

Nuclear structure for ^{24}Mg within *sd-shell* model space Hamiltonians

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Abstract – In this study, we assess the accuracy of the *sd-shell* Hamiltonians CW, USD, USDA and USDB in calculating the excited states in ^{24}Mg nucleus on the basis of recently reported experimental results. The assessments rely on the calculations of the energy levels, reduced electric quadrupole transition probabilities, and reduced magnetic dipole transition probabilities. We show a comparison between the four Hamiltonians calculations and demonstrate the possibility of confirming known states and suggesting new states.

Keywords: Shell model; OXBASH; USDA; USDB; CW; ^{24}Mg ; energy level

1. Introduction

Many methods have been used to calculate the nuclear states energies within higher numerical accuracy and to provide wave functions from which the calculation of other observables becomes applicable. The shell-model configuration mixing is the one of the most efficient methods used for this purpose where the conventional shell-model codes provide typically 1 keV of numerical accuracy. In this method the matrix is established upon all possible Slater determinants with diagonalization a relatively small subset of valence orbits [1]. The basic requirements for the shell-model configuration mixing calculations are a set of single-particle energies (SPEs) and two-body interaction matrix elements or two-body matrix elements (TBME). These sets have recently been called effective interaction or model space Hamiltonian. This model space Hamiltonian may be described in two ways: the first method is the “realistic” which is constructed for a given shell model space from known data on the free nucleon-nucleon force. The second method is “empirical” which is based in the parameters whose values are determined by agreement between shellmodel eigenvalue and measured level energies [2]. The matrix elements relate to the free nucleon–nucleon interaction and considering the matrix elements merely as parameters to be adjusted to achieve agreement with empirical spectroscopic results [3].

CW is an effective interaction embedded with OXBASH code for Windows [4]. The “particle” Hamiltonian or CW description of the lowest-lying states in the region $17 \leq A \leq 28$ by a fit to 200 level energies was taken predominantly from the $A = 18-24$ mass region. This Hamiltonian has provided realistic *sd-shell* ($0d_{5/2}$, $0d_{3/2}$, $1s_{1/2}$) wave functions from 63 two-body matrix elements and three SPEs for the above subshells [5, 6]. The Wildenthal interaction or “universal” *sd* (USD) Hamiltonian is set up by fitting 380 energy data with experimental errors of 0.2 MeV or less from 66 nuclei. The data were fitted from the lower and upper parts of the *sd-shell* by supposing that the simple mass dependence for the matrix elements was within [3, 7]:

$$\text{ME}(A)/\text{ME}(18) = (18/A)^{0.3} \quad (1)$$

where A is the mass number. This hypothesis enables USD to describe all *sd-shell* nuclei with acceptable results. The new USD interactions called USDA and USDB refine the derivation

of the USD Hamiltonian by an updated and complete set of energy data [8]. The Universal sd-shell Hamiltonians (USDA and USDB) were obtained by fitting 63 two-body matrix elements (TBME) and three single-particle energies to the experimental values for 608 energies of the ground states and low-lying excited states of sd-shell nuclei with $A = 16$ to 40. The USDA and USDB were used to calculate the configuration-active proton and neutron orbitals in the $0d_{5/2}$, $0d_{3/2}$, and $1s_{1/2}$ shells. For USDA, thirty linear combinations of one- and two-body matrix elements were varied, and the remaining 36 linear combinations were fixed at values of a renormalized G-matrix, with the resulting root-mean-squared deviation between experimental and theoretical energies being 170 keV. The USDB was derived from the same data as in the derivation of USDA, except that for USDB, 56 linear combinations were varied with 10 fixed at the G-matrix values with an improved root-mean-square (rms) deviation of 130 keV [8]. USDB provides the best fit to the data; however, USDA is the more conservative Hamiltonian, which is closest to the realistic Hamiltonian [8]. For this reason, the USDB interaction is used more than the USDA in many recent researches [9], but the calculation with the USDA and USDB predict an almost identical spectrum for the energy states especially in the ^{24}Mg region of chart with marked distinction for USDA [10, 11].

The ^{24}Mg nucleus has special significance in shell model applications. This significance caused by the position of this nucleus on the chart and its rich spectrum of excitations states. The ^{24}Mg nucleus is being sufficiently heavy to show a strong deformation and as well as having a light nucleus that can be calculated using the shell model [12]. This nucleus contains a small number of nucleons, such that its structure can be calculated with the shell model using the full sd-configuration space [12]. This number of nucleons allowed for the sd-shell orbital configurations to generated the angular momentum with maximum value 12 for this nucleus which matches what was found experimentally [10]. Many studies have been conducted to study the ^{24}Mg nucleus; some were experimental studies in which the high-spin spectrum represents an urgent need in many mode tests [10, 12]. Others were theoretical studies that used various methods. In addition to the shell model, the clustering model also has been used recently to elucidate the nuclear structure with numerous hypotheses that are compatible with this model [13-15].

In this work, we use effective CW, USD, USDA and USDB interactions to calculate the energy levels, reduced electric quadrupole transition probabilities, and reduced magnetic dipole transition probabilities for all available experimental data to the ^{24}Mg isotope.

The aim of this work is to study the effects of these Hamiltonians within the nuclear structure of even-even, $A=24$, magnesium isotopes. The precision of the Hamiltonians are illustrated in both the energy levels (the Hamiltonian eigenvalues) and the transition probabilities which mainly depend on the state wave functions (eigenvectors). For this precision, one can determine the differences among the four effective interactions depending on the independent variables J_n^+ , the angular momentum J and the sequence number n , which are used to calculate the Hamiltonian eigenvalues and eigenvectors. This study will also help to identify new states or confirming others. The confirming of any new states is based on the agreement between the theoretical and experimental data and the identification of new states is based on the agreement between the different Hamiltonians of a certain state using.

2. Shell model calculations

The calculations have been conducted using the code OXBASH for Windows. The code uses an m-scheme Slater determinant basis. Using a projection technique, wave functions with good angular momentum J and isospin T are constructed. The SD model spaces consists of $0d_{5/2}$, $1s_{1/2}$, and $0d_{3/2}$ above the $Z = 8$ and $N = 8$ closed shells for protons and neutrons, respectively. The SPEs for the four Hamiltonians are listed in Table 1, while the TBME values can be found in the reference for every Hamiltonian as shown in Table 1.

Table 1 single-particle energies (SPEs) for every Hamiltonian used in this work (MeV)

Hamiltonian	0d3/2	0d5/2	1s1/2	Reference
CW	0.877	-4.15	-3.28	[6]
USD	1.647	-3.948	-3.164	[7]
USDA	1.979	-3.943	-3.061	[8]
USDB	2.1117	-3.9257	-3.2079	[8]

2.1 Energy Levels

The methods are used in this work for comparison between the theoretical and the experimental energies are based on the spin sequences and energy gaps and state-to-state correspondences [2]. A comparison has been made for the first three sequences, Figs 1-3, between the energy obtained from the four effective interactions calculations and the states obtained from all available experimental data for $0 \leq J \leq 12$ and T (isospin) = 0 with non-negative-parity values. The using of the first three sequences exhibit is a good illustration pattern due to the energy gaps between the energy states in these sequences with the same J values. It is certainly assists to study the change in the accuracy of the Hamiltonians for each sequence. The calculated energy levels and experimental states are presented in Figures 1 to 3. The calculated values from USDA and USDB are plotted on the left of the experimental data, whereas the USD and CW values are plotted on the right. Levels with '()' correspond to cases in which the spin and/or parity of the corresponding states are not well established experimentally.

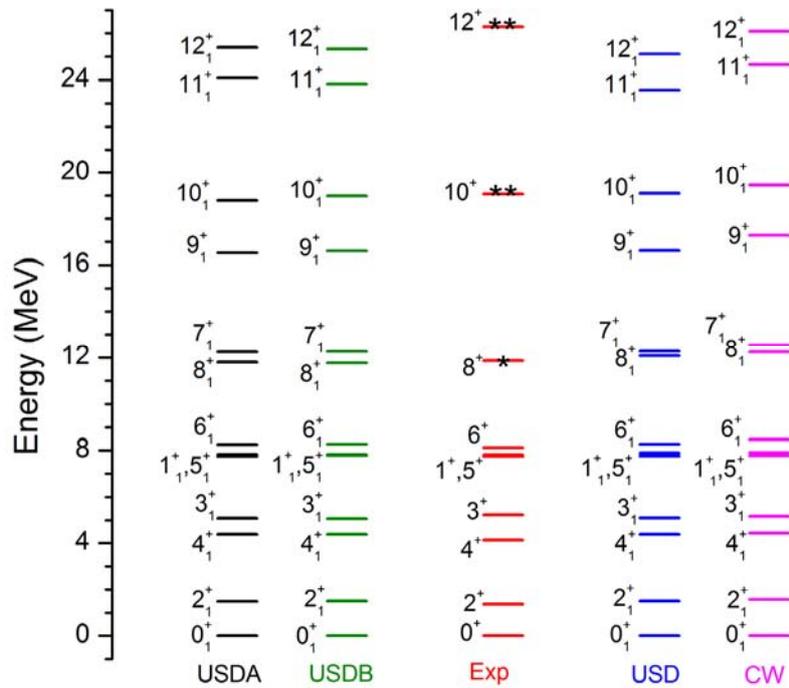


Figure 1. (Color online) Comparison of the experimental energy levels with the present theoretical work of the first sequence for ^{24}Mg nucleus. The experimental data (—) are taken from [16, 17], while (*) from [18] and ** from [10].

No variation is found between the results of the four interactions in the first sequence for $J \leq 10$, as shown in Fig. 1, with a good agreement can be observed with the experimental states. The good agreement between experimental and theoretical states indicates to the possibility of identify a new states with $J=7, 9$ and 11 at approximately energies 12.331, 16.758 and 24.035 MeV with average variations 0.8%, 1.5% and 1.3% between the four Hamiltonians values, respectively.

In Fig. 2, states with $J=0^+$ show difference between experimental and theoretical values. The predictions of the four Hamiltonians are higher than experimental values with average 1.031 MeV. With exception for this discrepancy, the second sequence calculations show also a good agreement with the experimental states for all Hamiltonians values. The doublet consisting of two states with $J = 3^+$ and 6^+ at energies 9.45 and 9.52 MeV [17], respectively, have been unconfirmed experimentally. The predictions of the Hamiltonians show a good confirmation for these states especially within USDB and USD calculations. The shell model calculations suggested a new state with $J=5^+$ at approximately energy 10.642 MeV with average variations 1.8% between the four Hamiltonians values.

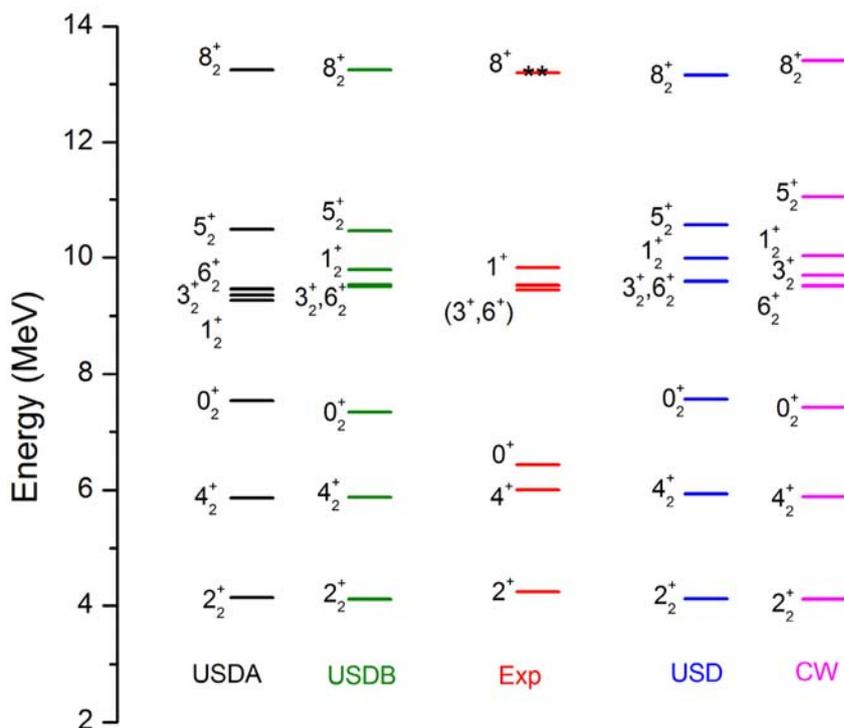


Figure 2. (Color online) Comparison of the experimental energy levels with the present theoretical work of the second sequence for ^{24}Mg nucleus. The experimental data (—) are taken from [16,17], while ** from [10].

The third sequence results show variance in some J states, as shown in Fig. 3. This variance is found with states $J = 0^+, 1^+,$ and 3^+ , wherein the USDA and USDB are more convergent than the other interactions. This variance illustrates the effect of the n values on the accuracy of the Hamiltonians results particularly with the CW values. The third sequence experimental data shows two unconfirmed states with $J=6^+$ and 8^+ at energies 12.002 and 14.153 MeV, respectively [17], for $J=6^+$ a theoretical confirmation appeared from the USD and CW Hamiltonians. Whereas state with $J=8^+$ has been confirmed by the all Hamiltonians results which was identical to the experimental results of the reference [10]. In

this sequence also the calculations suggested a new state with $J=5^+$ at approximately energy 12.424 MeV with average variations 1.1% between the four Hamiltonians values.

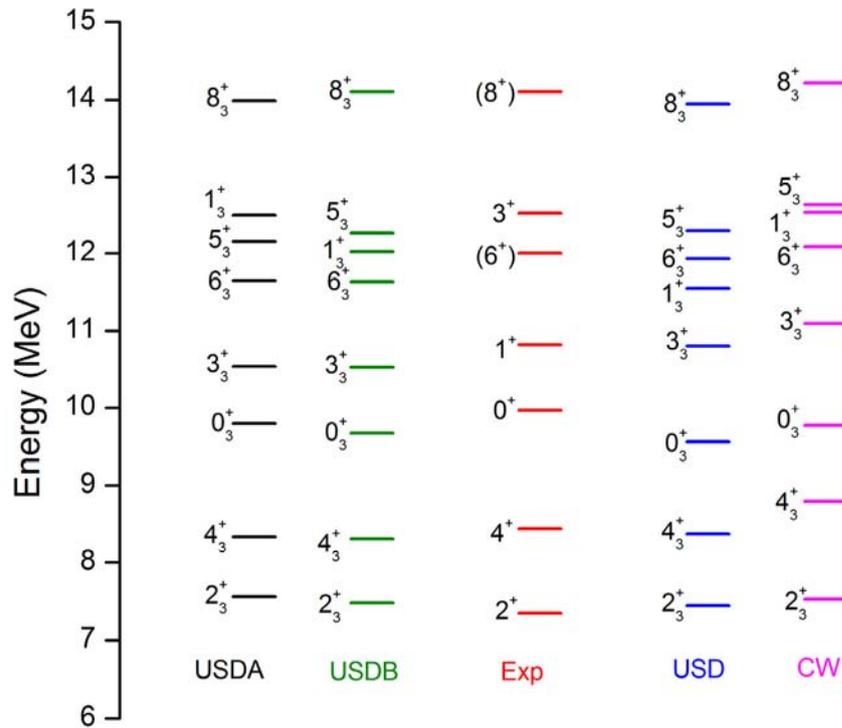


Figure 3. (Color online) Comparison of the experimental energy levels with the present theoretical work of the third sequence for ^{24}Mg nucleus. The experimental data are taken from [16, 17].

The higher sequence states for $J = 0^+$ to 8^+ are shown in Figs. 4 and 5. Theoretical calculations have been performed by using USDA and USDB according to the extent of available experimental energies and each J value is compared separately. The calculations are performed depending on the J states energy range; therefore the numbers of the theoretical states (n) are identified for each J value. In the $J=0^+$ calculations, one can see that there are clear differences between the USDA and USDB predictions with a clear preference for the USDA values. On the other hand, it is clear that experimental data have emerged a number of states larger than the theoretical states in this energy range. This means that we need to expand the model space to get more energy states within the intended range [11]. The same was found also in the $J=1^+$ calculations and for $J=2^+$ at energy <15.33 MeV. Where, in the $J=3^+$ results and for $J=2^+$ at energy >15.33 MeV the number of theoretical states are larger than the experimental (44 theoretical states between 15.33 MeV and 21.25 MeV; the maxima experimental energy for $J=2^+$ [19]; conversely there are only 3 experimental). This difference between the theoretical and experimental states clearly points to the possibility of the existence many states with $J=2^+$ and 3^+ in this energy range.

The calculation for states with $J=1^+$ and 3^+ have made in two isospin values 0, and 1. The experimental data show many states with $J=1^+$ and $T=1$, these states have a good agreement with their counterpart theoretical states. It is worth mentioning that a remarkably agrees between the USDA and USDB predictions for $T=1$ with $J=1^+$ and 3^+ , but in the same spectrum, we find varied between theoretical values with $T=0$. The comparison between experimental and theoretical values in Fig. 4 did not show any discrimination for any Hamiltonian due to the discrepancy between the experimental and theoretical values in $J=0^+$

spectrum, overcrowding values in the $J=1^+$ and 2^+ spectrum and the lack of experimental data in $J=3^+$ spectrum. In contrast, these calculations confirmed the presence of some energy states, as the states with $J=0^+$ at energy 13.198 MeV and $J=3^+$ at energy 11.314 MeV [17].

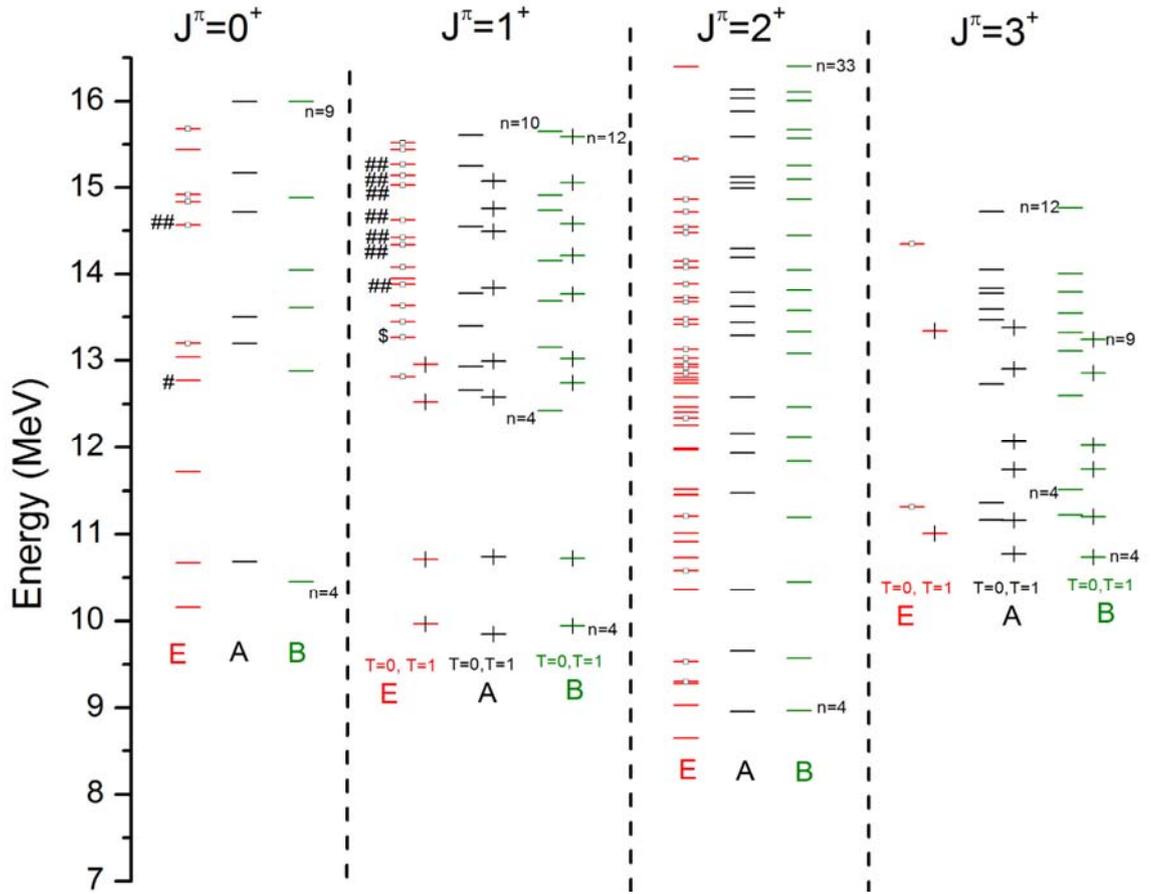


Figure 4. (Color online) Comparison between the calculations and the experimental energy levels for sequences higher than three with $J=0^+$ to 3^+ of the ^{24}Mg nucleus. E are the experimental data, A and B are theoretical levels using USDA and USDB, respectively. Experimental data (—) are taken from [16, 17] while (#) from [20], (##) from [19] and (\$) from [21]. Levels with + have $T=1$ and levels with (\square) are not well established experimentally. n is the theoretical sequence number.

The overcrowding of the theoretical and experimental states for $J=4^+$, 6^+ and 8^+ in Fig 5 prevented again the possibility of discrimination preference one of the Hamiltonians, USDA or USDB, but the theoretical calculations indicated to the many energy intervals have theoretical states higher than the experimental which are giving an indication of the need for more experimental works in these intervals. The shell model calculations confirmed the possibility of the existence many states in Fig 5. This confirmation was based on the existence of the energy gaps and state-to-state correspondences. This states are : 9.516 and 10.82 MeV [17] in the $J=4^+$ spectrum, 13.85, 14.673 and 15.62 MeV [17] in the $J=6^+$ spectrum, and 16.3 [19], 20.25 [10], and the doublet consisting of two states at 23.545, 23.601 MeV and 23.763, 23.78 MeV [19] in the $J=8^+$ spectrum.

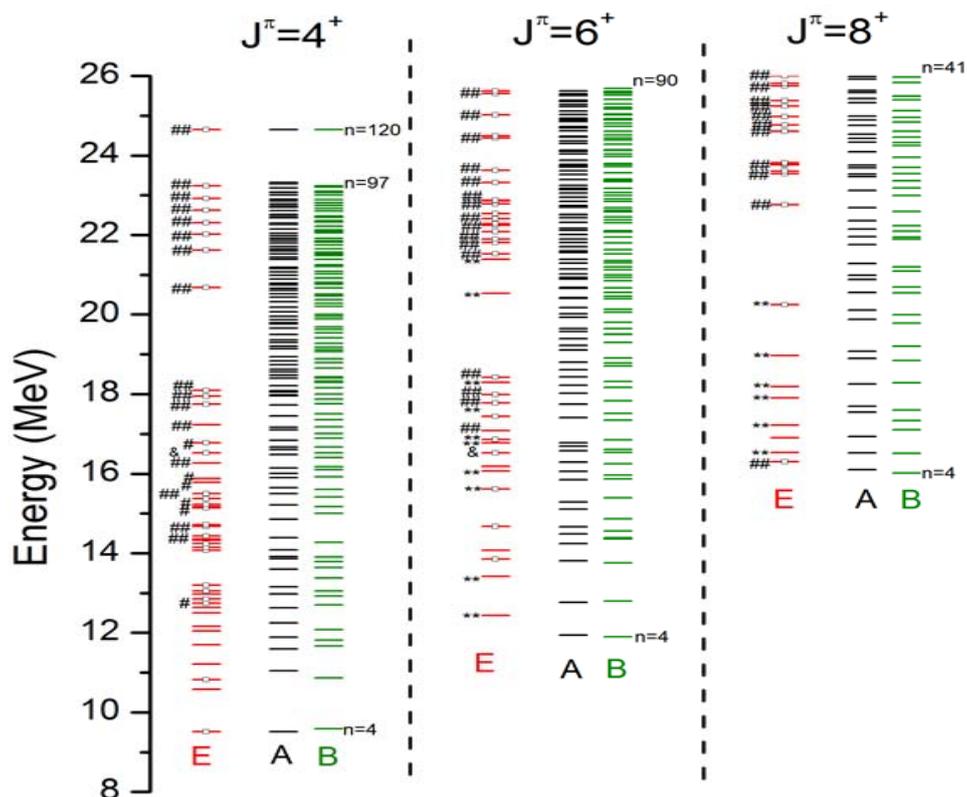


Figure 5. (Color online) Comparison between experimental energy levels and the energy levels calculated in the present theoretical work for the ^{24}Mg nucleus for sequences higher than three with $J=4^+, 6^+$ and 8^+ . E are the experimental data, A and B are theoretical levels using USDA and USDB, respectively. Experimental data (–) are taken from [16, 17] while(**) from [10], (#) from [20], (##) from [19] and (&) from [22]. Levels with (□) are not well established experimentally. n is the theoretical sequence number.

The experimental data in reference [17] show many states with $J=2^+, 3, 4^+$. The comparison with the theoretical states obtained by using the four Hamiltonians indicates that the USDA results have the best description for these states. These energy states and the corresponding USDA calculations are present in Table 2.

Table 2 Theoretical and new experimental energy for states with $J=2^+, 3, 4^+$ in ^{24}Mg spectrum.

Experimental		USDA		
J	Energy(MeV)	J	n	Energy (MeV)
$2^+, 3, 4^+$	9.302	3	2	9.363
	9.532	4	4	9.518
	10.581	3	3	10.538
	(11.293)	3	5	11.361
	12.339	4	8	12.248
	12.399	2	10	12.577
	12.919	4	10	12.98
13.473	3	7	13.465	

2.2 Reduced electric and magnetic transition:

Transition rates are a sensitive indicator for most modern effective interactions developed to describe the sd-shell region. This sensitivity resulting from the adoption of transition rates on the single particle wave function (Hamiltonianeigenvectors) [1]. In this section, the theoretical and experimental reduced electric quadrupole transition probability $B(E2)$ (in units of $e^2 fm^4$) and reduced magnetic dipole transition probability $B(M1)$ (in units of μ^2 , μ Bohr magneto) values for Mg^{24} isotope are presented in Table 3. The symbols n_i and n_f in table 2 represent the sequences of the closest theoretical J states to the experimental data.

The comparison between theoretical and experimental $B(E2)$ shows an advantage for USDA and USDB calculations for many states, but in general the four Hamiltonians results are acceptable. The reduced magnetic dipole transition probabilities $B(M1)$ results gave a clear advantage to the USDA calculations compared to the other Hamiltonians results.

Table 3 Theoretical and experimental $B(E2)$ and $B(M1)$ values for ^{24}Mg . Experimental data taken from [17]

Experimental							Theoretical $B(E2) e^2 fm^4$			
E_i (MeV)	J_i	E_f (MeV)	J_f	$B(E2) e^2 f$	n_i	n_f	USDA	USDB	USD	CW
0.0	0	1.368	2	383(53)	1	1	341.61	343.5	347	310.1
1.368	2	0.0	0	88.41(10)	1	1	68.32	68.70	62.98	62.03
4.122	4	1.368	2	160.37(4)	1	1	91.22	89.99	83.72	78.84
4.238	2	1.368	2	14.80(4)	2	1	13.08	13.36	13.7	12.21
4.238	2	0.0	0	7.98(19)	2	1	6.78	6.38	5.60	6.77
5.235	3	4.238	2	238.50(8)	1	2	120.8	121.11	122.5	119.2
5.235	3	1.368	2	10.28(3)	1	1	11.04	10.39	9.07	10.83
6.432	0	5.235	2	36.60(14)	2	2	13.41	13.30	10.95	12.95
6.432	0	1.368	2	2.63(10)	2	1	0.60	0.17	0.04	0.078
7.348	2	0.0	0	2.76(23)	3	1	0.31	0.43	0.47	0.341

Experimental							Theoretical $B(M1) \mu^2$			
E_i (MeV)	J_i	E_f (MeV)	J_f	$B(M1) \mu^2$	n_i	n_f	USDA	USDB	USD	CW
4.238	2	1.368	2	1.61×10^{-5} (8)	2	1	1.6×10^{-6}	1.5×10^{-8}	1.7×10^{-7}	1.4×10^{-7}
5.235	3	4.238	2	6.2×10^{-4} (17)	1	2	2.4×10^{-4}	2.4×10^{-4}	1.04×10^{-4}	2.1×10^{-4}
5.235	3	1.368	2	3.7×10^{-5} (11)	1	1	1.2×10^{-6}	6.0×10^{-6}	1.9×10^{-7}	4.2×10^{-7}
7.747	1	0.0	0	1.39×10^{-3} (20)	1	1	1.3×10^{-3}	6.9×10^{-4}	7.5×10^{-5}	4.8×10^{-4}

3. Summary

In this study, the empirical sd-shell Hamiltonians, CW, USD, USDA and USDB which embedded with OXBASH code for Windows are used to calculate the structure of ^{24}Mg nucleus. The calculation results are compared with the recently available experimental data. The comparisons are based on calculated energy levels, reduced electric quadrupole transition probabilities, and reduced magnetic transition dipole probabilities. The energy states

adopted in this research are of all available experimental data with non-negative parity. Some states have been confirmed and some new ones are suggested as we listed in Table 4.

The comparison between the Hamiltonians results showed the effect of the sequence number (n) on the consistency of the Hamiltonians calculations. This is clear from the remarkable consensus in the first and second sequence between all Hamiltonians states, while the CW calculations becomes higher than others in the third sequence. The same effect also can be seen in the comparison between the USDA and USDB calculation for higher sequence numbers.

Table 4 The energy states which are confirmed/suggested in this work. The column “Hamiltonian” shows the best Hamiltonian predicted closest energy value and the “Average” refers to the adoption of an average value from all the Hamiltonians.

Energy _{Th.} (MeV)	Hamiltonian	J	n	Energy _{exp} (MeV)	Reference	Status
12.331	Average	7	1	-		<i>suggested</i>
16.758	Average	9	1	-		<i>suggested</i>
24.035	Average	11	1	-		<i>suggested</i>
9.511	USDB	3	2	9.457	[17]	<i>confirmed</i>
9.532	USDB	6	2	9.527	[17]	<i>confirmed</i>
10.642	Average	5	2	-		<i>suggested</i>
11.932	USD	6	3	12.002	[17]	<i>confirmed</i>
14.096	USDB	8	3	14.153	[17]	<i>confirmed</i>
12.424	Average	5	3	-		<i>suggested</i>
13.192	USDA	0	5	13.198	[17]	<i>confirmed</i>
11.361	USDA	3	5	11.314	[17]	<i>confirmed</i>
9.518	USDA	4	4	9.516	[17]	<i>confirmed</i>
10.863	USDB	4	5	10.820	[17]	<i>confirmed</i>
13.812	USDA	6	7	13.850	[17]	<i>confirmed</i>
14.661	USDA	6	9	14.673	[17]	<i>confirmed</i>
15.85	USDA	6	12	15.620	[10]	<i>confirmed</i>
16.103	USDA	8	4	16.300	[19]	<i>confirmed</i>
20.106	USDA	8	13	20.250	[10]	<i>confirmed</i>
23.47	USDA	8	24	23.545	[19]	<i>confirmed</i>
23.535	USDA	8	25	23.601	[19]	<i>confirmed</i>
23.687	USDA	8	26	23.763	[19]	<i>confirmed</i>
23.753	USDA	8	27	23.780	[19]	<i>confirmed</i>

The results of B(E2) and B(M1) calculations are show a good agreement with the experimental data. The B(E2) values did not show preference for any one of the Hamiltonians, but B(M1) values showed a simple preference for the conservative Hamiltonian USDA.

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