Int. J. Adv. Eng. Pure Sci. 2020, 32(4): 473-477
DOI: 10.7240/jeps.714481

RESEARCH ARTICLE / ARAŞTIRMA MAKALESİ

Investigation of Nuclear Structures of Self-conjugate Zn, Ge, Se, Kr, Sr Nuclei

Öz-eşlenik Zn, Ge, Se, Kr, Sr Çekirdeklerinin Nükleer Yapılarının İncelenmesi

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Abstract
The nuclear structure of the atomic nuclei can be theoretically investigated by using the nuclear shell model. Generally, a doubly closed-shell nucleus has been considered as inert core and the nucleons outside the core are taken into account in the calculation. It is assumed that the nucleons in the inert core do not move but each valence nucleon out of the core moves under an average potential created by the others. The self-conjugate (N=Z) medium mass nuclei region is one of the regions for the investigation of several phenomena because of the maximum spatial overlap of neutrons and protons. In this study, the structures of the medium mass N=Z nuclei have been analyzed in the scope of the nuclear shell model by using KSHELL computer code. In the calculations, doubly magic ^{56}Ni were taken as core, and the $2p_{3/2}$, $1f_{5/2}$ ve $2p_{1/2}$ single-particle orbits were used as valence orbits. Different two-body interactions (*jun45* and *f5pvh*) have been taken into account. The results have been compared with each other and the available values existing in the literature.
Keywords: Nuclear shell model, jun45, f5pvh, N=Z nuclei, energy level, deformation.

Öz
Atom çekirdeklerinin nükleer yapıları, nükleer kabuk modeli kullanılarak teorik olarak incelenebilir. Genel olarak, bir çift-çift kapalı kabuk çekirdeği durağan kor (inert kor) çekirdek olarak kabul edilir ve bunun dışındaki nükleonlar hesaplamalarda dikkate alınır. Kor çekirdekteki nükleonların hareket etmediği, ancak kor dışındaki valans nükleonlarının, diğerleri tarafından yaratılan ortalama bir potansiyel altında hareket ettiği varsayılmaktadır. Öz-eşlenik (N=Z) orta ağırlığa sahip kütleli çekirdeklerin bölgesi, nötronların ve protonların azami uzaysal çakışması nedeniyle, bazı nükleer olguların araştırılması için uygun bölgelerden birisidir. Bu çalışmada, orta ağırlıktaki N=Z çekirdeklerinin nükleer yapı özellikleri, nükleer kabuk modeli kapsamında KSHELL bilgisayar kodu kullanılarak araştırılmıştır. Hesaplamalarda kor çekirdek olarak çift sihirli ^{56}Ni ele alınmış ve valans orbitalleri olarak $2p_{3/2}$, $1f_{5/2}$ ve $2p_{1/2}$ tek parçacık seviyeleri kullanılmıştır. Farklı iki cisim etkileşmeleri (*jun45* ve *f5pvh*) ele alınmıştır. Sonuçlar birbirleriyle ve literatürdeki mevcut değerlerle karşılaştırılmıştır.
Anahtar Kelimeler: Nükleer kabuk modeli, jun45, f5pvh, N = Z çekirdekler, enerji seviyesi, deformasyon

I. INTRODUCTION

Many nuclear properties of nuclei can be obtained from the mean-field approximation in which protons and neutrons move independently from each other in a common potential. The field is generated as a result of the interaction among nucleons [1-5]. Atomic nuclei at N=Z line at the nuclide chart are very interesting in nuclear structure studies due to protons and neutrons (nucleons) occupy the same orbits. They are unique to study several phenomena such as shape coexistence along the N=Z line and the role of pairing correlation of neutron and proton. Furthermore, these nuclei are in the rp-process pathway [6]. In order to investigate the nuclear structure including N=Z nuclei, the nuclear shell model (SM) is one of the successful models [7-14]. Several phenomena can be predicted by using this model such as the energy of the excited states, their spin/parity, the electromagnetic transition probabilities and electromagnetic moments. In this model, protons and neutrons are filling the single-particle orbits in increasing order of energy, resulting in the concept of shell structure and shell closures.

Complete determination of the nuclear level schemes is an important issue for both experimentalists and theoreticians. In this way, theoretical models can be improved by the comparison of the experimental values thus extending the predictive power of the theoretical approach further away of the stability. In a simplified approach, the nuclear SM can be considered as similar to the electronic shell model of the atoms. Analogously, valence nucleons in the nuclei which are located out of inert core are responsible of the nuclear properties. The nuclei

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Submitted: 04.04.2020, **Revised:** 11.06.2020, **Accepted:** 08.08.2020

having the particular numbers of protons and/or neutrons (2, 8, 20, 28, 50, 82, 126) are called closed-shell nuclei and these nuclei are generally used as an inert cores in the calculations. Closed-shell nuclei are often very stable and have completely different properties compared with their neighbours. It is assumed that the nucleons in the inert core do not move, whereas each valence nucleon out of the core moves under the average potential by the others. Therefore, only valence nucleons are taken into account in the calculations.

For the SM calculations, there are many computer codes exist in the literature such as KSHELL [15], NuShellX [16], REDSTICK [17], BIGSTICK [18], ANTOINE [19] and Oxbash [20]. The investigated self-conjugate Zn, Ge, Se, Kr, Sr nuclei have been studied previously via different theoretical models [21-23]. In this paper, the first 2^+ and 4^+ excited state energies, reduced electric transition probabilities (B(E2) from 0^+ to 2^+ state, quadrupole deformation parameters (β), $R_{4/2}$ ratios of medium mass N=Z nuclei have been calculated and investigated by using KSHELL shell model code [15]. For this aim, shell model calculations with two different two-body interactions (*jun45* and *f5pvh*) have been performed and the results have been compared with each other and the literature data. These effective interactions are appropriate for the investigation of the nuclear properties for the nuclei in the upper pf-shell and N=Z nuclei in this shell [24]. Also, it was stated that the shell model with *jun45* describes very well the expected properties of the N=Z nuclei lie in this shell [25]. The KSHELL 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. Depending on the memory availability of the computer used, M-scheme matrices with dimensions of up to tens of billion elements can be diagonalized. In the calculations of the present study, doubly magic ^{56}Ni nuclei were taken as inert core and $2p_{3/2}$, $1f_{5/2}$ ve $2p_{1/2}$ single-particle orbits form the valence orbits. Two different Hamiltonians for two-body interactions have been used. The results have been compared with each other and the available values in the literature.

II. MATERIAL AND METHOD

The model space above the ^{56}Ni closed-shell is suitable for the investigation of medium mass N=Z nuclei. The model space used in the calculations consists of $2p_{3/2}$, $1f_{5/2}$ ve $2p_{1/2}$ valence orbits. The valence nucleons are distributed in these three orbits in order to minimize the energy for a determined spin. Because, the nucleons in the core with J=0 do not move from the core and the valence nucleons do not move into the core, we did not consider the nucleons in the closed-shells. In Figure 1, we have illustrates the model space and core for protons and neutrons used in this work. The Hamiltonian of the valence nucleons is given by the following equation,

$$H = E_0 + \Sigma\varepsilon_i + \Sigma\langle ab;JT|V|cd;JT\rangle \qquad (1)$$

where E_0 is the energy of the inert core, ε_i is single-particle energies that the nucleons in the *i*th orbits interact with the core and the last term $\langle ab;JT|V|cd;JT\rangle$ is two-body matrix elements for the valence particles. Here, the nucleon pairs in *a*, *b* and *c*, *d* orbits are coupled to spin and isospin quantum numbers *J* and *T*. For two-body interaction, *f5pvh* [26] and *jun45* [25] commonly used interaction Hamiltonians have been used separately in the calculations. Although the regions where the interactions are successful are explained in detail at the relevant papers, we have used these interactions for all N=Z nuclei in the pf-shell. The purpose is to see the success of the interactions for each nucleus and comparing the results with each other. The single-particle energies for *f5pvh* interaction are -10.27 MeV, -9.42 MeV and -9.05 MeV for the $2p_{3/2}$, $1f_{5/2}$ ve $2p_{1/2}$ orbitals, respectively. The interaction Hamiltonian is defined by a set of 63 two-body matrix elements. For *jun45* interaction, the single-particle energies are -9.83 MeV, -8.71MeV and -7.84 MeV for the $2p_{3/2}$, $1f_{5/2}$ ve $2p_{1/2}$ orbitals. Although this interaction also includes the $g_{9/2}$ orbit above the $p_{1/2}$, we have not taken into account this orbit for the exact comparison with the former one. The full interaction file contains 334 two-body matrix elements. 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 e_n =0.5e and e_p = 1.5e, respectively.

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

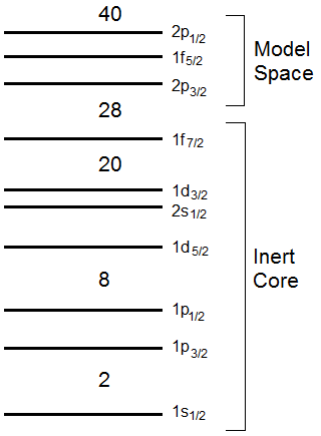

Figure 1. Single-particle levels of nucleons grouped to form model space above the ^{56}Ni core for the calculations

III. RESULTS AND DISCUSSIONS

Due to the fundamental information about the nuclear structure in even-even nuclei comes from the first two excited states. In Figure 2, we have shown the first 2^+ and 4^+ state energies from SM calculations for the investigated ^{60}Zn, ^{64}Ge, ^{68}Se, ^{72}Kr and ^{76}Sr nuclei (N=Z) in comparison with the experimental data [27]. To analyze nuclear structure, these levels have to be known accurately. The first 2^+ energies of nuclei can be used as an indicator of collective behavior. Generally, light nuclei have higher energy values for the first 2^+ state. While the mass numbers of nuclei increase, the 2^+ energy values decrease. Until atomic number 34, this behavior is seen in this work. From our calculations, the results for 2^+ energy values stay nearly constant after atomic number 34 for *jun45* interaction and slightly increase for *f5pvh* interaction. For ^{60}Zn isotope, the first 2^+ excited level energies from different interactions are compatible with the experimental value. However, *f5pvh* gives closer value to the experimental value. For ^{64}Ge isotope, the result from *f5pvh* is still close to the experimental value, but *jun45* gives results far from it. The result of the calculations made using the *f5pvh* interaction and the experimental value is very close to each other for the ^{68}Se isotope, whereas the calculated result by *jun45* interaction is very far from them. For these three isotopes, theoretical results from the both interactions are lower than the experimental values. For ^{72}Kr isotope, the result is still lower than the experimental value for *jun45* interaction, but *f5pvh* gives larger value. For the last investigated N=Z isotope ^{76}Sr, the first 2^+ experimental energy value is very low and not certainly determined in the literature. This corresponds to the deformed shell gap at the nucleon number 38. The theoretical value from *jun45* is closer to this low value. Besides, both theoretical results are seen as larger than the low experimental value.

In the figure, we have also shown the first 4^+ excited state energies for the isotopes under investigation. For ^{60}Zn isotope, the result from *f5pvh* interaction is very close to the experimental value. For ^{64}Ge and ^{68}Se isotopes, *f5pvh* gives almost the same value as the experiment. After these isotopes, *jun45* starts to give results closer to the experimental data. For ^{72}Kr isotope, *jun45* value is very close to the experimental value. However, as in the 2^+ state, results from both theoretical calculations are not compatible with the experiment for ^{76}Sr. Again, the experimental value is ambiguous at this state for ^{76}Sr isotope. However, with the increasing number of valence nucleons, divergence from experimental results is inevitable. Therefore, the difference between the low energy 2^+ and 4^+ levels observed in the collective nuclei is the expected result.

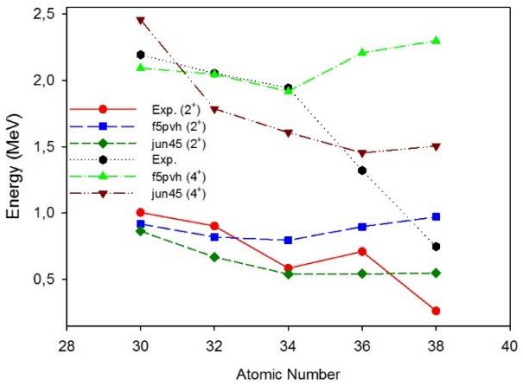

Figure 2. The calculated first 2^+ and 4^+ excited state energies for ^{60}Zn, ^{64}Ge, ^{68}Se, ^{72}Kr, and ^{76}Sr isotopes in comparison with the experimental data [27].

We have also calculated the ratios of 4^+ to 2^+ energies ($R_{4/2}$) for the investigated nuclei (Figure 3). This ratio can take different value as < 2.0, ~2.0-2.2, ~2.7 and ~3.33 for non-collective, spherical-vibrator, transitional and rigid-rotor structured nuclei, respectively. For ^{60}Zn and ^{64}Ge, both theoretical with *f5pvh* interaction and experimental results are close to each other and they indicate that these nuclei are spherical vibrators whereas according to the calculations with *jun45*, these are transitional. For ^{68}Se, the theoretical result with *jun45* interaction is closer to the experimental value which indicates this nucleus is rigid-rotor. For ^{72}Kr, both theoretical results are far from the experimental value. According to the experimental value, this nucleus can be a spherical vibrator but to the theoretical results, it is transitional. For ^{76}Sr, both theoretical with *jun45* interaction and experimental results are very close to each other. All the results indicate that this nucleus is transitional. Generally, by using *jun45* interaction in the calculations, we have obtained slightly larger values than *f5pvh*.

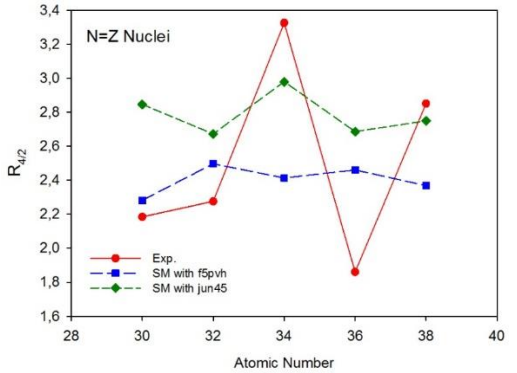

Figure 3. $R_{4/2}$ ratios for ^{60}Zn, ^{64}Ge, ^{68}Se, ^{72}Kr, and ^{76}Sr isotopes in comparison with the experimental data [27].

We have also calculated reduced electric transition probability from the ground state to the first 2^+ state B(E2) which is shown in Figure 4. Both theoretical results are in good agreement for ^{64}Ge and ^{68}Se with the available adopted values in the literature [28]. For ^{60}Zn, there is no adopted value in the literature. For ^{72}Kr and ^{76}Sr, the theoretical results stay nearly constant, but the adopted values start drastically to increase which shows an increase of collectivity. We have also given the B(E2) values from other theoretical models in the figure which are taken from Raman [29]. As is seen in the figure that only HFB+BCS results are in harmony with both SM calculations.

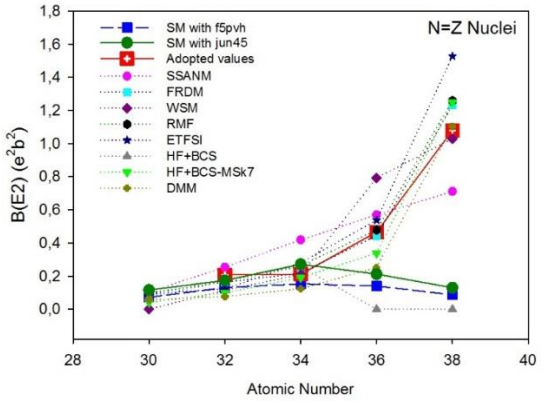

Figure 4. B(E2) values for ^{60}Zn, ^{64}Ge, ^{68}Se, ^{72}Kr, and ^{76}Sr isotopes.

Finally, in Figure 5, we have shown the quadrupole deformation parameters for the nuclei. The positive value of β_2 is related to prolate shape while the negative value of β_2 corresponds to the oblate shape of nuclei. As can be seen in the figure that all the nuclei under investigation have prolate shape. There is no adopted value for ^{60}Zn nuclei in the literature. According to the adopted values, ^{72}Kr and ^{76}Sr are very deformed nuclei, but for both theoretical calculations by *f5pvh* and *jun45* interactions, these are less deformed. Additionally, according to the common literature result [30], the ^{68}Se nucleus has an oblate shape.

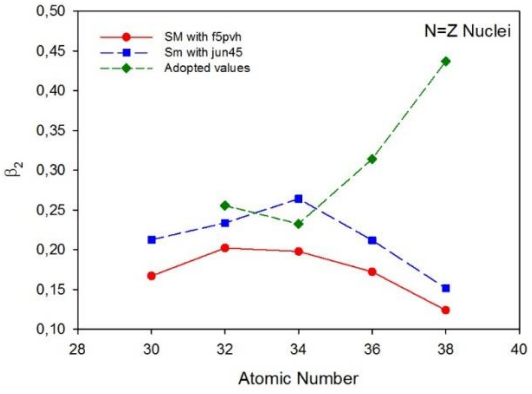

Figure 5. Quadrupole deformation parameters (β_2) for ^{60}Zn, ^{64}Ge, ^{68}Se, ^{72}Kr and ^{76}Sr nuclei

IV. CONCLUSIONS

In this study, nuclear structures of ^{60}Zn, ^{64}Ge, ^{68}Se, ^{72}Kr and ^{76}Sr medium mass N=Z nuclei have been investigated within the nuclear shell model by calculating first 2^+ and 4^+ energies, the ratios between these energies, reduced electric transition probabilities from the ground state to first 2^+ state and quadrupole deformation parameters. KSHELL computer code was used for the calculations on these isotopes with two different two-body interaction Hamiltonians (*f5pvh* and *jun45*). The results have been compared with each other and the available literature data. For ^{60}Zn, ^{64}Ge, ^{68}Se nuclei, the results from theoretical calculations are in harmony with the literature data. However, with the increasing number of valence nucleons, divergence from experimental results is inevitable. Therefore, the divergence from experimental values for the low energy 2^+ and 4^+ levels observed in the collective nuclei is the expected result. *F5pvh* interaction generally gives closer results than *jun45* interaction for these nuclei. Furthermore, the B(E2) values are theoretically calculated in this study whose data do not exist in the literature. In the future, it is planned to extend this work to the heavier N=Z nuclei (^{80}Zr, ^{84}Mo, ^{88}Ru, ^{92}Pd, ^{96}Cd, and ^{100}Sn) in the same shell.

Acknowledgment

This work is supported by the scientific research project fund of Sivas Cumhuriyet University under project number F-616.

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