{49}Ti and ^{49}Sc nuclei. These are several shell model codes available in the literature for the calculations such as Kshell (Shimizu, 2013), NuShell (Brown and Rae, 2014), Redstick (Ormand and Jhomnson, 2000), Bigstick (Jhonson et al. 2018), Antoine (Caurier and Nowacki, 1999) and Oxbash (Brown, 2004). In the present work, we have used Kshell code for the calculations. This code enables us to perform nuclear shell-model calculations with M-scheme representation with the thick-restart Lanczos method. It can compute energy levels, spin, isospin, magnetic and quadrupole moments, *E2/M1* transition probabilities, and one-particle spectroscopic factors.

MATERIAL and METHODS

In this paper, some nuclear properties of ^{49}Fe, ^{49}Mn, ^{49}Cr, ^{49}V, ^{49}Ti and ^{49}Sc nuclei have been calculated in the scope of the nuclear shell model by using Kshell code. The *fp* model space above the ^{40}Ca closed-shell nuclei is suitable for the calculations (Fig.1) because the nuclei under investigations have proton/neutron numbers are above nuclear magic number 20. This model space consists of $f_{7/2}$, $p_{3/2}$, $f_{5/2}$ and $p_{1/2}$ orbits for valance nucleons. The valance nucleons can occupy these orbits randomly in different combinations. A total of 20 available positions exist for the occupation of the nucleons. We did not consider the nucleons in the closed shells and they do not contribute to the results of the calculations. Valance nucleons move in a finite number of j-orbits. Due to the difficulty of not knowing the individual interactions between the nucleons, an average potential created by other nucleons takes part in the works instead. Thus, the problem under the nuclear shell model is reduced to the many-body problem that takes into account all the nucleons in the nucleus,

to a few-body problem that takes into account only the valence nucleons. The Hamiltonian of the valance nucleons is given by

$$H = \sum_{ij}^{A} \epsilon_i a_i^+ a_j + \frac{1}{4} \sum_{ijkl}^{A} \langle ij|V|kl\rangle a_i^+ a_j^+ a_k a_l \quad (1)$$

Here the ϵ_i values are single-particle energies that the nucleons interact with the core. The particle destroyed in orbit *j* is created in orbit *i* by annihilation (*a*) and creation (a^+) operators. The two-body interaction term (<*ij*|*V*|*kl*>) says that particles destroyed in *k* and *l* orbits are created in orbits *i* and *j*. In the literature, several matrix element sets for the two-body interactions for different models spaces exist. In the present calculations, two different commonly used two-body interaction matrix element sets (*gxpf1a* and *kb3g*) have been used and the results have been compared with each other and the available literature values. The single-particle energies are -8.6240 MeV, -5.6793 MeV, -1.3829 and -4.1370 MeV for the $f_{7/2}$, $p_{3/2}$, $f_{5/2}$ and $p_{1/2}$ orbits in *gxpf1a*. For the *kb3g*, these values are -8.6 MeV, -6.6 MeV, -2.1 and -4.6 MeV. The two-body interactions include 518 matrix elements. The energy levels of the nucleus can be calculated by solving the Hamiltonian equation (Eq.2) using the many-body wave function (Ψ) defined by Slater determinants for nucleons.

$$H\Psi = E\Psi \quad (2)$$

Reduced quadrupole transition probability (*B(E2)*) and magnetic transition probability (*B(M1)*) values between the energy levels are in particular importance in nuclear structure studies (Bohr, 1969). They are related to the nuclear lifetime, deformations and shapes of the nuclei, quadrupole and magnetic moments, etc. In this study, these values have also been calculated for the *A=49* isobars whose experimental data is very limited in the literature.

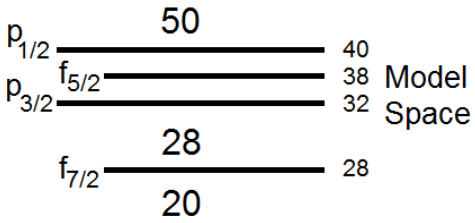

Fig 1. Single particle orbits in model space above ^{40}Ca core considered in the calculations

3. RESULTS and DISCUSSION

We have calculated nuclear-excited energy levels, spins/parities, *B(E2)* and *B(M1)* values for ^{49}Fe, ^{49}Mn, ^{49}Cr, ^{49}V, ^{49}Ti and ^{49}Sc nuclei which are A=49 isobars. Among them, ^{49}Fe - ^{49}V and ^{49}Cr - ^{49}Mn are the mirror pairs of each other by exchanging proton and neutron numbers. The calculated energy levels are presented in Tables 1-3 in comparison with the exiting experimental values in the literature from NNDC database (Kinser et al.1996). For proton-rich ^{49}Fe isotope (left of Table 1), the energy values for only the first two excited levels from experiments exist in the literature. Additionally, the spin and parity values for these levels have not been determined. Ground state spin and parity have been assigned as $7/2^-$ from both calculations. The two theoretical calculations give close results to these available experimental data, but *gxpf1a* results are slightly closer than *kb3g*. The other theoretically calculated energy level values for both calculations are similar to each other. For ^{49}Mn isotope (right of Table 1), more *kb3g* results are closer to the available

experimental data. Also, the excited level parity values could not be determined precisely in the literature. We have supported (-) parities for these levels in our calculations. The experimentally unknown levels have also been predicted by the theoretical model.

Table 1. Calculated energy levels, spin/parities of ^{49}Fe (left) and ^{49}Mn (right) in comparison with the available experimental data

^{49}Fe Exp.		Gxpf1a			Kb3g		
Spin	Energy	Spin	Energy	Diff.	Spin	Energy	Diff.
(7/2-)	0	7/2-	0	0	7/2-	0	0
-	90	5/2-	87	**-3**	5/2-	95	5
-	153	3/2-	152	**-1**	3/2-	165	12
		11/2-	966		11/2-	954	
		9/2-	1113		9/2-	1099	
		1/2-	1517		1/2-	1470	
		5/2-	1562		5/2-	1513	
		3/2-	1656		3/2-	1610	
		15/2-	2045		15/2-	2126	
		5/2-	2195		7/2-	2160	

^{49}Mn Exp.		Gxpf1a			Kb3g		
Spin	Energy	Spin	Energy	Diff.	Spin	Energy	Diff.
5/2-	0	5/2-	0	0	5/2-	0	0
7/2(-)	261	7/2-	175	-86	7/2-	234	**-27**
9/2(-)	1059	9/2-	1106	**47**	9/2-	1161	102
11/2(-)	1541	11/2-	1349	-192	11/2-	1442	**-99**
		3/2-	2052		3/2-	2145	
13/2(-)	2481	13/2-	2232	-249	1/2-	2284	
		7/2-	2278		3/2-	2308	
		3/2-	2310		13/2-	2373	**-108**
		1/2-	2389		7/2-	2416	
		5/2-	2705		5/2-	2579	

For ^{49}Cr isotope (left of Table 2), both theoretical results have been predicted ground state correctly. The low-lying levels have been determined more precisely for this isotope. For ^{49}V isotope (right of Table 2), *kb3g* gives mostly closer results to the experimental values. The ambiguous second $3/2^-$ level spin and parity values have been supported by two calculations in this study.

Table 2. Calculated energy levels, spin/parities of ^{49}Cr (left) and ^{49}V (right) in comparison with the available experimental data

^{49}Cr Exp.		Gxpf1a			Kb3g		
Spin	Energy	Spin	Energy	Diff.	Spin	Energy	Diff.
5/2-	0	5/2-	0	0	5/2-	0	0
7/2-	271	7/2-	175	-96	7/2-	234	**-37**
9/2-	1084	9/2-	1106	**22**	9/2-	1161	77
11/2-	1562	11/2-	1349	-213	11/2-	1442	**-120**
3/2-	1741	3/2-	2052	**311**	3/2-	2145	404
13/2-	2500	13/2-	2232	-268	1/2-	2284	
7/2-	2503	7/2-	2278	-225	3/2-	2308	-305
3/2-	2613	3/2-	2310	**-303**	13/2-	2373	**-127**
		1/2-	2389		7/2-	2416	**-87**
		5/2-	2705		5/2-	2579	

^{49}V Exp.		Gxpf1a			Kb3g		
Spin	Energy	Spin	Energy	Diff.	Spin	Energy	Diff.
7/2-	0	7/2-	0	0	7/2-	0	0
5/2-	91	5/2-	46	-45	5/2-	95	**4**
3/2-	153	3/2-	176	23	3/2-	165	**12**
11/2-	1022	11/2-	928	-94	11/2-	954	**-68**
9/2-	1155	9/2-	1070	-85	9/2-	1099	**-58**
		1/2-	1423		1/2-	1470	
5/2-	1515	5/2-	1493	-22	5/2-	1513	**-2**
(3/2-)	1643	3/2-	1646	**3**	3/2-	1610	-33
15/2-	2263	15/2-	1965	-298	15/2-	2126	**-137**
7/2-	2182				7/2-	2160	**-22**

Whereas for ^{49}Ti isotope (left of Table 3), *gxpf1a* gives closer results to the experimental values. The ambiguous $9/2^-$ level spin and parity values have been supported in this work. In the literature, the first and second excited state spin and parity values have been assigned as $3/2^-$ and $11/2^-$, respectively. Whereas in our calculations, the values for these levels seem displaced. For the last nucleus under investigation ^{49}Sc (right of Table3), low-lying levels are well calculated by *kb3g* and the higher ones are generally well calculated by *gxpf1a*. Ground state spin and parities have been assigned correctly and ambiguous spin and parities have partially been supported mostly by *gxpf1a*.

Table 3. Calculated energy levels, spin/parities of ^{49}Ti (left) and ^{49}Sc (right) in comparison with the available experimental data

^{49}Ti Exp.		Gxpf1a			Kb3g		
Spin	Energy	Spin	Energy	Diff.	Spin	Energy	Diff.
7/2-	0	7/2-	0	0	7/2-	0	0
3/2-	1382	11//2-	1515	**-27**	11//2-	1637	95
11/2-	1542	3/2-	1540	**158**	3/2-	1682	300
(9/2-)	1610	9/2-	1680	**70**	9/2-	1826	216
5/2-	1762	5/2-	1738	**-24**	5/2-	1877	115
		3/2-	2095		3/2-	2244	
		7/2-	2240		7/2-	2408	
15/2-	2506	15/2-	2447	**-59**	1/2-	2500	
		1/2-	2540		15/2-	2644	138
		13/2-	2574		13/2-	2817	

^{49}Sc Exp.		Gxpf1a			Kb3g		
Spin	Energy	Spin	Energy	Diff.	Spin	Energy	Diff.
7/2-	0	7/2-	0	0	7/2-	0	0
3/2-	3085	3/2-	2767	-318	3/2-	3335	**250**
(9/2-)	3915	9/2-	3649	**-266**	11/2-	4210	**18**
(11/2-)	4192	11/2-	3752	-440	5/2-	4233	**-99**
7/2-	3809	7/2-	3761	**-48**	13/2-	4276	
5/2-	4072	13/2-	3851		9/2-	4383	336
5/2-	4332	5/2-	3911	**-161**	7/2-	4450	641
(9/2-)	4047	9/2-	4138	**91**	9/2-	4466	419
(15/2-)	4267	15/2-	4168	**-99**	1/2-	4582	**89**
1/2-	4493	1/2-	4201	-292	15/2-	4712	1555

The calculated *B(E2)* and *B(M1)* values from the ground state to the first excited states for the nuclei by using the nuclear shell model have been shown in Fig. 2. Only for ^{49}Cr and

^{49}Ti isotopes, *B(E2)* values exist in the literature. The calculated results for these isotopes are very close to each other and the available literature value. This value is an important quantity in seeing the collective behavior of nuclei and gives information about the nuclear structure. As seen in the figure that the high *B(E2)* values for the ^{49}Cr and ^{49}Mn isotopes indicate high collectivity for these nuclei. In the literature, there is no data for *B(M1)* values for the investigated nuclei. In our calculations, we have obtained these values for ^{49}Fe, ^{49}Mn, ^{49}Cr and ^{49}V isotopes. As is seen in Fig. 3 that, again for ^{49}Cr and ^{49}Mn, *B(M1)* values are larger. The results from *kb3g* are generally larger than *gxpf1a* especially for ^{49}Cr and ^{49}Mn.

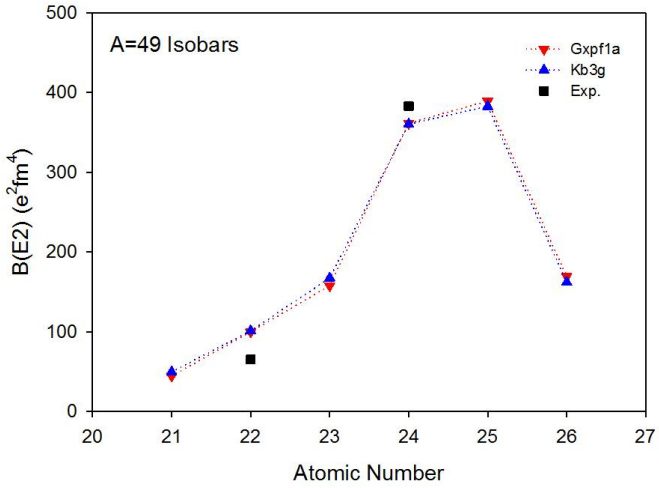

Fig. 2 *B(E2)* values for ^{49}Fe, ^{49}Mn, ^{49}Cr, ^{49}V, ^{49}Ti and ^{49}Sc nuclei

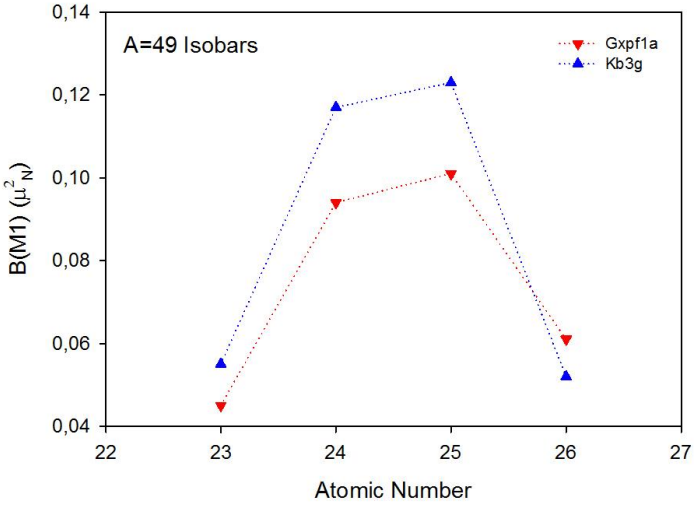

Fig. 3 *B(M1)* values for ^{49}Fe, ^{49}Mn, ^{49}Cr, ^{49}V, ^{49}Ti and ^{49}Sc nuclei

CONCLUSION

In this study, the energy levels, spins/parities, *B(E2)* and *B(M1)* values for ^{49}Fe, ^{49}Mn, ^{49}Cr, ^{49}V, ^{49}Ti and ^{49}Sc nuclei have been investigated in the scope of nuclear shell model. Kshell computer code has been used for the calculations. Two different parameter sets have been used for two-body interactions. The results have been compared with each other and the available literature data. Several energy states for these nuclei have not been investigated

experimentally in detail in the literature. Some unknown and ambiguous energy levels are predicted by the calculations in this study. Also, ambiguous levels have been supported by the calculations. Furthermore, most of the *B(E2)* and *B(M1)* values have been predicted the first time in this study.

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