Shape polarization and coexistence of high-K three-quasiparticle states in odd-mass N=106 isotones

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Abstract

Three-quasiparticle K-isomeric states in odd-mass N=106 isotones within the A~180 mass region are systematically investigated using configuration-constrained potential energy surface calculations. The calculations successfully reproduce the excitation energies and deformations of known high-K isomers in the nuclei from 175Tm to 181Re. For the nuclei closer to the Z=82 shell closure (183Ir, 185Au, and 187Tl), predictions for the configurations of observed and yet-to-be-observed isomers are provided. The results reveal strong shape polarization, where the three-quasiparticle states are driven to larger deformations compared to the often shape-soft or spherical ground states. A particularly rich spectrum of shape coexistence is predicted in 187Tl, where several high-K three-quasiparticle configurations with distinct prolate, oblate, and triaxial shapes are found to coexist at similar excitation energies. Notably, the oblate-deformed Kπ=29/2+ configuration at E_x = 1839 keV is proposed to be responsible for a long-lived isomer. This study provides a comprehensive picture of shape evolution and coexistence in high-K multi-quasiparticle states, offering valuable insights for future experimental research.

Full Text

Preamble

Shape polarization and coexistence of high-K three-quasiparticle states in odd-mass N = 106 isotones∗ Runyan Dong[1,2] and Changfeng Jiao[1,2,†] [1]School of Physics and Astronomy, Sun Yat-sen University, Zhuhai 519082, China [2]Guangdong Provincial Key Laboratory of Quantum Metrology and Sensing, Sun Yat-sen University, Zhuhai 519082, China

Three-quasiparticle K-isomeric states in odd-mass N = 106 isotones within the $A \sim 180$ mass region are systematically investigated using configuration-

constrained potential energy surface calculations. The calculations successfully reproduce the excitation energies and deformations of known high-K isomers in nuclei from ^{175}Tm to ^{181}Re. For nuclei closer to the $Z = 82$ shell closure (^{183}Ir, ^{185}Au, and ^{187}Tl), predictions for the configurations of observed and yet-to-be-observed isomers are provided. The results reveal strong shape polarization, where the three-quasiparticle states are driven to larger deformations compared to the often shape-soft or spherical ground states. A particularly rich spectrum of shape coexistence is predicted in ^{187}Tl, where several high-K three-quasiparticle configurations with distinct prolate, oblate, and triaxial shapes are found to coexist at similar excitation energies. Notably, the oblate-deformed $K^\pi = 29/2^+$ configuration at $E_x = 1839$ keV is proposed to be responsible for a long-lived isomer. This study provides a comprehensive picture of shape evolution and coexistence in high-K multi-quasiparticle states, offering valuable insights for future experimental research.

Keywords: Shape polarization, shape coexistence, high-K isomeric state, configuration-constrained potential energy surface.

INTRODUCTION

Atomic nuclei in the $A \sim 180$ mass region with neutron numbers close to midshell are characterized by an abundance of low-lying, high-seniority isomeric states. In this region, orbitals with large Ω, the projection of individual angular momentum onto the intrinsic symmetric axis, approach the neutron Fermi surface at moderate quadrupole deformations. This facilitates the formation of broken-pair states with high K values (where $K = \sum_i \Omega_i$) near the yrast line. According to electromagnetic transition selection rules, transitions of multipolarity λ are significantly hindered when $\Delta K > \lambda$. This so-called K-hindrance can lead to relatively long half-lives (on the order of nanoseconds or longer) [1, 2], resulting in the formation of "K isomers." One of the most well-known examples of high-K isomers is found in ^{178}Hf, where two 2-quasiparticle (qp) $K^\pi = 8^-$ isomers and a long-lived four-quasiparticle $K^\pi = 16^+$ isomer with a half-life of 31 years are observed [3, 4]. Since the occurrence of K isomers represents a combined effect of unpaired nucleons occupying high-Ω states and nuclear deformation, the study of K isomeric states is pivotal for understanding the interplay between the shell structure of "individual" nucleons and the collective behavior of a strongly correlated nucleus [1].

Another common feature associated with the $A \sim 180$ mass region is shape transition. Here, the ground-state (g.s.) shape can change from a well-deformed prolate ellipsoid with $\beta_2 \geq 0.28$ for ^{176}Yb to a very soft spheroid for ^{188}Pb [5]. Moreover, this shape softness gives rise to the novel phenomenon of shape coexistence, characterized by the emergence of low-lying states with different intrinsic shapes within a single nucleus. Generally, this originates from the combined effect of approaching the $Z = 82$ spherical shell closure and the deformed shell gaps around the neutron midshell at $N = 104$–106 due to quadrupole-quadrupole correlations, which has drawn considerable interest [6–8]. The most well-known example is the differently shaped 0^+ triplet observed in ^{186}Pb, corresponding to the coexistence of prolate, oblate, and spherical configurations [9, 10]. Coexisting 0^+ states in even-even Pt, Hg, Pb, and Po isotopes around the neutron midshell have been extensively studied [11–14].

In addition to shape changes resulting from collective correlations such as quadrupole-quadrupole interactions, unpaired nucleons are found to strongly polarize the nuclear shape [15]. Since K isomeric states involve high-Ω unpaired nucleons, shape polarization can produce considerable differences in shape between high-K states and ground states, leading to novel structures that involve both K isomerism and shape isomerism. For example, the two-quasineutron $K^\pi = 8^-$ ($\nu\{7/2^-[514] \otimes 9/2^+[624]\}$) isomeric states are systematically observed in the even-even $N = 106$ isotones between ^{174}Er and ^{188}Pb (see [16, 17] and references therein). Previous theoretical investigations have shown that while the g.s. are oblate-deformed with $|\beta_2| \approx 0.13$ for ^{186}Hg and spherical for ^{188}Pb, the $K = 8^-$ isomeric states are polarized to prolate deformations with $|\beta_2| \approx 0.25$. These $K = 8^-$ isomers with shapes different from those of the g.s. were later confirmed by measuring rotational bands built on them [18, 19]. Furthermore, it has been found that for shape-soft nuclei, shape changes—particularly in triaxial deformations—are important for understanding the observed behaviors of isomeric states, such as decay properties [5].

While shape evolution and coexistence of high-K states in even-even nuclei around the neutron midshell and $A \sim 180$ have been extensively studied, systematic investigations of structural properties such as shape-changing effects of 3-qp high-K states in their odd-proton neighbors are lacking. In odd-A nuclei, although the unpaired nucleon introduces additional complexity, it also serves as a sensitive probe of the underlying shell structure. The shape polarization effect induced by a single nucleon can be either parallel or opposed to that of the high-K 2-qp configuration, thereby amplifying or diminishing the shape difference between the 3-qp states and the g.s. Recently, 3-qp high-K isomers originating from the coupling between the odd proton and the aforementioned $K^\pi = 8^-$ configuration in even-mass cores have been observed in odd-mass $N = 106$ isotones from ^{175}Tm to ^{187}Tl (except ^{183}Ir) [20–26]. Additionally, substantial experimental data suggest that low-lying 1-qp states of neutron-deficient odd-mass Au and Tl isotopes exhibit shape coexistence [6–8]. However, the extent to which the observed 3-qp isomers involve shape isomerism in addition to K isomerism remains unclear, which has greatly stimulated our interest in pursuing theoretical studies on shape polarization and coexistence in 3-qp high-K states within this mass region.

In this work, we investigate the 3-qp K-isomeric states of odd-A nuclei in the $N = 106$ isotonic chain using the configuration-constrained potential energy surface (CCPES) method [27]. This method is a deformation-pairing self-consistent PES calculation that includes the axially asymmetric γ-degree of freedom. At prolate deformations, we focus primarily on high-K 3-qp configurations composed of the coupling of the unpaired proton with the $K^\pi = 8^-$ 2-qp configuration systematically observed in even-even $N = 106$ nuclei. We predict possible configurations of isomers in ^{185}Au and ^{187}Tl, with particular attention to the shape-polarization effect from multi-qp excitations. Furthermore, we explore high-K states with distinct shapes (oblate, prolate, and triaxial) that coexist at comparable excitation energies in ^{187}Tl, and analyze in detail the impact of different quasiparticle configurations on shape evolution.

II. THE MODEL

We employ the CCPES approach [27], based on the macroscopic–microscopic model. The macroscopic energy contribution was computed using the standard liquid-drop model [28] with parameters taken from Ref. [29]. The microscopic correction includes the Strutinsky shell correction [30] and the pairing correction. Single-particle levels required for microscopic energy calculations were obtained from a non-axial deformed Woods-Saxon potential [31] using a universal parameter set [32]. To avoid the collapse of pairing correlations in multi-quasiparticle states, we used the Lipkin-Nogami (LN) method [33] as an approximate particle-number projection incorporating monopole pairing. The pairing strength G was initially determined via the average-gap method [34, 35]. Although it is often further adjusted to reproduce the odd-even mass difference using a five-point formula, we note that irregularities may arise near magic numbers (e.g., Au and Tl isotopes) [34]. Therefore, following the recommendation of Ref. [34], closed-shell nuclei were excluded from the pairing strength calibration. For consistency, we adopted the standard pairing strength across all isotopes under investigation.

In the PES calculations, a deformation mesh in (β_2, γ) is used, with hexadecapole deformation β_4 variation at each mesh point. The intrinsic PES is assumed to be reflection-symmetric with respect to $\gamma = 0^\circ$; that is, the shape with $\gamma = -60^\circ$ is the same as that with $\gamma = 60^\circ$ for non-collective excitations. For broken-pair configurations, the microscopic energy incorporates contributions from unpaired nucleons occupying specific single-particle orbitals (see Ref. [27] for details). These orbitals are continuously tracked and adiabatically blocked throughout the deformation plane. Although Nilsson quantum numbers are not strictly conserved, their expectation values $\langle N \rangle$, $\langle n_z \rangle$, $\langle \Lambda \rangle$, and $\langle |\Omega| \rangle$ exhibit slow variation, allowing reliable configuration assignment. Therefore, each configuration is identified by computing the average Nilsson quantum numbers of the blocked orbitals. The total energy of a multi-qp state with unpaired nucleons can be decomposed into the deformation energy and the configuration energy, where the latter originates from qp excitations due to pair breaking and excitations of particles that define the specific configuration.

Quasiparticle excitations, particularly in deformation-soft nuclei, can induce significant shape polarization, resulting in an equilibrium deformation for the multi-qp state that differs from that of the ground state. The CCPES method effectively accounts for this polarization caused by the unpaired nucleon and offers a self-consistent description of both the deformation and excitation energy of multi-qp states [5, 36]. The excitation energy is computed as the energy difference between the PES minimum of the excited configuration and that of the ground-state configuration, enabling direct comparison with experimental values.

III. CALCULATIONS AND DISCUSSIONS

A. Systematics of 3-qp states involving $\nu\{9/2^+[624] \otimes 7/2^-[514]\}$

For nuclei in the $A \sim 180$ region, an abundance of high-K isomeric states has been discovered [37]. Among them, the two-quasineutron $K^\pi = 8^-$ ($\nu\{7/2^-[514] \otimes 9/2^+[624]\}$) isomeric states exist systematically in even-even $N = 106$ isotones, which have been investigated via configuration-constrained PES calculations in Ref. [5]. The calculated excitation energies agree well with experimental data, and strong shape polarizations have been found when approaching the $Z = 82$ shell closure. For odd-mass $N = 106$ isotones in this mass region, most observed 3-qp K isomers consistently involve a two-quasineutron configuration coupled to $K^\pi = 8^-$ states identified in the aforementioned even-even nuclei. For example, in nuclei such as ^{175}Tm [20, 38], ^{177}Lu [21, 39], ^{179}Ta [22, 40, 41], and ^{181}Re [23, 42], 3-qp K isomers have been assigned as the two-quasineutron $K^\pi = 8^-$ configuration coupled to the energetically lowest one-quasiproton configuration. Furthermore, in ^{181}Re, ^{179}Ta, and ^{177}Lu, meta-stable $K^\pi = 9/2^-$ states are found, assigned to the $\pi 9/2^-[514]$ configuration, leading to 3-qp states associated with the coupling of a $K^\pi = 8^-$ two-quasineutron configuration with $\pi 9/2^-[514]$ [21–23]. In ^{175}Tm, a K isomer that may involve coupling of the two-quasineutron $K^\pi = 8^-$ configuration with $\pi 7/2^-[523]$ has been found [20]. The half-lives of these isomers range from a few microseconds to several days, and the extent to which these high-K states are associated with shape polarization and shape isomerism remains an open question.

We have performed CCPES calculations on the 1-quasiproton and 3-qp states in $N = 106$ odd-mass isotones. Table 1 presents the calculated deformations and energies of the g.s., possible high-Ω 1-quasiproton, and low-lying high-K 3-qp states, compared with available experimental data. Our calculations reproduce the experimentally assigned spin-parity of the g.s. for these nuclei, except for ^{177}Lu, where the calculated lowest 1-quasiproton configuration is $\pi 9/2^-[514]$ rather than the experimentally assigned $\pi 7/2^+[404]$ [43]. However, the calculated $\pi 7/2^+[404]$ configuration lies only 259 keV above the $\pi 9/2^-[514]$ state. Given the strong dependence of 1-qp state energies on the ordering and spacing of single-particle levels, this deviation in their relative positions falls within an acceptable range.

Experimentally, the spin and parity of the g.s. of ^{183}Ir [44] and ^{185}Au [45–47] have been assigned to $5/2^-$ states built on the $\pi 1/2^-[541]$ configuration, while strong mixing between the $\pi 1/2^-[541]$ and $\pi 5/2^-[532]$ configurations attributed to Coriolis interactions has been proposed for the $5/2^-$ g.s. of ^{185}Au [48]. Our calculations show that the $\pi 1/2^-[541]$ configuration has the lowest energy, while the $\pi 5/2^-[532]$ state is about 500 keV higher. The present PES calculations indicate that these two low-lying 1-quasiproton states both have considerable triaxial deformations, which would reinforce substantial configuration mixing; however, configuration mixing calculations are beyond the scope of this work.

The present CCPES calculations also reasonably reproduce the high-Ω 1-qp isomeric states observed in odd-mass $N = 106$ isotones, except for the aforementioned deviation in ^{177}Lu. Notably, the CCPES calculations show that the $K^\pi = 9/2^-$ isomer of ^{185}Au and the $K^\pi = 11/2^-$ state of ^{187}Tl have moderate triaxial deformations with $\beta_2 \sim 0.2$, which are remarkably polarized compared with their g.s. This indicates the appearance of single-proton-induced shape polarization in shape-soft odd-proton nuclei when approaching the $Z = 82$ closed shell.

We now turn to the investigation of energetically low-lying 3-qp states in odd-mass $N = 106$ isotones, focusing primarily on 3-qp states consisting of the two-quasineutron $\nu\{7/2^-[514] \otimes 9/2^+[624]\}$ configuration coupled to different 1-quasiproton configurations, since the $K^\pi = 8^-$ isomeric states are systematically identified as the $\nu\{7/2^-[514] \otimes 9/2^+[624]\}$ configuration in even-even $N = 106$ isotones. As seen in Table 1, the calculated energies of these 3-qp states in ^{175}Tm, ^{179}Ta, and ^{181}Re agree well with experimental data. For ^{177}Lu, the calculated $K^\pi = 23/2^-$ $\pi 7/2^+[404] \otimes \nu\{9/2^+[624] \otimes 7/2^-[514]\}$ configuration is overpredicted, while the $K^\pi = 25/2^+$ $\pi 9/2^-[514] \otimes \nu\{9/2^+[624] \otimes 7/2^-[514]\}$ state is slightly underestimated. This can be attributed to the deviation of the $\pi 7/2^+[404]$ and $\pi 9/2^-[514]$ orbitals found in our calculations of the 1-quasiproton states.

Furthermore, the CCPES calculations predict candidate configurations for 3-qp isomeric states in odd-A $N = 106$ isotones when moving towards the $Z = 82$ shell closure. To date, no experimental evidence has been reported for three-quasiparticle high-K isomers in ^{183}Ir. We propose two possible high-K 3-qp states composed of two-quasineutron $\nu\{7/2^-[514] \otimes 9/2^+[624]\}$ coupled with proton configurations $\pi 1/2^-[541]$ and $9/2^-[514]$, respectively. For ^{185}Au, a new isomer at an excitation energy of 1504.2(4) keV with a half-life of 630(80) ns was recently identified in γ–γ coincidence analysis [26]. Possible spins for this isomer are constrained to a range from 13/2 to 21/2 based on Weisskopf estimates [26]. Our calculations suggest two possible 3-qp high-K configurations consistent with systematics of 3-qp configurations in lighter odd-mass $N = 106$ isotones. Both lie at excitation energies of about 1900 keV, which is somewhat overpredicted. However, Ref. [26] argued that the g.s. configuration of ^{185}Au is more likely $\pi 3/2^-[532]$, and the calculated energy differences of these two 3-qp states relative to the $3/2^-[532]$ configuration are 1444 and 1458 keV, respectively, in excellent agreement with observation.

For nucleus ^{187}Tl, two isomers with microsecond lifetimes ($T_{1/2} = 1.11$ μs and 0.69 μs) have been reported [24]. Spin-parities $J^\pi = 27/2^+$, $31/2^-$ are tentatively assigned to the isomer at 2584 keV with lifetime $T_{1/2} = 0.69$ μs based on the deduced total conversion coefficient [25]. Our calculation presents a $K^\pi = 27/2^+$, $\pi 11/2^-[505] \otimes \nu\{9/2^+[624] \otimes 7/2^-[514]\}$ configuration with an excitation energy of 2312 keV, in accord with the prolate high-K configuration suggested in Ref. [24]. This implies that the $T_{1/2} = 0.69$ μs isomer observed in ^{187}Tl involves the two-quasineutron $\nu\{9/2^+[624]\otimes 7/2^-[514]\}$ configuration, consistent with systematics of 3-qp isomers observed in lighter odd-mass $N = 106$ isotones, though further experimental data are required for unambiguous spin-parity and configuration assignment. We will discuss the other $T_{1/2} = 1.1$ μs isomer later in Sect. III B.

Intrinsic shape evolution is crucial for understanding the observed behavior of isomeric states, such as their decay properties. Previous studies [5] have demonstrated strong shape polarization in even-even nuclei with $A \sim 180$ and $N = 106$, especially in nuclei close to the $Z = 82$ shell closure. For systematic comparison, we plot the variation of β_2 and γ deformations of the high-K 3-qp states and the g.s. along the proton number Z in Fig. 1. When approaching the $Z = 82$ shell closure, the β_2 value of the g.s. gradually decreases, indicating evolution towards a spheroidal shape, whereas the 3-qp states are polarized to have distinct prolate shapes. The g.s. of ^{185}Au, for example, has a very γ-soft shape with an energy minimum at $\gamma \approx 24^\circ$, while the predicted two 3-qp high-K states both have approximately prolate shapes with $\gamma \approx 1^\circ$ and about a 60% increase in β_2 deformation. The nucleus ^{187}Tl has a spherical g.s. with a proton singly occupying the $\pi 3s_{1/2}$ orbital, while the calculated $K^\pi = 27/2^+$ $\pi 11/2^-[505] \otimes \nu\{9/2^+[624] \otimes 7/2^-[514]\}$ state is predicted to have a moderately axially-asymmetric shape with $\beta_2 \approx 0.23$ and $|\gamma| \approx 12^\circ$, exhibiting the greatest difference in quadrupole deformation between the 3-qp state and the g.s. In fact, the calculated high-K 3-qp configurations of ^{187}Tl present an ensemble of multiple nuclear shapes, which will be analyzed in detail in Sect. III B.

B. Shape coexistence in high-K 3-qp states of ^{187}Tl

Shape-coexisting configurations in this mass region are mainly attributed to the simultaneous appearance of large spherical and deformed shell gaps near the proton shell closure at $Z = 82$ and the neutron midshell at $N \approx 106$. Moreover, an unpaired nucleon occupying different single-particle orbitals polarizes the shape of the odd-A nucleus in different ways, leading to a more profound shape coexistence phenomenon. Abundant experimental data have demonstrated that differently-shaped configurations in these odd-A nuclei are observed not only in low-lying 1-qp states but also in higher-seniority isomeric states [7].

For ^{187}Tl, previous studies [49–52] have proposed coexistence of different nuclear shapes through analysis of observed low-lying collective structures. As the proton-hole neighbor of ^{188}Pb, the $I = 1/2^+$ g.s. of ^{187}Tl can be interpreted as the coupling of the $\pi 3s_{1/2}$ hole with the spherical 0_1^+ state of the ^{188}Pb core. The observed $K^\pi = 9/2^-$ and $K^\pi = 13/2^+$ isomeric states can be understood as filling the $\pi 9/2^-[505]$ and $\pi 13/2^+[606]$ intruder orbitals that are lowered with increasing oblate deformation, respectively [53, 54], while the rotational band built on the $I^\pi = 11/2^-$ state is suggested to be the prolate-deformed $\pi 11/2^-[505]$ configuration [24, 25]. The calculated deformations and excitation energies for these 1-quasiproton states are listed in Table 2. The CCPES calculations well reproduce the measured excitation energies and clearly show coexisting shapes for these 1-qp states. Note that the $\pi 11/2^-[505]$ configuration is predicted to have a considerable axially-asymmetric shape with $\gamma \approx 18^\circ$, which breaks K- and shape-hindrance and would explain why it decays rapidly to the oblate $K^\pi = 9/2^-$ isomeric state [24].

In addition to the high-Ω proton orbitals mentioned above, other deformation-driving high-j high-Ω orbitals, including high-Ω members of the proton $\pi h_{9/2}$ shell and high-Ω members of neutron $\nu h_{9/2}$, $\nu i_{13/2}$, and $\nu f_{7/2}$ shells, appear close to the proton and neutron Fermi surfaces at both oblate and prolate sides. Couplings of these high-Ω orbitals form energetically low-lying high-K 3-qp configurations that are polarized to different shapes. We summarize the calculated deformations and excitation energies of possible high-K 3-qp configurations in Table 2. Coexisting different types of intrinsic shape are obtained for various high-K 3-qp configurations from the CCPES calculations. Fig. 2 depicts typical PESs corresponding to 3-qp configurations with spherical, γ-soft prolate, oblate, and axially-asymmetric shapes.

Among them, the lowest prolate high-K 3-qp state given by the CCPES is the $K^\pi = 27/2^+$, $\pi 11/2^-[505] \otimes \nu\{9/2^+[624] \otimes 7/2^-[514]\}$ configuration. The calculated PES for this configuration is shown in panel (b) of Fig. 2. As discussed in Sect. III A, this configuration is most likely assigned to the observed isomeric state with excitation energy $E_x = 2584.6$ keV and lifetime $T_{1/2} = 0.69$ μs. Experimentally, it is found that the 2584.6-keV isomer decays to the $I^\pi = 25^+$ member of a rotational band assigned to the low-Ω $\pi 1/2^+[660]$ configuration [24, 25]. To understand this transition, we also compute the deformation and excitation energy of the low-Ω $\pi 1/2^+[660]$ state (see Table 2). The calculated energy of the $\pi 1/2^+[660]$ state is 1216 keV, compatible with the estimated band-head energy of the observed rotational band. Note that both the $\pi 1/2^+[660]$ and $\pi 11/2^-[505] \otimes \nu\{9/2^+[624] \otimes 7/2^-[514]\}$ configurations have very soft axially-asymmetric deformations with $\gamma \sim 15^\circ$. The γ-soft shape breaks K-conservation and allows decay from the $K^\pi = 27/2^+$ state to the $I^\pi = 25^+$ state built on the $\pi 1/2^+[660]$ configuration. The CCPES calculations predict another $K^\pi = 27/2^+$ configuration consisting of $\pi 11/2^-[505] \otimes \nu\{9/2^-[505] \otimes 9/2^+[633]\}$ with smaller $\beta_2 \approx 0.18$ and larger $|\gamma| \approx 30^\circ$. However, the large axially-asymmetric deformation violates K-conservation and may prohibit formation of the K isomeric state.

Another interesting 3-qp state we predict is the $K^\pi = 29/2^+$, $\pi 13/2^+[606] \otimes \nu\{9/2^+[624] \otimes 7/2^+[633]\}$ configuration. As seen in panel (c) of Fig. 2, its calculated PES shows a minimum at oblate deformation of $\beta_2 \approx 0.19$ and $|\gamma| \approx 60^\circ$. The combination of high K value, axially symmetric shape, and low calculated energy of $E_x = 1839$ keV supports the existence of a long-lived K isomer. We therefore suggest that this $K^\pi = 29/2^+$ configuration could be assigned to the observed isomeric state with lifetime $T_{1/2} = 1.1$ μs, although the position and spin-parity cannot be firmly determined because γ rays linking this isomer to low-lying states are still missing [24, 25]. More recently, it has been found that this isomer decays to the low-lying $13/2^+$ isomer at 1061 keV [25], implying that the $T_{1/2} = 1.1$ μs isomeric state may be oblate-deformed and composed of the same $\pi 13/2^+[606]$ configuration, compatible with the predicted $K^\pi = 29/2^+$, $\pi 13/2^+[606] \otimes \nu\{9/2^+[624] \otimes 7/2^+[633]\}$ state. We thus propose that two long-lived 3-qp high-K isomeric states with different shapes coexist at intermediate excitation energies in ^{187}Tl. Further measurements of observables such as gyromagnetic ratios or electromagnetic transition properties of rotational bands built on these two long-lived states would help unambiguously determine the shapes and intrinsic structures of these observed isomers.

Other low-lying 3-qp high-K states are predicted by the CCPES calculations. Among them, the $K^\pi = 25/2^-$, $\pi 9/2^-[505] \otimes \nu\{9/2^+[624] \otimes 7/2^+[633]\}$ configuration is of particular interest due to its very low energy and high spin value. Since it is calculated to be energetically lower than the observed lowest $I^\pi = 13/2^+$ state, the predicted $K^\pi = 25/2^-$ state could form a “spin trap” [1]. As Dracoulis et al. [55] have pointed out, very low excitation energy could result in long-lived states that preferentially undergo β decay and thus be missed experimentally. This presents a challenge for both experimental and theoretical studies and, in effect, a test of model reliability.

IV. SUMMARY

We present a systematic theoretical study of shape polarization and coexistence in high-K 3-qp states of odd-mass $N = 106$ isotones (^{175}Tm, ^{177}Lu, ^{179}Ta, ^{181}Re, ^{183}Ir, ^{185}Au, ^{187}Tl) using the configuration-constrained potential energy surface (CCPES) method. The investigation focuses on 3-qp states formed by coupling a single proton to the systematic two-quasineutron $K^\pi = 8^-$ isomeric configuration known in even-even $N = 106$ cores. The calculations demonstrate excellent agreement with experimental data for well-established isomers in lighter isotones ($Z = 69$–75), validating the theoretical approach. As the proton number increases towards the $Z = 82$ shell closure, the ground states become progressively softer and less deformed, while the high-K 3-qp states exhibit significant shape polarization, maintaining well-defined prolate deformations. This leads to substantial shape differences between the isomers and ground states in nuclei like ^{185}Au and ^{187}Tl.

Furthermore, we analyze in detail the intrinsic shapes of 3-qp states in ^{187}Tl. The CCPES calculations identify a multitude of low-lying high-K configurations with distinctly different shapes (including prolate, oblate, and triaxial) coexisting within a narrow energy range. Two specific long-lived isomers observed in ^{187}Tl are assigned to configurations with different shapes: the $T_{1/2} = 0.69$ μs isomer is associated with a prolate-deformed $K^\pi = 27/2^+$ state, while the $T_{1/2} = 1.1$ μs isomer is proposed to be an oblate-deformed $K^\pi = 29/2^+$ state characterized by a high K value, an axial shape, and low excitation energy of 1839 keV, which favors a long lifetime. The study also predicts a very low-lying $K^\pi = 25/2^-$ 3-qp state in ^{187}Tl that could act as a "spin trap," presenting a challenge for future experimental detection.

In conclusion, this research provides a consistent and systematic description of high-K isomers in the $N = 106$ chain, highlighting the crucial role of unpaired nucleons in driving shape polarization and revealing a complex landscape of shape coexistence in neutron-deficient odd-mass nuclei near shell closures. The predictions offered herein serve as strong motivation and guidance for future spectroscopic studies.

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