Shape coexistence and tilted-axis rotation in neutron-rich hafnium isotopes

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We have performed tilted-axis-cranked Hartree-Fock-Bogoliubov calculations for a neutron-rich hafnium isotope ($^{182}$Hf) whose proton and neutron numbers are both in the upper shell region. We study whether the shell effects play a role in producing high-$K$ isomers or highly gamma-deformed states at high spin. In particular, the possibility of shape coexistence and the effect of wobbling motion are discussed.

Keywords: High-$K$ states, gamma deformation, wobbling motion, tilted axis cranking model

Hafnium isotopes ($Z = 72$) are best known as nuclei that have high-$K$ isomers (e.g., the $K^+ = 16^+$ isomer in $^{178}$Hf, with a half life $t_{1/2} = 31$ yr). From a viewpoint of the Nilsson model, a reason is that proton single-particle levels are filled up to the upper part of the shell where there are many high-$\Omega$ states at prolate deformation ($\Omega$ is the angular momentum projection on the nuclear symmetry axis). The presence of long-lived high-$K$ isomers indicates the existence of axial symmetry to make $K = \sum \Omega_i$, a good quantum number. With recent developments of experimental techniques, such as fragmentation and deep-inelastic reactions in populating high-spin states, the study of nuclei in the well deformed rare-earth region moves away from the $\beta$ stable line towards the neutron-rich isotopes. D’Alarcao et al. recently discovered several high-$K$ isomers in the neutron-rich hafnium isotope of $^{182}$Hf. For neutron-rich hafnium isotopes, whose neutron Fermi level is located in a similar position to the proton one (i.e., the upper half of the shell), we can expect an even more important role for high-$K$ isomeric states. At the same time, however, the empty nucleon states near the Fermi surfaces can be considered as hole states, and these may induce substantial gamma deformation which breaks the axial symmetry.

A few theoretical investigations of high angular momentum collective states have been reported for such neutron-rich hafnium isotopes: by means of a microscopic method (cranked Hartree-Fock-Bogoliubov method, or C-HFB), the possibility of a collective oblate deformation at high-spin ($I = 26\hbar$) in $^{180}$Hf was predicted; by means of a macroscopic-microscopic method (total routhian surface calculations, or TRS), the existence of non-collective prolate-deformed states becoming yrast, i.e., lowest in energy, for $J \gtrsim 10\hbar$ was shown in $^{182-186}$Hf. In the latter study, the collective oblate deformed states become yrast when quite high in spin ($I = 36\hbar$ in $^{182}$Hf). In both of the studies, the rotational states are treated only by the one-dimensional cranking model, but recent developments in the tilted-axis-cranking model allow for the possibility of further investigation of these neutron-rich hafnium isotopes.

In this paper, in a microscopic framework of the two-dimensional tilted-axis-cranked HFB method, we analyze the high-spin structures predicted for the neutron-rich hafnium isotope $^{182}$Hf (which has $N/Z = 1.53$).

First, the calculational procedure is briefly described. We solve the HFB equations with a 2d-cranking term self-consistently for $^{182}$Hf, following the method of steepest-descent. Nucleon numbers and the total angular momentum are constrained during the iterations: $\langle \hat{N}_r \rangle = N_r$ ($r = p, n$); $J_x = \langle \hat{I}_x \rangle = J \cos \theta, J_y = \langle \hat{I}_y \rangle = 0; J_z = \langle \hat{I}_z \rangle = J \sin \theta$. (Note that the tilt angle $\theta$ is measured from the $x$-axis to see the deviation of the rotation axis from the $x$-axis. In this study, it corresponds to a principal axis of the quadrupole deformation, perpendicular to the symmetry axis that is chosen to be the $z$-axis). We also constrain off-diagonal components of the quadrupole tensor such that the intrinsic coordinate axes coincide with the principal axes of the quadrupole deformation. See Ref. for details.

The one-dimensional cranking calculations (or 1d-cranking calculations), in which the rotation axis is fixed to be along the $x$-axis ($\theta = 0^\circ$), are performed as follows. First for $J = 0$, the Nilsson + BCS state is taken as a trial state. Then cranked HFB states, $\Psi_a(J)$, are calculated up to $J = 40\hbar$ with increments $\Delta J = 0.1\hbar$. This way of calculation is what we call “up-cranking” calculations. Then, using the up-cranking solution at $J = 40\hbar$ as a trial state, “down-cranking” calculations are similarly performed from $J = 40\hbar$ down to $J = 0$ to obtain $\Psi_d(J)$.

The calculations of tilted-axis-cranked HFB states (2d-cranked states, or $\Psi(\theta, J, \theta)$) are carried out by starting at a state $\Psi(J, \theta = 0^\circ)$, which are calculated through an up-cranking calculation, and performing a “forward” tilting calculation up to $\theta = 90^\circ$ with increments $\Delta \theta = 0.5^\circ$ for each (integer) $J$. Then in a similar manner we make “backward” tilting calculations from $\theta = 90^\circ$ to $\theta = 0^\circ$. At certain tilt angles, the forward and backward tilting results do show interesting differences, particularly, at high spins.
Our Hamiltonian consists of a spherical part \( H_0 \) and a residual part \( V_{\text{res}} \) employing the pairing-plus-Q \( \cdot \) Q interaction. In the hafnium isotopes the hexadecapole interaction can be important, but we have checked that our results below are not affected very much by including the interaction. Thus we omit it in the present study. The Hamiltonian is thus written,

\[
H = H_0 + V_{\text{res}} = \sum_{\tau=p,n} \sum_{i=1}^{N(\tau)} \epsilon_i \hat{c}_i^\dagger \hat{c}_i - \frac{1}{2} \kappa \sum_{\mu=-2}^{2} \hat{Q}_\mu \hat{Q}_\mu - \sum_{\tau=p,n} G_\tau \hat{p}_\tau^\dagger \hat{p}_\tau,
\]

in which \( \epsilon_i \) means a spherical Nilsson level and \( i \) runs all over the model space. Force parameters \( \kappa \) and \( G_\tau \) are determined in the framework of the Nilsson + BCS model by giving input parameters for the quadrupole deformation \((\beta_{\text{ini}}, \gamma_{\text{ini}})\) and gap energy \((\Delta_{\text{ini}})\). (Our definition of \( \gamma \) is taken from pp.8 in Ref. 11, and is opposite to the Lund convention in the sign.) In this paper, we employ a set of the input parameters based on the calculations by Möller et al. 12 because we find it gives a good agreement with experimental data. For \(^{182}\text{Hf}\), we employ \( \Delta_{\text{ini}}^p = 0.725 \text{ MeV} \), \( \Delta_{\text{ini}}^n = 0.625 \text{ MeV} \); \( \beta_{\text{ini}}^p = 0^\circ \); \( \beta_{\text{ini}}^n = 0.270 \) or 0.268. We will see soon the reason for the two values of \( \beta_{\text{ini}} \).

Our single-particle model space is almost the same as the choice of Kumar and Baranger 13 (two major shells in the spherical Nilsson model: \( N = 4, 5 \) for proton and \( N = 5, 6 \) for neutron), with two extra single-particle orbits, proton \( j_{13/2} \) and neutron \( j_{15/2} \). The single particle energies are the spherical Nilsson model energies with \( A \)-dependent Nilsson parameters 14.

First of all, let us discuss a principal axis rotation \((\theta = 0^\circ)\) in 1d- and 2d-cranking calculations. Fig.1 shows the energy spectra of one-dimensional up- and down-cranking states (\( \Psi_\uparrow(J) \) and \( \Psi_\downarrow(J) \), respectively) and the states of \( \theta = 0^\circ \) in the 2d-cranked calculations, \( \Psi^J(J, \theta = 0^\circ) \) that are obtained through the backward tilting procedure at a given value of \( J \). They are plotted also in the inset of Fig.1 together with the known experimental values of the g-band. The g-band is well reproduced by our one-dimensional cranking calculations.

We have two kinds of 1d-cranked states plotted in Fig.1. They are calculated with the same conditions except for the initial value of \( \beta_{\text{ini}} \). One (denoted as \( \text{“A”} \) in the graph) is obtained with the initial value of \( \beta_{\text{ini}} = 0.270 \) while the other (denoted as \( \text{“B”} \)) is with \( \beta_{\text{ini}} = 0.268 \). The small difference in \( \beta_{\text{ini}} \) gives almost no difference in the wave functions at low spin \(( J \lesssim 16h) \), but it does lead to a significant difference at high spins. The sensitive dependence of the high-spin HFB solutions to \( \beta_{\text{ini}} \) shows that the energy manifold in the variational space near the crossing regions has several local minima that are almost degenerate. The states \( \text{“A”} \) and \( \text{“B”} \) imply the possibility of band crossings \( \dag \), which correspond to the regions \( 17h \lesssim J \lesssim 26h \) and \( 22h \lesssim J \lesssim 31h \) respectively \( \dag \) in the calculations, but a substantial difference between the states is seen in the gamma deformation. Before the crossing regions both of the states have \( \gamma \approx 10^\circ \), while after the crossing regions the states \( \text{“A”} \) have near-prolate deformation with a negative gamma value (\( \gamma \approx -10^\circ \)) and the states \( \text{“B”} \) have oblate shape (\( \gamma \approx 60^\circ \)). (See Fig.2(a) for evolutions in gamma deformation for each solution). From an analysis of our numerical results, the oblate deformation is caused by the gradual alignments of both \( j_{13/2} \) neutrons and \( h_{11/2} \) protons, while, in addition to these alignments, the near-prolate deformation with \( \gamma \approx -10^\circ \) is caused by the quick alignment of \( j_{15/2} \) neutrons. (Note that the neutrons in the \( j_{15/2} \) orbits are not part of the usual Kumar-Baranger model space). The solution \( \text{“A”} \) is reported in this paper for the first time. Xu et al. found that there is no stable minimum corresponding to this solution in their TRS calculations 15. However, they performed their (1d) cranking calculations for given rotational frequencies \((\omega_x)\), while we have performed calculations for given (average) angular momentum vectors \((J_x, J_y, J_z)\).

In a spin region \( 23h \lesssim J \lesssim 35h \), the three kinds of states having different gamma deformations \((\gamma \approx \pm 10^\circ \text{ and } 60^\circ)\) are close to each other in energy. This result implies a manifestation of shape coexistence at high spin, or multi-band crossings among bands specified by different gamma deformations (or corresponding rotational alignments).

It is interesting to see the energies for the state \( \Psi^J(J, \theta = 0^\circ) \), which are represented by the thick solid line in Fig.1. The line has two discontinuities, at \( J = 27h \) and \( 34h \), implying two configuration changes. At lower spin \(( J \lesssim 26h) \), \( \Psi^J(J, \theta = 0^\circ) \) follows the 1d-cranking calculations which give rise to nearly prolate shape \((\gamma \approx 10^\circ \text{ at } J \approx 25h)\). Then at \( J = 27h \), the gamma deformation changes to \( \gamma \approx -10^\circ \), which is the same as \( \text{“A”} \). Finally, at \( J = 34h \), \( \Psi^J(J, \theta = 0^\circ) \) changes into the same state as \( \text{“B”} \), having oblate shape \((\gamma \approx 60^\circ)\). The result that the states having different gamma deformation are connected by the tilted-axis-cranking solutions indicates the impor-

\footnote{As Hamamoto et al. pointed out 15, the validity of the cranking model is questionable in the band crossing region because of the semi-classical aspects in the model. However, the model works well outside the crossing region and could explain qualitative features near the crossing region, such as alignments. For a more accurate analysis of the crossing region, we should employ the so-called “variation-after-projection” method 16, the generator coordinate method 18, or the diabatic method 19.}

\footnote{Note that we do not mean here that these values of the crossing angular momentum correspond exactly to the experimental values. In general, the simple self-consistent cranking calculations do not reproduce the value precisely 14.}
tance of the tilting degree of freedom ($\theta$) for the search for excited states near band crossings. In Fig.2(b), we show how the quadrupole deformations ($\beta$ and $\gamma$) evolve at $J = 34\hbar$ as we vary the tilt angle ($\theta$). The corresponding energy curves are plotted in Fig.3(a). There are three types of solutions with different gamma deformation: (i) the solution having no $\theta$-dependence in tilt angles for $\theta \lesssim 20^\circ$ is oblate ($\gamma \simeq 60^\circ$); (ii) the solution which shows a tilted rotation minimum at $\theta \simeq 10^\circ$ has negative gamma deformation ($\gamma \simeq -10^\circ$); (iii) the solution with a minimum at $\theta = 90^\circ$, which may correspond to high-$K$ states, has $0^\circ \lesssim \gamma \lesssim 10^\circ$.

The energy difference between the states of type (i) and (ii) is roughly constant and small ($\simeq 500$ keV), so that these two states can couple to form states with mixed deformation. The energy curves for these states are shallow in the range $0^\circ \leq \theta \leq 30^\circ$, so that fluctuations in the rotation axis, or wobbling motion, can be expected. However, gamma deformations for each state of type (i) and (ii) are quite constant against variation in the tilt angle up $\theta \simeq 30^\circ$. Therefore, rather than a picture in which states of type (i) and (ii) are coupled thorough the wobbling motion, we should have a picture where they are connected possibly through $\gamma$ tunnelling, and where the mixed states wobble around the tilted rotation minimum at $\theta \simeq 10^\circ$. Nevertheless, a coupling of these mixed states with states of type (iii), is possible through wobbling motion.

It is interesting to see in Fig. 3(a) the energy curve at $J = 40\hbar$ corresponding to the states of type (i) above. There are two minima at $\theta = 0^\circ$ and $90^\circ$, but the barrier height between them is only $\simeq 50$ keV, not visible in the plot. The corresponding deformation is collective oblate (the $y$-axis is the symmetry axis) and almost constant over the entire range of $\theta$. For a strict oblate symmetry, there would be no energy dependence on $\theta$. The projection of the nuclear deformation onto the $x-z$ plane is a circle, so that there is no preference for a direction of (collective) rotation in the $x-z$ plane. For finite triaxiality, it is important to consider wobbling motion in the $\theta$ direction.

From these discussions, we can deduce that the shape coexistence creates successive backbends (sudden changes in moments of inertia) in the excited rotational bands of $\theta \simeq 0^\circ$. The first backbend, which is caused by neutron $i_{13/2}$ alignment, in addition to alignments of neutron $i_{11/2}$ and proton $h_{11/2}$, is expected at lower spins, which corresponds to $17\hbar \lesssim J \lesssim 26\hbar$ in our calculations. The second one, which is caused by de-alignment of the $j_{15/2}$ neutrons and retaining alignments of the $i_{13/2}$ neutrons and $h_{11/2}$ protons, can be seen at higher spins (corresponding to $22\hbar \lesssim J \lesssim 31\hbar$ in the calculations). According to Fig.1, the second backbend can be more pronounced than the first one. It is also possible that these two backbends are mixed together to create one giant backbend as Hilton and Mang predicted [4], but according to our analysis three types of gamma deformations are involved: $\gamma \simeq \pm 10^\circ$ and $\simeq 60^\circ$.

Now, let us look at the calculated high-$K$ states. In Fig.1, states of $\theta = 90^\circ$, $\Psi^t(J, \theta = 90^\circ)$, are shown with “+” symbols. These states correspond to a local minimum at $\theta = 90^\circ$ in the energy curve (see Fig.3(b)). In our calculations, this minimum starts to appear at $J \simeq 8\hbar$, and becomes the lowest minimum at $J = 12\hbar$ and at higher spins. The $\theta = 90^\circ$ minimum may be considered approximately to correspond to a high-$K$ state, and the corresponding $z$-axis cranked state, or $\Psi^t(J, \theta = 90^\circ)$, is a simulation of nuclear rotation where single-particle angular momenta carry most of the total angular momentum. We have checked that the corresponding gamma deformation is almost zero as in Fig.2(b) which shows that there is axial symmetry for these states.

However, we should note that $J_z(= J \sin \theta)$ in the self-consistent cranking calculations is not an eigenvalue but just an expectation value, due to the rotational symmetry breaking by the mean field. Besides, in the tilted-axis-cranked HFB calculations, angular momenta are fully mixed in the sense that even a mixture among even and odd angular momenta happens. This is because the signature symmetry, a discrete subgroup ($D_2$) of the rotational group $O(3)$, is broken by tilted rotation [13]. We should therefore keep in mind that the mean-field description of high-$K$ states has a certain limitation.

Remembering the above remarks, let us look at our results for $\Psi^t(J, \theta = 90^\circ)$. The experimental energy of the isomer, which is tentatively assigned to $K^\pi = 13^+$, is $2.572$ MeV relative to the ground state energy, while the numerical values are $2.101$ MeV ($J = 12\hbar$), $2.255$ MeV ($J = 13\hbar$), and $2.408$ MeV ($J = 14\hbar$). Deformations of $\Psi^t(J = 13\hbar, \theta = 90^\circ)$, are calculated to be $\beta = 0.2661$ and $\gamma = 0.015^\circ$.

We can consider whether this isomer is yrast or not. (Experimentally, the $g$-band is identified only up to $8\hbar$ [1].) Xu et al. calculated that the non-collective prolate state would be yrast at $J = 13\hbar$ [8]. Our self-consistent calculations also show that $\Psi^t(J, \theta = 90^\circ)$ is lower in energy than principal axis rotation, $\Psi^t(J, \theta = 0^\circ)$, for $12\hbar \leq J \leq 34\hbar$, so that in this region the high-$K$ isomeric states can be favoured relative to the collective rotation. Let us use the term “tilted rotation” for the states with local minima, with $\theta \neq 90^\circ$. At $J = 13\hbar$ (see Fig.3(b)), there is tilted rotation ($\theta \simeq 15^\circ$) with an excitation energy of $2.593$ MeV, which happens to be quite close to the experimental value of the $K^\pi = 13^+$ isomer. Numerical deformation values for this minimum are $\beta = 0.2704$ and $\gamma = 4.62^\circ$, that is, the shape is nearly prolate. It is possible to consider the tilted rotation to describe a rotational member of a high-$K$ state. However, at this angular momentum, the potential energy curve is shallow in the whole range of $\theta$ (see Fig.3(b)), and the barrier height is the same order of magnitude as uncertainties from the mean-field approximation. The question as to whether the high-$K$ state should be described as either a tilted rotation state or a $z$-axis cranked state $\Psi^t(J, \theta = 90^\circ)$ (or coupling of them) should be answered by a quantum
mechanical calculation by using angular momentum projection (and/or the generator coordinate method), which we plan to study in the future. At this moment, the description of high-$K$ states in the framework of self-consistent tilted-axis-cranking calculations is reasonably good up to an accuracy of several hundred keV, but more detailed studies are surely necessary.

For these shallow energy curves, we can consider the wobbling motion to relate and cause transitions between high-$K$ isomers and low-$K$ states such as the $g$-band. For the energy curve at $J = 13\hbar$, there are three minima at $\theta = 0^\circ$ (principal axis rotation), $\theta = 15^\circ$ (tilted rotation), and $\theta = 90^\circ$ (possible high-$K$ states) within 600 keV. If the first minimum represents a rotational member in the $g$-band and the third (and/or second) minimum represents the one in a high-$K$ band, then the corresponding band crossing is expected to show (experimentally) a strong coupling as evidence for a realization of the wobbling motion.

In summary, we have performed tilted-axis-cranked HFB calculations for $^{182}$Hf, and investigated high-spin states near the yrast line up to $J = 40\hbar$. For our parameter set, the comparison of the experimental data for the $g$-band and a high-$K$ isomeric state ($K^\pi = 13^+$) with our calculation gives a reasonable agreement within the framework of the mean-field approximation. With our modified single-particle model space based on Kumar-Baranger’s choice, we found a new HFB solution with near-prolate deformation ($\gamma \simeq -10^\circ$) involving $j_{15/2}$ neutron alignment at high spin ($J \gtrsim 17\hbar$). We discussed the possibility of shape coexistence among three states in principal axis rotation with different gamma deformation: two with near-prolate shapes ($\gamma \simeq \pm 10^\circ$) and the other with oblate shape ($\gamma \simeq 60^\circ$). An analysis of the possible backbends in yrare states was also given. In addition, we discussed the effect of wobbling motion as a coupling mode between low-$K$ and high-$K$ states.

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FIG. 1. Energy spectrum near the yrast line obtained through the tilted-axis-cranking calculations. In the large graph, we show the energy with an arbitrary subtraction of rotational energy, $0.005 J(J+1)$ MeV for $10 \hbar \leq J \leq 40 \hbar$, in order to see excited structures in detail. In the small graph, the energy curve (without subtraction) is shown for the full range of angular momentum $0 \hbar \leq J \leq 40 \hbar$. Experimental values for the g-band (open circle) and a $K^\pi = (13^+)$ isomer (asterisk) are plotted for a comparison. One-dimensional up- and down-cranking are depicted by upward and downward triangles, respectively. When the up- and down-cranking results are the same, the triangles are superposed to give the stars. Two kinds of 1d-cranked calculations are shown as “A” and “B”, which are obtained by $\beta_{ini} = 0.270$ (open triangles) and 0.268 (closed triangles), respectively. “A+B” means that the two 1d-cranking solutions “A” and “B” give similar results. Also “u+d” means that the up- and down-cranking calculations show no differences. The thick solid line indicates states of $\theta = 0^\circ$ obtained in the 2d-up-cranking calculations ($\Psi_t(J, \theta = 0^\circ)$) while plus signs denote 2d-up-cranking states $\Psi_t(J, \theta = 90^\circ)$. The tilted rotation minima are represented by diamonds (see Fig.3(b)).
FIG. 2. (a) Gamma deformation in 1d- and 2d-cranking calculations are shown with respect to $J (= J_x)$. The symbols are the same as those in Fig.1. (b) Gamma and beta values at $J = 34\hbar$ in the 2d-cranking calculations are shown with respect to $\theta$. “Fwd” means the forward tilting calculations, while “Bwd” means the backward calculations.
FIG. 3. Energy curves with respect to tilt angle $\theta$. (a) energy curves at $J = 34\hbar$ and $40\hbar$. Three states having different gamma deformation are energetically close in the range $0^\circ \leq \theta \leq 40^\circ$. For $J = 40\hbar$ there are two minima, at $\theta = 0^\circ$ and $90^\circ$, the barrier height between them being only about 50 keV. (b) energy curve at $J = 13\hbar$. For $12\hbar \leq J \leq 20\hbar$, there are three minima at $\theta = 0^\circ, 90^\circ$, and $\simeq 15^\circ$. The last minimum implies tilted rotation. (c) energy curve at $J = 4\hbar$. In the low-spin region ($J < 12\hbar$), there is only one minimum, at $\theta = 0^\circ$, i.e., principal axis rotation.