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NUCLEAR PHYSICS

Effect of the Woods-Saxon Spin–Orbit Term on the Nuclear Spectra: ^{18}O Application

Serkan Akkoyun[1]

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Abstract
One of the successes in describing the nuclear structure correctly is taking into account the spin–orbit interaction. Thus, single-particle energies and nuclear magic numbers can be obtained accurately. The main subject of this study is to investigate how the strength of this spin–orbit interaction affects the nuclear structure, more specifically the nuclear spectra. In this study we carried out for this purpose, we obtained neutron single-particle energies by changing the strength of the spin–orbit term included in the Woods-Saxon potential. By using the neutron single-particle orbit energies in the calculations of the nuclear shell model, which we obtained for different strengths of spin–orbit term, we obtained the ground and low-lying excited states of the ^{18}O isotope. According to the results, we observed that spin–orbit interactions of different strength have a discernible effect on the nuclear spectra.

Keywords Nuclear shell model · Spin–orbit term · Woods-Saxon potential · Single-particle energy · Energy states

1 Introduction

The way to understand what is going on inside atomic nuclei is the subject of nuclear structure studies. One of the most successful and powerful models used for this purpose is of course the nuclear shell model [1–5]. The nuclear shell model allows for a microscopic description of the structure of the nucleus and it is based on the ansatz that each nucleon inside the nucleus moves independently in a spherically symmetric mean field generated by all other constituents. The mean field is usually described by a Woods-Saxon or a harmonic oscillator potential supplemented by a strong spin–orbit term. Nucleons arrange themselves in well-defined and separated energy levels. The shell model (SM) can be further improved by introducing the interacting shell model. According to the interacting shell model, the complex nuclear many-body problem is reduced to a simplified one where only few valence nucleons interact in the reduced model space above an inert core [6]. The valence nucleons interact with each other via two-body residual interaction, that is, the part of the interaction which is not accounted for in the central potential. The inclusion of the two-body interaction removes the degeneracy of the states which belong to the same configuration and produces a mixing of different configurations. The SM Hamiltonian consists of one- and two-body components. These are single-particle energies and the two-body matrix elements of the residual interaction, respectively.

The effects of the variation of single-particle energy values on the nuclear spectra are clearly seen in the calculations performed within the scope of the shell model. Therefore, it is important to examine the parameters affecting the single-particle energies. Ross et al. studied the effects of the surface diffuseness of the potential on the single-particle levels [7]. Takeuchi and Moldauer investigated the behavior of neutron single-particle bound states in the real part of the low-energy neutron optical model potential. They have systematically analyzed the effect of the changing of the nuclear radius on shell model single-particle levels [8]. Kanestrom and Koren performed more detailed shell model calculation using Woods-Saxon potential. The strength of the residual interaction treated as a free parameter and varied to obtain results fitting to experimental data. They showed that the shape of the potential outside the core may be of importance for the energy levels order [9]. Tanaka et al. investigated the effect of the spin–orbit potential on the single-particle levels in the super-heavy region. They concluded that a negative

✉ Serkan Akkoyun
sakkoyun@cumhuriyet.edu.tr

[1] Department of Physics, Faculty of Science, Sivas Cumhuriyet University, Sivas 58140, Turkey

symmetry term in the spin–orbit potential might result in an incomplete closing of the $Z=126$ shell gap [10].

A strong spin–orbit term is an important contribution to the nuclear mean field [11, 12]. As a result of the correct nuclear magic numbers that emerged by taking into account the existence of this term, it was possible to obtain results compatible with the experimental data on nuclear structure. The main aim of this study is to investigate of the spin–orbit contribution to the nuclear mean field on the nuclear spectra. For this purpose, neutron single-particle energies for ^{18}O are modified by the calculation of Woods-Saxon potential with different spin–orbit strengths. In other words, how the variation of spin–orbit interaction strength affects the neutron single-particle levels of ^{18}O isotope was systematically investigated. Then, how these varying single-particle energy levels affect the nuclear spectrum of the ^{18}O isotope was analyzed. For this purpose, the ground and excited state energies of the ^{18}O isotope were obtained by calculations performed within the scope of the nuclear shell model. In the shell model, the calculations were made by using different single-particle energy values in the shell model Hamiltonian. The reason for doing the analyses on this isotope is both its even-even structure and to minimize the contributions that may come from possible two-body interactions. Therefore, we preferred the isotope with the lowest possible number of valence nucleons (also electrically neutral nucleon to minimize Coulomb effects), since our main goal was to study spin–orbit interaction that causes the variation on the single-particle energies.

2 Materials and Methods

The nuclear shell model is one of the most appropriate tools to describe the low-energy structure of the atomic nucleus. In this model, nucleons are assumed to move in an independent central potential well. After the strong spin–orbit interaction proved to be an important component [11, 12], single-particle orbitals are correctly arranged and the nuclear magic numbers are identified [13]. Calculating nuclear energy levels in the scope of the nuclear shell model is a very difficult task. The main reason for the difficulty is that the nature of the interaction between free protons and neutrons, in other words the strong nuclear interaction, is not well known. If we consider a nucleus with a few valence nucleons outside the closed shells, the energies of the levels can be divided into three parts. The first is the binding energy of the closed shells (^{16}O in this study); the second is the sum of the kinetic energies of the valence nucleons and the single nucleon energies that include their interactions with the nucleons of the core (^{16}O). The third is the interaction of valence nucleons with each other. Of these, calculating the binding energies of closed shells is the most difficult, while the easiest to calculate is the interaction between valence nucleons. If these valence nucleons are in a single orbital, it is sufficient to know only the matrix elements of the effective interaction between the nucleons in that orbital. If the valence nucleons are distributed over several orbitals, differences between single-particle energies are also needed, which can often be taken from experimental data. One of the most important points in the shell model calculations is the selection of the effective interaction to be used between the valence nucleons [14].

Due to the difficulty of not knowing the individual interactions among nucleons, the many-body problem that takes into account all nucleons in the nucleus is reduced to a few-body problem that takes into account only valence nucleons. Since the interaction between nucleons is not clearly defined, the Hamiltonian can be arranged as given in Eq. (2), assuming that each nucleon moves at an average potential generated by the others.

$$H = \sum_{i=1}^{A} [T_i + U_i] + (\frac{1}{2}\sum_{i,j=1}^{A} V_{ij} - \sum_{i=1}^{A} U_i) \tag{1}$$

$$H = H_0 + H_{\text{residual}} \tag{2}$$

Here, H_0 is the single-particle energy (spe) of each nucleon under an average potential. Single-particle energies can be determined by choosing a central potential such as the harmonic oscillator, Woods-Saxon or Yukawa type. In order to calculate proton spe's to be used in the SM calculations, we have dealt with potential that consisted of a spin-independent central potential term, a spin–orbit potential term, and a Coulomb potential term for neutron interactions in Eq. (3) as

$$V(r) = V_o(r) + V_{so}(r)\vec{l}.\vec{s} + V_C(r) \tag{3}$$

where $V_o(r)$ is the spin-independent central potential, $V_{so}(r)$ is the spin–orbit potential, and $V_C(r)$ is the Coulomb potential. Explicit expression is given as in Eq. (4) with $R_0 = r_0 A^{1/3}$ $R_{so} = r_{so} A^{1/3}$. It can be explicitly written in Eq. (4) as

$$V(r) = \frac{V_0}{1+[\frac{\exp(r-R_0)}{a_0}]} + \frac{1}{r}\frac{d}{dr}\frac{V_{so}}{1+[\frac{\exp(r-R_{s0})}{a_{s0}}]}\vec{l}.\vec{s} + V_C(r) \tag{4}$$

where, e is the magnitude of the electron charge, Z is the proton number, ℓ is the orbital quantum number, s is the spin quantum number, V_i is the potential parameter, R_i is the radius, R_c is the Coulomb radius, ai is the surface thickness, and $V_c(r)$ is the Coulomb interaction potential inside and outside of the nucleus. In this study, to compute the spe's, we have used *wspot* software [15] which runs according to above formalism in the equations [1].

In the shell model calculations in order to obtain ground and excited state energies, the calculations were performed in matrix formalism for multi-particle systems. The dimensions of the Hamiltonian matrix increase to very high orders (10^{10}) as the size of the model space and the number of nucleons increase. To obtain the eigenvalues, the matrices are diagonalized using appropriate algorithms such as Lanczos and the solution is reached. For this purpose, there are many computer codes developed to make nuclear shell model calculations in the literature. In the calculations performed in this study, Kshell code [16] was used. Running on the Linux operating system, this code enables performing nuclear shell model calculations with M-scheme representation using the Lanczos method.

3 Results and Discussions

In order to investigate the effect of the spin–orbit term in Woods-Saxon (WS) potential on the energy levels of the nuclei, we have taken into account *usdb* interaction [17] in the shell model calculations for ^{18}O isotope. In the beginning, the parameters of the WS potential with the spin–orbit term are set to give the closest values to the sd-shell neutron spe values used in *usdb* interaction. These parameters are given in Table 1. The corresponding spe's are $+2.113$, -3.212, and -3.919 MeV for $d_{3/2}$, $s_{1/2}$, and $d_{5/2}$ orbits, respectively, whose *usdb* equivalents are 2.112, -3.208, and -3.926 MeV. The spe's have been computed by using *wspot* code [15] in considering the Woods-Saxon potential as given in Eq. (4). Since the average proton-neutron potential is stronger than the average neutron-neutron or proton-proton potential, V_0 parameter is modified for proton and neutron by taken into account the V_1 modification parameter (for more details about the formulation, we refer the readers to Brown [15]).

It is clear that altering the potential parameter of the spin–orbit term (V_{so}) will not affect the $s_{1/2}$ orbital because its orbital angular momentum quantum number is 0, whereas the other orbits $d_{3/2}$ and $d_{5/2}$ in the sd-shell are influenced by this change. Increasing the V_{so} term increases the neutron spe value of the $d_{3/2}$ orbit and decreases that of the $d_{5/2}$ orbit. Neutron spe values and their dependence on the spin–orbit strength for the ^{18}O isotope are shown in Fig. 1. Thus, the gap between these two orbits increases as is seen in the figure. When this parameter is 0, that is, there is no spin–orbit interaction, the neutron spe values of these two orbitals are the same and are -1.741 MeV. We have investigated the neutron spe values for $d_{3/2}$ and $d_{5/2}$ orbits by increasing this parameter from 0 to 30 MeV. It is seen that a 6-unit increase in this parameter value causes a shift in energy values approximately between 0.5 and 1.5 MeV.

Table 1 WS parameters in order to obtain neutron spe values for the sd-shell closing to the values used in *usdb* interaction

Parameter	Value
V_0	-47 MeV
V_1	-24 MeV
V_{so}	18.37 MeV
$r_0 = r_{so}$	1.297 fm
$a_0 = a_{so}$	0.916 fm
r_C	1.2 fm

In the first stage, we have investigated the ground-state energy of ^{18}O isotope relative to the ^{16}O core nucleus via the shell model calculations. As expected, it has been observed that with the increase of the spin–orbit potential parameter, the ground-state binding energy also increases. Because the increase of this parameter decreases the neutron single-particle energy value of the $d_{5/2}$ orbital. Although the change in the $d_{5/2}$ orbital is linear, it is seen in Fig. 2 that there is a slight deviation from the linearity in the change of the ground-state energy. Within the scope of shell model calculations, since all two neutrons are terms for spe levels in the shell model Hamiltonian matrix, it is inevitable to see the effect of other spe values other than the $d_{5/2}$ orbital on the ground-state binding energy. However, since this study focuses on spin–orbit interaction, the effect of $s_{1/2}$ level on ground-state energy has not been investigated. Therefore, we examined the contribution of the shifts of each of the $d_{5/2}$ and $d_{3/2}$ orbitals in the sd model space to the change of ground-state energy. The increase in the V_{so} parameter, which indicates an increase in the spin–orbit interaction, caused the $d_{5/2}$ neutron single-particle energy to decrease as well. As a result, as expected, the ground-state binding energy of the ^{18}O nucleus increased. However, the increase in the V_{so} value causes the $d_{3/2}$ neutron spe orbit to increase. As a result of this level moving away from the $d_{5/2}$ level, the ground-state binding energy of the ^{18}O isotope decreases as seen in Fig. 2. Moving the $d_{3/2}$ level away from the $d_{5/2}$ level causes a decrease in the eigenvalues of the Hamiltonian; that is, the ground-state binding energy decreases. As can be seen from the figure, the simultaneous variation of these two single-particle orbits ($d_{3/2}+d_{5/2}$) with respect to V_{so} was also investigated. Changing the spin–orbit term together for both orbitals resulted in a net increase in the ground-state binding energy, whereas the increase of V_{so} term only at $d_{5/2}$ level increased the energy, while the increase of V_{so} at $d_{3/2}$ decreased the energy.

Figure 3 shows the effects of spin–orbit interaction on the nuclear spectrum of ^{18}O. Nuclear excited states, especially high-level ones, appear to be highly sensitive to the strength of spin–orbit interaction. In this figure, where the experimental spectrum [18] of ^{18}O is given and the spectra obtained from the change in the intensity of the spin–orbit interaction are compared, the value of $V_{so} = 18.37$ MeV is the coefficient that gives the closest value to the current theoretical calculations, as stated before. While the experimental value for the first excited 2^+ level is 1.982 MeV, the value obtained with the potential coefficient $V_{so} = 18.37$ MeV is 1.998 MeV, which is the closest to the experimental value among the others.

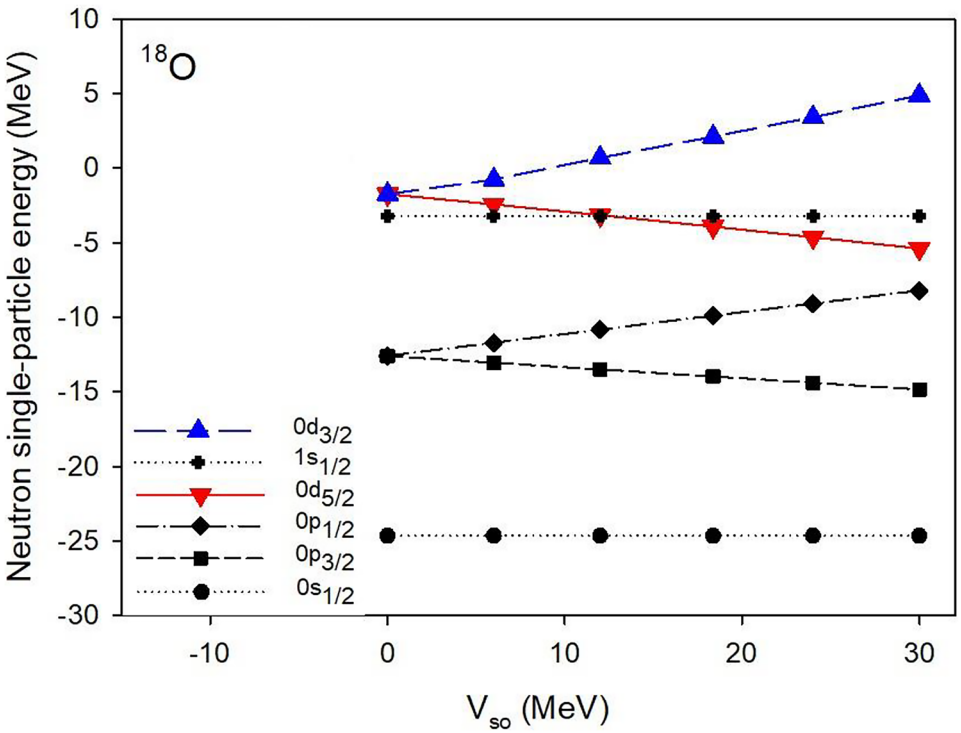

Fig. 1 Evolutions of the sd-shell neutron spe for ^{18}O isotope by the altering of potential parameter (V_{so}) in Woods-Saxon spin–orbit term

While the experimental energy of the first excited 4^+ level was 3.555 MeV, the closest value to this value was obtained as 3531 MeV, again from the $V_{so}=18.37$ MeV spin–orbit interaction potential. Moreover, for this excited level, the spin–orbit interaction weakens and takes the values of $V_{so}=0$ or 6, causing the first excited 0^+ level to fall below this level. When the first excited 0^+ levels are examined, the energy of this level is 3.739 MeV, which is closest to the experimental value in the absence of spin–orbit interaction ($V_{so}=0$). The experimental value is 3.634 MeV, which is very close to the

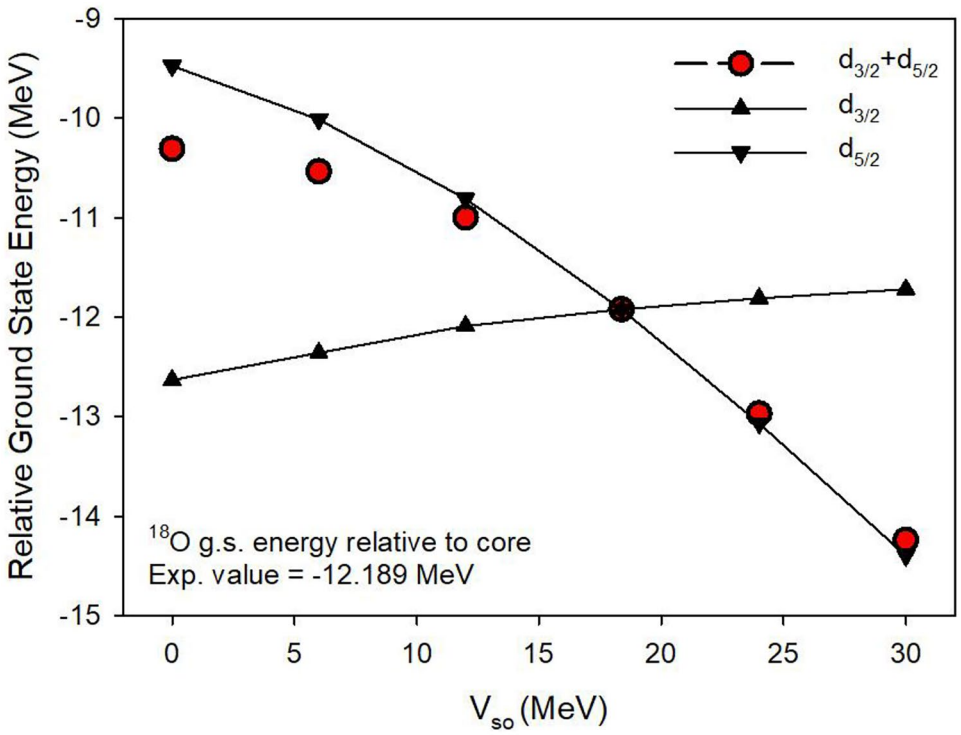

Fig. 2 Effects of the shifting of the neutron single-particle energy levels on the relative ground-state energy for ^{18}O isotope

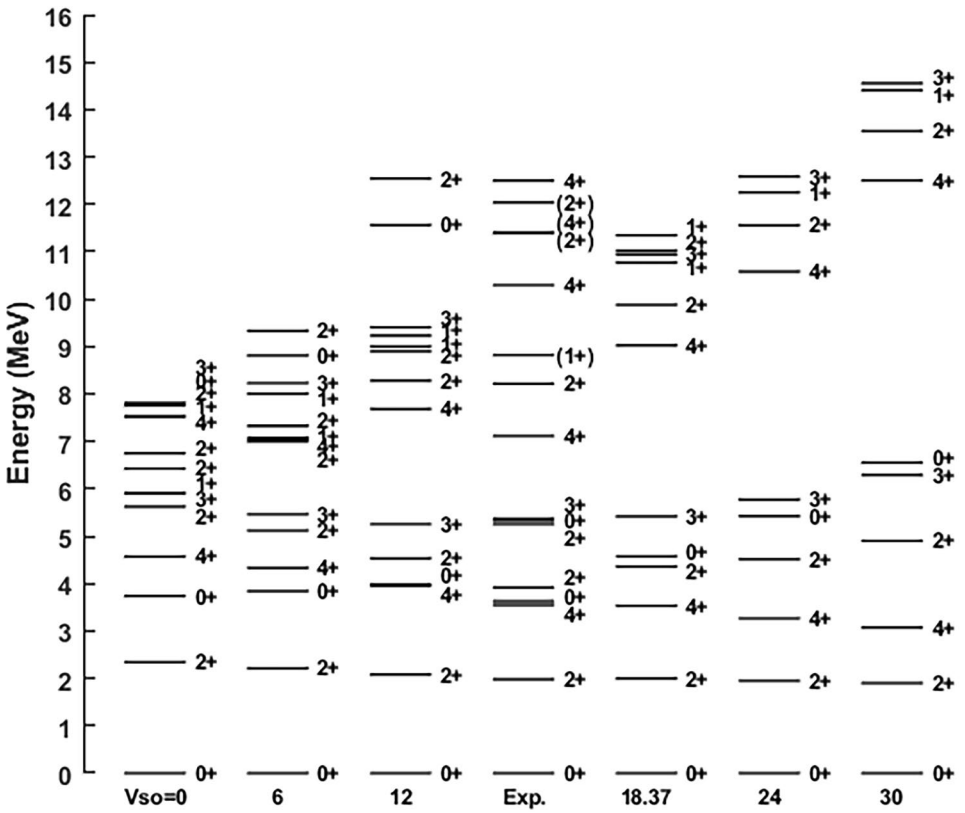

Fig. 3 Excited energy levels of ^{18}O isotope according to the different spin–orbit interaction parameters in comparison with the experimental data [18]

lower level of 4^+. For this level, it is seen in Fig. 3 that the energy values are quite high at values where the V_{so} potential coefficient value is higher than 18.37 MeV. The experimental energy value of the second excited 2^+ level is 3.920 MeV. It is seen that the energy value of this level increases with the increase or decrease of the $V_{so}=18.37$ MeV value. Among others, the closest value to the experimental value was obtained for this level as 4.358 MeV using $V_{so}=18.37$ MeV. When we make a comparison of the third 2^+ excited level, it is seen that the closest value to the experimental value of 5.255 MeV is 6.429 MeV, which is obtained in the case of $V_{so}=0$ where there is no spin–orbit interaction. The energies of the second excited 0^+ and first excited 3^+ levels located very close to this level are 5.336 and 5.374 MeV, respectively. Although this second 0^+ level could not be calculated in all theoretical calculations, the energy of the first excited 3^+ level was calculated with the parameter $V_{so}=18.37$ MeV as closest to the experimental data.

When the higher excited states are examined, it is seen that the results of the calculations where the V_{so} value is less than 18.37 MeV, that is, the spin–orbit interaction is weaker, are located at lower levels in terms of energy. Of these levels, the closest to the experimental second excited 4^+ level is the one from the calculations made with $V_{so}=6$. While the experimental energy value of the fourth excited 2^+ level was 8.213 MeV, the closest value was obtained as 8.277 MeV with the parameter $V_{so}=12$. In the literature, the experimental energy value of the first excited 1^+ level with ambiguity in spin and parity value is 8.817 MeV, and this value was calculated as 9.000 MeV in the calculations performed with $V_{so}=12$.

In our study, to see the effect of spin–orbit interaction strength, we examined the E2 transition probabilities from the ground state to the first excited 2^+ level and from the first excited 2^+ state to the first excited 4^+ state, over B(E2) values [19]. As can be seen from Table 2, both transition probabilities depend on the spin–orbit interaction potential parameter. The 0^+ to 2^+ transition probability, which was 25.1 e^2fm^4 in the absence of spin–orbit interaction, decreased with the increase of spin–orbit interaction and reached 16.3 e^2fm^4 for $V_{so}=30$. Similarly, for the 2^+ to 4^+ transition which was 8.6 e^2fm^4 in case of $V_{so}=0$, decreased to 4.6 e^2fm^4 for $V_{so}=30$. The current adopted value for 0^+ to 2^+ transition in the literature is given as 43 e^2fm^4. As can be seen, in the calculations carried out within the scope of the shell model, the B(E2) transition probabilities were also found to be smaller compared to the literature value. This is also known from previous studies and seen from the literature [19]. However, our main purpose in this study was to see how this transition probability value changes with the change of the term V_{so}.

Table 2 Calculated B(E2) values according to different V_{so} parameters. The adopted literature value is 43 e^2fm^4 [19]

V_{so}	B(E2) 0^+ to 2^+ (e^2fm^4)	B(E2) 2^+ to 4^+ (e^2fm^4)
0	25.1	8.6
6	24.4	8.0
12	22.6	6.7
18.37	20.1	5.8
24	18.1	5.2
30	16.3	4.6

4 Conclusions

In general, it is seen that the results of the calculations performed with the $V_{so} = 18.37$ MeV spin–orbit interaction give closer results to the experimental data for many excited levels. However, our main motivation in this study was to examine the effects of variation of the spin–orbit interaction intensity on the nuclear spectra. With this effect, it is seen that excited levels shift as expected. With this shift, it was observed that the levels obtained from the calculations made with different spin–orbit interaction parameters sometimes approached the experimental energy level values. As a result, the increase of the spin–orbit potential parameter caused the levels above the first excited 4^+ level to shift upwards. The first excited 2^+ and 4^+ levels showed a decreasing trend with the increase of this parameter. On the other hand, when the V_{so} parameter dropped below 18.37 MeV and approached 0, it caused an increase in the first excited 2^+ and 4^+ levels, while a decrease in the first excited 0^+ level. It is seen that the subsequent second excited 2^+ and first excited 3^+ levels increase with decreasing V_{so}. Looking at the higher excited levels, it is seen that the energy of the second excited 4^+ level decreases with the decreasing V_{so} parameter, but increases again at the value of $V_{so} = 0$. For the levels above this level, it was seen that the levels went down with the decreasing V_{so} parameter.

Declarations

Competing Interests The author declares no competing interests.

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