Deformation and its influence on *K* isomerism in neutron-rich Hf nuclei

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We investigate the influence of deformation on the possible occurrence of long-lived *K* isomers in Hf isotopes around $N = 116$, using configuration-constrained calculations of potential-energy surfaces. Despite having reduced shape elongation, the multiquasiparticle states in ^{186,188}Hf remain moderately robust against triaxial distortion, supporting the long expected occurrence of exceptionally long-lived isomers. The calculations are compared with available experimental data.

Atomic nuclei have special stability at some proton or neutron numbers named magic numbers. Analogously, there exist some *K*-magic (*K* is the total angular momentum projection onto the symmetry axis of a deformed nucleus) numbers associated with exceptionally long-lived high-*K* isomers [1,2]. Such isomers are formed through broken-pair or multiquasiparticle (multi-qp) excitations. The long half-life usually originates from a combination of relatively low excitation energy, high *K* value, and well-deformed axially symmetric shape. These factors favor the conservation of the *K* quantum number and hence the hindrance of decay to low-*K* states. The best known *K*-magic number is probably $Z = 72$, where $K^\pi = 8^-$ isomers with the configuration $\pi^2\{7/2^+[404] \otimes 9/2^-[514]\}$ systematically occur in $^{170-184}$Hf, with half-lives ranging from nanoseconds to hours [3,4]. The neutron number $N = 106$ is another well-known *K*-magic number. Here $T_{1/2} > 1\ \mu$s $K^\pi = 8^-$ isomers with the configuration $\nu^2\{7/2^-[514] \otimes 9/2^+[624]\}$ are observed from ^{174}Er to ^{188}Pb [5]. These scarce long chains of isomers provide unique opportunities for systematic study. The doubly *K*-magic nucleus ^{178}Hf manifests itself with the occurrence of a 31 yr $K^\pi = 16^+$ isomer based on the coupling $\nu^2_{8^-} \otimes \pi^2_{8^-}$. The possible stimulated release of the stored energy (2.4 MeV) in the isomer has been associated with proposals for a clean reservoir of nuclear energy and γ-ray lasers [1,2,6].

Exceptionally long-lived isomers have been predicted to also occur in neutron-rich Hf isotopes due to favorable conditions, i.e., low energy and high *K* value [2,7,8]. With a $K^\pi = 18^+$ isomeric state from the configuration $\nu^2_{10^-}\{9/2^-[505] \otimes 11/2^+[615]\} \otimes \pi^2_{8^-}$, ^{188}Hf seems to be a doubly *K*-magic nucleus [2]. Experimentally, projectile-fragmentation [9] and deep-inelastic [10] reactions have been employed to explore this region, such as the observation of a 240 μs isomer with the configuration $\nu^2_{10^-}$ in ^{190}W [9,10]. A major advance was achieved recently using storage-ring mass measurements [4], where long-lived isomers were observed in neutron-rich Hf isotopes up to ^{186}Hf, with $N = 114$. Nevertheless, the predicted doubly *K*-magic character of ^{188}Hf, with $N = 116$, remains to be confirmed.

However, another important factor, deformation, for the emergence of *K* isomers, could be much different between ^{178}Hf and the nuclei around ^{188}Hf. With neutron number $N = 106$ at the midshell between spherical magic numbers 82 and 126, ^{178}Hf is well deformed, having a shape that favors the formation of long-lived isomers. In contrast, a reduced shape elongation is expected in ^{188}Hf because the neutron number $N = 116$ is far away from the midshell. Generally, a smaller β_2 deformation is more susceptible to shape fluctuation toward triaxiality that induces *K* mixing. It is still an open question to what extent the deformation influences the occurrence of exceptionally long-lived *K* isomers in neutron-rich Hf isotopes. In the present work, we investigate these high-*K* isomeric states using configuration-constrained calculations of potential-energy surfaces (PES) [11,12], a model that properly treats the deformations of multi-qp states.

In our model, the single-particle levels are obtained from the deformed Woods-Saxon potential with the universal parameter set [13,14]. To avoid the spurious pairing phase transition encountered in the usual BCS approach, we use the Lipkin-Nogami (LN) treatment of pairing [15], with pairing strength G determined by the average-gap method [16]. The configuration energy [11] in the LN approach can be written as

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

where S is the proton or neutron seniority for a specified configuration (i.e., the number of blocked orbits with index k_j), and N is the proton or neutron number. The orbits with index k_j are blocked at each point of the $(\beta_2, \gamma, \beta_4)$ [11] or $(\beta_2, \beta_4, \beta_6)$ [12] deformation lattice, which is the so-called configuration constraint. This is achieved by calculating and identifying the average Nilsson quantum numbers for every orbit involved in a configuration. The total energy of a configuration consists of a macroscopic part, which is obtained from the standard liquid-drop model [17], and a microscopic part resulting from the Strutinsky shell correction [18], $\delta E_{\mathrm{shell}} = E_{\mathrm{LN}} - \tilde{E}_{\mathrm{Strut}}$.

The minimum of the PES gives the energy, deformation, and pairing property of a multi-qp state.

Figure 1 displays the calculated excitation energies and deformations of high-K isomeric states in even-A $^{176-192}$Hf isotopes. Our calculations satisfactorily reproduce the excitation energies of the π^2 8^- isomers observed in $^{176-182}$Hf [19]. It should be noted that the observed 4 s isomer in ^{178}Hf has a mixed configuration of 64% $\nu^2_{8^-}$ and 36% $\pi^2_{8^-}$ [20], resulting from the interaction between the two close-lying $\nu^2_{8^-}$ and $\pi^2_{8^-}$ configurations. The experimental excitation energy of the unperturbed $\pi^2_{8^-}$ state, 1.35 MeV [5], is well reproduced by our calculation of 1.35 MeV. The calculation of the 8^- state in ^{184}Hf gives an excitation energy of 1.23 MeV, which is in good agreement with the measured value of 1.26 MeV [4]. This indicates the association of the isomer with the $\pi^2_{8^-}$ configuration, which is consistent with the suggestion in Ref. [4].

The calculated excitation energy of the $K^\pi = 8^-$ state suddenly increases at $N = 118$, as shown in Fig. 1. Here there occurs a ground-state phase transition from prolate shape to oblate shape. Our prediction is consistent with other calculations (see, e.g., Refs. [21,22]). In contrast, Möller *et al.* predict that ^{190}Hf is still prolate deformed [23], indicating that the prediction of the neutron number for the prolate-to-oblate transition is model dependent. The 8^- state in ^{190}Hf is calculated (see Fig. 1) to be at an excitation energy of 1.86 MeV, but has a prolate shape, distinct from the oblate shape of the ground state. Also, the calculated β_4 deformations are much different between the isomeric state and the ground state. A combination of K isomerism and shape isomerism may happen in ^{190}Hf, analogous to that predicted for the ν^2 8^- isomer in ^{186}Hg [24]. Whether or not the higher excitation energies and smaller β_2 deformations predicted for the more neutron-rich Hf isotopes will lead to the termination of the $K^\pi = 8^-$ isomer chain at $N \approx 118$ remains to be determined.

Figure 1 also shows the lowest-lying 4-qp high-K isomeric states in $^{176-190}$Hf isotopes that are formed through the coupling of ν^2 (see Table I) with $\pi^2_{8^-}$. For ^{188}Hf, the $K^\pi = 18^+$ state has calculated excitation energy close to that of the $K^\pi = 16^-$ state. The calculated excitation energies are reasonably in accord with experimental data of $^{176-182}$Hf. The observed 2.48 MeV isomer in ^{184}Hf is likely the lowest-lying 4-qp 15^+ state. The calculated excitation energy of the 17^+ state is closer to the experimental data, but it can barely be long-lived because of the possibility to decay to the 15^+ state. The newly observed isomer in ^{186}Hf was tentatively associated with the 17^+ configuration in Ref. [4] based on blocked-Nilsson + LN calculations with fixed deformations. That significantly underestimated the measured excitation energy. In our calculations, the inclusion of deformation effects does not remove this discrepancy.

The discrepancy in ^{186}Hf could lie in both experiment and theory. Experimentally, the data for the 4-qp isomer in ^{186}Hf, obtained from just two ions, need to be confirmed. Furthermore, the mass measurements do not give a complete picture of the low-lying intrinsic states and do not provide spectroscopic information. Theoretically, our calculations do not include the residual spin-spin interaction [7] that can
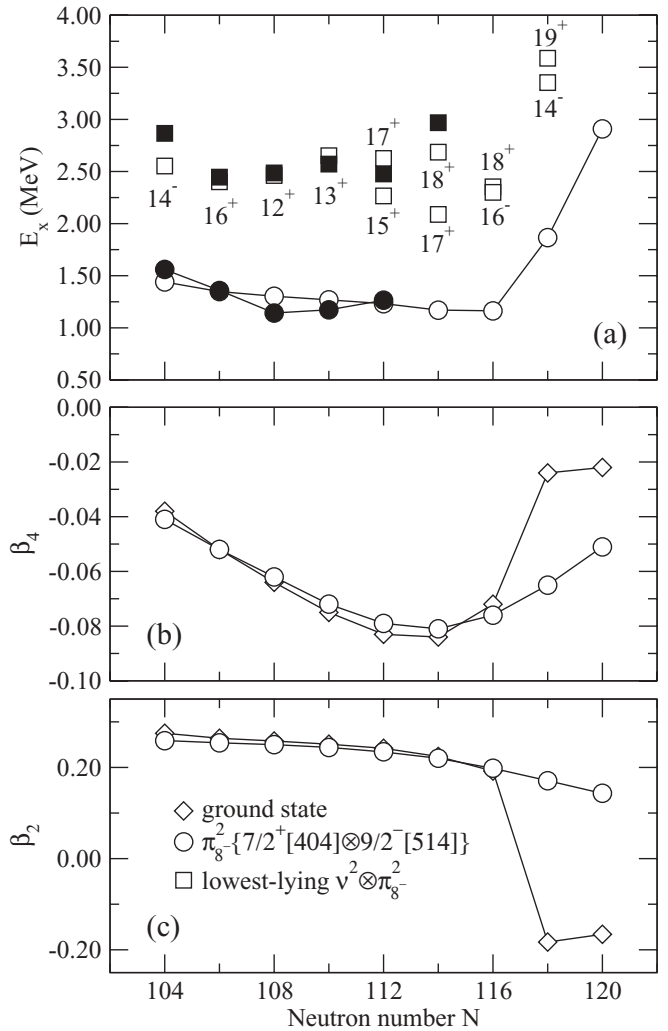

FIG. 1. Excitation energies (a), hexadecapole deformations (b), and quadrupole deformations (c) for multi-qp isomeric states in Hf isotopes. Open and filled symbols show the calculated and experimental values [4,5,19], respectively. The data for the 2-qp state in ^{178}Hf ($N = 106$) corresponds to an unperturbed $\pi^2_{8^-}$ state (see text). Note that no experimental configuration is available for the nuclei with $N \geqslant 112$. The deformations of 4-qp states (not shown for clarity) are similar to those of the corresponding 2-qp states. For all the multi-qp states, $\gamma \approx 0$ and $\beta_6 \approx 0$. The same configurations are connected by lines to guide the eye. See Table I for the neutron configurations ν^2 of the 4-qp isomeric states.

change the calculated excitation energy by up to several hundred keV. (We note that all the neutron configurations listed in Table I have energetically favored spin-antiparallel couplings except for the 17^+ state in ^{186}Hf.) In addition, the Woods-Saxon single-particle levels could become less accurate when moving away from the stability line. It has been remarked previously that the observed 1-qp states in odd-A W nuclei approaching $N = 114$ begin to deviate considerably from the predictions of the Nilsson model [25]. Our model cannot generate the correct state orderings in ^{187}W either, which implies a decreasing validity of the present Woods-Saxon potential parameters in the neutron-rich nuclei.

TABLE I. Neutron configurations of the $\nu^2 \otimes \pi^2_{8^-}\{7/2^+[404] \otimes 9/2^-[514]\}$ isomeric states.

Nucleus	$K^\pi_{\text{4-qp}}$	$K^\pi_{\nu^2}$	Neutron configuration ν^2
^{176}Hf$_{104}$	14^-	6^+	$5/2^-[512] \otimes 7/2^-[514]$
^{178}Hf$_{106}$	16^+	8^-	$7/2^-[514] \otimes 9/2^+[624]$
^{180}Hf$_{108}$	12^+	4^-	$9/2^+[624] \otimes 1/2^-[510]$
^{182}Hf$_{110}$	13^+	5^-	$1/2^-[510] \otimes 11/2^+[615]$
^{184}Hf$_{112}$	15^+	7^-	$3/2^-[512] \otimes 11/2^+[615]$
	17^+	9^-	$11/2^+[615] \otimes 7/2^-[503]$
^{186}Hf$_{114}$	17^+	9^-	$11/2^+[615] \otimes 7/2^-[503]$
	18^+	10^-	$11/2^+[615] \otimes 9/2^-[505]$
^{188}Hf$_{116}$	18^+	10^-	$11/2^+[615] \otimes 9/2^-[505]$
	16^-	8^+	$7/2^-[503] \otimes 9/2^-[505]$
^{190}Hf$_{118}$	14^-	6^+	$9/2^-[505] \otimes 3/2^-[501]$
	19^+	11^-	$9/2^-[505] \otimes 13/2^+[606]$

These parameters are determined by fitting the properties of nuclei near the stability line. Finally, the pairing strength could be another factor influencing the calculated excitation energy. An enhancement of about 10% (relative to the value obtained from the average-gap method) for both protons and neutrons is obtained for ^{190}W by fitting experimental odd-even mass differences [26]. This increment in pairing strength can result in an increase of the calculated excitation energy by ≈ 400 keV for the $\nu^2_{10^-}$ state. Unfortunately, such a fitting process is not available for the neutron-rich Hf nuclei due to the absence of mass data required to calculate the odd-even mass differences. The above-mentioned problems in residual interaction, single-particle energy, and pairing strength still await proper treatment to obtain a more complete and accurate description of the neutron-rich Hf nuclei.

In Fig. 2, we plot the excitation energy relative to a rigid rotor for the 4-qp isomeric states. It has been found that the degree of K hindrance increases in a simple manner with decreasing excitation energy relative to a rigid rotor
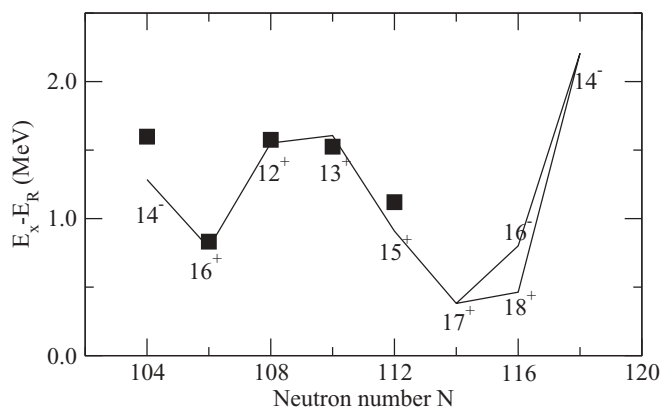

FIG. 2. Excitation energy relative to a rigid rotor for the lowest-lying 4-qp isomeric states in even-A Hf isotopes. Calculated and experimental values [4,19] are represented by lines and squares, respectively. The data point for ^{186}Hf is not shown, as the K value is unclear. Note that the 16^- state in ^{188}Hf has a larger $E_x - E_R$ value than the 18^+ state because of the smaller angular momentum.

[1,2,27]. This is because a relatively low excitation energy is often associated with low statistical K mixing due to the low level density [27], favoring the conservation of the K quantum number. Figure 2 shows two minima at $N = 106$ and $N \approx 116$, which is mainly ascribed to the closeness of the two single-particle orbits occupied by the unpaired neutrons and coupled to high K. The minimum at $N \approx 116$ is even lower than that at the K-magic number $N = 106$, where the well-known 31 yr $K^\pi = 16^+$ isomer occurs. This, although consistent with the prediction in Ref. [2], needs to be confirmed by further work because of the uncertainty in our calculations of excitation energy around $N = 116$ (see above). It is the remarkably low energy together with the high K value that indicates the possible emergence of exceptionally long-lived isomers [2,7,8].

Nevertheless, these isomeric states have smaller β_2 deformations than ^{178}Hf. It is usually easier for a less elongated shape to fluctuate toward γ distortion. Axially asymmetric deformation is intimately involved with K mixing because there is then no axis of symmetry on which to define a K projection. Some high-K isomers with very low hindrance in decay have been found to have γ deformations (see, e.g., Ref. [11]). Even though a K isomer has axially symmetric shape, it can decay by tunneling through triaxial shapes [28]. The softness against γ deformation facilitates such a decay mode. To see the degree of γ softness accompanied by small β_2 deformation, we calculate the potential-energy curves as a function of γ deformation for Hf isotopes, as shown in Fig. 3. The doubly K-magic nucleus ^{178}Hf can be treated as a benchmark, to which the neutron-rich nuclei are compared. The qualitative comparison can be barely influenced by the potential inaccuracy in pairing strengths and single-particle levels. It can be seen that the ground states of neutron-rich Hf isotopes become increasingly soft against triaxial distortion with decreasing β_2 deformations. With $|\beta_2| < 0.2$, ^{188,190}Hf have remarkably flat ground-state potential wells. However, the multi-qp states in ^{186,188}Hf show enhanced stiffness in the potential wells compared to the corresponding ground states. The isomeric states in ^{188}Hf have potential wells not much different from those in ^{186}Hf where a long-lived isomer has been observed [4], though the depth of the potential wells
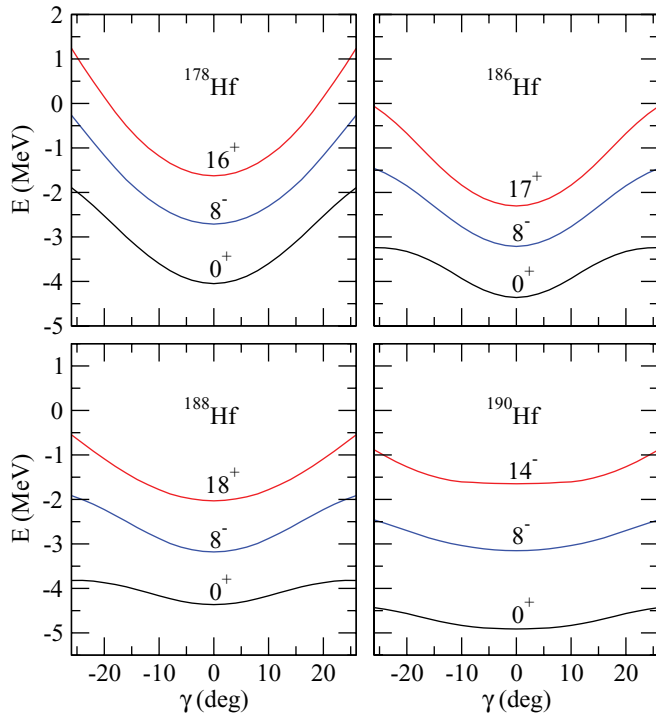
FIG. 3. (Color online) Calculated potential-energy curves as a function of γ deformation. The energy is minimized with respect to β_2 and β_4 deformations. The true minimum of the oblate-deformed ground state in ^{190}Hf is at $\gamma = -60°$ in the Lund convention.

in both are moderately reduced with respect to ^{178}Hf. This, together with the favorable conditions in energy and K value, points to the possibility of very long-lived isomers in ^{186,188}Hf.

The neutron-rich Hf isomeric states are expected to decay through β^- emission competing with γ-ray transitions [2,4].

The $K^\pi = 8^-$ isomers in ^{178,180}Hf mainly decay to the 8^+ member in the ground-state band by K-forbidden $E1$ transitions [19]. For neutron-rich nuclei, the 8^+ state would lie higher in energy than the isomer due to reduced β_2 deformation. Instead, the isomers would decay to the 6^+ member by slower $M2/E3$ transitions, making the β^--decay channel competitive. A similar situation could happen for the 4-qp isomeric states where the major γ-transition channel is open to the members in the rotational band built upon the $K^\pi = 8^-$ isomer. Spectroscopic measurements may soon be available owing to the quick development of experimental techniques.

In summary, the multi-qp states in neutron-rich Hf isotopes are investigated by using configuration-constrained PES calculations, with attention paid to see the influence of deformations on the occurrence of long-lived isomers. Isomeric states with relatively low excitation energy and very high K value are predicted in Hf isotopes at $N \approx 116$. In spite of having small β_2 deformations, the multi-qp states in ^{186,188}Hf remain moderately robust against γ distortion, favoring the formation of long-lived isomers. Further work in both experiment and theory is needed to study the isomeric structures in neutron-rich Hf isotopes, through the $N \approx 116$ prolate-oblate shape-transition region.

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