Rotational properties in even-even superheavy $^{254-258}$Rf nuclei based on total-Routhian-surface calculations

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Abstract: High-spin yrast structures of even-even superheavy nuclei $^{254-258}$Rf are investigated by means of total-Routhian-surface approach in three-dimensional ($\beta_2, \gamma, \beta_1$) space. The behavior in the moments of inertia of $^{256}$Rf is well reproduced by our calculations, which is attributed to the $j_{15/2}$ neutron rotation-alignment. The competition between rotationally aligned $i_{13/2}$ proton and $j_{15/2}$ neutron is discussed. High-spin predictions are also made for its neighboring isotopes $^{254,256}$Rf.

Key words: rotational properties, total-Routhian-surface calculation, moment of inertia, band crossing

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1 Introduction

Both experimentally and theoretically, studies of superheavy nuclei, with $Z \gtrsim 104$, are a fast developing piece of nuclear physics [1–2]. These nuclei are stabilized by a shell-correction energy, which originates from the clustering of single-particle orbitals and the occurrence of regions of low level density. The structures and formation mechanism of shell-stabilized nuclei are governed by the similar physics responsible for the predicted stability of an island of superheavy nuclei around $Z = 114, N = 184$ (also $Z = 120, 124, or 126$, depending on theoretical models and the parametrization employed) [3, 4, 5]. The precise location of the proposed new magic numbers depends on the single-particle structure sensitively. Presently, the related single-particle levels of the new spherical shell cannot be directly investigated through the use of both in-beam and decay spectroscopy because the production cross sections of these nuclei with $Z \gtrsim 110$ are very small.

However, a great number of spectroscopy measurements have been carried out to study yrast and non-yrast level structures, including high-K isomers, for the deformed nuclei of the transfermium mass region, typically with $Z \approx 100, N \approx 150 – 160$ [4, 5, 6]. High-spin rotational bands have been observed in many of them (e.g. $^{247,249}$Cm [6], $^{248,249,250,252}$Cf [7], $^{250}$Fm [8, 9], $^{252}$Md [9, 10], $^{254}$No [10, 11], $^{254}$Lr [11]). Theoretically, the nuclear properties of the transfermium nuclei have been systematically investigated using various theoretical methods such as the macroscopic-microscopic models and the self-consistent mean-field models (see Refs. [4, 5, 12–20] and references therein). Though these nuclei are not really superheavy ones, they are at the gateway to the superheavy mass region. In particular, their high-spin information can provide an indirect way to study the single-particle states of the next spherical shell above $^{208}$Rf, because some of them are strongly down-sloping and thus can come close to the Fermi surface in the deformed region [21]. Moreover, these high-spin states also may give information on the fission barrier at high angular momentum which is important for understanding the produced mechanism for the heaviest elements [13].

For the superheavy isotopes, spectroscopic studies are in a preliminary stage and detailed information on high-spin properties is still scarce [22]. Nevertheless, the ground-state band in the $Z = 104$ isotope $^{250}$Rf, the first even-even superheavy element for which high-spin data now exist, was recently reported by Greenlees et al. [23]. Soon afterwards, the kinematic and dynamic moments of inertia of the ground-state band in $^{250}$Rf was studied by using a particle-number conserving method based on a cranked shell model [24]. It is conceivable that with the help of the new generation detector systems and radioactive beam facilities [25, 26], the experimental spectroscopic borders of this region will soon be expanded towards even heavier nuclei. In the present work, we aim to understand the high-spin states in the nucleus $^{256}$Rf using self-consistent total-Routhian-surface...
(TRS) approach based on Woods-Saxon (WS) potential and predict the rotational behaviors of its neighboring even-even isotopes $^{254,258}$Rf. Part of the aim of this work is to test the predictive power of present model in superheavy nuclei, although generally successful in other mass regions. The different polarization effects and functional forms of the densities may occur in superheavy region. These effects can be naturally incorporated within the self-consistent nuclear mean-field models, but the preconceived knowledge about the expected densities and single-particle potentials, which fades away towards superheavy region, is required in the macroscopic-microscopic investigations [3].

2 The model

The TRS approach [27–29], which is based on the cranked shell model [30,31], accounts well for the overall systematics of high-spin phenomena in rapidly rotating medium and heavy mass nuclei. The total Routhian, which is called "Routhian" rather than "energy" in a rotating frame of reference, is the sum of the energy of the non-rotating state and the contribution due to cranking. The energy of the non-rotating state consists of a macroscopic part that is obtained from the standard liquid-drop model [32] and a microscopic term representing the Strutinsky shell correction [33]. Single-particle energies needed in the calculation of the quantal shell correction are obtained from a triaxial WS potential [34,35] with the parameter set widely used for cranking calculations. During the diagonalization process of the WS hamiltonian, the oscillator states with the principal quantum number $N \leq 12$ and $14$ have been used as a basis for protons and neutrons, respectively. The nuclear shape is defined by the standard parametrization in which it is expanded in spherical harmonics [33]. The deformation parameters include $\beta_2, \gamma, \text{ and } \beta_4$ where $\gamma$ describes nonaxial shapes. The pairing correlation is treated using the Lipkin-Nogami approach [36] in which the particle number is conserved approximately. This avoids the spurious pairing phase transition encountered in the simpler BCS calculation. Not only monopole but also doubly stretched quadrupole pairings are considered. The quadrupole pairing is important for the proper description of the moments of inertia, though it has negligible effect on energies [37]. The monopole pairing strength, $G$, is determined by the average gap method [38] and the quadrupole pairing strengths are obtained by restoring the Galilean invariance broken by the seniority pairing force [24,39]. The 80 single-particle levels, the respective 40 states just below and above the Fermi energy, are included in the pairing windows for both protons and neutrons. The Strutinsky quantal shell correction is performed with a smoothing range $\gamma = 1.20\hbar\omega_0$, where $\hbar\omega_0 = 41/A^{1/3}$ MeV, and a correction polynomial of order $p = 6$.

The nuclear system is cranked around a fixed axis (the x-axis) at a given rotational frequency $\omega$. Pairing correlations are dependent on rotational frequency and deformation. The resulting cranked-Lipkin-Nogami equation takes the form of the well known Hartree-Fock-Bogolyubov-like (HFB) equation [29]. For a given rotational frequency and point of deformation lattice, pairing is treated self-consistently by solving this equation using a sufficiently large space of WS single-particle states. Certainly, symmetries of the rotating potential can be used to simplify the cranking equations. In the reflection-symmetric case, both signature, $r$, and intrinsic parity, $\pi$ are good quantum numbers. The solution characterized by $(\pi, r)$ provides simultaneously the energy eigenvalue from which it is straightforward to obtain the energy relative to the non-rotating state. After the numerical calculated Routhians at fixed $\omega$ are interpolated using cubic spline function between the lattice points, the equilibrium deformation can be determined by minimizing the calculated TRS. The absolute minimum of the TRS corresponds to the solution for an yrast state. Secondary ones correspond to other solutions, which may be yrast at higher spins.

3 Results and discussions

![Fig. 1. Calculated Woods-Saxon single particle levels near the Fermi surface of $^{256}$Rf$_{152}$ (a) for protons and (b) for neutrons. The positive (negative) parity levels are denoted by solid (dot-dash) lines.](image)

To test the validity of current nuclear potential, single-particle levels calculated for $^{256}$Rf$_{152}$ are shown in Fig. 1 for protons and neutrons, respectively. The typical spherical and deformed shell gaps can clearly be seen, which indicate the best candidates for spherical and deformed nuclei. As an example, the combination of the $Z = 108$ and $N = 162$ gaps at $\beta_2 \approx 0.24$ leads to $^{256}$Hf$_{162}$, which was predicted to be doubly magic deformed nucleus [40]. The effect of the known deformed shell at the
neutron number N=152 is also reproduced in the results for the mass region. The properties of the single-particle structures are in good agreement with previous study by Sobiczewski et al\textsuperscript{41}. The present results are also supported by the microscopic corrections calculated by Möller et al\textsuperscript{42}, which are related to single-particle level density (Low level density results in the large correction energy). In Fig. 3 the unique-parity high-j intruder orbitals are 1i_{13/2} proton and 1j_{15/2} neutron orbitals. The proton (neutron) Fermi surface is just above $\pi$ (0.03+$\nu$)

$^{254}$Rf is expected to be identified, which can provide a test for current nuclear model. Experiments on quasiparticle excitations for $^{256}$Rf have been performed by Jeppesen et al\textsuperscript{43} and by Robinson et al\textsuperscript{44}. However, the search for 2-quasiparticle states is not very successful, even their experimental results and interpretation are in disagreement and conflict. Up to now, there is no convincing evidence for the existence of 2-quasiparticle states in $^{256}$Rf, additional experimental investigation is thus highly desirable.

The present TRS calculations based on the WS potential are performed in the lattice of quadrupole ($\beta_2, \gamma$) deformations with hexadecapole ($\beta_4$) variation, since our previous investigation\textsuperscript{48} with the inclusion of reflection-asymmetric deformation degrees of freedom shows that there is no octupole instabilities at normal deformed minima for the lighter Rf isotopes. In Fig. 2, the evolutions of calculated $\beta_2$, $\beta_4$ and $\gamma$ deformations with increasing rotational frequency are displayed for even-even $^{254-258}$Rf nuclei studied here. These nuclei are predicted to have well-deformed prolate shapes with very small $\gamma$ deformation. Note that the calculated ground-state $\beta_2$ deformations, typically $\approx 0.24$, are basically consistent with the previous results given by Möller et al\textsuperscript{42} and by Sobiczewski et al\textsuperscript{41}. The associated $\beta_4$ deformations are rather stable and decrease slightly with increasing rotational frequency. In our opinion, the decrease of $\beta_2$ as a function of rotational frequency is due to the mixing between the $g^{-}$-band and a 2-quasiparticle ($\pi_{13/2}$ or $\nu_{15/2}$ quasi-particles) aligned band. It seems that a rapid decrease of $\beta_2$ appears after a critical frequency $\approx 0.3$ MeV, which indicates the band crossing frequency. For prolate deformed nuclei, the rotation-induced deoccupation of the antialigned high-$j$ low-$\Omega$ quasiparticle orbitals can cause the nucleus to become less deformed\textsuperscript{49}. The $\pi_{13/2}$ alignment and the $\nu_{15/2}$ alignment seem to produce slightly triaxial shapes.

In principle, the study of multi-quasiparticle excitations can be used to determine the excitation energies and ordering of the single-particle states near the Fermi surface. For example, two 2-quasiproton isomeric states are reported in $^{254}$No by Herzberg et al\textsuperscript{45}, one with a K-value and parity of $K^\pi = 8^- (9/2^+ [521] \otimes 7/2^- [514])$ and the other with a $K^\pi = 3^+ (1/2^- [521] \otimes 7/2^- [514])$. The excitation energies of the 3$^+$ and 8$^-$ states were found at 0.988 and 1.296 MeV, which indicate the single-particle energy of 1/2$^-$ [521] orbital is lower than that of 9/2$^+ [624]$ orbital. Similarly, 2-quasiparticle isomeric states in $^{256}$Rf are expected to be identified, which can provide a test for current nuclear model.
symbols). Experimental data are taken from Ref. 22.

Figure 3 shows the kinematic and dynamic moments of inertia, \( J^{(1)} \) (\( J^{(1)} = \hbar^2 (2I - 1)/E_i(I) \)) and \( J^{(2)} \) (\( J^{(2)} = 4\hbar^2/[E_i(I) - E_n(I - 2)] \)), for the ground-state bands of even-even nuclei \( ^{254-258}\text{Rf} \), which usually can provide useful information on the energies of single-particle orbitals, particularly of those with high \( j \). The level spins adopted here are obtained from Zhang et al 22, which are further confirmed by Zhang et al 23. One can see that the agreements of the moments of inertia for \( ^{256}\text{Rf} \) between theory and experiment are to a great extent excellent. The moments of inertia \( J^{(1)} \), \( J^{(2)} \) show a gradual increase, reflecting a large-interaction band crossing, and essentially no difference among even-even \( ^{254-258}\text{Rf} \) nuclei, especially at low frequency. The upbending phenomena due to the alignment of \( \beta \) neutrons and \( i_{13/2} \) protons are clearly seen in Fig. 3. In general, the changes in the moments of inertia can be well understood in terms of the changing deformations \( \omega \) and pairing correlations. The quadrupole deformation \( \beta_2 \) usually has an important effect on the moments of inertia. However, from the \( \omega \) dependences of \( \beta_2 \) in Fig. 2, we observe a nearly constant behavior for the low-spin region and a sudden decrease in the high-spin states where rotation-alignment occurs. Obviously, the increase in moment of inertia, as shown in Fig. 3, cannot be explained by an increasing deformation \( \beta_2 \). It should be attributed to a decrease in the nucleon pairing correlations due to the Coriolis anti-pairing (CAP) effect. The slightly negative \( \gamma \) deformation may result in a change in the moment of inertia.

To understand the changing properties in the moments of inertia, we display the calculated collective angular momenta for even-even \( ^{254-258}\text{Rf} \) nuclei in Fig. 4 together with proton and neutron components. As expected, the aligned angular momentum shows a similar changing trend to the moment of inertia (Note that its slope means the moment of inertia \( J^{(2)} \)). It can be seen that a substantial increase of the total aligned angular momentum is due to the neutron contribution, though both proton and neutron components increase gently with increasing frequency. A sudden rise in the aligned angular momentum indicates additional contribution from the rotation-alignment of a pair of high-\( j \) neutrons. In this mass region, the related high-\( j \) single-particle states are proton \( i_{13/2} \) and neutron \( j_{15/2} \) orbitals. About 30 years ago, the alignment properties of these orbitals in the actinides were surveyed by Frauendorf et al 31, 50 and by Simon et al 51, 52. Moreover, the behavior of the simultaneous alignment of protons and neutrons has been noticed in different nuclei such as in \( ^{235}\text{U} \) and \( ^{237}\text{Np} \) 31. Recently, several studies 3, 21, 53 indicated the alignments of \( i_{13/2} \) proton and \( j_{15/2} \) neutron pairs are also strongly competitive in some transfermium nuclei (heavy actinides). For example, it was pointed out that the proton and neutron alignments take place simultaneously in the lighter No isotopes (e.g. in \( ^{252,254}\text{No} \)), while the \( j_{15/2} \) neutrons win in the competition between proton- and neutron-alignment in the heavier No isotopes (e.g. in \( ^{254,258}\text{No} \)) 22. Figure 4 shows that the first band crossing is most likely to be ascribed to rotation-alignment of a pair of \( j_{15/2} \) neutrons for the lighter \( ^{254}\text{Rf} \) nucleus and there is a possible competition in rotation-alignment between high-\( j \) intruder protons and neutrons for \( ^{256,258}\text{Rf} \), because the proton and neutron upbending frequencies seem to be somewhat close to each other.
sentenced as follows: (+,+1/2) solid lines, (+,−1/2) dotted lines, (−,+1/2) dashed-dotted lines, and (−,−1/2) dashed lines.

The diagram of the quasi-particle routhians versus rotational frequency is a convenient way to display the interplay between rotation and microscopic structure. By studying the quasi-particle diagram, as shown in Fig. 5, one can see the relevant quasi-particles are those from the unique-parity high-j intruder orbitals with π_13/2 for protons and ν_15/2 for neutrons. The ν_15/2 band crossing in 256Rf is calculated to occur slightly earlier than that for π_13/2, which indicates a competitive behavior to some extent. In contrast, our calculation predicts that the alignment of the 1_15/2 neutron pair is more favored than the π_13/2 alignment in 254,258Rf. Moreover, similar to the situation in N = 152 254No isotope [18], a delayed alignment is calculated to occur in 256Rf.

4 Summary

In the present work, we have studied the evolution properties of the deformations and moments of inertia for even-even 254−258Rf nuclei by using self-consistent TRS method based on WS potential in (β_2,γ,β_3) deformation space. Our results are compared with previous calculations and available experiments. It is shown that the single-particle potential is still valid in the superheavy region and the deformed shell gaps (e.g. at N = 152 and 162) are well reproduced. Calculated moments of inertia of 256Rf are in good agreement with experiments and the up-bending is attributed to rotation-alignment of 1_15/2 neutron pair, showing a competitive property to some extent. Our prediction of rotational properties for 254,258Rf awaits future experimental confirmation. It is clear, however, that high-spin experiments on 254,258Rf, whose correction energies are smaller than that of the deformed magic number N = 152 256Rf nucleus, will meet a great challenge due to the large fission probabilities.

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