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Description of Shape Coexistence and Mixed-Symmetry States in ^{96}Mo Using IBM-2 *

Cheng-Fu Mu(穆成富)**, Da-Li Zhang(张大立)**

Department of Physics, Huzhou University, Huzhou 313000

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We investigate the level structure and E2, M1 electromagnetic transition properties in an even–even ^{96}Mo nucleus within the framework of the proton–neutron interacting boson model (IBM-2). The calculated results of the IBM-2 can reproduce the recent new experimental data on ^{96}Mo both qualitatively and quantitatively. It is found that both shape coexistence and mixed-symmetry states in ^{96}Mo can be simultaneously described very well with the IBM-2 by taking into account that the relative energy of d neutron bosons is different from that of proton bosons.

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Since the discovery of the atomic nucleus, how protons and neutrons are bound to atomic nuclei has attracted the interest of several generations of physicists.[1–5] The structures of medium mass nuclei are a recent hot research topic in nuclear structure physics due to their rich characteristics.[6–10] As typical medium mass nuclei, molybdenum isotopes have been investigated theoretically and experimentally.[11–17] Mo isotopes can be considered as a good probe for studying the mixed-symmetry (MS) states, which mainly occur in ^{94}Mo[11], and shape coexistence, which mainly occurs in ^{98}Mo.[15] Recently, the low-spin states of ^{96}Mo have been investigated in $\gamma\gamma$ angular correlation in-beam experiments.[12] From their experimental results, Thomas *et al.* found that there are not only MS states but also some characters of shape coexistence in ^{96}Mo. Many theoretical investigations have been carried out of even–even Mo isotopes, e.g., the mapped interacting boson model based on the Gogny energy density functional.[18] The properties of MS states in Mo isotopes were studied in Refs. [19,20] using the proton–neutron interacting boson model (IBM-2). Sambataro *et al.*[21] discussed the configuration-mixing effect in Mo isotopes for the first time, which can give a basic description of the low-lying structure in ^{96}Mo, whereas they only discussed some $E2$ transitions due to the limited experimental data available at that time and did not calculate the $M1$ transition. However, it was found that the IBM-2 can also explain the experimental data of nuclei without configuration mixing by taking into account the fact that the relative energy of d neutron bosons is different from that of proton bosons.[22] In recent years, the above method has been applied to discuss the shape coexistence close to $N = 50$ in the neutron-rich isotopes ^{80}Ge[23] and in the ^{100}Mo nucleus.[24] The properties of MS states in the ^{94}Mo nucleus have also been systematically investigated.[25] The above theoretical works concentrate either on shape coexistence or on MS states. The goal of this study is to simultaneously describe the shape coexistence and the MS states in ^{96}Mo through the IBM-2 by considering the relative energy of d neutron bosons to be different from that of proton bosons.

The microscopic foundation of the interacting boson model (IBM) is based on collective fermion pairs of valence nucleons.[26] The properties of low-lying states of even–even nuclei can be approximately described by a system of interacting pairs of valence nucleons with angular momentum $l = 0$ (s-boson) and $l = 2$ (d-boson). The IBM-2 is an extended version of the original IBM, which differentiates neutron bosons from proton bosons. The eigenvectors of the neutron and proton entities can couple symmetrically or antisymmetrically. The first case containing fully symmetric (FS) states is equivalent to IBM-1 states. The latter case with antisymmetric coupling of the neutron and proton is the well-known MS state.[28] The general form of the IBM-2 Hamiltonian applied in our calculation is as follows:[26]

$$\begin{aligned}\hat{H} =& \varepsilon_\pi \hat{n}_{d\pi} + \varepsilon_\nu \hat{n}_{d\nu} + \kappa_{\pi\nu}\hat{Q}_\pi \cdot \hat{Q}_\nu \\ &+ \kappa(\hat{Q}_\pi \cdot \hat{Q}_\pi + \hat{Q}_\nu \cdot \hat{Q}_\nu) \\ &+ \omega_{\pi\nu}\hat{L}_\pi \cdot \hat{L}_\nu + \omega_{\nu\nu}\hat{L}_\nu \cdot \hat{L}_\nu + \hat{M}_{\pi\nu}, \end{aligned} \quad (1)$$

where $\varepsilon_{d\rho}$ is the excitation energy of the d-boson (for neutron bosons ($\rho = \nu$) and proton bosons ($\rho = \pi$), respectively), and $\hat{n}_{d\rho} = d^\dagger_\rho \cdot \tilde{d}_\rho$ represents the number operator of the d-boson. The explicit expression of the quadrupole operator $\hat{Q}_\rho$ is given by the usual form $\hat{Q}_\rho = (s^\dagger_\rho \tilde{d}_\rho + d^\dagger_\rho s_\rho)^{(2)} + \chi_\rho (d^\dagger_\rho \tilde{d}_\rho)^{(2)}$. The parameter $\kappa_{\pi\nu}$ is the strength of the quadrupole-quadrupole interaction between neutron–boson and proton–boson. In the fourth term, $\hat{Q}_\pi \cdot \hat{Q}_\pi$ and $\hat{Q}_\nu \cdot \hat{Q}_\nu$ stand for

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**Corresponding author. Email: zdl@zjhu.edu.cn; muchengfu@zjhu.edu.cn

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the quadruple interactions between like-bosons with the strength parameter κ. The fifth term denotes the dipole proton–neutron and the sixth terms represents neutron–neutron interactions, where L_ρ is the angular momentum operator having the form $\hat{L_\rho} = \sqrt{10}[d^\dagger_\rho \cdot \tilde{d_\rho}]^{(1)}$. The explicit form of the Majorana operator in the last term is $\hat{M}_{\pi\nu} = \lambda_2(s^\dagger_\pi d^\dagger_\nu - s^\dagger_\nu d^\dagger_\pi)^{(2)} \cdot (s_\pi \tilde{d}_\nu - s_\nu \tilde{d}_\pi)^{(2)} + \sum_{k=1,3} \lambda_k (d^\dagger_\pi d^\dagger_\nu)^{(k)} \cdot (\tilde{d}_\pi \tilde{d}_\nu)^{(k)}$, where λ_k $(k = 1, 2, 3)$ are the strength parameters.[22] The Majorana interaction can separate the MS states from FS states. The $E2$ transition operator is expressed as[26,29]

$$\hat{T}^{(E2)} = e_\pi \hat{Q}_\pi + e_\nu \hat{Q}_\nu, \tag{2}$$

where the operator $\hat{Q}_\rho$ takes the same form as in Eq. (1). For consistency, we also choose the same χ_ρ contained in the operator $\hat{Q}_\rho$ as in the Hamiltonian, and e_ρ is the effective quadrupole charge of interacting bosons. The $M1$ transition operator is defined as

$$\hat{T}^{(M1)} = \sqrt{3/4\pi}(g_\nu \hat{L_\nu} + g_\pi \hat{L_\pi}), \tag{3}$$

where g_ρ is the gyromagnetic ratio of interaction bosons. We refer to Refs. [26,27] for more discussion in detail on the Hamiltonian and the transition operators of the IBM-2. The numerical calculation of energy spectrum was accomplished by using the computer code NPBOS.[30]

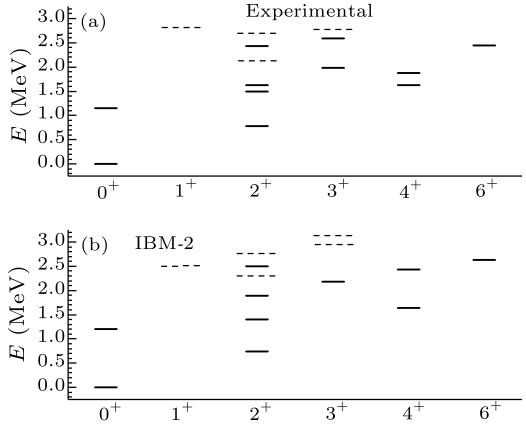

Fig. 1. The experimental levels (upper panel) are compared with the calculated results (lower panel) for ^{96}Mo. The MS states having an F-spin quantum number of $F_{\max} - 1$ predicted by the IBM-2 are marked with the dashed lines. The experimental results are taken from Refs. [12,13].

In this study, we take the doubly closed-shell $^{100}_{50}\mathrm{Sn}_{50}$ as the inert core. For a $^{96}_{42}\mathrm{Mo}_{54}$ nucleus, eight valence protons are the hole-like type, whereas four valence neutrons are the particle-like type, the different types of valence neutrons and protons are inclined to drive the nucleus to exhibit opposite intrinsic quadrupole deformation. These types of nuclei correspond to $SU^*(3)$ or $O(6)$ or an intermediate case.[31] As discussed in Ref. [22], the interaction between the valence neutrons and protons occupied in the different orbitals is an important deformation driving force in the Mo isotopes. We take $\varepsilon_\nu \neq \varepsilon_\pi$ to reflect this effect of different orbitals. According to the above consideration, we perform a parameter scanning procedure to reproduce the energy spectrum and the electromagnetic properties of the ^{96}Mo nucleus, especially for MS states. The IBM-2 parameters adopted in our calculation are expressed as follows: $\varepsilon_\nu = 0.9\,\mathrm{MeV}$, $\varepsilon_\pi = 0.7\,\mathrm{MeV}$, $\kappa_{\pi\nu} = -0.05\,\mathrm{MeV}$, $\kappa = -0.010\,\mathrm{MeV}$, $\chi_\pi = -\chi_\nu = 0.900$, $\omega_{\pi\nu} = 0.175\,\mathrm{MeV}$, $\omega_{\nu\nu} = 0.11\,\mathrm{MeV}$, $\lambda_1 = 0.6\,\mathrm{MeV}$, $\lambda_2 = 0.24\,\mathrm{MeV}$, and $\lambda_3 = 0.25\,\mathrm{MeV}$.

Figure 1 shows a comparison of the experimental energy levels and the calculated results, where the dashed lines represent the MS states. The correspondence between theoretical and experimental levels appears to be satisfactory. For ^{96}Mo, the experimental value of characteristic ratio $R_{4/2} = E(4^+_1)/E(2^+_1)$ is 2.09, and the calculated result is 2.23. In the $\mathrm{U}_{\pi\nu}(5)$ dynamical limit of the IBM-2, the characteristic ratio $R_{4/2}$ has the limit of 2.00, which corresponds to spherical nuclei. The characteristic ratio $R_{4/2}$ is 2.50 for the $O(6)$ symmetry. For an axial rotor ($SU(3)$ symmetry), the ratio $R_{4/2} = 3.33$.[32] Both the experimental characteristic ratio $R_{4/2}$ and the calculated $R_{4/2}$ indicate that ^{96}Mo is a nearly spherical nucleus with a weak deformation. However, the ratio $R_{4/2}$ is not the only criterion for determining the shapes of nuclei. We will discuss the other criteria from the electromagnetic transitions further.

Table 1. The calculated R ratio and the corresponding F-spin values. The experimental level energies (taken from Refs. [12,13]) compared with the results from the IBM-2 calculations are shown as well.

	E_{Exp} (MeV)	E_{IBM} (MeV)	F	R
0^+_1	0.000	0.000	2	0.998
0^+_2	1.148	1.200	2	0.996
1^+_1	2.806	2.513	1	0.498
2^+_1	0.778	0.736	2	0.959
2^+_2	1.498	1.403	2	0.976
2^+_3	1.626	1.888	2	0.879
2^+_4	2.096	2.253	1	0.527
2^+_5	2.426	2.497	2	0.831
2^+_6	2.700	2.752	1	0.503
3^+_1	1.978	2.177	2	0.897
3^+_2	2.594	2.972	1	0.488
3^+_3	2.736	3.124	1	0.423
4^+_1	1.628	1.644	2	0.833
4^+_2	1.870	2.426	2	0.828
6^+_1	2.440	2.629	2	0.614

In the IBM-2, Arima *et al.* introduced a new quantum number F-spin to distinguish the MS states from the FS states,[33] which is the correspondence of nucleon isospin and characterizes the neutron–proton symmetry. The FS states have a maximum of F-spin $F_{\max} = (N_\pi + N_\nu)/2$ and a minimum $F_{\min} = |N_\pi - N_\nu|/2$. The MS states are characterized by $F = F_{\max} - 1, F_{\max} - 2, \ldots, F_{\min}$. To qualitatively

describe the F-spin nature of a state $|s\rangle$, one can introduce an important quantity

$$R = \langle s \parallel F^2 \parallel s\rangle F_{\max}(F_{\max}+1), \qquad (4)$$

as a measure of the mixing F-spin states.[19] Generally, if the ratio R is larger than 90%, the corresponding states can be considered as FS states. If the ratio $R < 60\%$, one can think that the MS components dominate the state. The explicit calculated level energies are listed in Table 1. The 2_4^+ state is the lowest-lying MS state, and the calculated energy is 2.253 MeV, slightly higher than the corresponding experimental value of 2.096 MeV. As can be seen from Table 1, the R ratios are less than 60% for the 2_4^+, 2_6^+, 3_3^+ and 1_1^+ states, and all of them are the MS states, which have been identified experimentally as the MS excitations from their characteristics of electromagnetic transition.[13] We will discuss the transition properties in the following. The calculated R value can describe the corresponding MS components very well. It is noteworthy that the predicted $R = 48.8$ for the 3_2^+ state implies that this state contains more MS components, but experimental data on the absolute $M1$ transitions of 3_2^+ state are currently unavailable, and new experimental data are needed to determine its MS properties for future experiments.

The effective boson charges in the $T(E2)$ operator are determined by normalizing the calculated $B(E2)$ values to the corresponding experimental data. In this study, we take $e_\nu = 0$ for simplicity and only fit the parameter e_π. Fitting to the experimental result of $B(E2, 2_1^+ \to 0_1^+) = 20.7(4)$ W.u. for ^{96}Mo nucleus, we obtain $e_\pi = 0.111eb$. For the magnetic transitions, we set $g_\nu = 0$ and vary g_π to reproduce $B(M1, 2_4^+ \to 2_1^+) = 0.17(2)\mu_N^2$. The obtained g_π is $1.15\mu_N$, which is very close to the naked value of $1.0\mu_N$. In Table 2, we compare the calculated electromagnetic transition strengths $B(E2)$ and $B(M1)$ for ^{96}Mo with the available experimental data. From Table 2, one can see that most of the calculated $B(E2)$ transition probabilities can well reproduce the experimental data.

Another observable related with shape character is $B(E2, 4_1^+ \to 2_1^+)$, which is the transition between the pure FS states and represents strongly collective $E2$ transition. The calculated value of $B(E2, 4_1^+ \to 2_1^+)$ is 31.02 W.u., the experimental value is 41(7) W.u., and the difference between them is acceptable. The calculated ratio $B_{4/2} = B(E2, 4_1^+ \to 2_1^+)/B(E2, 2_1^+ \to 0_1^+) = 1.52$, which is slightly lower than the $U(5)$ limit of 2 for a large N limit, the experimental value of $B_{4/2}$ is 1.98. The ratio $B_{4/2}$ of Ref. [12] is 1.25. In the IBM-1 space with finite number of bosons $N = 3$, $B_{4/2}$ ratio equals 4/3 for the $U(5)$ limit. Therefore, the $E2$ transition strength of ^{96}Mo also deviates from the $U(5)$ limit.

Table 2. Experimental and calculated $E2$ and $M1$ transition strengths for the ^{96}Mo nucleus. The $E2$ transition strengths are given in units of W.u., and the $M1$ transition strengths are given in units of μ_N^2. The experimental data are taken from Refs. [12,13].

$J_i^\pi \to J_f^\pi$	B(E2)		B(M1)	
	Experiment	IBM-2	Experiment	IBM-2
$0_2^+ \to 2_1^+$	51(7)	18.02		
$1_1^+ \to 0_1^+$			$0.040^{+0.006}_{-0.005}$	0.035
$2_1^+ \to 0_1^+$	20.7(4)	20.47		
$2_2^+ \to 0_1^+$	$1.0^{+0.2}_{-0.1}$	0.0		
$2_2^+ \to 0_2^+$	< 93.2	2.04		
$2_2^+ \to 2_1^+$	13.9(28)	24.46	0.082^{+8}_{-7}	0.001
$2_3^+ \to 2_1^+$			< 0.067	0.022
$2_4^+ \to 0_1^+$	0.081(11)	1.16		
$2_4^+ \to 0_2^+$	5.0^{+22}_{-17}	1.58		
$2_4^+ \to 2_1^+$	0	0.22	0.17(2)	0.168
$2_4^+ \to 2_2^+$	0	1.58	<0.08	0.052
$2_5^+ \to 2_1^+$	2.9^{+8}_{-9}	0.15	0.0056^{+19}_{-21}	0.001
$2_5^+ \to 2_2^+$	6.1^{+11}_{-14}	0.19	0.0003(3)	0.020
$2_6^+ \to 2_1^+$	$2.0^{+0.6}_{-0.5}$	3.05	0.007(2)	0.019
$2_6^+ \to 2_2^+$	6.1^{+11}_{-14}	0.28	$0.10^{+0.02}_{-0.01}$	0.083
$3_3^+ \to 2_1^+$	$0.0016^{+0.0003}_{-0.0002}$	0.098	$0.028^{+0.003}_{-0.002}$	0.019
$3_3^+ \to 2_2^+$	2.3(4)	1.71	0.06(1)	0.042
$4_1^+ \to 2_1^+$	41(7)	31.02		
$4_2^+ \to 2_1^+$	2(1)	0.10		
$4_2^+ \to 2_2^+$	26(11)	14.39		
$4_2^+ \to 2_3^+$	< 32	5.48		
$4_2^+ \to 4_1^+$	0.2(1)	8.58	$0.015^{+0.008}_{-0.006}$	0.013

The computed $E2$ transition strength of $B(E2, 2_2^+ \to 2_1^+) = 24.46$ W.u. is in agreement with the experimental data 13.9(28) W.u. within the experimental uncertainty. To discuss the shape character, we introduce the other characteristic quantity $B_{2/2} = B(E2, 2_2^+ \to 2_1^+)/B(E2, 2_1^+ \to 0_1^+)$. The values of $B_{2/2}$ for a large boson number are 2 for the $U(5)$ limit and 10/7 for the $O(6)$ limit.[34] However, the ex-

perimental data have some uncertainty for ^{96}Mo. The data from Ref. [12] gives $B_{2/2} = 0.67$, while in Ref. [13] the result was $B_{2/2} = 2.85$, and our calculation gives $B_{2/2} = 1.19$. Both the experimental and calculated values of $B_{2/2}$ imply that ^{96}Mo nucleus is located in the transitional region between the $O(6)$ and $U(5)$ dynamical limits. For the interband $E2$ transition, the calculated $B(E2, 0_2^+ \to 2_1^+) = 18.02$ W.u. is a better theoretical result compared with other theoretical calculations, although it is one third of the corresponding experimental data. The calculated intraband $E2$ decay strength from the 4_2^+ state to the 2_2^+ state of the $B(E2, 4_2^+ \to 2_2^+)$ value is 14.39 W.u., and this predicted result is slightly smaller than the experimental value 26(11) W.u. The calculated $E2$ transition strength from the 4_2^+ state to the 4_1^+ state is $B(E2, 4_2^+ \to 4_1^+) = 8.58$ W.u., which belongs to the interband transition, and the corresponding experimental data is too small and has a great deal of uncertainty. In Ref. [13] the authors gave the value $B(E2, 4_2^+ \to 4_1^+) = 330^{+178}_{-132}$ W.u. The previous experimental data of $B(E2, 4_2^+ \to 4_1^+) = 12^{+5}_{-4}$ W.u. agrees with our calculation.[35] Further experimental work is needed to reduce the uncertainty.

For magnetic transitions, the comparison between the calculated $M1$ transition strengths and the available experimental data for ^{96}Mo are also shown in Table 2. For the $M1$ decay from the 1_1^+ state to the 0_1^+ state, the calculated transition strength of $B(M1, 1_1^+ \to 0_1^+) = 0.035\ \mu_N^2$ agrees with the experimental value $0.040^{+0.006}_{-0.005}\mu_N^2$ within the experimental uncertainty. The 1_1^+ state is the so-called scissors mode, which is a two-phonon MS state.[36] The experimental identification of MS excitation is characterized by three aspects.[37] The first is strong $M1$ transitions between the FS and MS states with the transition matrix element of about $1\mu_N$. The second is weakly collective $E2$ transitions between the MS and FS states, which is a few percent of $B(E2, 2_1^+ \to 0_1^+)$. The third criterion is strongly collective $E2$ transitions between MS states, with typical strength for collective $E2$ transitions between FS states. From Table 2, in view of the weakly collective $E2$ transitions of $B(E2, 2_4^+ \to 2_1^+)$ and the enhanced $M1$ transition strength of $B(M1, 2_4^+ \to 2_1^+)$, one can interpret the 2_4^+ state as the MS state. Absolute electromagnetic decay strengths provide a solid basis for the identification of MS states.[38] From the above discussion on the transition properties of the 2_4^+ state, one can identify the 2_4^+ state as a one-phonon MS state $2^+_{1,\mathrm{ms}}$ in ^{96}Mo. In the meantime, the $2_4^+ \to 2_2^+$ $M1$ transition strength is very small, the experimental value is $0.08\mu_N^2$, the calculated value is $0.052\mu_N^2$, and both the results imply that $M1$ transition takes place between two states with different phonon numbers. Therefore, the 2_2^+ state is a two-phonon FS state, which agrees with the predicted value 0.976 of R ratio. For deformed rotational nuclei, the $M1$ transition of $B(M1, 1_1^+ \to 0_1^+)$ dominates the MS transition.[13] However for ^{96}Mo, $B(M1, 2_4^+ \to 2_1^+)$ is larger than $B(M1, 1_1^+ \to 0_1^+)$. This means that ^{96}Mo belongs to one of the dynamical limits: either γ-soft or vibrational nucleus.

Table 2 lists the calculated $B(M1, 3_3^+ \to 2_2^+)$ and $B(M1, 2_6^+ \to 2_2^+)$, which agree with the experimental data in the same order of magnitude. In Ref. [36], Otsuka discussed the $M1$ transitions between low-lying collective states using the IBM-2. In the $O(6)$ limit, the $4_2^+ \to 4_1^+$ $M1$ transition is forbidden because they are totally symmetric states. However, the experimental value is $B(M1, 4_2^+ \to 4_1^+) = 0.015^{+0.008}_{-0.006}\mu_N^2$, the calculated value is $0.013\mu_N^2$. The reason can be explained such that the $O(6)$ limit can be reached only under the condition $\chi_\pi = \chi_\nu = 0$. Although the Hamiltonian (1) with $\chi_\pi = -\chi_\nu \neq 0$ can bring about an energy structure that is almost indistinguishable from the $\chi_\pi = \chi_\nu = 0$ case, the difference between them is not negligible, and $\chi_\pi = -\chi_\nu \neq 0$ results in more MS components into low-lying states. Therefore, there exists the sizeable $B(M1, 4_2^+ \to 4_1^+)$. The nonzero $B(M1, 4_2^+ \to 4_1^+)$ indicates that the ^{96}Mo nucleus has the deviation from the $O(6)$ structure.

In summary, we have investigated the level structures and electromagnetic transition properties in ^{96}Mo using the IBM-2 by considering $\varepsilon_\nu \neq \varepsilon_\pi$. The calculated excitation energies for almost all of the low-lying states can reproduce the recent new experimental data. The IBM-2 calculations for the 2_4^+, 2_6^+, 3_3^+ and 1_1^+ MS states are in good agreement with the corresponding experiment data. The calculations also imply that ^{96}Mo is a weakly deformed transitional nucleus and the characteristics of $U(5)$ and $O(6)$ coexist in ^{96}Mo. It is shown that shape coexistence and the MS states in ^{96}Mo can be simultaneously well described using the IBM-2 by considering the relative energy of d neutron bosons to be different from that of proton bosons.

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