Araştırma Makalesi / Research Article

Nuclear Shell Model Calculations for Ca Isotopes

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Abstract
Energies of nuclear excited states of nuclei, nuclear spin/parity and transition probabilities between nuclear levels can be calculated in the scope of nuclear shell model. The nuclei having magic numbers are used as inert core in the calculations. It is assumed that the nucleons in the inert core do not move outside from the core. Only valance nucleons out of the core are considered in the shell model calculations. In this study, the nuclear energy levels of even-even $^{42-56}$Ca isotopes have been calculated by the nuclear shell model using KShell computer code. This code enables us to perform nuclear shell-model calculations with M-scheme representation. In the calculations, doubly magic ^{40}Ca isotope was taken as core. For the neutrons, $0f_{7/2}$, $1p_{3/2}$, $0f_{5/2}$ and $1p_{1/2}$ orbits are considered as model space. Excited nuclear level spins, parities and energies have been obtained for Ca isotopes. The results have been compared with the available experimental values in the literature.

Keywords: Shell Model, energy levels, spin/parity, electromagnetic transitions, Ca.

Ca İzotopları için Nükleer Kabuk Modeli Hesaplamaları

Öz
Nükleer uyarılmış durum enerjileri, nükleer enerji/parite ve nükleer seviyeler arasındaki geçiş olasılıkları nükleer kabuk modeli kapsamında teorik olarak hesaplanabilir. Sihirli sayıları olan çekirdekler, hesaplamalarda kor çekirdek olarak kullanılır. Kor çekirdekteki nükleonların çekirdek dışına çıkmadığı varsayılmaktadır. Kabuk modeli hesaplamalarında sadece değerlik nükleonları dikkate alınır. Bu çalışmada, çift-çift $^{42-56}$Ca izotoplarının enerji seviyeleri, KShell bilgisayar kodu kullanılarak nükleer kabuk modeli kapsamında hesaplanmıştır. Bu kod, M şema gösterimi ile nükleer kabuk modeli hesaplamaları yapmaya olanak sağlar. Hesaplamalarda, çift sihirli ^{40}Ca izotopu kor çekirdek olarak alındı. Nötronlar için $0f_{7/2}$,$1p_{3/2}$, $0f_{5/2}$ and $1p_{1/2}$ yörüngeleri model uzay olarak kabul edildi. Ca izotopları için uyarılmış nükleer seviye spinleri, pariteleri ve enerjileri elde edildi. Sonuçlar literatürdeki mevcut deneysel değerlerle karşılaştırıldı.

Anahtar kelimeler: Kabuk Modeli, enerji seviyeleri, spin/parite, elektromanyetik geçişler, Ca.

1. Introduction

In order to understand structure of the atomic nuclei, nuclear shell model is one of the best methods. The fpg-shell nuclei lying between 20 to 50 atomic numbers are one of the interesting region in nuclear physics studies. Determinations of the energy levels, spin and parities of nuclei are important for nuclear properties of nuclei. By this purpose, usage of different nuclear models serves us to understanding of nuclear structure containing many physical properties of the nuclei. Among them, nuclear shell-model (SM) is one of the most featured and successful nuclear models. It is similar to the electronic shell model for atoms. Analogously, valance nucleons (protons or neutrons) in a nucleus play a role for the determination of nuclear properties. The valance nucleons are located out of closed nuclear shells. Generally double magic nuclei are considered as inert core which are closed nuclei. As is known, nuclei with magic numbers are most stable and have completely different properties comparing with their neighbors [1-7].

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Calcium element has 20 proton numbers which is one of the nuclear magic numbers. The doubly-magic ^{40}Ca isotope is very stable and taken into account in the calculations as an inert core. By considering additional neutrons above this core, nuclear structure studies have been performed. In the scope of the nuclear shell model, many investigations for Ca isotopes have been performed existing in the literature [8-11]. In this paper, first three excited level energies of even-even Ca isotopes have been calculated by using Kshell shell model computer code [12]. This code enables us to perform nuclear shell-model calculations with M-scheme representation with the thick-restart Lanczos method. The code is easily used on a Linux PC with a many-core CPU and OpenMP library. It is also used on a state-of-the-art massive parallel computer with hybrid MPI+OpenMP parallel programming. It can compute energy levels, spin, isospin, magnetic and quadrupole moments, E2/M1 transition probabilities, and one-particle spectroscopic factors. Up to tens of billions M-scheme dimension is capable, if enough memory is available on the computers. By using this code, several calculations have been performed by our group in pf shell [13, 14].

2. Material and Method

For the calculation of the first three (2^+, 4^+, 6^+) excited energy levels of even-even Ca isotopes, nuclear shell model has been taken into account. For this task, Kshell computer code [12] has been used. There are many useful open codes in the literature which is written for the nuclear shell model calculations such as NuShell [15], Redstick [16], Bigstick [17], Antoine [18], Oxbash [19], etc. This model space consists of $0f_{7/2}$, $1p_{3/2}$, $0f_{5/2}$, $1p_{1/2}$ and $0g_{9/2}$ valence orbitals. In the study, $0f_{7/2}$,$1p_{3/2}$, $0f_{5/2}$ and $1p_{1/2}$ orbits for the neutrons are considered as model space. We have considered double magic ^{40}Ca isotope as a core. The nucleons in the core with J=0 do not move from the core. Valance nucleons move in a finite number of j-orbits and their Hamiltonian of the valance nucleons is given by Eq. (1).

$$H = E_0 + \sum_i \varepsilon_i a_i^+ a_j + 1/2 \sum_{ijkl} \langle ij|V|kl\rangle a_i^+ a_j^+ a_l a_k \tag{1}$$

where E_0 is the energy of the inert core, ε_i is single particle energies (SPE) of the valance orbits and $<ij|V|kl>$ term is two-body matrix elements (TBME) of residual interaction amongst the valance particles. In this work, different interactions for fpg shells (fpd6, gxpf1a and kb3g) have been taken in the calculations, separately. The SPE's for these different interactions are given in Table 1. Each interaction Hamiltonians consist of 518 elements. No truncation has been performed in the calculations. In the investigation of nuclear shapes, reduced electric quadrupole transition probability (B(E2)) and quadrupole deformation parameter (β_2) are the indicators. The β_2 showing the deformation of the nuclei can be calculated by Eq.2. The neutron and proton effective charges have been taken as en =0.5e and ep = 1.5e, respectively.

$$\boldsymbol{\beta_2} = \frac{4\pi}{3ZR_0^2}[B(E2)/e^2]^{\frac{1}{2}} \tag{2}$$

Table 1. Single particle energies for fpd6, gxpf1a and kb3g interactions

	Single Particle Energies		
	Fpd6	**Gxpf1a**	**Kb3g**
1	-8.3876	-8.6240	-8.6000
2	-6.49520	-5.6793	-6.6000
3	-1.89660	-1.3829	-2.1000
4	-4.47830	-4.1370	-4.6000

3. Results and Discussion

The nucleons of the core for the calculations are 20 protons and 20 neutrons with J=0, T=0 ground state configuration of ^{40}Ca nucleus. The additional neutrons are distributed over all possible combinations of the $0f_{7/2}$,$1p_{3/2}$, $0f_{5/2}$ and $1p_{1/2}$ orbitals for Ca isotopes. For all isotopes, ground state spins have been calculated in accordance with the experimental values. For even-even $^{40-56}$Ca isotopes, we have shown first there (or two) experimental [20] and shell model calculated energies in Table 2. As can be clearly seen in the tables that one of the calculated excited level energies are closer to the experimental values.

For ^{42}Ca isotope, the results from gxpf1a interaction for 2^+ level and fpd6 interaction for 4^+ and 6^+ levels are closer to the experimental values. For ^{44}Ca isotope, the results from kb3g interaction for 2^+ level, gxpf1a interaction for 4^+ level and fpd6 interaction for 6^+ level are closer to the experimental values. For ^{46}Ca isotope, the results from gxpf1a interaction for 2^+ level and fpd6 interaction for 4^+ and 6^+ levels are closer to the experimental values. For ^{48}Ca isotope, only first two levels have been calculated. The results from gxpf1a interaction for 2^+ and for 4^+ levels are closer to the experimental values. In the calculation of kb3g interaction, the level order is interchanged. For ^{50}Ca isotope, again only first two levels have been calculated. The kb3g interaction for 2^+ and gxpf1a interaction for 4^+ levels give closer results to the experimental values. For this isotope, there is unambiguity in 4+ level spin in the experimental value. For ^{52}Ca isotope, only first level experimental energy value exists in the literature. We have calculated first two and fpd6 interaction gives closer result to the experimental value. For ^{54}Ca isotope, only first level experimental energy value exists in the literature and also there is unambiguity in the spin value. We have calculated first two levels and fpd6 interaction gives closer result to the experimental value. For ^{56}Ca isotope, no experimental energy value exists in the literature. We have calculated first two levels by using different interactions.

Table 2. Experimental and Shell Model calculated first three energy levels for $^{42-56}$Ca isotope

	^{42}Ca			
	Fpd6	**Gxpf1a**	**Kb3g**	**exp**
2^+	1781	**1438**	1370	1525
4^+	**2709**	2269	2365	2572
6^+	**3145**	2711	2782	3189
	^{44}Ca			
	Fpd6	**Gxpf1a**	**Kb3g**	**exp**
2^+	1619	1361	**1248**	1157
4^+	2552	**2105**	2033	2283
6^+	**3187**	2694	2715	3285
	^{46}Ca			
	Fpd6	**Gxpf1a**	**Kb3g**	**exp**
2^+	1576	**1279**	1177	1346
4^+	**2757**	2236	2229	2575
6^+	**3119**	2631	2610	2974
	^{48}Ca			
	Fpd6	**Gxpf1a**	**Kb3g**	**exp**
2^+	3658	**3735**	4231 (**4^+**)	3832
4^+	4134	**4264**	4238 (**2^+**)	4503
	^{50}Ca			
	Fpd6	**Gxpf1a**	**Kb3g**	**exp**
2^+	1325	1192	**1060**	1027
4^+	3748	**4459**	4143	(**4^+**) 4515
	^{52}Ca			
	Fpd6	**Gxpf1a**	**Kb3g**	**exp**
2^+	**2749**	2258	2349	2563
4^+	3242	5014	3901	-
	^{54}Ca			
	Fpd6	**Gxpf1a**	**Kb3g**	**exp**
2^+	1470	2957	1317	(**2^+**) 2043
4^+	2404	5326	2851	-
	^{56}Ca			
	Fpd6	**Gxpf1a**	**Kb3g**	**exp**
2^+	1366	942	1064	-
4^+	2456	1252	1574	-

We have plotted first 2^+ excited level energies for Ca isotopic chain according to the mass number (Figure 1). As is seen in the figures that N=28 shell closure is observed for all calculations since ^{48}Ca isotope is doubly-magic. The N=32 subshell closure is also seen but N=34 closure is enhanced in gxpf1a interaction. The results from gxpf1a interaction, N=34 subshell closure in ^{54}Ca is confirmed. This appears because the neutron $f_{5/2}$ orbital lies relatively high above the $p_{1/2}$ orbital in this interaction. No significant N=34 subshell closure is predicted by kb3g and fpd6 effective interactions. We have also calculated reduced electric transition probability from the ground state to the first 2^+ state B(E2) which is shown in Figure 2. Gxpf1a and kb3g interactions give similar results to each other, whereas results from fpd6 is a bit larger. Also, according to results from fpd6 interaction, higher collectivity is seen for ^{56}Ca isotope. The quadrupole deformation parameters (β) for Ca isotopes have been calculated theoretically for Ca isotopic chain. All Ca isotopes are almost spherical in shape to the shell-model calculations. The values are in the order of $1x10^{-1}$.

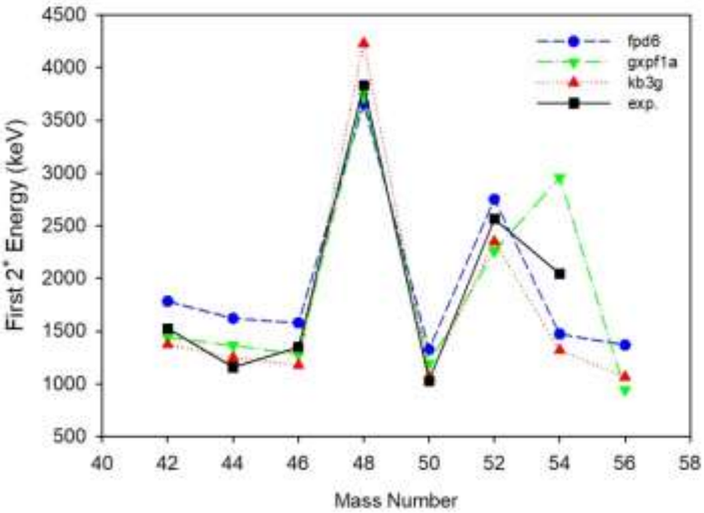

Figure 1. First 2^+ excited levels of even-even Ca isotopes from experiments, fpd6, gxpf1a and kb3g interactions

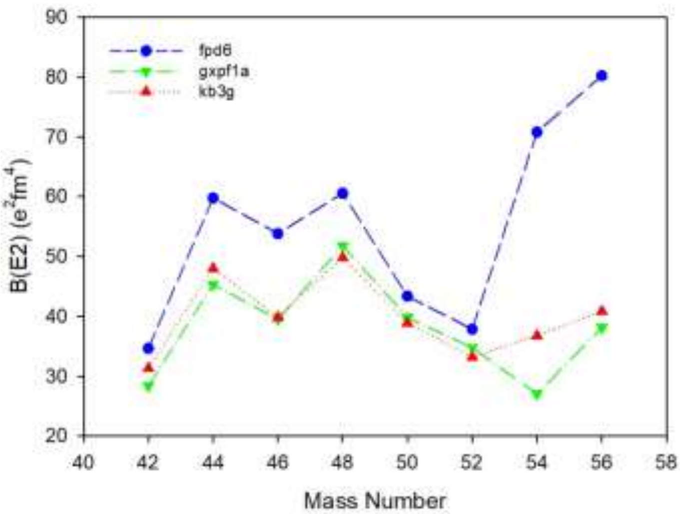

Figure 2. B(E2) values of even-even Ca isotopes from fpd6, gxpf1a and kb3g interactions

4. Conclusion

In this work, ground state and excited states energy levels of even-even Ca isotopes have been calculated by using Kshell computer code in the scope of nuclear shell model. It has been seen that the results from different interaction Hamiltonians are close to the experimental values which are available in the literature in some cases. For $^{48-50}$Ca isotopes there are no experimental values in the literature for 6^+

energy levels. For $^{52-54}$Ca isotopes there are no experimental values in the literature for both 4^+ and 6^+ energy levels. For very neutron rich ^{56}Ca isotope, there are no experimental values in the literature for the excited energy levels. We have also calculated these missing values by using the nuclear shell model. According to the B(E2) calculations with fpd6 interaction, the ^{56}Ca isotopes are the most collective among the others having the higher B(E2) value.

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Authors' Contributions

Yasemin Ayhan performed the theoretical calculations with the computer code. The results were interpreted by all authors and the article was written.

Statement of Conflicts of Interest

There is no conflict of interest between the authors.

Statement of Research and Publication Ethics

The author declares that this study complies with Research and Publication Ethics.

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