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SHELL MODEL CALCULATIONS FOR ^{18,19,20}O ISOTOPES BY USING USDA AND USDB INTERACTIONS

The shell model (SM) is used to calculate the energy levels and transition probabilities $B(E2)$ for $^{18,19,20}O$ isotopes. Two interactions (USDA and USDB) are used in the SDPN model space. We assume that all possible many-nucleon configurations are defined by the $0d_{5/2}$, $1s_{1/2}$, and $d_{3/2}$ states that are higher than in ^{16}O doubly magic nucleus. The available empirical data are in a good agreement with theoretical energy levels predictions. Spins and parities were affirmed for new levels, and the transition probabilities $B(E2;\downarrow)$ are predicted.

Keywords: shell model, OXBASH code, energy levels, model space, $B(E2;\downarrow)$.

1. Introduction

The nuclear shell model represents an important step to the understanding of the nuclear structure. In shell-model studies, for many of existing conventional interactions, it is difficult to reproduce simultaneously the drip lines of carbon and oxygen isotopes, as well as some other properties such as the excitation energies, spins, parities, and $B(E2;\downarrow)$.

The model is one of the cornerstones for a comprehensive understanding of nuclei. Strong efforts in this field are aimed at unraveling the driving forces behind structural departures from the well-established traditional shell model, which have been observed mostly in nuclei with a large proton and neutron excesses [1–3]. The realistic nucleon-nucleon (NN) interactions needs to be renormalized, when applying to the shell-model calculations because of the short-range correlation and medium effects [4]. The effective most successful empirical interactions are chosen to be the isospin-conserving USDA and USDB ones [5], because the universal interaction is still lacking in the shell model, and the predictive power is restricted in small regions. It has been demonstrated that one may obtain a reliable multipole Hamiltonian from the G-matrix, but the monopole Hamiltonian is often incorrect [6]. It introduces a simple Hamiltonian capable of describing the collective nuclear properties through an extensive range of nuclei, and it is based on somewhat general algebraic group theoretical methods [7]. The calculations were performed, by using the shell model program OXBASH code. The OXBASH program includes a set of computational codes, which are based on the ability to measure the energy levels, by forming the ground-state matrices with dimensions up to 2,000,000 and the JT matrix with dimension up to 100,000. The version of this code is 2005-8, which can be installed and used on any operational system without using any other additional software [8–10].

2. Theory

The available successful nuclear shell model can explain many of the properties of the stable nuclides. The shell-model wave functions are obtained, by assuming initially that the nucleons are moving inside an average potential well created by all of the nu-

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cleons, called the mean field. The shell model allows for the configuration mixing beyond the mean field approximation and involves the assumptions underlying the configuration mixing calculations. We note that they will be affected by their application to nuclei near the drip lines [11]. The modern shell-model calculations also take the residual nucleon-nucleon interactions into account. In the extreme single-particle shell model, the single-particle wave functions can be obtained by solving the Schrödinger equation with the mean field potential, and energy levels for particles with quantum numbers (n, l, j) result. The quantum number (n) represents the number of nodes in the radial wave function, l is the orbital angular momentum, and j is the total angular momentum that results from the coupling of the intrinsic nucleon spin $s = \frac{1}{2}$ to the orbital angular momentum to obtain the two possibilities $j = l \mp \frac{1}{2}$ [12]. Some even-even nuclei have the first excited states, which lie at a relatively high excitation energy as compared to the neighboring even-even nuclei. This is an indication that the gap between single-particle levels is relatively large for both protons and neutrons for these particular Z and N values. These values of Z and N are the magic numbers in the nuclear shell model. In the simplest approximation, these nuclei are modeled by closed-shell configurations. Shell-model calculations start with the assumption that one or more of these magic nuclei is inert, since they have a closed-shell configuration [13]. I will restrict myself mainly to a region of light nuclei, for which the most work on the configuration mixing has been carried out. This will include nuclei up to $Z = 8$ and $N = 8$. For these nuclei, we can expect many new experimental results out to the proton and neutron drip lines over the next decade. A shell-model calculation with some choice of inert cores can be considered successful, if it can describe a large subset of the observed energy levels and transitions for the nuclei covered by the model space with Hamiltonians and operators, which are close to those expected from the properties of free nucleons [14]. The shell model calculations were performed with the program OXBASH [15], by using the SDPN model space for ^{18,19,20}O nuclei. The model space indicates the orbit and the truncation within that set of orbitals, which is assumed for a given calculation. Generally, the best and most complete results are obtained, when the model space is as large as possible. However, the computation time increases exponentially with the size of the model space, and empirical Hamiltonians are better determined in smaller model spaces. Thus, the choice of a model space is a compromise between what one would like to describe and what is computationally practical. The specific distribution of n valence particles over a given set of valence orbits will be called a partition. The complete or "full" model space includes all possible partitions for a given set of orbits [16].

3. Results and Discussions

In the present work, we have calculated the energy levels and reduced transition probabilities of $B(E2;\downarrow)$ for ^{18,19,20}O nuclei, by using OXBASH code which can calculate the energies, one- and two-nucleon spectroscopic factors, one- and two-body transition densities, and cluster overlaps. The package of programs DENS can be used to generate the spherical harmonic-oscillator, Woods–Saxon, and HF radial wave functions, densities, and binding energies. They can then be combined with the output of OXBASH to obtain the transition densities associated with the beta decay, electromagnetic transitions, and electron scattering. Together, OXBASH and DENS form a powerful set of tools for nuclear structure calculations. The goal of the code OXBASH is to reduce the dimensions of the matrix to be diagonalized by projecting the angular momentum onto the m-scheme basis, and, therefore, focusing on states with definite angular momentum and isospin, if desired, and parity [17]. The SDPN model space consists of configurations $0d_{5/2}$, $1s_{1/2}$, and $0d_{3/2}$above the ^{16}O closed core for protons $(Z = 8)$ and $(N = 8)$ neutrons, respectively. We assess the accuracy of the *sd*-shell Hamiltonians with USDA and USDB in calculating the excited states. The basic inputs to the most shell model configuration mixing codes are the single-particle matrix elements (SPE) and the two-body matrix elements (TBME). For example, in the *sd* shell, there are three SPE and 63 TBME. This input for the *sd*-shell determines the energies and wave functions for about 10 levels in the mass region (A = 16-40) [18]. The shell-model configuration mixing is carried out by diagonalizing a Hamiltonian, which is usually specified by a set of numbers for the single-particle energies

(SPE) and the two-body matrix elements (TBME) for n particles in a given model space. Such configuration mixing does not explicitly involve the radial wave functions (they are only implicit in the SPE and TBME). The configuration mixing is in terms of the multiparticle "angular" structure in the model space. To apply shell-model configuration mixing results to the calculation of one-body densities such as those for electromagnetic transitions, the radial wave functions must be separately introduced: one may use the mean-field, Woods–Saxon or harmonic oscillator radial wave functions, depending upon the physical situation. It is conventional in the shell-model configuration mixing calculations to use the same set of SPE and TBME over the entire mass region covered by the model space with at most a smooth scaling of TBME. For example, the USD interaction in the shell model space takes the form

$$\mathrm{TBME}(A) = \mathrm{TBME}(A = 18)(A/18)^{-0.3}, \qquad (1)$$

where the power was determined empirically [19, 20]. The scaling is a result of the change of the (implicit) radial wave function as a function of the mass A.

The calculation of transition probabilities in nuclear physics is a problem, whose study has developed substantially in the last decade. This is because we are continually challenged by new experimental results for several nuclei. The transition rates represent a sensitive test for the most modern effective interactions that have been developed. The transition probability calculation in the present work was carried out with the use of the harmonic oscillator potential (HO, b), where $b < 0$ for each in-band transition and application USDA and USDB interactions for ^{18,19,20}O nuclei in the SDPN model space. Previous studies of low-lying states and transition probabilities for isotopes in the *sd*-shell region were performed by Kaneko *et al.* [21] and Mohammadi *et al.* [22].

3.1. Energy levels

Shell model calculations for low-lying energy states of neutron-rich oxygen ^{18,19,20}O isotopes have been performed within the space model $0d_{5/2}$, $1s_{1/2}$, and $0d_{3/2}$ with neutrons($N = 10, 11, 12$), respectively, for the above isotopes.

For ^{18}O nucleus, the predictions with the use of USDA and USDB interactions for the first sequence $\{0^+_1,\ 2^+_1,\ 4^+_1\}$ are presented in Table 1 and show a good agreement with the experimental data[23]. The states (2^+_2 and 3^+_1) were predicted with energies close to the experimental values, whereas our results for the states (0^+_2, 4^+_2, 2^+_3, and 2^+_4) give higher energies than experimental ones. With USDA and USDB interactions, the agreement with experimental data is reasonable for the energy levels {10.595, 10.820, 11.130, 14.450, and 15.950} MeV. We associate these energies with the states $\{1^+_1,\ 3^+_2,\ 1^+_2,\ 0^+_3$, and $2^+_5\}$, for which the angular momentum and parity are yet unknown experimentally.

For ^{19}O nucleus, the order of $\{5/2^+_1,\ 3/2^+_1,\ 1/2^+_1,\ 9/2^+_1,\ 7/2^+_1,\ 5/2^+_2$, and $3/2^+_2\}$ states is well reproduced with the USDA and USDB interactions. The comparison with experimental data [23] is given in Table 2. Experimentally, the energy level 5.384 MeV was identified at the state $9/2^+_2$. Theoretically, the the energy of the state $5/2^+_3$ with both interactions appeared close to the recent experimental value. We have predicted the angular momentum and parity for

Table 1. **Comparison of the experimental excitation energies [23] and excitation energies predictions for ^{18}O nucleus by using USDA and USDB interactions**

J^+	Theoretical values for E, MeV		Experimental values	
	USDAPN	USDBPN	E MeV	J^+
0^+_1	0.000	0.000	0.000	0^+
2^+_1	2.023	1.998	1.982	2^+
4^+_1	3.354	3.527	3.554	4^+
2^+_2	4.151	4.360	3.920	2^+
0^+_2	4.273	4.592	3.633	0^+
3^+_1	5.388	5.426	5.377	3^+
4^+_2	8.904	9.019	7.116	4^+
2^+_3	9.955	9.881	5.254	2^+
1^+_1	10.068	10.770	10.595	–
3^+_2	10.342	10.941	10.820	–
2^+_4	10.995	11.031	8.213	2^+
1^+_2	11.022	11.355	11.130	–
0^+_3	15.207	15.009	14.450	–
2^+_5	15.753	16.220	15.950	–

Table 2. **Comparison of the experimental excitation energies [23] and excitation energies predictions for ^{19}O nucleus by using USDA and USDB interactions**

Theoretical values for USDAPN		Experimental values		Theoretical values for USDBPN		Experimental values	
J^π	E, MeV	E, MeV	J^π	J^π	E, MeV)	E, MeV	J^π
$5/2_1^+$	0	0	$5/2^+$	$5/2_1^+$	0	0	$5/2^+$
$3/2_1^+$	0.278	0.096	$3/2^+$	$3/2_1^+$	0.118	0.096	$3/2^+$
$1/2_1^+$	1.422	1.471	$1/2^+$	$1/2_1^+$	1.567	1.471	$1/2^+$
$9/2_1^+$	2.286	2.371	$9/2^+$	$9/2_1^+$	2.370	2.371	$9/2^+$
$7/2_1^+$	2.921	2.779	$7/2^+$	$7/2_1^+$	2.883	2.779	$7/2^+$
$5/2_2^+$	3.362	3.153	$5/2^+$	$5/2_2^+$	3.216	3.153	$5/2^+$
$3/2_2^+$	3.618	4.109	$3/2^+$	$3/2_2^+$	3.802	4.109	$3/2^+$
$5/2_3^+$	4.951	4.702	$5/2^+$	$9/2_2^+$	5.097	5.384	$\underline{9/2}$,11/2,13/2
$9/2_2^+$	5.075	5.384	$\underline{9/2}$,11/2,13/2	$5/2_3^+$	5.196	4.702	$5/2^+$
$3/2_3^+$	6.193	5.540	$3/2^+$	$3/2_3$	6.081	5.540	$3/2^+$
$7/2_2^+$	7.409	7.508	–	$7/2_2^+$	7.198	7.508	–
$5/2_4^+$	7.806	7.806	–	$1/2_2^+$	7.861	7.806	–
$11/2_1^+$	7.947	7.947	–	$5/2_4^+$	7.868	7.947	–
$1/2_2^+$	8.067	8.048	–	$11/2_1^+$	7.986	8.048	–
$3/2_4^+$	8.586	8.561	–	$3/2_4^+$	8.838	8.561	–
$7/2_3^+$	9.335	9.324	–	$7/2_3^+$	9.456	9.324	–
$5/2_5^+$	9.584	9.560	–	$5/2_5^+$	9.595	9.560	–
$9/2_3^+$	9.599	–	–	$9/2_3^+$	9.772	–	–
$3/2_5^+$	10.061	9.930	–	$3/2_5^+$	10.359	9.930	–
$7/2_4^+$	10.063	9.980	–	$9/2_4^+$	10.708	9.980	–
$5/2_6^+$	10.372	–	–	$7/2_4^+$	10.745	–	–
$1/2_3^+$	10.783	–	–	$5/2_6^+$	10.800	–	–
$9/2_4^+$	10.804	–	–	$1/2_3^+$	11.243	–	–
$3/2_6^+$	10.831	–	–	$3/2_6^+$	11.279	–	–
$5/2_7^+$	11.978	11.250	–	$5/2_7^+$	11.954	11.250	–
$3/2_7^+$	12.051	11.580	–	$3/2_7^+$	12.577	11.580	–
$7/2_5^+$	12.317	–	–	$7/2_5^+$	12.608	–	–
$5/2_8^+$	14.648	–	–	$5/2_8^+$	14.593	–	–
$9/2_5^+$	14.780	–	–	$9/2_5^+$	15.101	–	–
$7/2_6^+$	15.502	–	–	$7/2_6^+$	15.564	–	–
$1/2_4^+$	16.143	–	–	$1/2_4^+$	16.061	–	
$3/2_8^+$	16.520	–	–	$1/2_5^+$	16.711	–	–
$5/2_9^+$	16.786	–	–	$3/2_8^+$	17.356	–	–
$1/2_5^+$	17.096	–	–	$5/2_9^+$	17.366	–	–
$5/2_{10}^+$	17.216	–	–	$5/2_{10}^+$	17.645	–	–
$3/2_9^+$	17.573	–	–	$3/2_9^+$	17.993	–	–
$3/2_{10}^+$	21.582	–	–	$3/2_{10}^+$	21.902	–	–

Table 3. **Comparison of the experimental [24] and theoretical predictions excitation energies for ^{20}O nucleus by using USDA and USDB interactions**

Theoretical values for USDAPN		Experimental values		Theoretical values for USDBPN		Experimental values		Theoretical values for USDAPN		Experimental values		Theoretical values for USDBPN		Experimental values	
J^π	E (MeV)	E (MeV)	J^π	J^π	E (MeV)	E (MeV)	J^π	J^π	E (MeV)	E (MeV)	J^π	J^π	E (MeV)	E (MeV)	J^π
0_1^+	0	0	0^+	0_1^+	0	0	0_1^+	2_8^+	12.607	–	–	0_4^+	12.562	–	–
2_1^+	1.810	1.673	2^+	2_1^+	1.746	1.673	2_1^+	4_7^+	12.738	–	–	4_6^+	12.702	–	–
4_1^+	3.472	3.570	4^+	4_1^+	3.619	3.570	4_1^+	3_6^+	12.921	–	–	4_7^+	12.918	–	–
2_2^+	4.047	4.042	2^+	2_2^+	4.154	4.042	2_2^+	2_9^+	12.988	–	–	3_6^+	13.088	–	–
0_2^+	4.887	4.456	0^+	1_1^+	5.114	5.002	–	0_4^+	13.000	–	–	1_5^+	13.182	–	–
1_1^+	5.044	5.002		2_3^+	5.157	5.234	2^+	1_5^+	13.100	–	–	6_2^+	13.327	–	–
2_3^+	5.240	5.234	2^+	4_2^+	5.269	4.850	4^+	6_2^+	13.336	–	–	2_9^+	13.427	–	–
4_2^+	5.246	4.850	4^+	3_1^+	5.352	–	–	3_7^+	13.337	–	–	2_{10}^+	13.770	–	–
3_1^+	5.249			0_2^+	5.378	4.456	0^+	2_{10}^+	13.610	–	–	4_8^+	14.037	–	–
4_3^+	7.324	7.754	4^+	4_3^+	7.384	7.754	4^+	4_8^+	13.621	–	–	3_7^+	14.099	–	–
5_1^+	7.397			5_1^+	7.469	–	–	1_6^+	13.688	–	–	0_5^+	14.273	–	–
2_4^+	7.819	5.304	2^+	2_4^+	8.177	5.304	2^+	3_8^+	14.573	–	–	1_6^+	14.491	–	–
4_4^+	8.536	8.554	4^+	4_4^+	8.580	8.554	4^+	0_5^+	14.659	–	–	3_8^+	15.009	–	–
3_2^+	8.866			2_5^+	8.636	–	–	5_4^+	15.023	–	–	5_4^+	15.141	–	–
2_5^+	8.875	10.125	2^+	3_2^+	8.767	10.125	2^+	3_9^+	15.175	–	–	3_9^+	15.818	–	–
1_2^+	9.691			0_3^+	9.669	5.387	0^+	1_7^+	15.381	–	–	4_9^+	15.919	–	–
0_3^+	10.153	5.387	0^+	1_2^+	10.108	–	–	4_9^+	15.457	–	–	1_7^+	16.115	–	–
3_3^+	10.176	–	–	2_6^+	10.112	–	–	4_{10}^+	16.296	–	–	4_{10}^+	16.482	–	–
2_6^+	10.225	–	–	6_1^+	10.391	–	–	6_3^+	17.011	–	–	6_3^+	17.173	–	–
6_1^+	10.273	–	–	3_3^+	10.403	–	–	3_{10}^+	17.454	–	–	3_{10}^+	17.806	–	–
1_3^+	10.786	–	–	2_7^+	11.124	–	–	1_8^+	17.806	–	–	1_8^+	18.281	–	–
2_7^+	11.126	–	–	5_2^+	11.318	–	–	5_5^+	17.963	–	–	5_5^+	18.499	–	–
5_2^+	11.266	–	–	1_3^+	11.401	–	–	0_6^+	18.596	–	–	0_6^+	18.726	–	–
1_4^+	11.338	–	–	5_3^+	11.641	–	–	0_7^+	18.990	–	–	0_7^+	19.589	–	–
5_3^+	11.562	–	–	1_4^+	11.783	–	–	1_9^+	20.161	–	–	1_9^+	20.679	–	–
3_4^+	12.072	–	–	4_5^+	11.995	–	–	5_6^+	20.549	–	–	5_6^+	20.728	–	–
4_5^+	12.147	–	–	3_4^+	12.206	–	–	0_8^+	21.044	–	–	0_8^+	21.529	–	–
3_5^+	12.232	–	–	3_5^+	12.365	–	–	1_{10}^+	22.252	–	–	1_{10}^+	22.518	–	–
4_6^+	12.293	–	–	2_8^+	12.510	–	–	0_9^+	30.866	–	–	0_9^+	31.276	–	–

the experimental levels such as {7.508, 7.806, 7.947, 8.048, 8.561, 9.324, 9.560, 9.930, 9.980, 11.250, and 11.580} MeV with the use of USDA and USDB interactions. A number of new energy levels have been predicted for this nucleus for the states { $9/2_3^+$, $5/2_6^+$, $1/2_3^+$, $9/2_4^+$, $3/2_6^+$ and $7/2_5^+$ to $3/2_{10}^+$} that were not well established experimentally.

For the ^{20}O nucleus, we got an acceptable agreement with the USDA and USDB for the states {2_1^+, 4_1^+, 2_2^+, 2_3^+, 4_2^+, 4_3^+, and 4_4^+} with recent experimental values [24] shown in Table 3. The new energy levels are expected for this nucleus in the states {5_1^+, 3_2^+, 1_2^+, and 3_3^+ to 0_9^+} were not well established experimentally.

3.2. Reduced electric quadrupole transition probability B(E2). Calculations

The reduced probabilities of $B(E2;\downarrow)$ transitions have been predicted for ^{18,19,20}O nuclei within the nuclear shell model, by employing USDA and USDB interactions. With the harmonic oscillator potential (HO, b), the transition probabilitues were calculated for $b < 0$. The comparisons of the calculated $B(E2;\downarrow)$ values with the experimental data [23, 24] are given in Table 4 for all nuclei under study. From this comparison, a reasonable compatibility with the experimental data for the states $(2_1^+ \to 0_1^+)$ and $(4_1^+ \to 2_1^+)$ for ^{18}O nucleus and $(1/2_1^+ \to 5/2_1^+)$ for ^{19}O nucleus, as well as for ^{20}O, is obtained. The angular momentum and parity for some experimental levels and expected new energy levels have been assigned for the nuclei in $(2_1^+ \to 0_1^+)$ states. For the ^{18,19,20}O nuclei, the new transitions $B(E2;\downarrow)$ have been predicted with USDA and USDB interactions.

Table 4. **Comparison of the experimental [23, 24] and theoretical predictions of transition probabilities $B(E2)$ in unit) e^2 fm^4s for ^{18,19,20}O isotopes by using USDA and USDB interactions**

Isotopes	$(J_i^+ \to J_f^+)$	Theoretical $B(E2)$, e^2 fm^4		Experimental $B(E2)$, e^2fm^4
		USDA results	USDB results	
^{18}O	$2_1 \to 0_1$	18.30	19.47	9.302 ± 9
	$4_1 \to 2_1$	15.35	15.57	3.334 ± 6
	$3_1 \to 2_1$	0.719	0.765	–
	$3_1 \to 4_1$	11.40	11.280	–
	$1_1 \to 2_1$	3.378	2.545	–
	$1_1 \to 3_1$	6.811	5.599	–
^{19}O	$3/2_1 \to 5/2_1$	45.53	46.63	–
	$1/2_1 \to 5/2_1$	13.74	10.75	1.746 ± 12
	$9/2_1 \to 5/2_1$	12.43	12.42	–
	$7/2_1 \to 5/2_1$	14.83	16.579	–
	$7/2_1 \to 9/2_1$	16.93	16.23	–
	$11/2_1 \to 7/2_1$	6.993	7.874	–
	$11/2_1 \to 9/2_1$	4.663	5.095	–
^{20}O	$2_1 \to 0_1$	12.80	13.35	5.804 ± 7
	$4_1 \to 2_1$	4.184	4.456	–
	$1_1 \to 2_1$	3.742	3.217	–
	$3_1 \to 2_1$	2.076	2.336	–
	$3_1 \to 4_1$	2.828	2.156	–
	$3_1 \to 1_1$	1.502	1.486	–
	$5_1 \to 4_1$	5.178	7.098	–
	$5_1 \to 3_1$	6.650	6.289	–
	$6_1 \to 4_1$	0.722	0.829	–
	$6_1 \to 5_1$	3.931	3.971	–

4. Conclusions

Using the OXBASH code with USDA and USDB interactions and the SDPN model space for ^{18,19,20}O nuclei, we have predicted low-lying levels (energies, spins, and parities) and the reduced probabilities of the $B(E2;\downarrow)$ transitions. We conclude that the shell model configuration mixing is very successful in this region. We believe that the OXBASH program can be applied to other isotopes.

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РОЗРАХУНОК ^{18,19,20}О ІЗОТОПІВ ПО ОБОЛОНКОВІЙ МОДЕЛІ З ВИКОРИСТАННЯМ УСДА І УСДБ ВЗАЄМОДІЙ

Р е з ю м е

Використовується оболонкова модель для розрахунку рівнів енергії і ймовірностей переходів $B(E2)$ для ^{18,19,20}О ізотопів. У СДПН модельному просторі розглянуті УСДА і УСДБ взаємодії. Передбачається, що всі можливі багатонуклонні конфігурації визначені $0d_{5/2}$, $1s_{1/2}$, і $d_{3/2}$ станами вище, ніж у двічі магічного ядра ^{16}О. Розраховані рівні енергії добре узгоджуються з експериментальними даними. Підтверджено значення спінів і парності для нових рівнів, і передбачено ймовірності переходів $B(E2)$; $\downarrow$).