Prolate-oblate shape coexistence at high spin in ^{175}Hf

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The recent experimental observation of collective rotational bands up to $I > 60\hbar$ in ^{175}Hf presents theoretical challenges. It is shown here that total Routhian surface calculations are able to explain the yrast high-spin behavior, with collective oblate states favored at $I \sim 35\hbar$ and strongly deformed prolate states at the highest spins. The collective oblate rotation terminates in noncollective prolate states. Comparisons are made with ultimate cranker calculations, and theoretical quadrupole moments are evaluated.

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Shape is a basic nuclear property. Nuclear shapes may change as a function of angular momentum and excitation energy, and different shapes may coexist at the same spin and similar energies [1–3]. However, the oblate shape is relatively rare [2,4], and its collective rotation is mainly observed as a low-spin phenomenon in weakly deformed nuclei. Nevertheless, in transitional nuclei a considerable number of collective oblate rotational bands have been identified, principally composed of $\Delta I = 1$ sequences [5,6] built on rotation-aligned quasiparticles. The best such examples in nuclei with well-deformed (prolate) ground states are, perhaps, in ^{134}Nd [7] and ^{136}Sm [8], but the information is sparse. In the present work, recent data on the well-deformed nucleus ^{175}Hf [9] are interpreted as evidence for collective oblate rotation at $I \sim 35\hbar$.

There has already been considerable interest in the shapes of hafnium ($Z = 72$) isotopes at high angular momentum. The stable hafnium isotopes have mass numbers $A = 176-180$. On the neutron-rich side of stability, it has been predicted [10,11] that well-deformed, collective oblate rotation, with triaxiality parameter $\gamma \approx -60^\circ$ in the Lund convention, may form the yrast structure (i.e., the structure with lowest energy as a function of angular momentum) above $I \sim 15\hbar$. Although such behavior has not yet been identified experimentally, this could simply be a consequence of the difficulty in studying neutron-rich nuclei at high angular momentum. On the neutron-deficient side, it has been proposed [12] that triaxial superdeformed (TSD) shapes, with $\gamma \approx +30^\circ$, dominate the observed high-spin structure. However, gaps in the identified γ-ray transitions, connecting the high-spin and low-spin structures, have left many open questions.

The recent discovery of $\Delta I = 2$ rotational bands in ^{175}Hf, connected by γ-ray transitions to the low-spin states, enables for the first time the excitation energy and spin values in hafnium isotopes to be reliably determined up to $I \sim 60\hbar$ [9]. In related work, the quadrupole moments were measured for high-spin bands in ^{174}Hf and ^{175}Hf, and these were found [9,13] to be larger than expected from theoretical estimates based on the ultimate cranker (UC) model. In the light of these emerging results, the present work addresses the high-spin behavior of ^{175}Hf by comparison with total Routhian surface (TRS) model calculations. In contrast to the UC results [9], no TSD minimum is found. Rather, there is competition between a strongly deformed prolate minimum and an oblate minimum.

For the TRS calculations, the single-particle energies are obtained from the deformed Woods-Saxon potential [14], with the Lipkin-Nogami (LN) treatment of pairing [15]. This avoids the spurious pairing phase transition encountered in the simpler BCS approach. The pairing strength G is determined by the average-gap method [16]. The total energy of a configuration consists of a macroscopic part, which is obtained from the stardard liquid-drop model [17], and a microscopic part, resulting from the Strutinsky shell correction [18], $\delta E_{\rm shell} = E_{\rm LN} - \tilde{E}_{\rm Strut}$. Calculations are performed in the lattice of quadrupole (β_2, γ) deformations with hexadecapole (β_4) variation. For a given rotational frequency, pairing is treated self-consistently by solving the cranked LN equation at any given point of the deformation lattice and then the equilibrium deformation is determined by minimizing the obtained TRS (for details, see, e.g., Refs. [19,20]). Quadrupole pairing in doubly stretched coordinate space [21] has a negligible effect on energies but is included (with the strength determined by restoring the local Galilean invariance) because it has an important influence on collective angular momenta [20].

TRS diagrams for ^{175}Hf are shown in Fig. 1 at specific rotational frequencies, $\hbar\omega = 0.4$, 0.5, 0.6, and 0.7 MeV, corresponding to the spin range $I \sim (30-60)\hbar$. The oblate minimum ($\gamma \approx -60^\circ$) is evident. It is interesting to note that this minimum can, in the calculations, be consistently traced through to the heavier hafnium isotopes [11] where it occurs at significantly lower energy. In essence, low-K, rotation-aligned oblate structures compete at these nucleon numbers ($Z \approx 72$, $N \approx 110$) with high-K prolate configurations, which typically form isomers. In Fig. 1, for ^{175}Hf, the high-K prolate minimum is also evident, at $\gamma \approx -120^\circ$. This is indeed related to the experimental observation of high-K isomers in ^{175}Hf [22,23]. However, an appropriate theoretical description of high-K states requires configuration-constrained calculations [11], which will be the subject of a separate report.

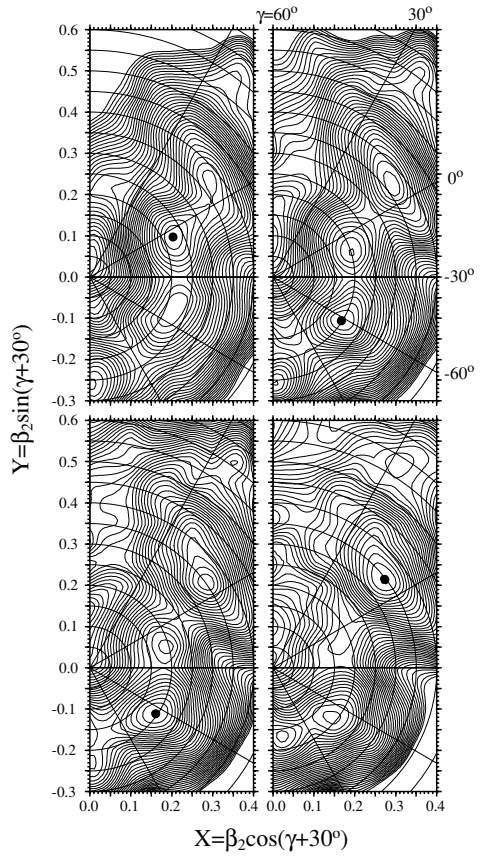

FIG. 1. Total Routian surfaces for ^{175}Hf negative-parity states, at $\hbar\omega = 0.4$ and 0.5 MeV (upper panels) and 0.6 and 0.7 MeV (lower panels) corresponding to $I \sim (30\text{–}60)\,\hbar$. The black dot represents the overall minimum in each panel, and the contours are at 200-keV intervals.

The experimental [9] and theoretical energies of rotational states are compared in Fig. 2. According to the TRS calculations, which agree qualitatively with the experimental data, the following interpretation may be given. At low spin, collective prolate rotation is yrast ($\gamma \approx 0^\circ$), here represented by the $7/2^+[633]$ one-quasiparticle band. At $I \sim 30\hbar$, collective oblate rotation (band 1, $\gamma \approx -60^\circ$) becomes yrast. However, this is taken over by strongly deformed, collective prolate rotation at the highest spins (band 2, $\beta_2 \approx 0.36$) and the oblate structure terminates in noncollective prolate states ($\gamma \approx -120^\circ$). This latter novel feature of oblate-to-prolate termination contrasts with the well-studied termination of collective prolate rotation in noncollective oblate states ($\gamma \approx +60^\circ$) [24].

The kinematic moments of inertia depend on the energy-versus-spin gradients of Fig. 2, so that although the calculated and experimental moments of inertia for the $7/2^+$ band and band 2 are in quite good agreement, the variation with spin for band 1 is poorly reproduced. This may be a consequence of the high dependence of the oblate band on rotation-aligned quasiparticles, with successive proton and neutron alignments calculated at $I \sim 30\hbar$ and $40\hbar$, respectively. Nevertheless, the overall agreement is good in the sense that the band 1 moment of inertia is intermediate between the values for

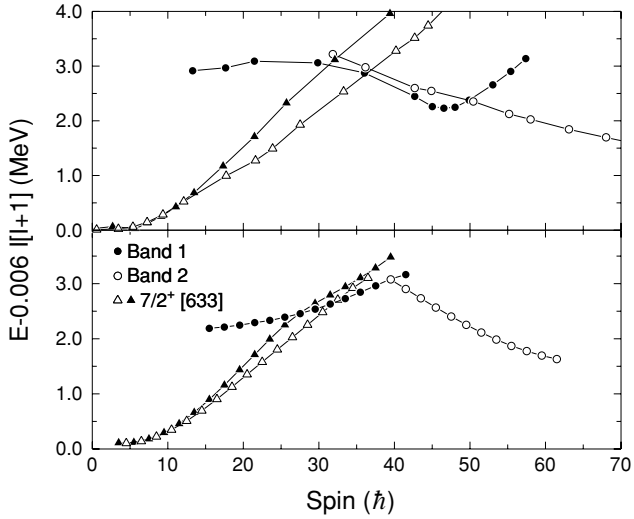

FIG. 2. Energy as a function of spin for rotational bands in ^{175}Hf, relative to an arbitrary rotor with fixed moment of inertia. (Top) Theoretical values from TRS calculations. (Bottom) Experimental values from Ref. [9]. Bands 1 and 2 have negative parity.

the $7/2^+$ band and band 2. (Moment-of-inertia comparisons from UC calculations have not been reported for ^{175}Hf [9].)

It is also notable that the TRS calculations, in contrast to the UC calculations [9,13], give no potential-energy minimum at $\beta_2 \approx 0.45$, $\gamma \approx 30^\circ$, for either negative- or positive-parity states in ^{175}Hf. (The shallow triaxial minimum that develops at $\beta_2 \approx 0.6$ is far from yrast—about 4.5 MeV above yrast at $I = 50\hbar$.) The origin of this difference between TRS and UC calculations is a significant issue, and some comparison with the situation in ^{163}Lu is appropriate. The nuclide ^{163}Lu has probably the best-studied TSD structures, and the large deformation was first associated with the proton $1/2^+[660]$ intruder orbital by Schmitz *et al.* [25,26] aided by TRS calculations. Later, this potential-energy minimum was seen to correspond to a TSD minimum from UC calculations [27,28]. However, the UC minimum was a little more deformed and more triaxial ($\epsilon_2 \approx 0.41$, $\gamma \approx 21^\circ$) than the TRS minimum [26] ($\beta_2 \approx 0.37$, $\gamma \approx 14^\circ$; note that $\epsilon_2 \approx 0.94\beta_2$). In the present work, TRS calculations have been repeated for ^{163}Lu, and these agree with the deformation values reported in Ref. [26]. Indeed, we have performed TRS calculations for several nuclides in this mass region and find that ^{163}Lu gives the most favorable TSD minimum, especially at low rotational

TABLE I. Average deformation parameters and quadrupole moments (in e b) for yrast structures in ^{175}Hf. The modulus $|Q_{\text{macro}}|$ is calculated with the macroscopic formula [29] using the given β_2, γ values; Q_{micro} is the sum of the single-particle contributions. The experimental values, $|Q_{\text{exp}}|$, are from Refs. [9,13].

Spin range	β_2	γ°	$\lvert Q_{\text{macro}}\rvert$	Q_{micro}	$\lvert Q_{\text{exp}}\rvert$
$(0\text{–}20)\hbar$	0.26	0	7.0	7.8	—
$(20\text{–}35)\hbar$	0.23	−45	6.8	−7.3	∼9
$(35\text{–}60)\hbar$	0.36	7	9.2	11.1	∼13

TABLE II. Variation with spin of energy, deformation parameters, and quadrupole moments (in e b) for calculated yrast and near-yrast collective structures in ^{175}Hf.

Band	$\hbar\omega$ (MeV)	I ($\hbar$)	E (MeV)	β_2	γ°	Q_{20}	Q_{22}	Q_{micro}
$\frac{7}{2}^+$[633]	0.2	9	0.85	0.27	−1	8.0	0.0	8.0
	0.3	18	2.97	0.25	−4	7.4	0.3	7.6
	0.4	24	5.04	0.24	−4	7.0	0.3	7.2
Band 1	0.3	22	5.97	0.24	−40	−5.9	−2.7	−8.1
	0.4	36	10.86	0.22	−50	−5.6	−1.2	−6.5
	0.5	45	14.68	0.20	−62	−5.2	0.3	−5.0
Band 2	0.4	36	11.02	0.38	11	12.8	−1.7	11.4
	0.5	45	14.90	0.37	7	12.3	−1.1	11.4
	0.6	55	20.70	0.35	6	11.7	−1.0	10.9

frequency. Another favored case from the TRS calculations is ^{165}Ta.

A further point of comparison concerns the collective oblate minimum. Although this is absent in ^{163}Lu with both UC and TRS calculations, it is present in ^{175}Hf with both calculation methods. However, only with the TRS method is the oblate minimum in ^{175}Hf found to become deep enough to be yrast, albeit over a limited spin region.

Detailed yet significant differences between the potential-energy minima from UC and TRS calculations thus seem to be pervasive and most likely arise from the mean-field potentials themselves (Nilsson and Woods-Saxon, respectively, the latter being more realistic). These can affect, in particular, the relative energies of the high-j intruder orbitals, which play key roles in generating both rotation alignments and large deformations. The different treatments of pairing correlations may also play a role (cf. Ref. [27] for details of the UC method). The present work highlights the need for an improved understanding of these differences, but further analysis goes beyond the scope of this Brief Report.

An important observable is the transition quadrupole moment Q_t, which can be estimated from the collective shape of the nucleus according to the "macroscopic" formula

$$Q_t = 6ZeA^{2/3}(15\pi)^{-1/2}r_0^2\beta_2(1+0.360\beta_2)\cos(30^\circ+\gamma)$$

with radius parameter $r_0 = 1.20$ fm [29]. This is called Q_{macro} in the present work. However, it is known that, in principle, the quadrupole moments should be determined from the "microscopic" wave functions (i.e., from the expectation values of the quadrupole operator using the calculated wave functions). This is what is done to obtain Q_{micro} in the present work. The values are compared in Table I, which also includes preliminary experimental data [9,13]. It is evident that Q_{micro} is reasonably close to the experimental values (and closer than Q_{macro}), lending support to the present interpretation. The evaluation of Q_{micro} follows the method of Laird *et al.* [30] with $Q_{\text{micro}} = Q_{20} + \sqrt{\frac{2}{3}}Q_{22}$. Table II gives additional details about the calculated shapes and quadrupole moments, including their variation with spin, which may be useful for future comparison with experimental data.

In summary, recent experimental results are compared with TRS calculations, giving a good description of high-spin rotational bands in ^{175}Hf. Collective oblate rotation ($\beta_2 \approx 0.23$) is suggested to form the yrast structure at $I \sim 35\hbar$, but this mode terminates in noncollective prolate states, and highly deformed ($\beta_2 \approx 0.36$) collective prolate rotation becomes yrast.

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