PREDICTION OF MIXING FORMALISM FOR THE ENERGY SPECTRA AND QUADRUPOLE TRANSITION RATES OF ^{98}Mo NUCLEUS

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This paper presents a detailed investigation of both normal and intruder states in ^{98}Mo nucleus in the $E \leq 3$ MeV. We considered all reported intruder energy levels for this nucleus, 0_2^+, 2_1^+, 4_1^+, 4_2^+, 2_2^+, and also the quadrupole transitions which originated from these levels. A mixing formalism based on the combination of U(5) and O(6) dynamical symmetries of the interacting boson model is used in the Hamiltonian and wavefunctions for, respectively, N- and $(N+2)$-boson spaces. The weight of each space is determined by the calculation of theoretical quadrupole transition rates and compared with their experimental counterparts. By using these weights, the expectation values of the pure U(5) and O(6) Hamiltonians and also the total Hamiltonian that contains these limits and mixing terms are calculated for different levels, too. The results show that normal energy levels and quadrupole transition between them can be described satisfactory in comparison with experimental counterparts by using the pure U(5) Hamiltonian in the only N-boson space. For intruder levels and quadrupole transition originating from them or holding between normal and intruder states, the mixed formalism of Hamiltonian and wavefunctions increases the efficiency of theoretical formalisms and suggests exact results.

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1. Introduction

The even mass nuclei located near the proton or neutron closed shells were thought to be vibrational and, therefore, classified as spherical nuclei. For numerous years, the theoretical explanation of the configuration of nuclei possessing 38, 40, and 42 protons, along with neutron numbers exceeding 50, has posed a significant challenge. Within this specific range, these nuclei exhibit remarkable characteristics, including a swift shift from vibrations to

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a structure reminiscent of rotation, as well as notably low-energy first excited 0^+ states that exhibit robust E2 transitions to the initial 2^+ states [1]. Within the $A = 100$ mass region, there exist a number of nuclei that have been extensively examined in relation to the concept of shape coexistence [2–5]. The shape coexistence refers to the occurrence of two or more distinct nuclear shapes, which arise from the pure normal valence configuration and the normal $2p$–$2h$ (intruder) configuration [6, 7]. The conclusions of such studies, as well as the presence of similar phenomena in other regions in the vicinity of closed shells, suggest that $2p$–$2h$ proton excitations could play an essential role in explaining the nature of intruder level in these nuclei, for example, the Mo isotopes [8, 9]. As a signature for such situations, the existence of an extra state between two-phonon states reports as the most suggested one and is proposed by different studies to describe these intruder states with the new configuration. In the interacting boson model (IBM), as the most commonly used algebraic framework for the investigation of such phenomena, a combination of different boson spaces and, therefore, the corresponding Hamiltonians of at least two dynamical limits is the method that is successful in describing of intruder levels. Federman and Pittle [10] have conducted an investigation of the rotational characteristics of Zr isotopes using the shell model framework. Their findings indicate that the rotational structure emerges gradually as neutrons are added, superimposed upon the first excited 0^+ states observed in lighter isotopes. This development is attributed to a robust monopole–monopole interaction between protons and neutrons, leading to both deformation of these states and a significant reduction in their energy. The authors have also drawn similar conclusions regarding the Mo isotopes using the Hartree–Fock–Bogoliubov method. The Zr isotopic chain, particularly in the range of $N = 50$–56, exhibits a remarkable demonstration of shape coexistence and shape transition, as recently have been elucidated in the case of ^{94}Zr nucleus [11]. In these isotopes, the 0_1^+state and the very low-lying 0_2^+ state are characterized by a strong mixing of protons. Such arrangements specifically have involved both $0p$–$0h$ and $2p$–$2h$ excitations, where protons are promoted from the pf shell to the $g_{9/2}$ orbital. Similarly, in the molybdenum isotopes starting from $N = 50$, the nuclear shape progressively evolves from a spherical form, and at around $N \approx 60$ and substantial deformation occurs due to an enhanced proton–neutron residual interaction [10]. The concept of shape coexistence can be applied to these nuclei and, particularly, to the ^{98}Mo nucleus with regard to proton excitations from the pf shell ($Z = 28$–40) to the $\pi g_{9/2}$ orbit [12, 13]. In Ref. [14], Thomas *et al.* have shown the uncovered evidence of two extensively blended configurations in the ^{98}Mo nucleus. The first one is the typical $2p$–$0h$ proton configuration which is associated with a rather U(5) vibrational pattern. The second one is the intruder $4p$–$2h$ configuration which is formed through excitations crossing the $Z = 40$ sub-shell closure and exhibiting characteristics properties similar to an O(6)γ-soft structure. The depiction of ^{98}Mo within the context of shape coexistence finds support from the examination of two-proton separation energies among even–even nuclei in the $A = 100$ region [15]. For nuclei located near closed shells, such as the Mo isotopic chain, normal states are described by the pure U(5) Hamiltonian which applies to the N-boson space, N is the total number of bosons in the considered nucleus. On the other hand, for such extra states between two-phonon states, the $(N+2)$-bosons spaces are suggested, which correspond with the O(6) dynamical limit [16–21]. Another sensitive parameter to the nuclear structure is the electromagnetic transition probability which, due to the available experimental data, the electric quadrupole transition, and its probability, $B(\mathrm{E2})$, is the most used one. By using these quadruple transition rates, a requirement is suggested to show the necessity to consider mixing of two different spaces. Two common approaches in the investigation of such situations, since nuclei contain both normal and intruder states, are the standard harmonic vibrator (HV) in the framework of the shell model, and the use of a pure U(5) dynamical symmetry description in the IBM. If the predictions of these two methods for quadruple transition rates fulfil the following requirements [12]:

$$\frac{N}{N-n_d+1} B\left(\mathrm{E2}; n_d \rightarrow n_d-1\right)_{\mathrm{IBM}} = B\left(\mathrm{E2}; N_{ph} \rightarrow N_{ph}-1\right)_{\mathrm{HV}} ,$$

where n_d is the number of d bosons, we can conclude that a pure U(5) formalism would describe both energy levels and transition rates satisfactory in comparison with the experimental counterparts. On the other hand, deviation from this pattern shows that we have to mix two configurations [22–28]. Consequently, it is necessary to consider interaction and mixing between two configurations in the framework of IBM and for nuclei such as ^{98}Mo, where the U(5) symmetry have been used for normal states and O(6) symmetry for intruder states [29–32].

It is well known that the $^{90}_{40}\mathrm{Zr}_{50}$ nucleus behaves as a closed-shell nucleus. If this were strictly the case, an IBM calculation of molybdenum isotopes would assume $1_\pi = 1$ proton boson and $N_v = 1, 2, \ldots$ neutron bosons for, respectively, ^{94}Mo, ^{96}Mo, ... However, it is also well-known that it is not really a closed shell but it rather represents a sub-shell closure. In the language of Duval and Barrett [9], this means, excitations of pairs from below to above $Z = 40$ are easily possible. If only one pair is excited from below to above $Z = 40$, the corresponding interaction boson configuration has $N_\pi = 3$ [1]. The authors of [29–32] have described the various aspects of such mixings in different nuclei. The results of Sambataro and Molnár in Ref. [1] have suggested a weak mixing for the ^{98}Mo nucleus, while a strong mixing is observed in the ^{96}Mo and ^{100}Mo nuclei. Again, a weak mixing is proposed for ^{102}Mo and ^{104}Mo with interchanging in the role of $N_\pi = 1$ and $N_\pi = 3$ configurations. Also, they have shown that the spectra belonging to two different configurations are simply superimposed on each other when they do not insert the mixing in their calculations. The process of mixing changes the sequence of the states and generates a particularly significant impact on states. Due to the significant energy spacing between the $N_\pi = 1$ configuration levels, only a few low-lying levels are associated with this configuration, primarily in the case of the ^{96}Mo nucleus. In this nucleus, the majority of the dominant components in the 2_1^+ and 0_2^+ states belong to the $N_\pi = 3$ configuration. Interestingly, the state is predicted to mostly belong to the $N_\pi = 1$ configuration, which is the only instance where this occurs. The level structures of ^{98}Mo and ^{100}Mo are quite similar, with two levels, and exhibiting close energy proximity, followed by another pair of levels, and also closely spaced but separated from the remaining levels. However, the crucial distinction between these two cases is that in the lighter isotopes, the state is predominantly associated with the $N_\pi = 3$ configuration, while in the heavier isotopes, the state is primarily attributed to the $N_\pi = 1$ configuration. An intriguing phenomenon is observed in the case of ^{102}Mo and ^{104}Mo nuclei in the ground state as well as the states belonging to the $N_\pi = 3$ configuration. On the other hand, the intruder state corresponds to the $N_\pi = 1$ configuration. It is also noteworthy that while states in the $N_\pi = 1$ configuration exhibit vibrational characteristics (associated with the U(5) limit of IBM), states in the $N_\pi = 1$ configuration display γ-unstable behaviour (related to the O(6) limit of IBM). This implies that the configuration mixing can occur between any two distinct collective structures, without being limited to a spherical- and axially-deformed structure. Experimental evidences which describe the unusual properties related to some of quadrupole transition probabilities, *e.g.*, $\frac{B(\mathrm{E2};0_2^+\to 2_1^+)}{B(\mathrm{E2};2_1^+\to 0_1^+)}$ ratio and the value of $2_1^+ \to 0_1^+$ transition can be found at the neutron number $N = 56$ by looking at the nature of involved states. In fact, in the ^{98}Mo nucleus, the 2_1^+ and 0_2^+ states mostly belong to the $N_\pi = 3$ configuration, however, the 0_1^+ state is mostly of $N_\pi = 1$ configuration [1]. References [33, 34] have shown that to describe this nucleus, we need to consider the combination of symmetries, and as the nucleus becomes heavier, the deformation of the nucleus will increase, so ^{100}Mo is more deformed than ^{98}Mo. In this paper, we consider the mixing between states by using such selection rules that have been introduced by Lehmann and Jolie [35, 36]. We used the U(5) symmetry for normal states and O(6) symmetry for the intruder states. As the first step, we expanded the wavefunctions of the intruder states and determined the weight of each N- and $(N + 2)$-bosons space by calculating the quadrupole transition rates originating from the intruder states and comparing them with their experimental counterparts. Then, by using these weights of each space, we calculated the expectation values of mixed Hamiltonian for both normal and intruder states. For the first time, all reported intruder states, 0_2^+, 2_1^+, 2_2^+, 4_1^+, 4_1^+, levels that were named intruder γ level are considered.

2. Methods and results

2.1. Transition rates

The low-lying energy spectra of many medium-to-heavy mass nuclei show regular features which can be explained remarkably well by different models. Different models, which are defined based on the geometrical aspect, such as the Bohr and Mottelson collective model [37] or the interaction boson model (IBM) [35, 36, 38, 39] which were defined by using the algebraic operators, are employed to investigate the characteristic properties of different nuclei such as energy spectra and different transition probabilities. For nuclei located near closed shells, advanced experimental techniques suggest some new energy levels and transitions that do not obey a special pattern offered by predictions of a single symmetry. Mixing of different symmetries is known as the technique used to investigate such systems with high accuracy. In this paper, we considered the ^{98}Mo nucleus that is supposed to be a spherical nucleus, corresponding to U(5) dynamical symmetry of IBM. Some levels and B(E2) values which are determined by using the predictions of this limit are not in agreement with the available experimental data. The existence of some energy levels and especially transitions originated from these extra levels or occurred between them and normal states cannot be described by the patterns of this symmetry proved that other symmetries have to be added and combined with U(5) symmetry. The results of some investigation which used the predictions of the shell model for such nuclei suggest a two particle–two hole ($2p$–$2h$) excitation which is equivalence to a new configuration, $(N+2)$-bosons space, in the IBM framework together with N-bosons space. For nuclei such as the Mo isotopic chain for which the normal states are described satisfactory by U(5) dynamical symmetry in the N-boson space, the $(N+2)$-space corresponding with the O(6) dynamical symmetry must be added. In this paper, we present a new procedure for the investigation of such intruder states and related quadrupole transition rates. Firstly, we show the disadvantages of using only the predictions of U(5) symmetry in the description of different quadrupole transition rates originating from intruder states or happening between normal and intruder levels. Also, all reported intruder states for ^{98}Mo nuclei, *e.g.* 0_2^+, 2_1^+, 2_2^+, 4_1^+, 4_2^+, are analyzed for the first time in this study. The electric quadrupole transition can be defined as [29, 30]

$$T_\mu^{(\mathrm{E2})} = e_2 \left(\left[s^\dagger \times d + d^\dagger \times s \right] + \chi'' \left[d^\dagger \times d \right]_\mu^2 \right) , \tag{1}$$

and its probability is determined as follows:

$$B\left(\mathrm{E2}; J_i \to J_f\right) = \frac{1}{2J_i + 1} \left| \langle J_f, \zeta \| T(E2) || J_i, \xi \rangle \right|^2 , \tag{2}$$

where ξ and ζ are the other quantum numbers which depend on dynamical symmetries selected to describe normal and intruder states. The results for such quadrupole transition rates of the ^{98}Mo nucleus, which are their experimental values are listed in Table 1. Theoretical values in this table are calculated by using the wavefunctions for different states that are labeled by only the quantum numbers of U(5) dynamical limit as:

$$|\psi\rangle = |N, n_d, \nu, L\rangle ,$$

where N is the total boson number, n_d, v, and L are, respectively, the quantum numbers of U(5), O(5), and O(3) symmetry groups. The effective charge

Table 1. E2 transition rates of the ^{98}Mo nucleus. Experimental values are taken from Ref. [40] and theoretical predictions are yielded by using wavefunctions in the N-bosons space, which correspond with U(5) dynamical symmetry.

Transition	Exp. {W.u.}	Th. {W.u.}
$2_1^+ \to 0_1^+$	21.4_{-10}^{+11}	14.4
$2_1^+ \to 0_2^+$	280	—
$2_2^+ \to 2_1^+$	47.8_{-100}^{+132}	21.5
$4_1^+ \to 2_1^+$	$49.1_{-4.5}^{+5.5}$	21.59
$2_3^+ \to 2_2^+$	4.7_{-23}^{+189}	4.11
$2_3^+ \to 0_2^+$	7.8_{-34}^{+286}	10.08
$2_4^+ \to 2_1^+$	1.7	—
$6_1^+ \to 4_1^+$	10.1	32.39
$0_3^+ \to 2_2^+$	1	1.02
$3_1^+ \to 4_1^+$	$\prec 0.40$	6.17
$3_1^+ \to 2_2^+$	1	15.42
$4_2^+ \to 4_1^+$	1	10.28
$4_2^+ \to 2_2^+$	0.88	11.32
$4_4^+ \to 2_3^+$	1	9.25
$4_4^+ \to 4_1^+$	0.33	—

and dimensionless parameters of Eq. (1) are respectively, $e = 1.897$ {W.u.} and $\chi = -0.266$, and are extracted in comparison with experimental values by using the MATLAB software.

The results of this table show that a pure U(5) configuration in the N-bosons space and corresponding wavefunctions are successful in the describing only intra-band quadrupole transitions between different levels of the ground band of energy. The best agreement is yielded for $2_1^+ \rightarrow 0_1^+$ transition where the uncertainty of theoretical predictions in comparison to the experimental counterpart is 0.01%. Also, this technique is unable to predict acceptable theoretical predictions for such a quadrupole transition which happened between normal and intruder states. On the other hand, for intra-band transitions and especially for such transitions originating from or ending in intruder states, the efficiency of this method reduces significantly. For some transitions, experimental data are available, however, they could not be described by the pure U(5) symmetry. A mixing formalism in IBM which is based on the combination of two N- and $(N+2)$-bosons spaces is the common method which has been used widely in different studies [8, 9] and [16–18, 41–45] for which we follow the same processes. To this aim, we consider the expansion of $|\psi_k\rangle = \sum_{k=1}^{2} a_{ki}|\psi_k\rangle$, where the summation indices are referred to U(5) and O(6) dynamical symmetries, respectively, for $k = 1$ and 2. In this step, we used the additional requirements on the quantum numbers of SO(5) and SO(3) symmetries which was introduced by Heyde *et al.* [29] as

$$\Delta L = |L_N - L_{N+2}| = 0 \quad \text{and} \quad \Delta v = |v_N - v_{N+2}| = 0\,. \tag{3}$$

By using these requirements, we expanded the wavefunctions of intruder states. Also, we applied the same processes for some normal states for which our previous pure U(5) formalism did not predict exact results for the quadrupole transitions originating from them or holding between these levels and intruder ones as follows:

$$\begin{aligned}
&\left|0_2^+\right\rangle = a^{0_2^+}{}_{22}\left|\psi_{\mathrm{O}(6)}\right\rangle + a^{0_2^+}{}_{12}\left|\psi_{\mathrm{U}(5)}\right\rangle, \quad &&\left|2_1^+\right\rangle = a^{2_1^+}{}_{11}\left|\psi_{\mathrm{O}(6)}\right\rangle + a^{2_1^+}{}_{21}\left|\psi_{\mathrm{U}(5)}\right\rangle,\\
&\left|0_1^+\right\rangle = a^{0_1^+}{}_{21}\left|\psi_{\mathrm{O}(6)}\right\rangle + a^{0_1^+}{}_{11}\left|\psi_{\mathrm{U}(5)}\right\rangle, \quad &&\left|2_3^+\right\rangle = a^{2_3^+}{}_{12}\left|\psi_{\mathrm{O}(6)}\right\rangle + a^{2_3^+}{}_{22}\left|\psi_{\mathrm{U}(5)}\right\rangle,\\
&\left|2_2^+\right\rangle = a^{2_2^+}{}_{11}\left|\psi_{\mathrm{O}(6)}\right\rangle + a^{2_2^+}{}_{21}\left|\psi_{\mathrm{U}(5)}\right\rangle, \quad &&\left|4_1^+\right\rangle = a^{4_1^+}{}_{11}\left|\psi_{\mathrm{O}(6)}\right\rangle + a^{4_1^+}{}_{21}\left|\psi_{\mathrm{U}(5)}\right\rangle,\\
&\left|2_4^+\right\rangle = a^{a_4^+}{}_{12}\left|\psi_{\mathrm{O}(6)}\right\rangle + a^{2_4^+}{}_{22}\left|\psi_{\mathrm{U}(5)}\right\rangle, \quad &&\left|4_3^+\right\rangle = a^{4_3^+}{}_{12}\left|\psi_{\mathrm{O}(6)}\right\rangle + a^{4_3^+}{}_{22}\left|\psi_{\mathrm{U}(5)}\right\rangle,\\
&\left|4_2^+\right\rangle = a^{4_2^+}{}_{11}\left|\psi_{\mathrm{O}(6)}\right\rangle + a^{4_2^+}{}_{21}\left|\psi_{\mathrm{U}(5)}\right\rangle,\\
&\left|4_4^+\right\rangle = a^{4_4^+}{}_{12}\left|\psi_{\mathrm{O}(6)}\right\rangle + a^{4_4^+}{}_{22}\left|\psi_{\mathrm{U}(5)}\right\rangle.
\end{aligned} \tag{4}$$

We considered states from the same classifications, normal or intruder, to determine the $B(\text{E2})$ values by considering the mixing of states. Also, the selection rules for different terms in Eq. (2) are $\Delta n_d = 1$ and 0 for, respectively, $[s^\dagger \times \tilde{d}]^2$ and $[d^\dagger \times \tilde{d}]^2$ terms to have non-zero values and, therefore, restrict our selected mixing states. After calculating the expectation values of these two terms, we compared our results with their empirical counterparts to extract different parameters introduced in Eqs. (4) together with parameters of Eq. (1), namely e and χ, whose different $a_{i,j}^{J_n^\pi}$ coefficients for the considered normal and intruder states are listed in Table 2.

Table 2. The coefficients of Eqs. (4). We used them to expand different normal and intruder states of ^{98}Mo nucleus in the N- and $(N+2)$-boson spaces.

$a_{11}^{2_1^+} = 0.87$	$a_{11}^{22^+} = 0.952$	$a_{11}^{0_1^+} = 0.654$	$a_{11}^{4_1^+} = 0.989$	$a_{11}^{4_1^+} = 0.961$
$a_{21}^{2_1^+} = -0.487$	$a_{21}^{2_2^+} = -0.308$	$a_{21}^{0_1^+} = -0.731$	$a_{21}^{4_1^+} = -0.147$	$a_{21}^{4_2^+} = -0.276$
$a_{22}^{2_3^+} = 0.87$	$a_{22}^{2_4^+} = 0.952$	$a_{22}^{0_2^+} = 0.654$	$a_{22}^{4_3^+} = 0.989$	$a_{22}^{4_4^+} = 0.961$
$a_{12}^{2_1^+} = 0.487$	$a_{12}^{2_4^+} = 0.308$	$a_{22}^{0_2^+} = 0.731$	$a_{12}^{4_3^+} = 0.147$	$a_{12}^{4_4^+} = 0.276$

Now, by using these constants, theoretical predictions for different quadrupole transitions of the ^{98}Mo nucleus are determined and presented in Table 3. Also, the effective charge in this formalism yields as $e = 2.762$ {W.u.} and $\chi = -0.866$.

The results of mixing formalism show significant improvement in comparison with the prediction of pure U(5) symmetry. More exact results are obtained for such intra- and inter-bands quadrupole transitions, since pure U(5) formalism is unable to make any predictions for them or gives more than 100% uncertainties in comparison with corresponding experimental results. Also, for the majority of quadrupole transitions which hold between normal and intruder levels or originated from intruder levels, this technique makes acceptable predictions and increases the efficiency of theoretical frameworks for the investigation in such situations. These results confirm that we could not explain all features in such nuclei just by considering the two isolated coexisting systems and it is necessary to consider the interaction between two configurations. Also, this improvement in theoretical predictions by using mixing of symmetries is significant even for such transitions between normal states that are known as pure U(5) states. The acceptable agreement between experimental values and theoretical predictions confirms the strong mixing between both configurations. The results of such mixing formalism of different symmetries makes it possible to provide theoretical predictions for some transitions for which isolated symmetries could not give any acceptable results.

Table 3. Similar to Table 1, the E2 transition rates of the ^{98}Mo nucleus. Theoretical predictions are yielded by using the mixing of two N- and $(N+2)$-bosons spaces. All transitions are expressed in {W.u.}.

Transition	Exp.	Theory (U(5))	Theory (MS)
$2_1^+ \to 0_1^+$	21.4^{+11}_{-10}	14.4	20.07
$2_1^+ \to 0_2^+$	280	—	220
$2_2^+ \to 2_1^+$	47.8^{+132}_{-100}	21.59	35.71
$4_1^+ \to 2_1^+$	$49.1^{+5.5}_{-4.5}$	21.59	33.14
$2_3^+ \to 2_2^+$	4.7^{+189}_{-23}	4.11	4.61
$2_3^+ \to 0_2^+$	7.8^{+286}_{-34}	10.08	9.41
$2_4^+ \to 2_1^+$	1.7	—	1.85
$6_1^+ \to 4_1^+$	10.1	32.39	8.99
$0_3^+ \to 2_2^+$	1	1.02	1.02
$3_1^+ \to 4_1^+$	< 0.40	6.17	0.28
$3_1^+ \to 2_2^+$	1	15.42	3.10
$4_2^+ \to 4_1^+$	1	10.28	1.22
$4_2^+ \to 2_2^+$	0.88	11.32	1.79
$4_4^+ \to 2_3^+$	1	9.25	1.88
$4_4^+ \to 4_1^+$	0.33	—	0.16

2.2. Energy spectra

The energy levels together with transition rates are regarded as observables that are sensitive to the nuclear structure and different studies [8, 9, 16–18, 41–46] show that it is necessary to consider the mixing of different configurations to make an acceptable description of these observables. A combination of different Hamiltonians where each term is proportional to a specific symmetry and an extra term for mixing of these symmetries, is the most usual method widely employed by different authors to make an exact description of normal and intruder states. For nuclei such as the molybdenum isotopic chain located near the $Z = 50$ proton closed shell, a combination of U(5) and O(6) dynamical symmetries is the most commonly used formalism. These symmetries correspond, respectively, with N- and $(N+2)$-boson spaces which are used for the description of normal and intruder states. We need another mixing potential of these two spaces to consider their interactions. In this study, we used the most general Hamiltonian of IBM for these limits and the final form of this mixed Hamiltonian is

$$\hat{H} = \hat{P}_N^{\dagger} \hat{H}_{\mathrm{U}(5)} \hat{P}_N + \hat{P}_{N+2}^{\dagger} \hat{H}_{\mathrm{O}(6)} \hat{P}_{N+2}^{\dagger} + \hat{V}_{\mathrm{mix}}^{N,N+2}, \tag{5}$$

where $\hat{P}_N$ and $\hat{P}_{N+2}$ are the projection operators into N- and $(N+2)$-bosons spaces and stand for the $\hat{V}_{\mathrm{mix}}^{N,N+2}$ interaction between these spaces. In the first stage and to show the necessity of using such mixing formalism, we applied each of pure U(5) and O(6) Hamiltonians separately. To this aim, we used the Hamiltonian of U(5) dynamical symmetry as [35, 36, 38, 39]

$$\hat{H}_{U(5)} = t_1 \hat{C}_{1\mathrm{U}(5)} + t_2 \hat{C}_{2\mathrm{U}(5)} + t_3 \hat{C}_{2\mathrm{O}(5)} + t_4 \hat{C}_{2\mathrm{O}(3)} \tag{6}$$

in the N-bosons space, where different states are described in terms of expectation values, $|N, n_d, \tau, L\rangle$. The Hamiltonian gives then:

$$E_{\mathrm{U}(5)} = t_1 n_d + t_2 n_d\,(n_d + 4) + t_3 \tau(\tau + 3) + t_4 L(L + 1)\,. \tag{7}$$

In the first step, we used this equation to reproduce all of the normal and intruder states. The constants are extracted in comparison with experimental data as $t_1 = 687.27$, $t_2 = -44.486$, $t_3 = 9.14$, and $t_4 = 9.41$ (all in keV). The predictions of U(5) symmetry for different levels of the ^{98}Mo nucleus are listed in Table 4.

The predictions of U(5) symmetry are in satisfactory agreement with their experimental counterparts for only normal states. Still, for intruder levels, the differences between theoretical predictions and empirical data are significant and the accuracy of these predictions is apparent for the levels of the ground band of energy. On the other hand, the lack of efficiency is apparent for such predictions of this pure U(5) symmetry in the excited energy levels. We can see disagreement for levels such as 0_2^+, 2_1^+, 2_2^+, 4_1^+, 4_2^+ that are classified as intruder levels. These results confirm the prediction of other authors and also our results for the quadrupole transition rates which suggested a mixing of at least two different symmetries for more exact description of energy levels in the ^{98}Mo nucleus. In this way and before using the mixed Hamiltonian, Eq. (5), we repeated the same procedure in the calculation of considered energy levels by using the prediction of U(5) symmetry for normal states and O(6) dynamical symmetry for intruder states, separately, to show possible advantages/disadvantages of this formalism, too. The most general form of Hamiltonian in the O(6) dynamical symmetry limit is defined as [35, 36, 38, 39]

$$\hat{H}_{\mathrm{O}(6)} = t'_1 \hat{C}_{2\mathrm{O}(6)} + t'_2 \hat{C}_{2\mathrm{O}(5)} + t'_3 \hat{C}_{2\mathrm{O}(3)}\,. \tag{8}$$

Table 4. Experimental values of different energy levels together with predictions of U(5) symmetry, Eq. (7). All energies are in keV.

Level	Experimental	U(5) symmetry
0_2^+	734.75	1196.6
2_1^+	787.26	717.5
2_2^+	1432.18	1344.4
4_1^+	1509.74	1476.1
2_3^+	1758.32	1754.4
0_3^+	1962.81	1825.9
3_1^+	2017.36	1938.8
0_4^+	2037.26	2037.3
2_4^+	2206.74	2349.6
4_2^+	2223.74	2014.1
2_5^+	2333.03	2185.1
4_3^+	2333.32	2481.3
6_1^+	2343.26	2221.0
4_4^+	2419.48	2316.8
5_1^+	2506.10	2575.4
6_2^+	2678.49	2688.3
8_1^+	2853.71	2970.5

We calculated the expectation values of this Hamiltonian in the $(N+2)$-bosons space, where different states are described in terms of expectation values of this Hamiltonian as $|N+2,\sigma,\tau,L\rangle$

$$E_{\mathrm{O(6)}} = t'_1\sigma(\sigma+4) + t'_2\tau(\tau+3) + t'_3 L(L+1)\,. \tag{9}$$

In Ref. [35], Lehman and Jolie, have considered σ as a constant coefficient as to ignore the effect of the Casimir operator of the O(6) dynamical limit. In this study, we used the standard formula of the O(6) dynamical symmetry limit as have been introduced in Ref. [20] but to follow the same idea of Ref. [35], σ is assumed as N, *e.g.* the possible maximum value. This value is constant for all states and essentially shows the same effect as an energy shift. Now, the parameters of Eq. (9) are extracted in comparison with experimental data in the MATLAB software via the least square technique, whose values are $t'_1 = 23.88$, $t'_2 = 36.50$, and $t'_3 = 19.62$ (all in keV). A comparison between theoretical predictions determined by U(5) and O(6) dynamical symmetries, respectively, are listed in Tables 4 and 5 and presented in figure 1.

Table 5. Experimental values of different energy levels together with predictions of pure O(6) symmetry. All energies are in keV.

Level	Experimental	O(6) symmetry
0_2^+	734.75	1421.3
2_1^+	787.26	1028.0
2_2^+	1432.18	1247.0
4_1^+	1509.74	1521.7
2_3^+	1758.32	1904.0
0_3^+	1962.81	—
3_1^+	2017.36	1656.7
0_4^+	2037.26	—
2_4^+	2206.74	2342.0
4_2^+	2223.74	1813.7
2_5^+	2333.03	—
4_3^+	2333.32	2178.7
6_1^+	2343.26	2245.3
4_4^+	2419.48	2616.7
5_1^+	2506.10	2374.9
6_2^+	2678.49	2610.3
8_1^+	2853.71	3189.9

Predictions of O(6) dynamical symmetry improve theoretical results for such levels which are known as intruder levels, 0_2^+, 2_1^+, 2_2^+, 4_1^+, 4_2^+, in comparison with U(5) dynamical symmetry. A comparison between Table 5 and Table 4 shows apparent improvement in the theoretical results for the excited states in the ^{98}Mo nucleus, but for the levels of the ground-energy band, our previous summary about the spherical nature of such levels has been verified. We have compared our results by using pure U(5) and O(6) with the previous studies on the ^{98}Mo nucleus and especially the work of Sambataro and Molnár in Ref. [1]. Due to different experimental data which have been used by them and in this study, it is impossible to compare their predictions for different energy levels separately but our results describe the energy levels and quadrupole transitions with high accuracy and reduce the variation. Moreover, they do not consider all of the reported intruder levels and related quadrupole transitions which have been included in our analyses and, therefore, a general comparison is not available. To reach a complete and exact description of all energy levels, we considered both U(5) and O(6) dynamical symmetries together in the mixing term, Eq. (5). The mixing

Hamiltonian considered in this study, similar to what have been done in Refs. [35, 36] is

$$\begin{aligned}\hat{H} &= \hat{P}_N^{\dagger}\hat{H}_{U(5)}\hat{P}_N + \hat{P}_{N+2}^{\dagger}\hat{H}_{\mathrm{O}(6)}\hat{P}_{N+2}^{\dagger} + \hat{V}_{\mathrm{mix}}^{N,N+2}\,, \\ \hat{V}_{\mathrm{mix}}^{N,N+2} &= \alpha\left[s^{\dagger}\times s^{\dagger}+s\times s\right]^{0} + \beta\left[d^{\dagger}\times d^{\dagger}+d\times d\right]^{0} \\ \underline{\text{and is equal to}} &= \alpha\left(s^{\dagger}s^{\dagger}+d^{\dagger}\,d^{\dagger}\right)\,,\end{aligned}$$

where α is the constant that describes the mixing effect. The expectation values of different terms of this mixing Hamiltonian in both the N- and $(N+2)$-bosons spaces, respectively U(5) and O(6) dynamical symmetries, are determined as [35, 36, 47]

$$\left\langle [N+2],\sigma,\tau,L\left|s^{\dagger}\,s^{\dagger}\right|[N],n_d,\tau\,L\right\rangle = \sqrt{(N-n_d+1)(N-n_d+2)}B_{n_d}^{N+2,\sigma,\tau}\,, \tag{10}$$

$$\left\langle [N+2],\sigma,\tau,L\left|d^{\dagger}\,d^{\dagger}\right|[N],n_d,\tau\,L\right\rangle = \sqrt{(n_d-\tau+2)(n_d+\tau+5)}B_{n_d+2}^{N+2,\sigma,\tau}\,. \tag{11}$$

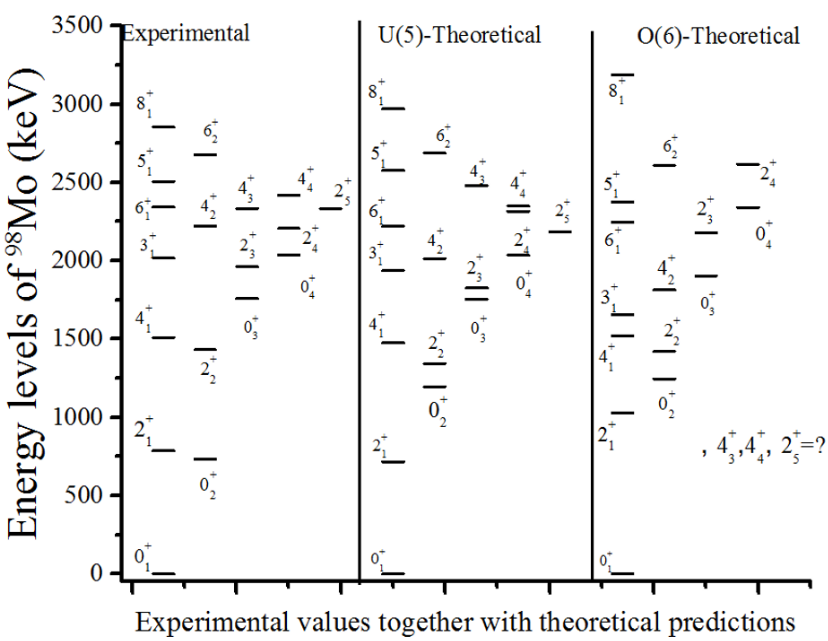

Fig. 1. Energy levels of the ^{98}Mo nucleus. The experimental values are taken from Ref. [40]. U(5)-theoretical and O(6)-theoretical are the results presented in Tables 4 and 5, respectively.

In this paper, we consider each of the above equations separately. The expansion coefficients for O(6) states in the U(5) basis $B_{n_d}^{N+2,\sigma v}$ are calculated for $\sigma = \sigma_{\max}$, the condition which in its final form is given as [47]

$$B_{n_d}^{\sigma\sigma\tau} = \sqrt{\frac{(\sigma+\tau+3)!(\sigma-\tau)!\left(\frac{1}{2}\left(n_d+\tau\right)+1\right)!}{2^{\sigma-\tau}(\sigma+1)!\left(\frac{1}{2}\left(n_d-\tau\right)\right)!\left(\sigma-n_d\right)!\left(n_d+\tau+3\right)!}}\,. \tag{12}$$

On the other hand, to determine the constant of mixing Hamiltonian, α, we use the $B(\mathrm{E2})$ values and the coefficient α_{ij} which is presented in Table 2. By using the relation between different a_{ij}s and the expectation values of pure U(5) and O(6) symmetries, respectively H_{11} and H_{22}, and the mixing term, $V_{\rm mix}^{N,N+2} = H_{21}$ we obtain as

$$\begin{aligned} a_{21} &= \frac{E_{\rm exp}-\langle H_{11}\rangle}{\sqrt{\left(E_{\rm exp}-\langle H_{11}\rangle\right)^2+\langle H_{12}\rangle^2}}\,, \\ a_{11} &= \frac{1}{\sqrt{\left[\left(\langle H_{11}\rangle-\langle H_{22}\rangle\right)^2+\left(\langle H_{11}\rangle-\langle H_{22}\rangle\right)\sqrt{\left(\langle H_{11}\rangle-\langle H_{22}\rangle\right)^2+4\langle H_{12}\rangle^2}\right]/2\langle H_{12}\rangle^2+2}}\,, \end{aligned}$$

which finally reduces to the following relation for the constant parameter of mixing Hamiltonian:

$$\alpha = \sqrt{\frac{E_{\rm exp}-\langle H_{11}\rangle - a_{21}^2\left[E_{\rm exp}-\langle H_{11}\rangle\right]^2}{a_{21}^2\langle H_{21}\rangle^2}}\,.$$

Now, by using the expectation value of mixing Hamiltonian, Eqs. (10)–(12), for each of the considered level in the ^{98}Mo nucleus, the prediction of total Hamiltonian, Eq. (5), which includes both U(5), O(6) dynamical symmetries together mixing term is yielded as

$$\begin{aligned} E_{\rm tot} &= t_1 n_d + t_2 n_d\left(n_d+4\right) + t_3\tau(\tau+3) + t_4 L(L+1) \\ &\quad + t_1'\sigma(\sigma+4) + t_2'\tau(\tau+3) + t_3' L(L+1) \\ &\quad + \alpha\left(\sqrt{\left(N-n_d+1\right)\left(N-n_d+2\right)} + \sqrt{\left(n_d-\tau+2\right)\left(n_d+\tau+5\right)}\right) \\ &\quad \times\sqrt{\frac{(\sigma+\tau+3)!(\sigma-\tau)!\left(\frac{1}{2}\left(n_d+\tau\right)+1\right)!}{2^{\sigma-\tau}(\sigma+1)!\left(\frac{1}{2}\left(n_d-\tau\right)\right)!\left(\sigma-n_d\right)!\left(n_d+\tau+3\right)!}}\,. \end{aligned} \tag{13}$$

In Eq. (13), n_d is considered as the quantum number of states in the framework of U(5) symmetry. Similar to what has been done for each of the pure symmetry, the constants of the energy equation are extracted in comparison with experimental data which are $t'_1 = 598.39$, $t'_2 = 84.864$, and $t'_3 = 2.53$ (all in keV), $t_1 = 1472.85$, $t_2 = -266.54$, $t_3 = 11.27$, and $t_4 = 17.34$ (all in keV), and $\alpha = 0.13$.

A comparison between the experimental energy levels of the ^{98}Mo nucleus together with theoretical predictions which are determined by mixing of symmetries formalism are listed in Table 6 and presented in figure 2.

Table 6. Predictions of total Hamiltonian, Eq. (13), together with experimental values of different energy levels and the α values which describe the effect of mixing Hamiltonian in different levels. The symbol "i" stands for intruder states. All energies are in keV.

Level	Experimental	Total Hamiltonian
0^+_{2i}	734.75	598.40
2^+_{1i}	787.26	952.99
2^+_{2i}	1432.18	1462.2
4^+_{1i}	1509.74	1497.6
2^+_3	1758.32	1355.51
0^+_3	1962.81	1879.5
3^+_1	2017.36	2430.7
0^+_4	2037.26	2222.6
2^+_4	2206.74	2096.3
4^+_{2i}	2223.74	2176.5
2^+_5	2333.03	1843.5
4^+_3	2333.32	2339.1
6^+_1	2343.26	2950.9
4^+_4	2419.48	2569.4
5^+_1	2506.10	2462.6
6^+_2	2678.49	2670.7
8^+_1	2853.71	3190.9

We can summarize the results of all tables and figures as follows:

(i) The total Hamiltonian describes the intruder energy levels with high accuracy in comparison with two pure U(5) and O(6) Hamiltonians. This means that such a combination of different dynamical symmetries together with mixing potential can be considered as the most exact formalism for studying such nuclei which have intruder states.

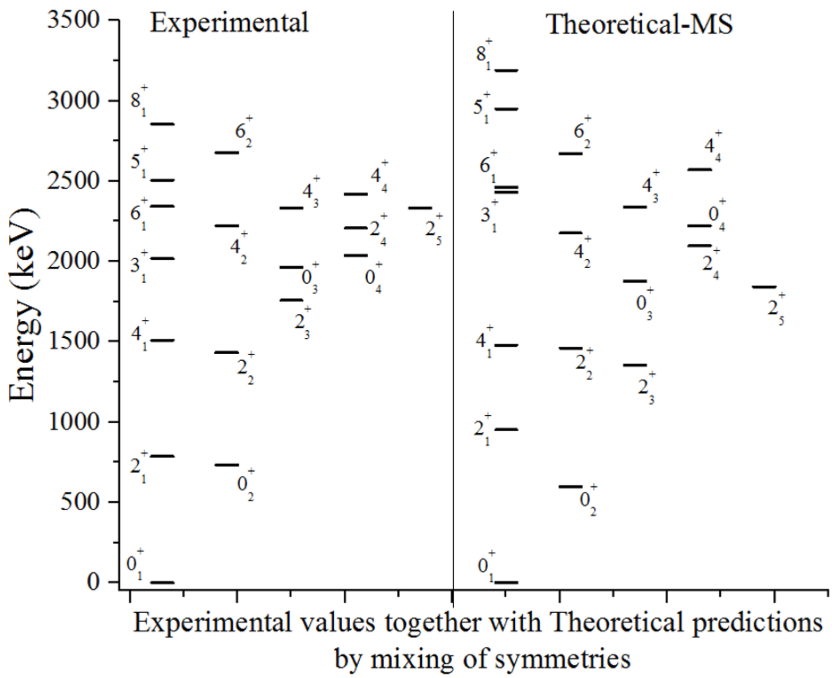

Fig. 2. Energy levels of the ^{98}Mo nucleus. The experimental values are taken from Ref. [40]. Theoretical-MS are the predictions of mixing formalism, Eq. (13).

(ii) A detailed comparison between the theoretical predictions in Tables 4, 5, and 6 shows that the pure U(5) Hamiltonian suggests the most exact predictions for the energy levels of the ground band in comparison to O(6) dynamical symmetry and the total Hamiltonian. For the excited energy levels in different bands, more accuracy is yielded by the predictions of O(6) dynamical symmetry.

(iii) Other exciting achievements shown in Table 6, are the values that describe the effect of mixing potential in different states. The minimum values are yielded for the energy levels of the ground band and the maximum values are suggested for intruder levels. This result confirms our idea about the pure spherical nature of the ground band and the necessity of using such a mixing term for the description of intruder levels. Also, we observed a straightforward relation between the spin of different normal states and α values, which suggests the maximum mixing effect for the $J = 6^+$ normal level. In the subsequent studies, we would consider such mixing Hamiltonians which contain high-rank tensors to analyse the possible relation between the mixing effect and the spin of considered states in detail and make an overall conclu-

sion. We have compared our results with the predictions of Fortune in Ref. [33] and Jalili Majarshin *et al.* in Ref. [34] which have considered this nucleus in the framework of a band-mixing. Our results for intruder states and quadrupole transition rates which originated from intruder levels, show better agreement with experimental counterparts. On the other hand, for excited energy levels in the $3^{\rm rd}$ and $4^{\rm th}$ bands of energies, their results are more exact due to their technique which mixed different levels of these bands without our considering requirements on the combination of states from the same type. In the next investigation, we would apply their methods and requirements to consider the possible effects of bands mixing in order to decrease variations between theoretical predictions and experimental data.

3. Summary and conclusions

This investigation presents detailed analyses of the quadrupole transition probabilities and energy levels of the ^{98}Mo nucleus. We considered all reported intruder levels for this nucleus and also tried a method based on the configuration mixing of N- and $(N+2)$-boson spaces in the description of transition rates. We expanded the wavefunctions of both normal and intruder levels in these two different spaces. We extracted the weight of each spaces via the theoretical calculation of transition rates and comparison with experimental counterparts. Apparent improvement in the exactness of theoretical predictions by using such a process in comparison with using only N or $(N+2)$ configurations, approves the necessity of using mixing formalisms in both wavefunctions and Hamiltonians. Also, we calculated different normal and intruder energy levels by using *(i)* only U(5), *(ii)* only O(6) dynamical symmetries, and *(iii)* total Hamiltonian containing both symmetries and mixing potential. We analyzed the advantages/disadvantages of these three Hamiltonians and concluded that the total Hamiltonian is the best choice for the description of intruder levels in the ^{98}Mo nucleus. We would investigate the possible relations between the spin of different intruder states and the weight of N- and $(N+2)$-boson spaces in the expansion of wavefunctions and the effect of mixing Hamiltonian in the following studies.

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