

## Limit to high-spin isomerism in hafnium isotopes

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Configuration-constrained nuclear shape calculations are used to show that reinforcing neutron and proton orbital structures create exceptional conditions for the formation of multiquasiparticle isomers in neutron-rich hafnium isotopes, with axially symmetric, prolate shapes. Highly excited, long-lived states are predicted. However, at angular momenta close to  $40\hbar$ , orbital alignment effects for collective oblate rotation lead to a deep potential minimum that competes energetically with the prolate multiquasiparticle states.

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Nuclear isomers are excited, metastable states [1]. In a recent compilation [2], more than 700 isomers were recorded as having half-lives greater than one millisecond. In the vast majority of these cases, the isomerism is a result of angular-momentum selection rules for the decay radiations, with high multipolarity radiations having low transition rates. In only one case is the transition rate so low that the isomer survives in nature:  $^{180}\text{Ta}$  has an  $I=9\hbar$ , 75 keV excitation with a half-life in excess of  $10^{15}$  yr for, potentially, multipolarity-eight (256-pole) electromagnetic decay to the  $I=1\hbar$  ground state.

The region of prolate-deformed nuclei around  $^{180}\text{Ta}$  ( $Z=73$ ,  $N=107$ ) is well known to contain some long-lived, highly excited ( $>1$  MeV) isomers, with the hafnium ( $Z=72$ ) isotopes being of particular note [1,3]. For example, there is a 31-yr,  $I^\pi=16^+$  isomer at 2.4 MeV in  $^{178}\text{Hf}$ , which has a stable ground state, and new isomers have recently been discovered in neutron-rich hafnium isotopes [4]. However, the angular-momentum and excitation-energy limits to the formation of such isomers remain to be determined, both as a result of the difficulty in obtaining appropriate experimental information, and due to the lack of a suitable, realistic theoretical framework. It is the latter aspect that is addressed in the present work. At the same time, significant experimental advances are being made with the use of deep-inelastic [4] and fragmentation [5] reactions.

In the general understanding, the formation of highly excited isomers in the prolate-deformed mass-180 region of nuclei is, to a large extent, due to the conservation of the angular-momentum projection quantum number  $K$ , associated with an axially symmetric shape, and long-lived isomers usually have low excitation energies compared to collective excitations of the same angular momentum [1]. The  $^{178}\text{Hf}$  31-yr isomer, for example, is yrast, i.e., the  $I^\pi=K^\pi=16^+$  isomer, at 2.4 MeV, is the lowest-energy  $I=16\hbar$  state in that nucleus. In the following, we are concerned, primarily, with the nuclear structure conditions that lead to long-lived, highly excited isomers. However, this study should also be seen in the wider context of investigations of the stimulated

deexcitation of isomers [1,6,7] and the consequent need to understand the mechanisms and limitations of the isomer formation.

In an early theoretical work by Åberg [3], it was shown how hafnium high- $K$  multiquasiparticle (i.e., many-broken-pair) excitations can be energetically lower than prolate collective rotations of the same angular momentum, and hence be yrast states. In contrast, Hilton and Mang [8] focused on the collective rotation of the  $^{180}\text{Hf}$  nucleus (without discussing multiquasiparticle states) and predicted, remarkably, that well-deformed oblate collective rotation coexists and becomes lower in energy than the prolate collective rotation in the high-spin region of  $I>26\hbar$ . Hence, the question arises as to whether the prolate noncollective isomers compete with the oblate collective rotation. The present work treats both collective and noncollective modes in a consistent theoretical framework, and demonstrates that multiquasiparticle states may remain yrast up to  $I\geq 40\hbar$ .

A realistic treatment of a multiquasiparticle state can be achieved with a configuration-constrained calculation of the potential-energy surface [9]. The single-particle energies are obtained from the deformed Woods-Saxon potential [10], with the Lipkin-Nogami (LN) treatment of pairing [11]. (This avoids the spurious pairing phase transition encountered in the usual BCS approach.) The pairing strength  $G$  is determined by the average-gap method [12,13]. The constrained configuration energy in the LN approach can be written as

$$E_{\text{LN}} = \sum_{j=1}^S e_{k_j} + \sum_{k \neq k_j} 2V_k^2 e_k - \frac{\Delta^2}{G} - G \sum_{k \neq k_j} V_k^4 + G \frac{N-S}{2} - 4\lambda_2 \sum_{k \neq k_j} (U_k V_k)^2, \quad (1)$$

with

$$N-S = \sum_{k \neq k_j} 2V_k^2, \quad (2)$$

where  $S$  is the proton or neutron seniority for a given configuration (i.e., the number of blocked orbitals with index  $k_j$ ), and  $N$  is the proton or neutron number.

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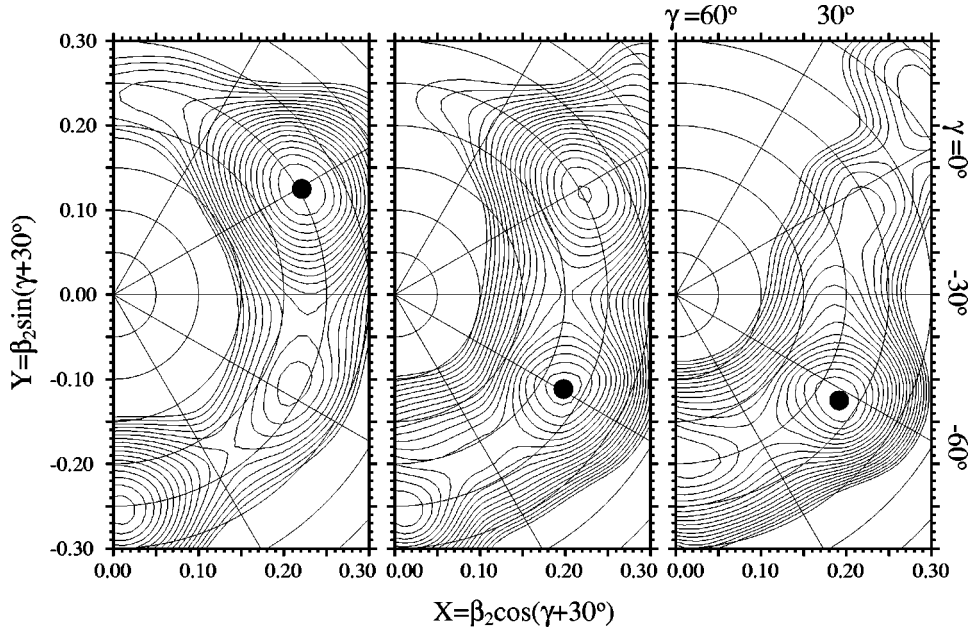


FIG. 1. Calculated total Routhian surfaces at  $\hbar\omega=0.2$  MeV (left),  $\hbar\omega=0.3$  MeV (center), and  $\hbar\omega=0.4$  MeV (right) for  $^{182}\text{Hf}$ , with 200 keV contours. For the first two panels, there are three potential-energy minima, corresponding to prolate-collective rotation ( $\gamma=0^\circ$ , top), oblate-collective rotation ( $\gamma=-60^\circ$ , middle), and prolate noncollective rotation ( $\gamma=-120^\circ$ , bottom). The absolute minimum in each panel is represented by a dot. For the third panel, the prolate-collective minimum disappears, and a highly deformed near-prolate state ( $\beta_2 \approx 0.38$ ,  $I \geq 45\hbar$ ) appears but its energy is far from yrast. Note that each potential-energy minimum has, in general, a different angular-momentum value; and the quantitative evaluation of the prolate noncollective mode requires a configuration-constrained approach where the potential-energy minimum is represented at  $\gamma \sim 0^\circ$  [9]. See also Table I.

The total energy of a configuration consists of a macroscopic part which is obtained from the standard liquid-drop model [14] and a microscopic part resulting from the Strutinsky shell correction [15],  $\delta E_{\text{shell}} = E_{\text{LN}} - \bar{E}_{\text{Strut}}$ . Calculations are performed in the lattice of quadrupole ( $\beta_2, \gamma$ ) deformations with hexadecapole ( $\beta_4$ ) variation. We have investigated low-lying high- $K$  states for the even hafnium isotopes. Results show that all the studied multiquasiparticle states have well-deformed prolate shapes. The axially symmetric shape is one of the important conditions for the existence of  $K$  isomers. The calculated excitation energies agree with the data for the observed isomers. For example, for the  $^{178}\text{Hf}$  31-yr isomer, the calculated energy of 2470 keV agrees well with the experimental value of 2447 keV [2]. Additional comparisons are given in Ref. [9].

In order to predict isomers, we also need to see whether the multiquasiparticle states are yrast. Therefore, for the competing collective rotational states we have performed pairing-deformation self-consistent total Routhian surface (TRS) calculations, i.e., for a given rotational frequency, pairing is treated self-consistently by solving the cranked LN equation at any given point of the deformation lattice ( $\beta_2, \gamma, \beta_4$ ) and then the equilibrium deformation is determined by minimizing the obtained TRS (for details, see, e.g., [16,17]). Quadrupole pairing in doubly stretched coordinate space [18] has a negligible effect on energies, but it is included (with the strength determined by restoring the local Galilean invariance) because it has an important influence on collective angular momenta [17].

Calculations for the mass-180 region show that oblate or

approximately oblate rotational states exist at high spin. The osmium ( $Z=76$ ) and platinum ( $Z=78$ ) isotopes have approximately oblate rotations with small deformations of  $\beta_2 < 0.20$  and become triaxial with increasing spin, which is consistent with the results of previous work [19]. The  $Z=72$  hafnium isotopes, however, have axially symmetric collective rotational bands. In the low-spin region, well-deformed prolate rotation is favored. However, at  $I \sim 20\hbar$  (depending on the neutron number) well-deformed ( $\beta_2 > 0.20$ ) oblate collective minima appear and become energetically lower than the prolate collective minima for heavy hafnium isotopes. As shown below for  $^{182}\text{Hf}$ , the prolate and oblate minima are, in general, well separated in the  $\beta_2 - \gamma$  quadrupole-deformation space. Therefore, our results are insensitive to shape-mixing effects (cf. Valor *et al.* [20]).

The appearance of energetically favored, oblate collective minima is in agreement with the previous Hartree-Fock-Bogoliubov results of Hilton and Mang [8] for  $^{180}\text{Hf}$ . We find that, for a range of isotopes covering at least  $^{178}\text{Hf}$  to  $^{186}\text{Hf}$ , the oblate rotation mode has a stable shape up to very high spins. The oblate rotation has a large kinematic moment of inertia of  $\sim 100\hbar^2 \text{ MeV}^{-1}$ , due to nucleon alignments (see later), which lead to the moment of inertia being slightly larger than the corresponding classical oblate rigid-body value of  $\sim 80\hbar^2 \text{ MeV}^{-1}$ . Figure 1 shows the calculated TRS's for the neutron-rich isotope,  $^{182}\text{Hf}$ . For this isotope, the calculated TRS displays a clear oblate minimum at  $\hbar\omega = 0.20$  MeV (see the left panel of Fig. 1). This minimum gets deeper with increasing rotational frequency and becomes the energetically favored collective state at  $\hbar\omega \approx 0.30$  MeV (see

TABLE I. Calculated energies and deformations for states in  $^{182}\text{Hf}$ .

$I^\pi$	$E$ (MeV)	$\beta_2$	$\beta_4$	$\gamma^a$
Prolate collective				
$0^+$	0.0	0.250	-0.073	$0^\circ$
$10^+$	1.40	0.251	-0.073	$-1^\circ$
$24^+$	6.40	0.230	-0.075	$-6^\circ$
Oblate collective				
$18^+$	4.80	0.235	0.002	$-55^\circ$
$28^+$	5.30	0.230	0.007	$-58^\circ$
$40^+$	10.45	0.238	0.017	$-65^\circ$
$50^+$	15.10	0.230	0.021	$-66^\circ$
Prolate multiquasiparticle <sup>b</sup>				
$8^-$	1.29 (1.174 <sup>c</sup> )	0.241	-0.063	$0^\circ$
$13^+$	2.61 (2.573 <sup>c</sup> )	0.239	-0.064	$0^\circ$
$15^+$	2.73	0.238	-0.064	$0^\circ$
$23^-$	4.52	0.229	-0.064	$0^\circ$
$29^+$	6.57	0.218	-0.053	$0^\circ$
$39^-$	10.23	0.205	-0.041	$10^\circ$

<sup>a</sup>Note:  $\gamma=0^\circ$  corresponds to prolate collective rotation, and  $\gamma=-60^\circ$  corresponds to oblate collective rotation. Also,  $\gamma=-120^\circ$  conventionally represents prolate noncollective rotation, and such minima can be seen in Fig. 1. However, the ‘‘prolate multiquasiparticle’’ values in the table come from the configuration-constrained approach, with  $\gamma=0^\circ$  representing the prolate noncollective (multiquasiparticle) mode [9].

<sup>b</sup>Nilsson configurations can be grouped as proton ( $\pi$ ) and neutron ( $\nu$ ) pairs with  $K^\pi=8^-$ :  $\pi^{8^-}$ ;  $13^+$ :  $\pi^{8^-} \otimes \nu^{5^-}$ ;  $15^+$ :  $\pi^{8^-} \otimes \nu^{7^-}$ ;  $23^-$ :  $\pi^{8^-} \otimes \nu^{7^-} \otimes \nu^{8^-}$ ;  $29^+$ :  $\pi^{8^-} \otimes \pi^{6^-} \otimes \nu^{7^-} \otimes \nu^{8^-}$ ;  $39^-$ :  $\pi^{8^-} \otimes \pi^{6^-} \otimes \nu^{8^-} \otimes \nu^{8^+} \otimes \nu^{9^+}$ ; with the following pairings:  $\pi^{6^-}=5/2[402]$ ,  $7/2[523]$ ;  $\pi^{8^-}=7/2[404]$ ,  $9/2[514]$ ;  $\nu^{5^-}=1/2[510]$ ,  $11/2[615]$ ;  $\nu^{7^-}=3/2[512]$ ,  $11/2[615]$ ;  $\nu^{8^-}=7/2[503]$ ,  $9/2[624]$ ;  $\nu^{8^+}=7/2[514]$ ,  $9/2[505]$ ;  $\nu^{9^+}=7/2[633]$ ,  $11/2[615]$ .

<sup>c</sup>Experimental excitation energies [4].

the central panel of Fig. 1). The angular-momentum values, energies, and shape parameters are given in Table I. The prolate collective mode terminates at  $\hbar\omega \sim 0.4$  MeV ( $I \sim 26\hbar$ ), i.e., where the potential energy minimum disappears (see the right panel of Fig. 1). A similar effect was previously noted in  $^{186}\text{Os}$  TRS calculations [21].

Comparison can now be made with configuration-constrained calculations. Figure 2 shows the energies of prolate-collective, oblate-collective, and multiquasiparticle excitations. We can see that at low spins prolate rotation is energetically favored, but at higher spins multiquasiparticle excitations become yrast. With increasing neutron number, the prolate-collective deformations ( $\beta_2$ ) decrease slightly, resulting in decreased moments of inertia and hence increased rotational excitation energies. In contrast, with increasing neutron number (i.e., raising the Fermi level) higher- $\Omega$  orbitals will condense around the Fermi level (where  $\Omega$  is the individual nucleon contribution to  $K$ ) which implies that multiquasiparticle states can gain more angular momentum at a given excitation energy. The above two facts lead to high- $K$  excitations being progressively more favored

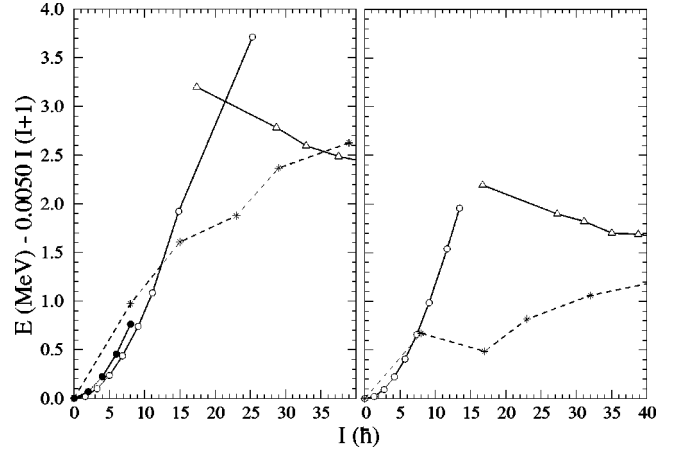


FIG. 2. The energies of prolate-collective (open circles), oblate-collective (open triangles), and prolate multiquasiparticle (stars) states for  $^{182}\text{Hf}$  (left) and  $^{186}\text{Hf}$  (right). For  $^{182}\text{Hf}$ , the filled circles are for the observed ground-state band [4]. An arbitrary constant-rotor energy has been subtracted at each spin value, to emphasize the different behaviors.

energetically than prolate-collective rotations, as the neutron number increases, and they are yrast over a large angular-momentum range for hafnium isotopes with  $N \geq 104$ . The very low excitation energies, combined with axially symmetric shapes, suggests high-multipolarity decays and long half-lives, though the slightly smaller  $\beta_2$  values for the more neutron-rich isotopes may lead to significantly increased  $K$  mixing. Only after reaching  $I \geq 35\hbar$  does the yrast status of the multiquasiparticle excitations become limited by oblate-collective rotation, for isotopes with  $104 \leq N \leq 110$  (see  $^{182}\text{Hf}$  in Fig. 2) and even this limitation does not appear to apply to the more neutron-rich isotopes (see  $^{186}\text{Hf}$  in Fig. 2). Although the calculated oblate bands become lower in energy with increasing neutron number, the multiquasiparticle excitations become lower still (comparing  $^{186}\text{Hf}$  with  $^{182}\text{Hf}$  in Fig. 2). In the present work, we restrict ourselves to the calculation of high- $K$  configurations with seniority up to 10 (corresponding to  $I \sim 40\hbar$ ) which appear to be within experimental reach. For angular momenta approaching  $40\hbar$ , some of the multiquasiparticle configurations can become slightly  $\gamma$  deformed (see Table I). The  $\gamma$  deformations may limit the half-lives of the isomers, due to the consequent  $K$ -mixing effects, but this also opens up interesting perspectives for stimulated deexcitations [1,6].

The appearance of deep oblate-collective minima is due to both neutron and proton rotational alignments. These reinforcing alignment effects lead to the special favoring of the oblate mode in the neutron-rich hafnium isotopes. In  $^{182}\text{Hf}$ , for example, two  $i_{13/2}$  neutrons align at  $\hbar\omega \approx 0.2$  MeV, two  $h_{11/2}$  protons align at  $\hbar\omega \approx 0.25$  MeV, and at  $\hbar\omega \approx 0.3$  MeV a second pair of  $i_{13/2}$  neutrons align. With increasing neutron number the  $i_{13/2}$  neutrons align earlier, which results in earlier crossings between prolate and oblate collective bands (comparing, for example,  $^{186}\text{Hf}$  with  $^{182}\text{Hf}$  in Fig. 2). It can be seen that both the multiquasiparticle and the oblate-collective states in  $^{186}\text{Hf}$  have significantly lower energies than those in  $^{182}\text{Hf}$ . Thus,  $^{186}\text{Hf}$  may provide the best case

for experimental investigation of very long-lived isomers and the oblate-rotation mode.

At prolate deformations, when valence nucleons lie in the bottom part (low- $\Omega$  region) of a high- $j$  subshell, usually one pair of low- $\Omega$  nucleons will align at  $I \sim 14\hbar$  due to strong Coriolis interactions, and the rotation-aligned bands (S bands) become yrast [22]. However, when nucleon numbers are increased and the upper orbitals (with high  $\Omega$ ) are filled, the prolate alignments will no longer be favored. In contrast, at oblate deformations it is the upper orbitals that have low- $\Omega$  values, and consequently oblate rotational alignments become favored. For the neutron-rich hafnium isotopes, the neutron Fermi level lies in the upper part of the  $i_{13/2}$  subshell (the  $N=82-126$  shell is about 70% filled) and, at the same time, the proton Fermi level lies in the upper part of the  $h_{11/2}$  subshell (the  $Z=50-82$  shell is also about 70% filled). Hence, both neutrons and protons favor oblate rotational alignments. It is no accident that the very same shell fillings that lead to very-high- $K$  yrast configurations also lead to competing oblate rotation-aligned states.

The reinforcing effect of neutron and proton shell fillings on nuclear shapes has been well documented in the mass-80 region [23]. For comparison with the mass-180 region, we performed calculations for the  $^{88}\text{Ru}$  nucleus, where a strong

reinforcing effect of the proton  $g_{9/2}$  and neutron  $g_{9/2}$  subshell fillings is expected, with the respective valence shells each approximately 70% filled (i.e., corresponding to the situation for  $^{186}\text{Hf}$ ). Similar oblate rotation is predicted. However, it is calculated to be far from yrast, and is therefore unlikely to be observed experimentally. Symmetric (proton and neutron)  $\sim 70\%$  shell filling appears not to be within experimental reach in any other region of medium-mass or heavy nuclei. Therefore, the neutron-rich hafnium isotopes constitute the most favorable candidates for the experimental verification of the predicted exotic mode of rigidlike oblate rotation.

In summary, significantly low excitation energies combined with prolate axially symmetric shapes lead to a prediction of the systematic existence of long-lived, multiquasiparticle isomers in the hafnium isotopes with  $N \geq 104$ . However, for  $I \geq 35\hbar$ , well-deformed oblate-collective rotation may take over as the energetically favored mode for accommodating angular momentum. Both the prolate and oblate modes depend on reinforcing neutron and proton contributions. The predicted structures appear to be within experimental reach.

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