Effects of high-order deformation on high-K isomers in superheavy nuclei

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Effects of high order deformation on superheavy high-K isomers

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Using, for the first time, configuration-constrained potential-energy-surface calculations with the inclusion of β_6 deformation, we find remarkable effects of the high order deformation on the high-K isomers in ^{254}No, the focus of recent spectroscopy experiments on superheavy nuclei. For shapes with multipolarity six, the isomers are more tightly bound and, microscopically, have enhanced deformed shell gaps at $N = 152$ and $Z = 100$. The inclusion of β_6 deformation significantly improves the description of the very heavy high-K isomers.

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By overcoming the strong Coulomb repulsion between the large number of protons, shell effects can lead to the so-called "island of stability" centered on a doubly magic nucleus beyond ^{208}Pb that has yet to be identified. On the way to the predicted island, new chemical elements up to $Z = 118$ [1, 2] have been synthesized, while the transfermium nuclei have been studied in detail through spectroscopy experiments [3]. Of special note in spectroscopy studies are multi-quasiparticle (multi-qp) high-K (K is the total angular momentum projection onto the symmetry axis) isomers whose decay to low-K states is inhibited due to K forbiddenness [4]. They provide a probe into the underlying single-particle structure around the Fermi surface. For example, the systematic observation of $K^\pi = 8^-$ isomers in $A \approx 250$ nuclei demonstrates the existence of $N = 152$ and $Z = 100$ deformed shell gaps [5]. Such information is vital for determining the nuclear potential that can then be used to predict properties of superheavy nuclei. Furthermore, superheavy high-K isomers can have enhanced stability against α decay and spontaneous fission due to unpaired nucleons [6], perhaps serving as stepping stones towards the "island of stability".

Among the $A \approx 250$ nuclei in which high-K isomers have been discovered, ^{254}No has been the focus of recent experiments due to its relatively high production rate. Two-qp and four-qp high-K isomers were first established by Herzberg *et al.* [7], Tandel *et al.* [8] and Kondev *et al.* [9]. Later these isomers were extensively studied by Heßberger *et al.* [10] and Clark *et al.* [11], with emphasis on the spectrum above the two-qp isomer. All the experiments agree on the existence of a four-qp isomer with a half-life in the region of 200 μs, but the suggested configurations are controversial. Heßberger *et al.* [10] and Clark *et al.* [11] derived different levels bridging the four-qp and two-qp isomers. More work is required, both experimental and theoretical, to confirm the ^{254}No high-spin level structure.

Theoretical descriptions of superheavy nuclei have made continuous progress [12] along with experiments. One important finding is that high order deformation, especially β_6, is significant in modeling very heavy nuclei [13, 14]. The inclusion of β_6 deformation can give extra binding energy in excess of 1 MeV, resulting in improved reproduction of experimental masses [13]. The ^{254}No moment of inertia calculated with the addition of β_6 deformation is 17% larger than the calculation with only β_2 and β_4 deformations [15]. Remarkable β_6 deformations were predicted in the $A \approx 250$ mass region, with the largest magnitude ($\beta_6 \approx -0.05$) in ^{254}No [15]. In this work, we investigate the high order deformation effects on ^{254}No high-K isomers.

Configuration-constrained potential-energy-surface (PES) calculations [16] have been applied to the three-dimensional deformation space (β_2, β_4, β_6) to determine the deformations and excitation energies of multi-qp states. Other frequently-used deformation degrees of freedom such as γ and β_3 are excluded as they are calculated to be negligible in ^{254}No. The observation of large hindrance in K-forbidden γ-ray transitions (that indicates approximately good K quantum numbers) in ^{254}No has confirmed that the nucleus is well deformed and axially symmetric [11]. Reflection asymmetry can significantly reduce the outer barrier beyond the second potential well of a prolate superheavy nucleus, but does not affect the first well [17]. In addition, ^{254}No has no indication of β_8 deformation [15]. Deformations with multipolarity higher than eight have been demonstrated to be negligible in calculations [14]. Therefore, it is justified for us to limit the calculations to the (β_2, β_4, β_6) deformation space.

We employ the axially deformed Woods-Saxon potential with the set of universal parameters [18] to provide single-particle levels. In order to reduce the unphysical fluctuation of the weakened pairing field (due to the blocking effect of unpaired nucleons) an approximate particle-number projection has been used by means of the Lipkin-Nogami method [19], with pairing strengths determined by the average gap method [20]. In the configuration-constrained PES calculation, it is required to adiabatically block the unpaired nucleon orbits that specify a given configuration. This has been achieved by calculating and identifying the average Nilsson quantum numbers for every orbit involved in a configuration [16]. The good quantum numbers of parity and Ω (the individual angular momentum projection onto the symmetry

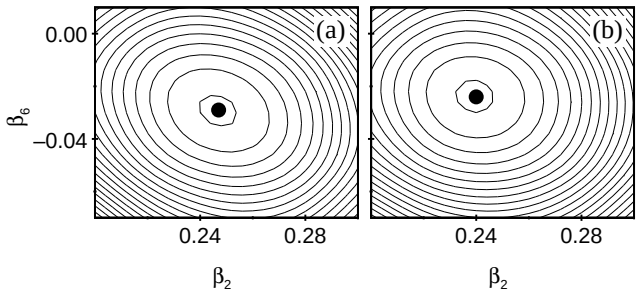

FIG. 1: Calculated PESs for ^{254}No ground state (a) and $K^\pi = 16^+\{\nu 9/2^-[734]\otimes\nu 7/2^+[613]\otimes\pi 7/2^-[514]\otimes\pi 9/2^+[624]\}$ state (b). At each point (β_2, β_6), the energy is minimized with respect to β_4. The energy interval between neighboring contours is 200 keV.

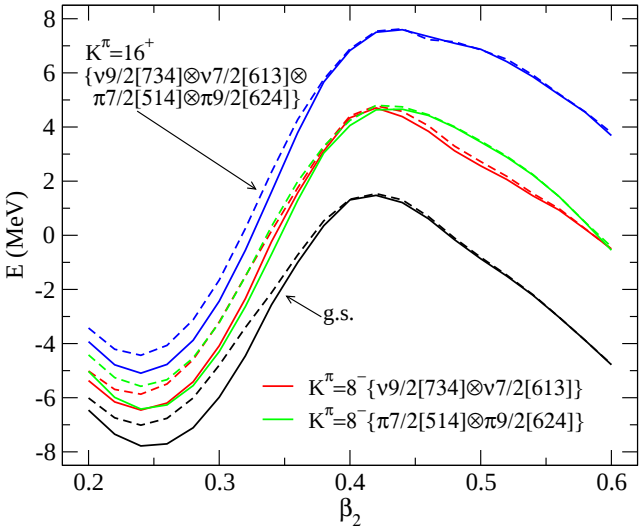

FIG. 2: (Color online) ^{254}No potential energy curves calculated with (solid lines) and without (dashed lines) β_6 deformation. The energy for each β_2 point is minimized with respect to deformations β_4 and β_6.

axis) facilitate the configuration constraint in (β_2, β_4, β_6) deformation space. The total energy of a state consists of a macroscopic part that is obtained with the standard liquid-drop model [21] and a microscopic part that is calculated by the Strutinsky shell-correction approach, including blocking effects. The configuration-constrained PES calculation can properly treat the shape polarization due to unpaired nucleons.

In Fig. 1, we display the calculated PESs for ^{254}No ground state (g.s.) and four-qp high-K state relevant to experiments (see below). The PESs show that the states have remarkable β_6 deformations. The g.s. β_6 deformation -0.029 is smaller in magnitude than -0.05 that was calculated by Muntian *et al.* [15]. This is because we employ the standard liquid-drop model with a sharp surface for the macroscopic energy, while Muntian *et al.* [15] used the Yukawa-plus-exponential model with a diffuse surface that is relatively soft against deformation. Since the latter treatment seems more realistic, our calculations may slightly underestimate the magnitude of the β_6 deformation and hence its effects. Fig. 1 also shows that the shape of ^{254}No is robust against multi-qp excitations, which verifies that the increase in moment of inertia of the high-K bands with respect to the g.s. band is due to the reduction of pairing rather than a change of deformation [11]. The influence of the high order deformation on the stability is significant. The g.s. obtains an extra binding energy of 0.8 MeV due to β_6 deformation. The multi-qp high-K states also have deeper potential wells than those calculated without β_6 deformation, as shown in Fig. 2. The depth increase for the $K^\pi = 8^-\{\pi 7/2^-[514] \otimes \pi 9/2^+[624]\}$ state reaches 0.856 MeV. Importantly, our calculations indicate that the β_6 deformation has no influence on the barrier peaks (see Fig. 2), so that the extra binding energy results in a net increase in fission barrier height. It is seen in Fig. 2 that the multi-qp states have wider and higher fission barriers than the g.s., implying enhanced stability against fission due to unpaired nucleons. This is consistent with the observed very small spontaneous fission branch of $\approx 10^{-4}$ for the two isomers in ^{254}No [10].

The multi-qp states calculated with and without β_6 deformation are compared with experimental data in Fig. 3. (Note: since the excitation energy data for the $K^\pi = 3^+, 8^-$ states from different experiments [7, 8, 10, 11] are similar, we adopt the earliest accurate data [7]; the detailed data from the most recent experiment [11] are used for the other states.) The $K^\pi = 3^+$ state is firmly assigned the proton two-qp configuration $\pi 1/2^-[521] \otimes \pi 7/2^-[514]$ through g factor measurement [7, 8, 11]. The $K = 3$ coupling is energetically favored over the $K = 4$ coupling due to the residual spin-spin interaction between the quasiparticles [22, 23]. According to the Gallagher-Moszkowski (GM) rule [22, 23], the spin-antiparallel coupling is energetically favored for two quasineutrons or two quasiprotons, while the spin-parallel coupling is lower in energy for the combination of a quasineutron and a quasiproton. The splitting energies for the $A \approx 180$ nuclei are found to be in the range of $\approx 100 - 400$ keV [24]. The energy is too small to substantially change the calculation of a multi-qp state. Our model in its present version does not include the residual spin-spin interaction. The calculations usually well reproduce the energetically favored coupling (see e.g. Refs. [6, 16]).

Our calculation of the $\pi 1/2^-[521] \otimes \pi 7/2^-[514]$ configuration with β_6 deformation gives an excitation energy of 0.965 MeV, in very good agreement with the experimental data 0.988 MeV [7]. The low excitation energy implies that the $\pi 1/2^-[521]$ and $\pi 7/2^-[514]$ orbits must be close in energy. In Fig. 4, we present the single-particle levels calculated with and without β_6 deformation. One can see in Fig. 4 that the two orbits become nearly degenerate due to β_6 deformation so that we obtain an improved reproduction of the state with the inclusion of the high order deformation. It is worth noting that β_6 de-

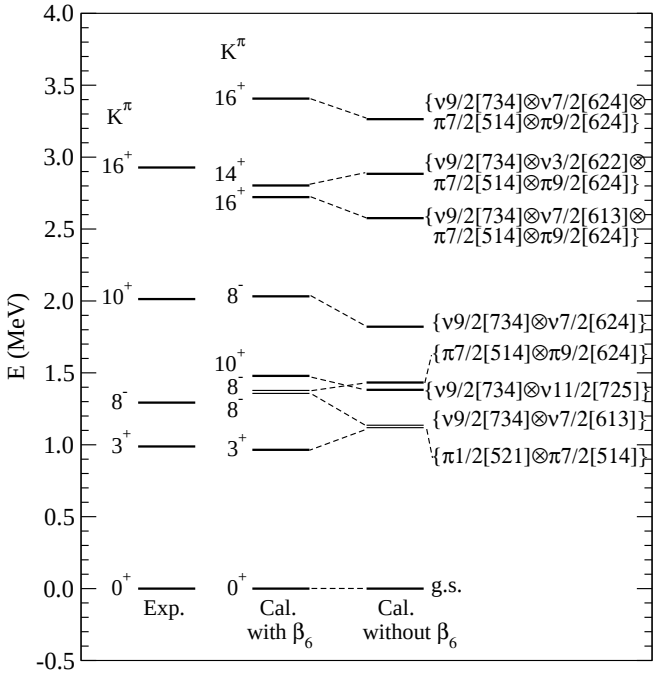

FIG. 3: Calculations of ^{254}No multi-qp states with and without β_6 deformation, compared with experimental data [7, 11].

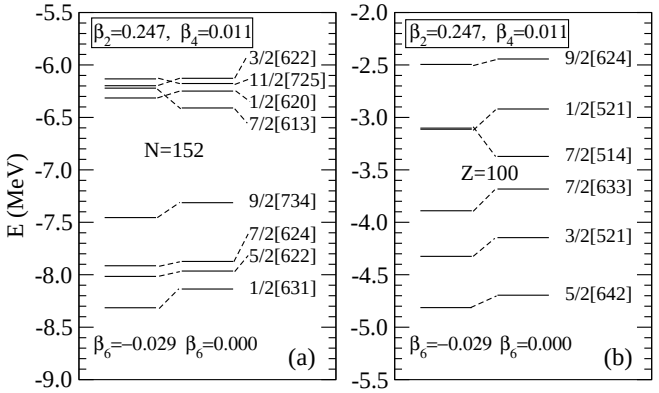

FIG. 4: ^{254}No neutron (a) and proton (b) single-particle levels calculated using the Woods-Saxon potential with the universal parameter set.

formation leads to an enlarged $Z = 100$ deformed shell gap, consistent with that predicted in Ref. [13]. Experiment [5] has confirmed the existence of the gap together with the stronger $N = 152$ gap. The $K^\pi = 3^+$ state is of special interest because the $\pi 1/2^-[521]$ orbit originates from the spherical orbit $2f_{5/2}$ whose position relative to the spin-orbit partner $2f_{7/2}$ determines whether $Z = 114$ is a magic number for the "island of stability". The good agreement between experiments and our calculations with β_6 deformation demonstrates the importance of the high order deformation in very heavy nuclei and the validity of the Woods-Saxon potential in this mass region.

Unlike the $K^\pi = 3^+$ state with its configuration unambiguously assigned, the observed 266 ms $K^\pi = 8^-$ isomer has its configuration controversially assigned in the literature. The proton two-qp configuration $\pi 7/2^-[514] \otimes \pi 9/2^+[624]$ is suggested for the isomer in Refs. [7, 8, 10], while the most recent experiment [11] favors a neutron two-qp configuration. There are two possible $K^\pi = 8^-$ neutron two-qp configurations, $\nu 9/2^-[734] \otimes \nu 7/2^+[613]$ and $\nu 9/2^-[734] \otimes \nu 7/2^+[624]$. Our calculation of the latter indicates that the state is too high in energy to be the isomer. The high energy is because both orbits lie below the large $N = 152$ shell gap. Therefore, it requires two neutrons to cross the gap to form the state. The configuration favors the formation of an isomer in $N = 150$ nuclei where the Fermi surface is between the two orbits. Indeed, low energy isomers with this configuration were systematically observed in $N = 150$ isotones [3]. For the other $K^\pi = 8^-$ neutron two-qp configuration, $\nu 9/2^-[734] \otimes \nu 7/2^+[613]$, the energy calculated with β_6 deformation is very similar to that of the proton two-qp configuration $\pi 7/2^-[514] \otimes \pi 9/2^+[624]$ (see Fig. 3). Both the calculated $K^\pi = 8^-$ states are in better agreement with experiments than those calculated without β_6 deformation. This is attributed to the β_6 deformation that enhances the $N = 152$ and $Z = 100$ deformed shell gaps, leading to increased separation of the $\nu 9/2^-[734]$ and $\nu 7/2^+[613]$ orbits and decreased separation of the $\pi 7/2^-[514]$ and $\pi 9/2^+[624]$ orbits. It should be noted that the $K = 8$ coupling for the neutron two-qp configuration is not the energetically favored one of the GM doublet. When considering the residual spin-spin interaction, the proton two-qp state, instead of the neutron two-qp state, could be the lowest $K^\pi = 8^-$ state. Nevertheless, they remain close to each other because the GM splitting energy is small. Experimental information such as the g factor is needed to distinguish between the two configurations for the $K^\pi = 8^-$ isomer.

The two low-energy $K^\pi = 8^-$ configurations can couple to form a four-qp $K^\pi = 16^+$ state, analogous to the well-known $K^\pi = 16^+$ isomer in ^{178}Hf [4]. Indeed, a four-qp 184 μs isomer has been observed. However, its configuration is less clear than those of the two-qp states. Two possible configurations, $K^\pi = 16^+\{\nu 9/2^-[734] \otimes \nu 7/2^+[624] \otimes \pi 7/2^-[514] \otimes \pi 9/2^+[624]\}$ and $K^\pi = 14^+\{\nu 9/2^-[734] \otimes \nu 3/2^+[622] \otimes \pi 7/2^-[514] \otimes \pi 9/2^+[624]\}$, were suggested in Ref. [7] and Ref. [8], respectively. The most recent experiment [11] preferred a spin-parity assignment of $K^\pi = 16^+$. Our calculations shown in Fig. 3 indicate that the configuration suggested in Ref. [7] is much higher than the four-qp $K^\pi = 16^+$ configuration involving the $\nu 7/2^+[613]$ orbit. This is due to the high energy of the $\nu 9/2^-[734] \otimes \nu 7/2^+[624]$ coupling, as discussed above. The $K^\pi = 14^+$ configuration with a low-Ω orbit $\nu 3/2^+[622]$ involved is calculated to be also higher than the $\nu 9/2^-[734] \otimes \nu 7/2^+[613] \otimes \pi 7/2^-[514] \otimes \pi 9/2^+[624]$ configuration. Consequently, the calculated lowest-lying $K^\pi = 16^+$ state is likely the 184 μs isomer due to its low energy and high K value, compatible with the experimental evidence of a $K^\pi = 16^+$ spin-parity as-

TABLE I: Theoretical deformations and excitation energies of multi-qp states in ^{254}No.

K^π	Configuration†	β_2	β_4	β_6	E_x(keV)
0^+	g.s.	0.247	0.011	-0.029	0
3^+	ab	0.247	0.011	-0.030	965
8^-	AB	0.241	0.012	-0.024	1357
8^-	bc	0.245	0.009	-0.028	1378
6^-	AE	0.247	0.010	-0.029	1427
10^+	AD	0.244	0.010	-0.027	1479
7^-	bd	0.246	0.010	-0.028	1481
8^+	cd	0.244	0.009	-0.027	1658
7^+	BC	0.242	0.014	-0.026	1774
9^-	CD	0.246	0.012	-0.028	1881
8^-	AC	0.243	0.014	-0.025	2032
9^-	BD	0.238	0.010	-0.022	2237
16^+	ABbc	0.240	0.010	-0.024	2722
14^+	AEbc	0.245	0.008	-0.028	2803
18^-	ADbc	0.242	0.008	-0.026	2845
17^+	ABCD	0.239	0.013	-0.023	3158
16^+	ACbc	0.241	0.012	-0.025	3407
25^-	ABCDbc	0.238	0.011	-0.023	4522
24^-	ABCDbd	0.239	0.013	-0.023	4631
25^+	ABCDcd	0.236	0.011	-0.021	4774

† Neutron orbits $9/2^-[734]$, $7/2^+[613]$, $7/2^+[624]$, $11/2^-[725]$, and $3/2^+[622]$ are represented by A, B, C, D, and E respectively. Proton orbits $1/2^-[521]$, $7/2^-[514]$, $9/2^+[624]$, and $7/2^+[633]$ are represented by a, b, c, and d respectively.

signment [11]. The excitation energy calculated with β_6 deformation is 2.722 MeV, which is close to the measured value of 2.928 MeV [11]. In Fig. 3, it can be seen that the inclusion of β_6 deformation increases the calculated energy, making it closer to the experimental value. Furthermore, the neutron component of unfavored residual interaction is expected to further increase the energy.

In addition to all the multi-qp states observed before, a two-qp $K^\pi = 10^+$ state was observed in the most recent experiment [11], with the configuration $\nu 9/2^-[734] \otimes \nu 11/2^-[725]$ suggested. Fig. 3 shows that the calculated excitation energy is 1.479 MeV, much lower than the experimental data 2.013 MeV [11]. However, the $K^\pi = 10^+$ state has unfavored spin-spin coupling that would increase the excitation energy. The energy increment could reach ≈ 400 keV as our calculated excitation energy can be taken as the value for the favored coupling.

As shown in Fig. 4, there exist several high-Ω orbits around the ^{254}No Fermi surface that can couple to many other high-K states. Table I summarizes the calculations with the inclusion of β_6 deformation. The calculated excitation energy of the six-qp $K^\pi = 25^-$ state is 4.522 MeV, comparable to 3.942 MeV, the excitation energy of the observed 24^+ g.s. band member [7]. The $K^\pi = 25^-$ state could be close to the yrast line (where the state has the lowest energy among the states with the same angular momentum), possibly forming an isomeric state.

In summary, the effects of the high order deformation, β_6, on the high-K isomers in ^{254}No are investigated by applying configuration-constrained PES calculations in $(\beta_2, \beta_4, \beta_6)$ deformation space. The isomers gain extra binding energy due to the β_6 deformation, implying enhanced stability against fission. The high order deformation rearranges the single-particle levels, leading to strengthened deformed shell gaps at $N = 152$ and $Z = 100$, which influences the properties of the multi-qp states. These effects are found to be significant. All the observed multi-qp states in ^{254}No are better reproduced by the calculations with β_6 deformation. This indicates the importance of the high order deformation in calculating multi-qp states in very heavy nuclei.

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