ЯДЕРНА ФІЗИКА
NUCLEAR PHYSICS

УДК 539.142+539.143 https://doi.org/10.15407/jnpae2023.03.219

A. K. Hasan, H. H. Abed*

Physics Department, College of Education for Girls, University of Kufa, Najaf, Iraq

*Corresponding author: baqrakeel87@gmail.com

STUDY OF THE NUCLEAR STRUCTURE FOR THE ^{18}O BY USING NuShellX@MSU CODE

In this study, the energy levels, electromagnetic transition probability, and charge density distribution of the ^{18}O nucleus were calculated using the NuShellX@MSU code within the sdpn-shell and using the effective USDEPN and WCPN interactions. The charge density distribution values were also reasonably consistent with existing experimental data. Comparing the theoretical and experimental results indicates that applying the nuclear shell model using the USDEPN and WCPN interactions is successful within the sdpn-shell.

Keywords: energy levels, electromagnetic transitions, charge density, NuShellX@MSU code.

1. Introduction

The nuclear shell model has proven to be a very successful tool for investigating the nuclear structure: using an appropriate selection of the remaining effective interaction, a shell model can compute various observations accurately and systematically [1]. The shell model was developed by Mayer and Jensen [2], and successfully used to assess nuclear structural properties such as rotation, parity, magnetic moment, etc. of relatively light and near closed-shell nuclei. It is one of the essential microscopic nuclear models and is considered the exporter and rationalization of other macroscopic nuclear models [3]. There are several standard effective interactions for light nuclei such as the Cohen-Kurath and USD interactions for p- and sd-shells, respectively. The analysis of neutron-rich sd-nuclei has been highly interesting in modern years as they introduce new aspects of nuclear structure [4, 5]. The nuclear shell model codes such as Oxbash [6], Antoine [7], NuShell [8], and NuShellX [9] and others, were used extensively for shell model calculations in the p shell, and sd-shell, and also in the fp-shell [10]. These codes are globally used to examine the structure of nuclei. The fundamental inputs to most shell model configuration mixing codes are groups of single-particle matrix elements (SPEs) and two-body matrix elements (TBMEs). These groups are described as "model-space Hamiltonians" or "effective interactions". The sd-model space contains the $0d_{5/2}$, $0d_{3/2}$, and $1s_{1/2}$ valence orbits. There are 3 SPEs and 63 TBMEs for this model space, which in the mass region of A = 16 - 40 can locate the energies and wave functions for about 106 levels [11]. In this research, the energy levels, electromagnetic transitions, and charge density distribution of the ^{18}O isotope were calculated using the two interactions USDEPN [9] and WCPN [9] within the sdpn-shell and using a NuShellX@MSU code. The isotope under study has been theoretically studied previously by [12 - 15].

2. Theory

NuShellX is a collection of computer programs created by Bill Rae [8] to obtain accurate energies, eigenvectors, and spectroscopic overlaps for low-lying states in computations using the shell model Hamiltonian matrix with extremely large basis dimensions. It makes use of a J-coupled proton-neutron basis and can take into account J-scheme matrix dimensions up to the order of 100 million. NuShellX@MSU is a collection of wrapper scripts created by Alex Brown [9] that generate input for NuShellX using model space and Hamiltonian data files.

In the classical shell model calculations, instead of calculating the system's overall energy, it is common to compute the energy levels for a single nucleon outside the doubly magical core relative to a closed shell. When there are several nucleons outside the core, energy is assumed to be an eigenvalue of the Hamiltonian H_0, and the overall Hamiltonian is expressed as [16]:

$$\mathrm{H} = \sum_{k=1}\left(H_0\right)_k + \sum_{k\le l} V_{kl}, \qquad (1)$$

where V_{kl} – the residual two-body interaction, this exists in addition to the typical shell model potential and which we may write as:

$$\sum_{k<l} V_{kl} =$$

$$= \Sigma_{JM} \Sigma_{j_a \ge j_b} \Sigma_{j_c \ge j_d} \langle j_a j_b | V_{12} | j_c j_d \rangle_J \, a^+_{JM}\left(j_a j_b\right) a_{JM}\left(j_c j_d\right), \qquad (2)$$

where < > – the matrix element of the residual two-body interaction; $a^{+}_{JM}\left(j_a j_b\right)$ – is an operator that creates a pair of nucleons in the single-particle states j_a and j_b with total angular momentum JM; $a_{JM}\left(j_a j_b\right)$ – the one that destroys a pair of particles in states j_c and j_d; it is the Hermitian adjoin operator to $a^{+}_{JM}\left(j_a j_b\right)$.

The transition probability $\lambda(\sigma L)$ for a gamma-ray emission of multipolarity L and letter σ is given by [17]:

$$\lambda\left(\sigma L, J_i \to J_f\right) = \frac{8\pi\left(L+1\right)}{\hbar L\left[\left(2L+1\right)!!\right]^2}\left(\frac{E_\gamma}{\hbar c}\right)^{2L+1} \times$$

$$\times B\left(\sigma L, J_i \to J_f\right), \qquad (3)$$

where $B(\sigma L)$ – the reduced transition probability; $E\gamma$ – the γ-ray energy.

With the use of the reduced matrix element $\langle \psi f \| M(\sigma L) \| \psi i \rangle$, the reduced transition probability may be expressed [16]:

$$B\left(\sigma L, J_i \to J_f\right) = \frac{1}{2J_i+1}\left|\langle \psi\, f \| M\left(\sigma L\right) \| \psi i\rangle\right|^2. \qquad (4)$$

The density distribution of a system containing A of nucleons gets [1]:

$$\rho_o(r) = \sum_{i=1}^{A} \left|\varphi_i(\vec{r})\right|^2. \qquad (5)$$

3. Results and discussions

The calculations for ^{18}O are done using the shell model in the Windows NuShellX@MSU code [9]; the model space used is sdpn with USDEPN and WCPN effective interactions, with neutrons (N = 2) above the ^{16}O close core for the above isotope. The goal of the current work is to use harmonic oscillator potential (HO, b), $b > 0$ for the ^{18}O isotope to compute energy levels and reduce electromagnetic transition probabilities, {$B(E2)$, $B(M1)$}. The calculations have accounted for the impacts of core polarization using the effective charges of both protons and neutrons.

3.1. Energy levels

The ground state of the ^{18}O nucleus is a closed ^{16}O nucleus with two neutrons outside the closed-shell distributed in the sd-shell, where $J = 0^+$ and $T = 1$. We have applied the two interactions USDEPN and WCPN to calculate the energy levels for the ^{18}O isotope using NushellX@MSUcode.

When applying effective interaction USDEPN, we conclude the following.

The total angular momentum and ground state parity of the 0^+_1 level was matched when compared with the available experimental values.

The agreement is appropriate for the values of energies calculated theoretically 1.988, 3.498, 4.359, 4.596, and 5.403 MeV corresponding to the angular momentum 2^+_1, 4^+_1, 2^+_2,0^+_2, and 3^+_1 when we compared it with the available experimental data.

The total angular momentum was confirmed only for experimental energy 10.24, 11.49, and 16.399 MeV which corresponds to angular momentum 1^-, 1^-, and 2^-. This study also confirmed the total angular momentum for values of uncertain experimental energy 10.99 MeV that corresponds to angular momentum 2^- but in a positive parity.

In our calculations, we expected that the total angular momentum and the parity of the experimental energies 9.030, 9.890, 10.82, and 15.23 MeV is 4^+_2, 2^+_3, 3^+_2,0^+_3 due to the convergence of measured values with our theoretical values.

We have observed from our calculations that the highest calculated energy value is theoretically 16.173 MeV while the highest experimental energy value is 36 MeV. Table 1 shows a comparison between the theoretical results and available experimental results [18] for the ^{18}O isotope by using the USDEPN interaction.

Table 1. **Comparison of the experimental excitation energies [18] and excitation energies predictions for the ^{18}O isotope by using USDEPN interaction**

J^+ (theoretical)	Energy (theoretical), MeV	Energy (experimental), MeV	J (experimental)
0_1	0	0	0^+
2_1	1.988	1.982	2^+
4_1	3.498	3.554	4^+
2_2	4.359	3.920	2^+
0_2	4.596	3.633	0^+
3_1	5.403	5.377	3^+
4_2	9.019	9.030	–
2_3	9.862	9.890	–

Continuation of Table 1

J^+ (theoretical)	Energy (theoretical), MeV	Energy (experimental), MeV	J (experimental)
1_1	10.779	10.24	$(0, 1, 2)^-$
3_2	10.882	10.82	–
2_4	11.042	10.99	(2^-)
1_2	11.276	11.49	$(0, 1, 2)^-$
0_3	15.001	15.23	–
2_5	16.173	16.399	$(3, 2)^-$

While applying the effective reaction WCPN to the ^{18}O isotope to calculate energy levels we conclude the following.

The total angular momentum and ground state parity of the 0_1^+ level was matched when compared with the available measured values.

The agreement is appropriate for the values of energies calculated theoretically 2.179, 3.782, 4.32, 4.439, and 5.726 MeV corresponding to the angular momentum $2_1^+, 4_1^+, 0_2^+, 2_2^+$, and 3_1^+ when we compared it with the available experimental data. Also, through our calculation, we got agreement that is appropriate for the value of energy calculated theoretically 10.555 MeV corresponding to the angular momentum 3_2^+, but in different parity.

The total angular momentum was confirmed only for experimental energy 9.270 and 11.49 MeV which corresponds to angular momentum 2^- and 1^-. This study also confirmed the total angular momentum for values of uncertain experimental energy 10.99 MeV that corresponds to angular momentum 2^- but in a positive parity.

In our calculations, we expected that the total angular momentum and the parity of the experimental energies 8.66, 10.820, 14.45, and 15.95 MeV is $4_2^+, 1_1^+, 0_3^+$, and 2_5^+ due to the convergence of measured values with our theoretical values. In our calculations, we have observed that the highest calculated energy value is theoretically 15.693 MeV while the highest experimental energy value is 36 MeV. Table 2 shows a comparison between the theoretical results and available experimental results [18] for the ^{18}O isotope by using WCPN interaction.

Table 2. **Comparison of the experimental excitation energies [18] and excitation energies predictions for the ^{18}O isotope by using WCPN interaction**

J^+ (theoretical)	Energy (theoretical), MeV	Energy (experimental), MeV	J (experimental)
0_1	0	0	0^+
2_1	2.179	1.982	2^+
4_1	3.782	3.554	4^+
0_2	4.32	3.633	0^+
2_2	4.439	3.92	2^+
3_1	5.726	5.377	3^+
4_2	8.75	8.66	–
2_3	9.466	9.270	$(0, 1, 2)^-$
3_2	10.555	10.396	3^-
1_1	10.823	10.920	–
2_4	10.928	10.99	(2^-)
1_2	11.341	11.49	$(0, 1, 2)^-$
0_3	14.135	14.45	–
2_5	15.693	15.95	–

3.2. Electromagnetic transition probability $B(E2)$ and $B(M1)$

Gamma-rays can be considered a kind of electromagnetic radiation that contains a changing electric field that leads to a changing magnetic field and vice versa. Radiation can be produced by an oscillating charge that causes the external magnetic field to fluctuate, or by changing the current or magnetic moment, which produced a changing magnetic field. The radiation emitted from the previous mechanism is called electric radiation (E), and the last leads to the generation of magnetic radiation (M) [19]. The electromagnetic transition probability has been calculated for the ^{18}O isotope within the nuclear shell model using USDEPN and WCPN interactions, for each in-band transition, the computation was performed using the harmonic oscillator potential (HO,

b), where $b > 0$. Core polarization effects were comprised by using effective charge $e_p = 1.450$, $e_n = 0.750$ for both interactions of the proton and neutron effective charges. Also, the *g*-factor was changed to obtain an agreement with the practical values of the ground state of the magnetic transitions ($g_s p = 7.500$, $g_s n = -5.500$) for both interactions respectively.

For USDEPN and WCPN interactions we found a good correspondence for the electric transitions $B(E2)$ $2_1 \rightarrow 0_1$, $B(E2)$ $4_1 \rightarrow 2_1$, $B(E2)$ $2_2 \rightarrow 0_1$, with available experimental data. Also, the magnetic transition $B(M1)$ compatibility was good for the transitions $B(M1)$ $2_1 \rightarrow 2_2$, $B(M1)$ $4_2 \rightarrow 4_1$, $B(M1)$ $2_4 \rightarrow 2_2$, $B(M1)$ $2_5 \rightarrow 2_2$, $B(M1)$ $2_5 \rightarrow 2_4$ with available experimental data. At the same time, the compatibility was reasonable for the rest of the transfers, and through our calculations, we also obtained new transitions for which there have been no experimental values until now. When comparing some of our results for the electrical transitions of the interaction USDEPN with the theoretical study [20] we found a good agreement for the transitions $B(E2)$ $2_1 \rightarrow 0_1$, $B(E2)$ $4_1 \rightarrow 2_1$, and the agreement was acceptable for the rest of the transitions. As for the interaction WCPN, our results were in good agreement with the transfers $B(E2)$ $2_1 \rightarrow 0_1$, $B(E2)$ $4_1 \rightarrow 2_1$, $B(E2)$ $2_4 \rightarrow 4_2$, $B(E2)$ $2_4 \rightarrow 0_1$, while the compatibility was acceptable for the rest of the transfers. Some of our results by using USDEPN interaction are listed in Tables 3 and 4 for electric and magnetic transition probabilities respectively and Tables 5 and 6 for WCPN interaction for electric and magnetic transition probabilities, respectively.

Table 3. **Comparison of the $B(E2)$ results by using USDEPN interaction in units e^2fm^4 for the ^{18}O isotope with the experimental data [18] and theoretical study [20]**

$J_i \rightarrow J_f$	$B(E2)$ Our results for USDEPN $e_p = 1.450$, $e_n = 0.450$	$B(E2)$ Experimental results [18]	$B(E2)$ Theoretical results [20]
$2_1 \rightarrow 0_1$	9.040	9.302	8.126
$4_1 \rightarrow 2_1$	7.206	3.334	5.884
$0_2 \rightarrow 2_1$	0.9204	47.635	12.049
$2_2 \rightarrow 0_1$	0.3607	3.642	4.483
$4_2 \rightarrow 2_2$	1.594	6.165	89.667
$2_4 \rightarrow 4_2$	3.019	6.725	1.961
$2_3 \rightarrow 0_2$	0.0144	64.448	67.250
$2_4 \rightarrow 0_1$	0.0661	2.522	0.168
$4_2 \rightarrow 2_1$	1.322	–	0.14

Table 4. **Comparison of the $B(M1)$ results by using USDEPN interaction in units μ^2 for the ^{18}O isotope with the experimental data [18]**

$J_i \rightarrow J_f$	$B(M1)$ Our results USDEPN $g_s p = 7.500$, $g_s n = -5.500$	$B(M1)$ Experimental results [18]
$2_2 \rightarrow 2_1$	0.2303	0.251
$4_2 \rightarrow 4_1$	2.1230	0.127
$2_4 \rightarrow 2_2$	0.3070	0.199
$2_5 \rightarrow 2_2$	0.0067	0.043
$2_5 \rightarrow 2_4$	0.0930	0.013
$3_2 \rightarrow 2_1$	0.2047	–
$1_2 \rightarrow 2_3$	3.6300	–
$1_2 \rightarrow 2_4$	7.8210	–

Table 5. **Comparison of the $B(E2)$ results by using WCPN interaction in units e^2fm^4 for the ^{18}O isotope with the experimental data [18] and theoretical study [20]**

$J_i \rightarrow J_f$	$B(E2)$ Our results for WCPN $e_p = 1.450$, $e_n = 0.450$	$B(E2)$ Experimental results [18]	$B(E2)$ Theoretical results [20]
$2_1 \rightarrow 0_1$	9.126	9.302	8.126
$4_1 \rightarrow 2_1$	7.065	3.334	5.884
$0_2 \rightarrow 2_1$	1.414	47.635	12.049

Continuation of Table 5

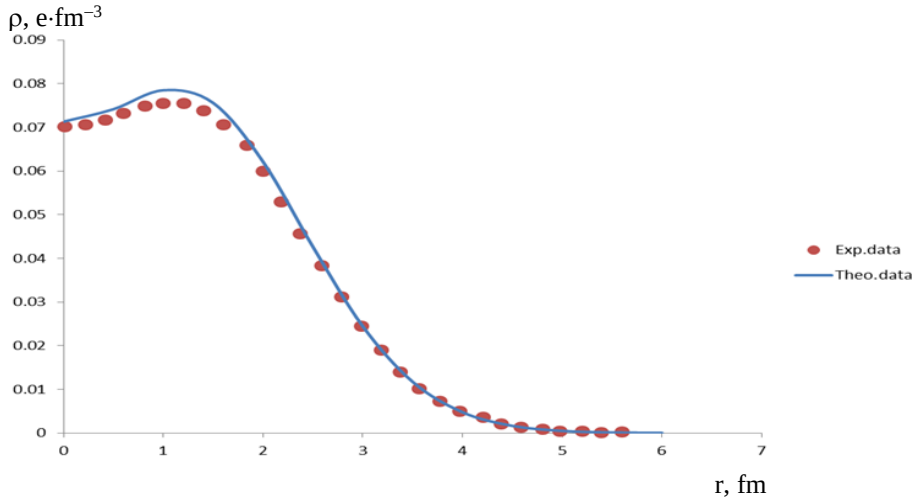
$J_i \to J_f$	$B(E2)$ Our results for WCPN $e_p = 1.450$, $e_n = 0.450$	$B(E2)$ Experimental results [18]	$B(E2)$ Theoretical results [20]
$2_2 \to 0_1$	0.349	3.642	4.483
$4_2 \to 2_2$	2.054	6.165	89.667
$2_4 \to 4_2$	2.308	6.725	1.961
$2_3 \to 0_2$	0.021	64.448	67.250
$2_4 \to 0_1$	0.0195	2.522	0.168
$4_2 \to 2_1$	1.5010	–	0.14

Table 6. **Comparison of the $B(M1)$ results by using WCPN interaction in units μ^2 for the ^{18}O isotope with the experimental data [18]**

$J_i \to J_f$	$B(M1)$ Our results WCPN $g_S p = 7.500$, $g_S n = -5.500$	$B(M1)$ Experimental results [18]
$2_2 \to 2_1$	0.2513	0.251
$4_2 \to 4_1$	2.1660	0.127
$2_4 \to 2_2$	0.3292	0.199
$2_5 \to 2_2$	0.0348	0.043
$2_5 \to 2_4$	0.1892	0.013
$3_2 \to 2_1$	0.1853	–
$1_2 \to 2_3$	2.4700	–
$1_2 \to 2_4$	6.0610	–

3.3. Charge density distribution

The charge densities of the ^{18}O isotope were calculated and shown in Figure. We notice from Figure that the value of the charge density at the center of the nucleus is 0.072 e·fm^{-3}, then begins to decrease down to r = 5 fm, and then its value is fixed at zero. The Figure shows a comparison of the theoretically calculated charge density distribution with the experiment results [13].



Comparison of the charge density distribution of the ^{18}O isotope with the experiment data [13].
(See color Figure on the journal website.)

4. Conclusions

The current study showed that the interactions USDEPN and WCPN used to calculate the energy levels, the electromagnetic transition probability, and the charge density distribution give results that are in acceptable agreement with the available experimental results. In our calculations, new energy levels have been obtained and many levels of energy have been confirmed for both interactions, Likewise, the $B(E2)$ and $B(M1)$ were reasonably compatible with the experimental values. Also, through our calculations, we concluded the value of the charge density distribution is at the center of the nucleus in 0.072 e·fm^{-3}, then begins to decrease, and then its value is fixed at zero. Finally, we got to the conclusion that the shell model configuration mixing in the sdpn-shell works quite well.

REFERENCES

1. R. Roy, B. Nigam. *Nuclear Physics. Theory and Experiment* (New York, John Wiley and Sons Inc., 1967).
2. M.G. Mayer. On closed shells in nuclei. II. Physical Review 75 (1949) 1969.
3. R.F. Casten. *Nuclear Structure from a Simple Perspective*. Vol. 13 (New York - Oxford, Oxford University Press, 1990) 391 p.
4. D.J. Dean et al. Effective interactions and the nuclear shell-model. Progress in Particle and Nuclear Physics 53(2) (2004) 419.
5. A.K. Hasan, A.N. Rahim. Study of Nuclear Structure of ^{24,26}Na isotopes by using USDB interaction. International Journal of Scientific and Research Publications 8(9) (2018) 169.
6. B.A. Brown et al. Oxbash for Windows PC. MSU-NSCL Report No. 1289 (USA, East Lansing, Michigan State University, 2004) 32 p.
7. E. Caurier, F. Nowacki. Present status of shell model techniques. Acta Physica Polonica B 30(3) (1999) 705.
8. B.A. Brown, W.D.M. Rae. "Nushell@MSU" MSU-NSCL Report (Upton, National Nuclear Data Center, Brookhaven National Laboratory, 2007).
9. B.A. Brown, W.D.M. Rae. The shell-model code NuShellX@MSU. Nuclear Data Sheets 120 (2014) 115.
10. A.D. Salman, S.A. Al-Ramahi, M.H. Oleiwi. Inelastic electron-nucleus scattering form factors for ^{64,66,68}Zn isotopes. AIP Conference Proceedings 2144(1) (2019) 030029.
11. B.H. Wildenthal. Empirical strengths of spin operators in nuclei. Progress in Particle and Nuclear Physics 11 (1984) 5.
12. A. Hasan. Shell model calculations for ^{18,19,20}O isotopes by using USDA and USDB interactions. Ukrainian Journal of Physics 63(3) (2018) 189.
13. H. De Vries, C.W. De Jager, C. De Vries. Nuclear charge-density-distribution parameters from elastic electron scattering. Atomic Data and Nuclear Data Tables 36(3) (1987) 495.
14. R.L. Lawson, F.J.D. Serduke, H.T. Fortune. Structure of low-lying positive-parity states of ^{18}O. Physical Review C 14 (1976) 1245.
15. G. Lévai, J. Cseh, W. Scheid. Semimicroscopic algebraic study of the α-cluster states of the ^{18}O nucleus. Physical Review C 46 (1992) 548.
16. P.J. Brussaard, P.W.M. Glaudemans. *Shell-Model Applications in Nuclear Spectroscopy* (North-Holland Publishing Company, 1977) 452 p.
17. M.A. Preston, R.K. Bhaduri. *Structure of the Nucleus* (Taylor & Francis Group LLC, 1975) 716 p.
18. D.R. Tilley et al. Energy levels of light nuclei A = 18 - 19. Nuclear Physics A 595(1) (1995) 1.
19. J. Lilley. *Nuclear Physics: Principles and Applications* (John Wiley & Sons, 2001) 416 p.
20. P. Descouvemont, D. Baye. Multiconfiguration microscopic study of α + ^{14}C molecular states. Physical Review C 31 (1985) 2274.

А. К. Хасан, Х. Х. Абед*

Факультет фізики, Коледж освіти для дівчат, Університет Куфи, Наджаф, Ірак

*Відповідальний автор: baqrakeel87@gmail.com

ДОСЛІДЖЕННЯ СТРУКТУРИ ЯДРА ^{18}O ЗА ДОПОМОГОЮ КОДУ NuShellX@MSU

У цьому дослідженні енергетичні рівні, ймовірність електромагнітних переходів та розподіл щільності заряду ядра ^{18}O розраховано за допомогою коду NuShellX@MSU з sdpn-оболонкою та з використанням ефективних взаємодій USDEPN та WCPN. Розподіл щільності заряду знаходиться в достатній згоді з існуючими експериментальними даними. Порівняння теоретичних і виміряних результатів показує, що застосування моделі ядерної оболонки з використанням взаємодії USDEPN і WCPN є успішним з sdpn-оболонкою.

Ключові слова: енергетичні рівні, електромагнітні переходи, густина заряду, код NuShellX@MSU.

Надійшла/Received 14.02.2023