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Shape evolution in ^{76,78}Kr nuclei at high spins in tilted axis cranking Hartree–Fock–Bogoliubov approach

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Abstract. A two-dimensional tilted axis cranking Hartree–Fock–Bogoliubov (CHFB) calculation is performed for ^{76}Kr and ^{78}Kr nuclei up to high spins $J = 30$ employing a pairing-plus-quadrupole (PPQ) model interaction Hamiltonian. Intricate details of the evolution of single particle structures and shapes as a function of spin have been investigated. The results show the existence of energy levels with high K quantum numbers lying close to the yrast line in both the nuclei. Such high K states should exhibit isomeric characteristics due to the K-selection rules for the γ-decays. Moreover, in ^{78}Kr a new band with $J = 20$–30 lying below the observed ground band is predicted.

Keywords. ^{76,78}Kr nuclei; high spin states; shape evolution; tilted axis cranking Hartree–Fock–Bogoliubov theory.

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1. Introduction

In a recent [1] one-dimensional cranking calculation for ^{76}Kr and ^{78}Kr nuclei, we have found that ^{76}Kr is prolate at spins $J \leq 12$ and becomes triaxial at higher spins, whereas ^{78}Kr remains prolate throughout up to $J = 24$. These shape changes appear to be consistent with the experimental results on change in moment of inertia as a function of rotational frequency. In the present study we aim at gaining further insight into the structural changes at high spins by allowing a wobbling motion of the rotational axis in the x–z plane (i.e., allowing the rotation axis to lie in the x–z plane). Thus, we extend our earlier investigations to spins up to $J = 30$ and perform a self-consistent 2D cranking HFB calculation [2–4]. In §2 some calculational details are presented and results are discussed in §3. Finally §4 contains summary and conclusions.

2. Some calculational details

A two-dimensional CHFB calculation is performed in the x–z plane such that the expectation values of the Cartesian components of the angular momentum $\langle \hat{J}_x \rangle = J\cos\theta$, $\langle \hat{J}_y \rangle = 0$ and $\langle \hat{J}_z \rangle = J\sin\theta$. Following our recent [1] x-axis cranking calculations for ^{76,78}Kr nuclei, an inert core of ^{40}Ca is assumed with the same basis space and spherical single particle energies (set A of table 1 in ref. [1]). Furthermore, instead of starting with a chosen set of interaction strengths, here one starts with a given value of the quadrupole deformation parameter and pairing gaps for the ground state, and then the interaction strengths are automatically fixed in the code [2,3]. We start with the values of the shape parameters in the ground state, as obtained in ref. [1].

In the present scheme of calculations, first a self-consistent HFB calculation is performed for the ground state ($J = 0$) to obtain the HFB wave functions. Then at $\theta = 0$ the one-dimensional x-axis cranking calculation is performed for a required J value of the angular momentum starting with the $J = 0$ input HFB solutions using an incremental step of $\Delta J = 0.1$ till the value J. In order to carry out the 2D cranking calculation, the CHFB wave function for a given J at $\theta = 0$ is used as the starting input with an angular incremental step of $\Delta\theta = 0.5°$ till 90°. We call this procedure of calculation a forward tilting calculation. After obtaining the CHFB solutions at 90°, a reverse tilting calculation is performed till $\theta = 0$. This is termed as backward tilting calculation. Sometimes the backward tilted cranking results may not coincide exactly with the forward cranking results. This is not a disadvantage, but in fact may be termed advantageous as it explores a wider area of the energy surface in the space of microscopic single-particle states.

3. Results and discussions

For the rotation of a spheroid we follow the convention that in an x-axis cranking calculation if the quadrupole asymmetry deformation parameter $\gamma = -60°$ at a certain value of J, it is termed as a 'rotation' about the oblate symmetry axis. Furthermore, cranking about z-axis with a value γ is equivalent to cranking about x-axis with a value $(120 - \gamma)°$. For ^{76}Kr and ^{78}Kr the results are presented below in separate subsections.

3.1 ^{76}*Kr*

The values of the shape parameters in the ground state are quadrupole deformation parameters $\beta = 0.345$, $\gamma = 0$, and pairing gaps $\Delta_{\rm p} = 1.017$ MeV and $\Delta_{\rm n} = 0.846$ MeV [1] with the quadrupole interaction strength $\kappa = 6.34557\times10^{-4}$ MeV $f_{\rm m}^{-4}$, and monopole pairing interaction strengths $g_{\rm p} = 0.25087$ MeV and $g_{\rm n} = 0.23706$ MeV for protons and neutrons, respectively. In the present x-axis cranking calculation with the PPQ interaction, the neutron pairing collapses at $J = 10$, whereas the proton pairing vanishes at $J = 20$. Study of the variation of energy as a function of θ shows no minimum for a tilt angle between the principal axes x and z. Rather, the minimum actually occurs for $\theta = 0$ corresponding to the x-axis cranking (xcr).

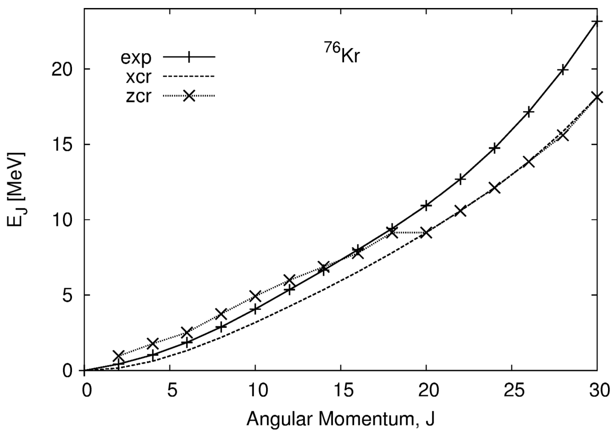

Figure 1. Energy as a function of angular momentum for x-axis and z-axis cranking calculations compared with experimental values [5] for ^{76}Kr.

For spins $J > 18$ the energy at $\theta = 0°$ and $90°$ become essentially the same with a maximum at $\theta \approx 45°$. In the following we present only our cranking results corresponding to the tilt angles $\theta = 0$ and $90°$.

In figure 1 the experimental [5] ground band energies are compared with the calculated ones. Like in our earlier work [1], here too the E_J vs. J curve obtained in the x-axis cranking calculation (labeled xcr) lies below the experimental one. The agreement in energy spectrum should improve considerably if particle number and angular momentum projections are carried out as these would lead to lowering of the ground state much more than the high-spin states. Furthermore, we find that the energies for $J \geq 20$ in xcr and zcr (z-axis cranking) are the same having a triaxial shape (γ varying from 10 to 25°) with the exception at $J = 28$ (rotation about the oblate symmetry axis, i.e., the spin generated by rotation alignment of multi-quasiparticle orbitals). For $J < 20$ the shape is prolate and the $J = K$ states lie about 1 to 2 MeV above the yrast line.

For $J = 28$ there are two energy solutions at $\theta = 0$ from forward and backward tilting (bxcr) calculations with difference in energy, $\Delta E = 0.25$ MeV. In table 1 the variation of β and γ with spin for $J \geq 16$ is listed for different cranking procedures. For $J = 2$–14 in xcr the values of β are 0.346, 0.348, 0.345, 0.330, 0.316, 0.301 and 0.283, respectively with γ changing from 0 to 4°. The bxcr and zcr results on β are qualitatively similar to that in xcr with an exception at $J = 28$ when $\beta = 0.07$. In bxcr the values of γ are similar to those as in xcr except at $J = 28$ when it is $-60°$. In zcr $\gamma = 0$ up to $J = 18$ and then for higher spins the shape becomes triaxial equivalently like in xcr except that at $J = 28$ it becomes 180°. Also a substantial decrease in the values of β at high spins implies a decrease in collectivity as observed recently by Valiente-Dobón *et al* [5]. Furthermore, as the energy difference between the two solutions for $J = 28$ at $\theta = 0$ is only about 0.25 MeV, one may term it as the coexistence of two shapes of ^{76}Kr at $J = 28$. Not only this, the lower solution corresponds to $J = K$ yrast state with a very high value of K, and should be expected to be isomeric due to the K-selection rule for the γ-decays.

3.2 ^{78}Kr

The values of the shape parameters in the ground state are $\beta = 0.323$, $\gamma = 0$, $\Delta_p = 1.0$ MeV and $\Delta_n = 1.062$ MeV [1] with the interaction strengths $\kappa = 5.87420 \times 10^{-4}$ MeV f_m^{-4}, $g_p = 0.24592$ MeV and $g_n = 0.23713$ MeV. The interaction strengths obtained for the two nuclei (^{76,78}Kr) are quite consistent within the expected A-dependence. In the x-axis cranking calculation, the neutron pairing collapses at $J = 8$, whereas the proton pairing vanishes at $J = 24$. Study of the energy $E_J(\theta)$ as a function of θ for this nucleus too does not show any energy minimum corresponding to a tilted axis rotation. For $J < 16$, in general, the results are similar to that for ^{76}Kr discussed above. But for all the $J \geq 16$ states we find two distinct energy solutions at $\theta = 0$ (for xcr and bxcr).

The variation of the shape parameters β and γ as a function of spin for $J = 16$–30 at $\theta = 0$ are presented in table 1 for certain cranking cases. In xcr the shape remains prolate at all spins. The values of β are 0.334, 0.357, 0.374, 0.376, 0.373, 0.369, and 0.363 for $J = 2$–14, respectively in xcr as well as in bxcr. On the other hand, in zcr the values of β are about 10% smaller than those in xcr for $J = 2$–14 and similar to those in bxcr for $J = 16$–30. The values of γ in zcr are equivalently similar to those in bxcr for $J = 16$–30 with a small difference at $J = 16$. In zcr we obtain $\beta = 0.130$ and $\gamma = 19.4°$ at $J = 16$. Thus, in zcr and bxcr calculations the value of β suddenly drops at $J = 16$ (also $\gamma > 0$) and tends to almost a zero value (spherical shape) for angular momenta $J = 28$ and 30.

Regarding the variation of the pairing gap Δ as a function of J, an interesting feature is observed: the roles of proton and neutron pairing get interchanged in zcr ($\theta = 90°$) calculation for $J = 16$–22, and Δ_n remains non-zero at $\theta = 0$ in the backward tilting calculation.

The states with $J = 16$ and 28 are very special. For the former the values of the shape parameters at $\theta = 0$ are $\beta = 0.354$, $\gamma = 0.0$, $\Delta_p = 0.653$ MeV and $\Delta_n = 0$ in the xcr case, and $\beta = 0.188$, $\gamma = 17°$, $\Delta_p = 0$ and $\Delta_n = 0.908$ MeV in the bxcr calculation. The exchanged roles of proton and neutron pairings are very

Table 1. Shape parameters β and γ at high spins. Values of γ are in degrees. For ^{78}Kr, $\gamma = 0$ in xcr at all spins.

	^{76}Kr		^{78}Kr		
J	β (xcr)	γ (xcr)	β (xcr)	β (bxcr)	γ (bxcr)
16	0.267	5.7	0.354	0.188	17.0
18	0.248	8.4	0.340	0.162	24.0
20	0.229	10.1	0.327	0.149	29.0
22	0.201	13.0	0.316	0.140	32.0
24	0.174	16.4	0.295	0.117	24.0
26	0.156	19.3	0.280	0.085	14.5
28	0.144	22.0	0.262	0.023	−60.0
30	0.135	24.6	0.241	0.056	15.0

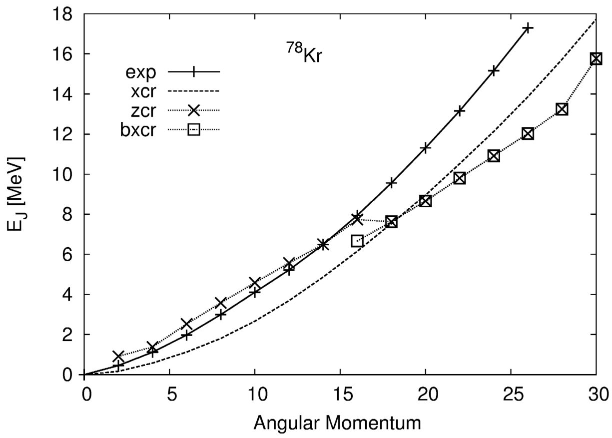

Figure 2. Same as figure 1 for ^{78}Kr with experimental data taken from [6]. Beyond $J = 18$ the zcr and bxcr results are found to be equivalent with triaxial shapes.

intriguing in the two cases when the difference in energy is only about 0.5 MeV with the prolate shape corresponding to the lower energy state.

The variation of energy as a function of J has been depicted in figure 2, where the bxcr curve is drawn only for $J = 16$–30. We find that for $J > 16$ the x-axis cranking levels do not remain the yrast. The $J = 20$–30 branch of the curve is like a forking observed recently at $J = 24$ [6], which is non-yrast just by about 0.037 MeV. The obvious question is as to why this branch is so far not observed experimentally. One possible reason may be that in heavy ion fusion reactions at high spins the entry state hits the ground band branch which is highly collective and cascades down fast to the ground state through stretched $B(E2)$ γ-decays. The other possibility is that in a more realistic treatment either at the Hamiltonian level or at the level of theoretical approach, this branch really lies above the ground band and it is already partially observed [6].

4. Summary and conclusions

Finally we would like to draw the following conclusions:

1. The present calculations show that up to $J = 30$ there does not exist any energy minimum in either of the two nuclei ^{76}Kr and ^{78}Kr corresponding to a tilted axis rotation. As far as experimental ground band is concerned, the xcr results remain the theoretical ground band results. However, for the high-spin states with triaxial shapes, cumbersome three-dimensional TAC calculations could be crucial.
2. In ^{76}Kr the $J = K$ states up to $J = 18$ are predicted to lie at only about 1–2 MeV above the yrast line. For $J = 20$–30 the levels become triaxial with the value of β decreasing gradually to almost a spherical shape. At $J = 28$ triaxial ($\beta = 0.144, \gamma = 22°$) and oblate ($\beta = -0.07$) shapes almost coexist

with a difference in energy of only about 0.25 MeV, the oblate solution being lower.

3. In ^{78}Kr also $J = K$ states (up to $J = 16$) lying close to the yrast line are predicted. At $J = 18$ the two energy values from xcr and zcr differ only by about 0.1 MeV, the xcr value being lower with shape parameters $\beta = 0.340, \gamma = 0.0, \Delta_{\rm p} = 0.624$ MeV and $\Delta_{\rm n} = 0$. On the other hand, for the upper (zcr) solution these parameters are $\beta = 0.162, \gamma = 24°, \Delta_{\rm p} = 0$ and $\Delta_{\rm n} = 0.81$ MeV. Thus, this is a case of shape coexistence not only in quadrupole shape but also the roles of proton and neutron pairing correlations are exactly opposite, a feature, to our knowledge, not reported so far.
4. The present investigations also predict a yrast forking branch in ^{78}Kr with $J = 20$–30.
5. In ^{76}Kr as well as in ^{78}Kr, the angular momentum $J = K = 28$ state is predicted to be isomeric due to the K-selection rules for the γ-decays.

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