Theoretical study of rotational and multi-phonon γ-vibrational structure in neutron-rich Zr, Mo, and Ru nuclei

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Abstract. A theoretical study for some neutron-rich nuclei in the A = 100−110 mass region is carried out by using the angular-momentum-projection technique implemented in the projected shell model. By assuming an axial symmetry in the deformed basis, the influence of the high-j h₁₁/₂ neutron orbital and the g₉/₂ proton orbital on the structure of strongly-deformed, neutron-rich even-even and odd-mass Zr isotopes is investigated. For even-even isotopes, the structure of multi-quasiparticle bands in ¹⁰²Zr is taken as an example and properties along the yrast line are analyzed in detail. For odd-neutron isotopes, the discussion is focused on the excited single-particle configurations. We also perform calculations by employing a triaxially-deformed basis to study multi-phonon γ vibrational bands in ¹¹⁰Mo and to interpret the anharmonicity observed in the one- and two-phonon γ vibrational bands in ¹¹⁴Ru.

1. Introduction

The study of neutron-rich nuclei is one of the current frontier topics in nuclear physics. An important issue is to understand those emerging subshell gaps, which cause substantial modifications of the intrinsic shell structure in nuclei with a neutron excess [1]. While information on collective excitations in low-spin states of neutron-rich nuclei is useful, a more comprehensive knowledge of these exotic nuclei requires the study of higher-spin states in which, owing to rotation alignment, quasi-particle (qp) configurations are dominant. For an yrast band consisting of the lowest states for each angular momentum, the aligning particles carry valuable information on the deformed single-particle orbitals. Therefore, investigations of high-spin spectra can yield knowledge of the intrinsic shell structure of single-particle levels.

Moreover, the investigation on the neutron-rich structure is crucially related to elucidating questions on nucleosynthesis in stars [2]. Shell model β-decay half-lives and neutron emission probabilities in the rapid neutron-capture process (r process) of nucleosynthesis have been found to differ significantly from those calculated by the traditional methods, thus calling for extensive applications of quantitative shell models in nuclear astrophysics [3].

Neutron-rich nuclei in the mass A = 100 − 110 region exhibit many interesting structural phenomena. Research in this mass region started more than four decades ago when Cheifetz
et al. [4] observed a sudden onset of deformation in Zr isotopes, and thereby discovered a new region of nuclei with large, stable deformation. This experimental finding was in line with theoretical predictions [5, 6]. For this mass region, the valence nucleons begin to fill the new region of nuclei with large, stable deformation. This experimental finding was in line with et al. [4]

In such an experiment, neutron-rich Zr and Mo isotopes were populated as fission fragments produced by the $^{238}$U$(\alpha, \gamma)$ fusion-fission reaction [12]. With these kinds of experiments, level schemes in this neutron-rich mass region have been largely expanded in the past five years or so. To mention some recent data to be discussed in the present article, information on the $\gamma/2[404]$ excited state in $^{101}$Zr was obtained by Urban et al. from the spontaneous fission of $^{248}$Cm [13]. The level scheme and new rotational bands in $^{102}$Zr were reported in Ref. [14] by Li et al. For $^{103}$Zr, Urban et al. identified a new rotational band with a proposed $3/2^+$ bandhead located at 26.8 keV [15]. In Ref. [16] by Yeoh et al., high spin levels of the very neutron-rich $^{104}$Zr nucleus were reinvestigated by measuring the prompt $\gamma$ rays in the spontaneous fission of $^{252}$Cf, and a new $4^-$ band was suggested with a bandhead energy at 1928.7 keV. Another important method to produce neutron-rich nuclei is through $\beta$ decay. In a recent experimental work [17], the neutron-rich nucleus $^{110}$Mo has been investigated by means of $\gamma$ ray spectroscopy following the $\beta$ decay of $^{110}$Nb, produced using in-flight fission of a $^{238}$U beam at 345 MeV/nucleon at the RIBF facility.

With increasing neutron number toward more neutron-rich regions, triaxial deformation and multi-phonon $\gamma$-vibrational structure develop. High-spin collective band structures in even-even $^{108,110,112}$Ru have been studied by measuring the prompt $\gamma$-rays emitted from the spontaneous fission or the induced fission of heavy nuclei [18, 19, 20, 21, 22, 23, 24, 25, 26, 27]. Besides the ground state bands, some collective bands such as one-phonon $\gamma$-vibrational bands and chiral doublet bands have been observed in $^{108,110,112}$Ru. The level scheme of $^{114}$Ru was first established by Shannon et al. [18] from the spontaneous fission of $^{248}$Cm. The ground state band and one-phonon $\gamma$-vibrational band were observed up to $10^+$ and $5^+$, respectively. Further, an observed anharmonicity between the one-phonon and two-phonon $\gamma$-vibrational bands [28] made the study of nuclei with triaxial deformation more interesting.

The experimentally identified multi-qp bands with diverse phenomena in structure can serve as an ideal testing ground for various theoretical models. A theoretical study of equilibrium shapes and high-spin properties for neutron-rich nuclei was performed by Skalski et al. [10] using potential energy surface (PES) and total routhian surface (TRS) methods. The systematics of one-qp configurations in odd-mass neutron-rich Sr, Zr, and Mo isotopes was studied by the Hartree-Fock-Bogoliubov plus equal filling approximation method with the Gogny energy density functional [29]. However, to describe the observed rotational bands, more quantitative model calculations are desired. Large-scale shell model calculations were carried out by Sieja et al. [30] for transitional Zr isotopes with $N < 60$, but due to limitations in model space they were unable to describe heavier isotopes with large deformation. In Ref. [31], Verma et al. applied the projected shell model [33] to describe the yrast lines in even-even $^{98-102}$Sr and $^{100-104}$Zr, and they obtained a good agreement with experimental data. Studies of electromagnetic transition probabilities confirmed the reliability of the model wave function. Nevertheless, a
more challenging task for shell-model type calculations is to study the interplay of many excited multi-qp bands in both even-even and odd-mass isotopes and with multi-phonon vibrational bands, which is a sensitive test for the single-particle structure and interactions in these nuclei.

Part of the results presented in this talk was originally published in Refs. [28, 32].

2. The theory with angular momentum projection

Angular momentum projection is nowadays a often-used many-body method in the structure study of heavy, deformed nuclei. The method is used for situations where a deformed mean-field is employed for description of deformed nuclei, in which the rotational symmetry is broken. In the present work, angular momentum projection is carried out for a chosen set of qp configurations built by the Nilsson+BCS states near the Fermi energy. The projected configurations are then used as a new basis to diagonalize a shell model Hamiltonian. This approach, referred to as the projected shell model (PSM) [33], follows the basic philosophy of the standard shell model approach. The only difference is that, in the PSM, a deformed basis is employed rather than a spherical one. This makes the truncation of the many-body basis very efficient, so that shell model calculations can be easily performed even for the heaviest systems. The PSM approach has been used to describe a broad range of nuclear phenomena such as the backbending in moment of inertia [34], the signature dependence [35, 36], super-deformed bands [37, 38], rotational bands in super-heavy nuclei [39, 40], and structure of neutron-rich nuclei [41, 42, 43, 44], with considerable success.

The PSM calculation uses deformed Nilsson single-particle states to build the model basis. As the valence space for this mass region, nucleons in three major shells (N = 3, 4, 5 for neutrons and N = 2, 3, 4 for protons) are activated.

Let |Φ⟩ denote the qp vacuum and a^†_ν and a^†_π the qp creation operators, with the index ν (π) being the neutron (proton) quantum numbers. Below, we list multi-qp configurations used in the present work for different types of nuclei. The multi-qp configurations for even-even nuclei, consisting of zero-, two-, and four-qp states, are

\begin{equation}
\{ |Φ⟩, a^†_ν a^†_σ |Φ⟩, a^†_ν a^†_μ a^†_π |Φ⟩, a^†_ν a^†_µ a^†_π a^†_σ |Φ⟩ \},
\end{equation}

and for odd-neutron nuclei, the multi-qp configurations, consisting of one- and three-qp states, are

\begin{equation}
\{ a^†_ν |Φ⟩, a^†_ν a^†_π a^†_σ |Φ⟩ \}.
\end{equation}

The PSM wave function can then be written as a superposition of (angular-momentum) projected multi-qp states

\begin{equation}
|Ψ^q_I_M⟩ = \sum_{K\kappa} f^q_{K\kappa} \hat{P}^I_M |Φ^q_\kappa⟩
\end{equation}

where |Φ^q_\kappa⟩ denotes the qp-basis given in (1) or (2), and \( \hat{P}^I_M \) is the angular momentum projection operator [33].

The PSM calculation employs a quadrupole plus pairing Hamiltonian, with inclusion of the quadrupole-pairing term

\begin{equation}
\hat{H} = \hat{H}_0 - \frac{1}{2} \chi_{QQ} \sum_{\mu} \hat{Q}^\dagger_{2\mu} \hat{Q}_{2\mu} - G_M \hat{P}^I \hat{P} - G_Q \sum_{\mu} \hat{P}^\dagger_{2\mu} \hat{P}_{2\mu},
\end{equation}

where \( \hat{H}_0 \) is the single-particle term which contains a proper spin-orbit force. The strength of the quadrupole-quadrupole force \( \chi_{QQ} \) is determined in a self-consistent manner so that it is related to deformation of the basis [33]. The monopole-pairing strength is taken to be \( G_M = |G_1 - G_2(N - Z)/A|/A \) for neutrons and \( G_M = G_1/A \) for protons. The quadrupole-pairing strength \( G_Q \) is, as usual, assumed to be proportional to \( G_M \).
The above description assumed an axially deformed mean-field to start with. One can extend the model without the restriction of the axial symmetry [33]. The so-called triaxial projected shell model (TPSM) [45] is a generalized version of the original PSM [33] by extending it to a triaxially deformed basis. By performing diagonalization in a basis constructed with three-dimensional angular-momentum-projection on triaxially deformed states, it is feasible for the model to describe γ vibrational states in a shell model framework [46]. In this way, one can achieve a unified treatment of ground-state band (g band) and multiphonon γ vibrational bands (γ band) in one calculation, and the results can be quantitatively compared with data. The TPSM calculation has been successfully performed for the study of interplay between quasi-particle excitations and the collective motion in even-even [47, 48, 49] and odd-mass nuclei [50].

The TPSM uses the triaxially-deformed Nilsson+BCS basis and performs exact three-dimensional angular-momentum-projection. The Nilsson potential in the TPSM case is written as

$$\hat{H}_0 - \frac{2}{3} \hbar \omega \left[ \varepsilon \hat{Q}_0 + \varepsilon' \frac{\hat{Q}_{+2} + \hat{Q}_{-2}}{\sqrt{2}} \right],$$

where $\hat{H}_0$ is the spherical single-particle Hamiltonian again with inclusion of appropriate spin-orbit forces. The axial and triaxial deformation parameters, $\varepsilon$ and $\varepsilon'$ in (5), are related to the conventional triaxiality parameter by $\gamma = \tan^{-1}(\varepsilon'/\varepsilon)$. It is to be noted that an intrinsic triaxial state in the TPSM is a rich superposition of different $K$ states. For instance, the triaxially deformed vacuum state is composed of $K = 0, 2, 4, ...$ configurations. The projected bands from these $K = 0, 2$, and $4$ intrinsic states are the dominant components of the ground, γ, and $2\gamma$ bands, respectively [46]. Finally, the TPSM calculation adopts the same Hamiltonian (4) as the PSM to carry out diagonalization in the projected triaxial basis.

3. Influence of high-$j$ orbitals on the structure of Zr isotopes

In this section, we apply the PSM to investigate the influence of the high-$j$ $h_{11/2}$ neutron orbital and the $g_{9/2}$ proton orbital on the structure properties of Zr isotopes with neutron number $N = 61-66$. In the calculation, one first determines deformed bases to start with. We construct our deformed bases with the quadrupole and hexadecapole deformation parameters suggested by Ref. [51] for the isotopes $^{101-106}$Zr, except for $^{104}$Zr for which a smaller $\varepsilon_2$ is used. These deformation parameters are listed in Table I.

3.1. The deformed Nilsson diagrams

Single-particle states near the Fermi surfaces at a deformed potential are important for low-lying multi-quasi-particle excited configurations. Since in the present work, we study systematical behavior of an isotopic chain which is sensitive to the shell filling of nucleons, it is useful to discuss the deformed single-particle states employed in the calculation.

We plot the Nilsson diagrams for neutrons and protons in Fig. 1, on which many of our later discussions are based. For simplicity, we take only the quadrupole deformation parameter.

### Table 1. Quadrupole and hexadecapole deformation parameters employed for generating the deformed bases.

| $\varepsilon_2$ | $\varepsilon_4$ |
|----------------|----------------|
| 0.333 | 0.013 |
| 0.333 | 0.027 |
| 0.342 | 0.033 |
| 0.320 | 0.013 |
| 0.333 | 0.060 |
| 0.333 | 0.073 |
| 0.36 | 0.36 |
$\varepsilon_2$ as the variable, while omitting $\varepsilon_4$ (although $\varepsilon_4$ is included in the calculation). In Fig. 1, solid curves denote the positive parity states while dashed curves are for the negative parity states. The dotted rectangles enclose the most important states near the Fermi surfaces in the deformation range of $\varepsilon_2 = 0.32 - 0.34$ for the nuclei discussed in this paper.

In Fig. 1(a) for protons, with proton number $Z = 40$ and in the deformation range $\varepsilon_2 = 0.32 - 0.34$, the $K = 1/2, 3/2,$ and $5/2$ states from the $\pi g_{9/2}$ intruder orbital fall into the dotted rectangle and are physically important. As we shall discuss later, the states with $K = 3/2$ and $5/2$ can construct a two-quasi-proton state with a total $K = 1$, which plays a role at high spins in even-even Zr isotopes. On the other hand, there are negative-parity orbitals from $\pi f_{5/2}^\nu$ and $\pi h_{11/2}^\nu$, which are coupled states to the rotating body. In Fig. 1(b) for neutrons, with neutron number $N = 61 - 66$ and in the deformation range $\varepsilon_2 = 0.32 - 0.34$, we see more states in the rectangle. These are the positive-parity $K = 9/2$ state of $\nu g_{9/2}$, $K = 3/2$ of $\nu g_{7/2}$, $K = 5/2$ of $\nu d_{5/2}$, and $K = 1/2$ of $\nu s_{1/2}$. There are also the negative-parity $K = 3/2, 5/2,$ and $7/2$ states from the $\nu h_{11/2}$ intruder orbital which strongly influence the band crossing in this region.

In the following, we take the even-even isotope $^{102}$Zr and the odd-mass isotope $^{101}$Zr as examples for a detailed comparison of the PSM results with the experimental data. Results and discussion for some other Zr isotopes have been presented in our recent paper [32].

### 3.2. $^{102}$Zr

$^{102}$Zr is an experimentally well-studied nucleus. The yrast band and 2-qp bands were measured early in Refs. [4, 11], and recently in Refs. [12, 14] by two independent groups. Hua et al. [12] populated neutron-rich isotopes as fission fragments produced by the $^{238}$U($\alpha, f$) fusion-fission reaction. Beside the yrast band, they observed two rotational bands with negative-parity built on 2-qp states, one of which was assigned as $K^\pi = 4^-$ and the other $5^-$. In the latest experimental work reported in Ref. [14], Li et al. measured the prompt $\gamma$ rays from a spontaneous fissioning $^{252}$Cf source. In addition to the previously known bands, they identified several new 2-qp
rotational bands, among which two positive-parity bands were found, with band head energies of 1386.3 and 1652.7 keV, respectively. Different explanations were given by the two groups concerning the nature of the partner band of the \( K^\pi = 5^- \) band, starting from an excitation of 1932 keV. In Fig. 2, the calculated yrast and 2-qp bands are shown and compared with these data. Furthermore, two bands with \( K^\pi = 7^+ \) and \( 7^- \) are predicted.

Near the neutron Fermi level of \(^{102}\)Zr, there are three qp orbitals from the \( N = 4 \) harmonic shell: \( K = 3/2 \) of \( g_{7/2} \), \( K = 5/2 \) of \( d_{5/2} \), and \( K = 9/2 \) of \( g_{9/2} \) (see Fig. 1(b)). They can couple to three 2-qp high-\( K \) states, namely, \( K^\pi = 6^+ \) 2-qp state of \( 9/2^+ [404] \otimes 3/2^+ [411] \), \( K^\pi = 4^+ \) 2-qp state of \( 3/2^+ [411] \otimes 5/2^+ [413] \), and \( K^\pi = 7^+ \) 2-qp state of \( 5/2^+ [413] \otimes 9/2^+ [404] \). We found that calculated \( 4^+ \) and \( 6^+ \) bands are consistent well with the observed band (6) and (7) in Ref. [14] although our calculated band head energies are somewhat higher than the experimental data. We note, however, that the calculation predicts that these two bands have a coupled character with a presence of both even and odd spins members while in experiment only even spin members were observed. The authors in Ref. [14] could not determine whether the \( 6^+ \) band is constructed by \( 9/2^+ [404] \otimes 3/2^+ [411] \) or \( 9/2^- [514] \otimes 3/2^- [541] \) configuration. According to the PSM calculation, the configuration of the \( 6^+ \) band is \( 9/2^+ [404] \otimes 3/2^+ [411] \). We believe that it is reasonable because for the other proposal the energy of the \( 9/2^- [514] \) state is very high, and the energy of the \( 9/2^- [514] \otimes 3/2^- [541] \) configuration will be much higher than the experimental \( 6^+ \) band.

The \( K = 5/2 \) state of the \( h_{11/2} \) orbital is found to be close to the neutron Fermi level of \(^{102}\)Zr. Therefore, possible low-lying 2-qp states with negative parity can be built by coupling this with the above mentioned \( N = 4 \) shell states, namely, a \( K^\pi = 4^- \) 2-qp state of \( 5/2^- [532] \otimes 3/2^+ [411] \), a \( K^\pi = 5^- \) 2-qp state of \( 5/2^- [532] \otimes 5/2^+ [413] \), and a \( K^\pi = 7^- \) 2-qp state of \( 5/2^- [532] \otimes 9/2^+ [404] \). By a comparison with data in Ref. [14], we found an excellent agreement between our calculated \( 4^- \) band and their experimental band (2). This confirms the assignment for this band given in Ref. [14] and in early experimental papers. Another band (band (4) in [14] and band (b) in [12]) with a band head energy \( \sim 1932 \) keV was observed in both experiments [12, 14]; however, the assigned configuration was different in these references. Within 4 MeV of excitation in the

![Figure 2. Calculated energy levels for \(^{102}\)Zr and comparison with available data taken from Refs. [12, 14]. This figure is taken from Fig. 2 of Ref. [32].](image-url)
Figure 3. (Color online) Band diagram for $^{102}$Zr. The 0-qp ground band, two 2-qp bands, and one 4-qp band energies are plotted against spin. Note that for these bands only even-spin states are plotted in order to avoid a strong zigzag pattern. This figure is redrawn from Fig. 6 of Ref. [32].

PSM calculation, we do not find a 2-qp state with $K^\pi = 8^+$. The theoretical band head energy of the 2-qp $K^\pi = 6^-$ band with the configuration $3/2^-[541] \otimes 9/2^+[404]$ is 3795 keV, which is much higher than the band head energy of band (b) in [12]. On the other hand, we predict that the $5^-$ band is also a coupled one, and should have both even-spin and odd-spin branches, as shown in Fig. 2.

We predict two high-$K$ configurations of $K^\pi = 7^+$ and $7^-$ bands with the neutron 2-qp configuration $5/2^+[413] \otimes 9/2^+[404]$ and $5/2^-[532] \otimes 9/2^+[404]$, respectively. These bands lie low in energy and could have a chance to be detected.

3.3. Discussion of band diagrams
From the Nilsson diagrams in Fig. 1, one sees that for the deformation range listed in Table I, the intruder orbitals $\nu 5/2[532]$ and $\nu 3/2[541]$ from the $h_{11/2}$ neutrons and $\pi 3/2[431]$ and $\pi 5/2[422]$ from the $g_{9/2}$ protons lie near the Fermi surfaces of the nuclei under consideration. For a description of the rotational behavior in these nuclei, 2-qp states based on these orbitals (with $K_{\nu 1} \pm K_{\nu 2}$ or $K_{\pi 1} \pm K_{\pi 2}$) should be taken into account. We expect that crossing of 2-qp bands with the ground band can change the structure of the yrast states. The picture can be conveniently demonstrated by band diagrams [33], in which band energies of each angular-momentum-projected configuration in (1) or (2) are plotted as a function of spin. The energy of a band $\kappa$ is defined by

$$E_\kappa(I) = \frac{\langle \Phi_\kappa | \hat{H} \hat{P}_I^{KK} | \Phi_\kappa \rangle}{\langle \Phi_\kappa | \hat{P}_I^{KK} | \Phi_\kappa \rangle}. \quad (6)$$

This represents the expectation value of the Hamiltonian with respect to a projected multi-qp state $\kappa$. After configuration mixing, a band may be modified due to interactions with other configurations.

In Fig. 3, we plot the 0-qp ground band, two 2-qp bands of neutron and proton, and a 4-qp band for $^{102}$Zr, which represent the most important states for each kind of configuration. Dots
Figure 4. Calculated energy levels for $^{101}$Zr and comparison with available data taken from Refs. [12, 13]. This figure is taken from Fig. 10 of Ref. [32].

3.4. $^{101}$Zr

A theoretical description for odd-mass nuclei is more challenging than for even-even nuclei because of the sensitivity of odd-mass systems to single-particle states. Due to different occupations of single particle orbitals, observed low-lying bands in the odd-mass Zr isotopes reflect more directly the single-particle structure in this mass region. For example, the configuration of the ground state in $^{101}$Zr is $\nu 3/2^+ [411]$, but with two additional neutrons in $^{103}$Zr, $\nu 5/2^- [532]$ becomes the favored ground state configuration. The systematics of one-quasiparticle configurations in neutron-rich Sr, Zr, and Mo odd-mass isotopes has recently been studied by Rodriguez-Guzman et al. with the Gogny energy density functional [29].

In the past, the PSM was applied to interpret the phenomena of signature splitting and signature inversion observed in rare-earth nuclei [36, 52]. In this section, calculations are performed for odd-mass Zr isotopes. Two aspects are discussed: One is the variation of single-particle configurations of $^{101}$Zr, and the other is to study signature splitting in one-quasiparticle rotational bands.
The level scheme for low-spin states in $^{101}\text{Zr}$ was studied early through $\beta$ decay of $^{101}\text{Y}$ [53]. Recently, single-particle and collective degrees of freedom in this nucleus have been discussed in Refs. [12, 13, 54, 55]. Especially in Ref. [54], the measured $g$ factor values are used to discuss the low-lying structure. In Ref. [13], the authors found a $T_{1/2} = 16(2)$ ns isomeric level in $^{101}\text{Zr}$ at 941.8 keV in a measurement of prompt $\gamma$-rays using the EUROGAM2 array. The level is interpreted as a $K$-isomer corresponding to the $9/2^+$ neutron-hole excitation. From the Nilsson diagram plotted in Fig. 1, one sees that the neutron $9/2^+$ state indeed intrudes into the $N = 60$ region at a quadrupole deformation about 0.30.

Calculated energy levels for $^{101}\text{Zr}$ are compared with experimental data in Fig. 4. Data of the positive-parity $\nu 3/2^+ [411]$ band and the negative-parity $\nu 5/2^- [532]$ band are taken from Ref. [12], and those of $\nu 9/2^+ [404]$ from Ref. [13]. As one can see, the data are reproduced pretty well by the PSM calculation. In agreement with the experiment [12], the $\nu 3/2^+ [411]$ 1-qp configuration is found to the lowest in energy. The $\nu 5/2^- [532]$ 1-qp configuration, on the other hand, is the lowest among all the calculated negative-parity ones. Another positive-parity 1-qp state $\nu 9/2^+ [404]$ appears at the correct energy as what data showed [13], thus supporting the experimental assignment for this band. In addition, a positive-parity band based on the 1-qp $\nu 5/2^+ [413]$ state and a negative-parity band on the 1-qp $\nu 3/2^- [541]$ state are predicted with the band head energy 0.767 MeV and 1.403 MeV, respectively.

In Ref. [13], Urban et al. also observed a band with the band head energy 1942.0 keV which decays to the $11/2^+$ level of the $9/2^+[404]$ band rather than to the $11/2^+$ level of the ground band. Through angular correlations the authors concluded that the 777.6 keV transition has a dipole character. In our calculation, there is a $K^\pi = 11/2^-$ 3-qp configuration which lies in the energy range of the discussion. In Fig. 4, we plot this $11/2^-$ band with the calculated band head energy at 2212 keV, which compares well with the experimental value of 1942.0 keV. The main component of this $11/2^-$ band is of a 3-qp structure, namely $\pi 5/2^+ [422] \otimes \pi 3/2^+ [440] \otimes \nu 5/2^- [532]$.

### 3.5. Signature splitting in 1-qp bands

An interesting observation in Figs. 4 is the irregular structures in some bands, such as those in the $\nu 5/2^- [532]$ band. In these bands, every two levels lie closer forming groups. In a plot of energy versus spin, a staggering or zigzag pattern can be seen. These irregularities are attributed to the decoupling effect [52] which is usually seen in rotational bands with a high $j$ and low $K$ state (e.g. $K = 1/2$ or $K = 3/2$) as the main configuration.

Signature is a quantum number specifically appearing in a deformed intrinsic system. It is related to the invariance of a system with quadrupole deformation under a rotation of 180° around a principle axis. For an odd-mass nucleus, depending on the total spin, the signature quantum number can take two different values. It is customary to assign

\[
\alpha_I = \frac{1}{2} (-1)^{I-1/2}
\]

as the signature quantum number for a state of spin $I$ of an odd-mass nucleus. A rotational band with a sequence of levels differing in spin by $1\hbar$ is now divided into two branches, each consisting of levels differing in spin by $2\hbar$ and classified by the signature quantum number $\alpha_I = \pm \frac{1}{2}$, respectively. For some bands, one observes experimentally an energy splitting for the two branches. The energetically favored branch is formed by those spin $I$ states that satisfy $I - j$ even, where $j$ is the total angular momentum of the corresponding single-particle state. Following this rule, the favored branch of the $\nu 5/2^- [532]$ ($j = 11/2$) band consists of the spin levels $I = 7/2, 11/2, 15/2, \ldots$.

In Fig. 5, some low-energy rotational bands in $^{101,103,105}\text{Zr}$ with a clear signature splitting are shown[32]. In this figure, energy differences of two adjacent levels of spin $I$ and $I - 1$ are plotted.
The energy difference $E(I) - E(I - 1)$ is compared between theory (squares) and experiment (open circles). The first row is for positive parity band in $^{101,103,105}$Zr and the second row is for negative parity band in $^{101,103,105}$Zr, respectively. This figure is redrawn from Fig. 14 of Ref. [32].

This quantity was suggested to extract information about triaxiality of a rotational band because in model calculations, the trend of signature splitting was found to be very sensitive to the $\gamma$ degree of freedom. As discussed in Ref. [12], with two more protons, the isotopes $^{104,106,108}$Mo and $^{103,105,107}$Mo have well-defined triaxial ground-state minima. One may ask whether the $\gamma$ degrees of freedom are present in Zr isotopes.

We show the lowest positive-parity bands respectively in $^{101,103,105}$Zr in the upper row of Fig. 5 and the lowest negative-parity band $\nu5/2^-[532]$ in the bottom row. For the positive-parity bands the staggering is found to be small. This feature is correctly reproduced by the calculation. As can be seen, the calculation agrees with the experiment very well for the $\nu3/2^+[411]$ band in $^{101,103}$Zr. For $^{107}$Zr, the $\nu5/2^+[413]$ band is predicted to have a smaller staggering because it has a larger $K$.

In the $\nu5/2^-[532]$ negative-parity band, the zigzag behavior is more obvious. Although this configuration has a larger $K$, the coupling with the low $K$, $\nu3/2^-[541]$ state leads to a stronger decoupling effect for the $K = 5/2$ band. For $^{101,103}$Zr where data for the $\nu5/2^-[532]$ band are available, the observed signature splitting is correctly described although the calculated staggering amplitude is smaller than the observation. A similar zigzag pattern for $^{105}$Zr is predicted.

Our PSM calculation has been carried out by assuming an axial symmetry in the deformed basis where each band can be assigned with a $K$ quantum number. The good agreement with data in various multi-quasiparticle bands discussed above has indicated that the Zr isotopes can be considered to sustain an axial symmetry reasonably well. In particular, the description of signature splitting in the odd-mass isotopes suggests that the triaxiality effect in these isotopes is small. The situation is different from that in neutron-rich Mo isotopes where larger effects with $\gamma$ deformation have been discussed [12]. For a correct description of the $\gamma$ deformation effects, the triaxial projected shell model (TPSM) must be employed [45]. In the following section, we shall apply the TPSM approach to investigated the triaxiality in $^{110}$Mo.
4. Triaxiality in very neutron-rich $^{110}$Mo

With increase of proton number, the ground state of Mo isotopes becomes triaxially deformed and $\gamma$-vibrational bands in these nuclei are found low in excitation [9, 12, 56, 57, 58]. The most neutron-rich Mo isotope for which spectroscopic information on the low-lying level structure has so far been obtained by $\beta$-decay [17] is $^{110}$Mo, in which a quasi-$\gamma$ band with a 494-keV bandhead energy was established experimentally.

To understand the $\gamma$-softness nature of $^{110}$Mo and explore properties of deformed nuclei at the prolate-to-oblate transition region, we perform TPSM calculations for $^{110}$Mo. The value of $\varepsilon$ is taken from Ref. [51]. As discussed below, the value of $\varepsilon'$ in our calculation has been chosen such that the bandhead energy of the experimental $\gamma$-band is reproduced.

As shown in Fig. 6(a), we first calculate the $2_{1}^{+}$ and $4_{1}^{+}$ states energy of the ground band as a function of $\varepsilon'$, with the quadrupole deformation parameter fixed at $\varepsilon = 0.30$. As one can clearly see from the figure, the energy curves of the $2_{1}^{+}$ and $4_{1}^{+}$ states of the ground band are flat in the region of $\varepsilon' = 0.10 - 0.20$, indicating that these states are soft with respect to triaxiality. This picture thus suggests that the nucleus does not have a well-defined triaxial deformation in its ground state configuration. In contrast, energies of the states of the $\gamma$-band depend sensitively on $\varepsilon'$, showing low excitation energies for large triaxiality. Therefore, in the present treatment, $\varepsilon'$ is an adjustable parameter which reproduces the $E(2_{2}^{+})$ of $\gamma$-band and is equal to 0.18. It is important to mention that with $\varepsilon' = 0.18$, $\gamma$-bandhead energy is calculated to be 475 keV and the corresponding experimental value is 494 keV, which well reproduces the experimental data.

On the other hand, as seen in Fig. 6(b), energy curves of the $2_{2}^{+}$ and $4_{2}^{+}$ states of the ground band decrease slowly in the deformation region of $\varepsilon = 0.25 - 0.35$; however, the $\gamma$-band energy $E(2_{2}^{+})$ increases with the axial symmetry deformation parameter. The suggested axial deformation $\varepsilon = 0.30$ in Ref. [51] is an appropriate value to reproduce data.

To compare theoretical energies with the experimental data, we plot the experimental and theoretical level energies in Fig. 7 for the yrast and one-phonon $\gamma$-band. Level energies of the two-phonon $\gamma$-band are predicted in the present TPSM calculation. It is evident from Fig. 7 that not only the energies of each band but also their relative positions of the bands are correctly reproduce.

**Figure 6.** Band head energies varying with the deformation parameter $\varepsilon'$, $\varepsilon$ and comparison with the experimental $E(2_{1}^{+})$, $E(4_{1}^{+})$ and $E(2_{2}^{+})$ in $^{110}$Mo.
Figure 7. Band head energies varying with the deformation parameter $\varepsilon'$ and comparison with the experimental band head energies of the $\gamma$-vibrational bands in $^{110}$Mo.

reproduced by the current TPSM calculation.

5. Anharmonicity of $\gamma$ vibration in $^{114}$Ru

For the more neutron-rich nucleus $^{114}$Ru with $Z = 44$ and $N = 70$, high spin levels have recently been obtained by measuring the prompt $\gamma$-rays in the spontaneous fission of $^{252}$Cf [28]. The ground state band and one-phonon $\gamma$-vibrational band were extended up to $14^+$ and $9^+$, respectively. Two levels were proposed as the members of a two-phonon $\gamma$-vibrational band.

The TPSM results compared with the experimental data are presented in Fig. 8. One can see that the experimental results are described reasonably well by the TPSM calculation. We note especially that the band head energies for bands (2) and (3) in Ref. [28] are precisely reproduced. The good agreement with the experimental data supports the interpretation for the bands (2) and (3) as $1$-$\gamma$ and $2$-$\gamma$ bands, respectively. The TPSM calculation suggests also that the data can only be quantitatively described when a positive quadrupole deformation combined with a large triaxiality ($\gamma = 27^\circ$) is assumed. To understand the TRS results in Ref. [59, 60], we have performed TPSM calculations by assuming an oblate shape (negative quadrupole deformation) for $^{114}$Ru. We find that such results cannot reproduce the current data, and in particular, the obtained $\gamma$-ray energies (moments of inertia) for the yrast band (band (1)) are not consistent with the data. We note that the TRS calculations for $^{114}$Ru [59, 60] yield only very shallow minima, suggesting a $\gamma$-soft nature for this nucleus.

Another interesting observation in the $1$-$\gamma$ and $2$-$\gamma$ bands of $^{114}$Ru is the pronounced anharmonicity. By anharmonicity we mean that the ratio of the energy levels $E(4^+_1)/E(2^+_2)$ deviate from two. One can see from TABLE I in Ref. [28] that the $E(4^+_1)/E(2^+_2)$ values in all the $^{108,110,112,114}$Ru isotopes are in accord with the systematics, but they are larger than the harmonic ratio two, and progressively increase toward heavy isotopes. The larger ratio indicates an increasing anharmonicity in $\gamma$ vibration. In order to understand the large anharmonicity observed in $^{114}$Ru, we present in Fig. 9 the calculated band head energies of the $1$-$\gamma$ and $2$-$\gamma$ bands varying with the triaxial deformation $\varepsilon'$. The axial deformation is fixed at $\varepsilon = 0.25$.

It is interesting to observe that the band head energies of the $\gamma$-bands are nearly constant from $\varepsilon' = 0.02$ to 0.08 and the ratio $E(4^+_1)/E(2^+_2)$ is close to two, indicating that the vibration is nearly harmonic. With increasing triaxiality $\varepsilon'$, the ratio increases and an anharmonicity
Figure 8. Calculated energy for $^{114}$Ru and comparison with available data.

Figure 9. Band head energies varying with the deformation parameter $\varepsilon'$ and comparison with the experimental band head energies of the $\gamma$-vibrational bands in $^{114}$Ru. This figure is redrawn from Fig. 6 of Ref. [28].

develops. The variation shows that the anharmonicity of $\gamma$-vibration is sensitively dependent on triaxial deformation. This picture is consistent with the conclusion of the early work of Davydov and Filippov [61]. At $\varepsilon' = 0.13$ or $\gamma = 27^\circ$, the agreement with the data becomes perfect. Thus the TPSM calculation naturally describes the anharmonicity found by the experimental data, and suggests that the triaxial degree of freedom plays an important role in the $\gamma$-vibrational bands of $^{114}$Ru.
6. Summary
PSM calculations have been performed for the neutron-rich even-even and odd-even Zr isotopes with neutron number $N = 61 - 66$ in the $A \sim 100$ region. The current experimental data of the yrast bands and excited 1- and 2-qp bands have been reproduced well by the calculations. Furthermore, we have predicted some high-$K$ 2-qp bands in even-even isotopes at low excitations, which may be found by future experiments. The phenomenon signature splitting in the odd-neutron 1-qp bands has been discussed. By discussing the signature splitting, we have concluded that the nuclei studied in this paper could be regarded as axially symmetric systems.

The TPSM approach has been employed to study the $\gamma$-soft nature in very neutron-rich $^{110}$Mo. Its $\gamma$-soft picture can well be painted by the variation of yrast and $\gamma$-vibrational band energies versus triaxial deformation parameter $\varepsilon'$. The 2-$\gamma$-vibrational band is predicted from our calculation.

The TPSM calculations were used to describe the multi-phonon $\gamma$-vibrational band energy levels. The TPSM calculations indicate a good agreement between theoretical and experimental results when using a triaxial deformation in $^{114}$Ru but not for an oblate deformation. The anharmonicity can well be described by our TPSM theory. The results suggest that the triaxial degree of freedom plays an important role in the $\gamma$-vibrational bands of $^{114}$Ru. The present results have enriched the concept of $\gamma$-vibration and we hope that, in the future, more states of such kind will be identified experimentally.

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