Evolution of shape and rotational structure in neutron-deficient $^{118-128}$Ba nuclei

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Received January 30, 2016; Revised April 19, 2016; Accepted April 26, 2016; Published June 30, 2016

The evolution of shape and rotational structure along the yrast line in even–even $^{118-128}$Ba isotopes has been systematically investigated by means of pairing self-consistent Woods–Saxon–Strutinsky calculations using the total Routhian surface approach in $(\beta_2, \gamma, \beta_4)$ deformation space. Based on deformation Routhian curves at different rotational frequencies, the shape instability and softness are evaluated and/or predicted in detail, particularly in the $\gamma$ direction. The backbending or upbending behavior due to the alignments of neutron or proton $h_{11/2}$ orbitals in moments of inertia can be basically reproduced, indicating the necessity for the adjustment of the pairing force strength to the experimental data. It is found that the competition between the proton and neutron alignments may depend sensitively on nuclear shape (e.g., in $^{126}$Ba). In addition, the evolution and transition between vibrational and rotational collective modes along the yrast line are investigated on the basis of the centipede-like E-GOS (E-gamma over spin) curves, showing that the existing disagreement between theory and experiment may be to some extent attributed to a lack of the vibration mechanism in the present model.

Subject Index D11, D12, D13

1. Introduction

The evolution of shape and structure with nucleon number and spin is one of the most significant topics in nuclear structure research. As is well known, different intrinsic shape asymmetries may occur in the nuclear ground and/or excited states. Moreover, considerable effort has been made to reveal the mechanism of spontaneous symmetry breaking and to obtain conclusive evidence [1]. Indeed, an abundance of observed phenomena connected with different nuclear deformations are found in nuclei, for instance, according to the measurements of certain multipole moments. A great deal of evidence of nuclear shape phase transition has also been observed [2]. There exists shape phase transition in some isotopes from vibration to axial rotation or $\gamma$-unstable rotation with respect to the variation of neutron number [3]. Different characteristics may even be involved in one mode of collective motion. For example, along the yrast line there exists transition between rotations with different relations between angular momentum and rotational frequency, which is referred to as band crossing (exhibiting backbending) [4].

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In fact, in the 1970s, the band crossing (popularly known as “backbending”) between rotational bands was discovered at angular momentum \( I \sim 14\hbar \) in \(^{160}\text{Dy}\) \[5\], which was interpreted as being due to the decoupling of a pair of high-\(j\) nucleons from the rotating nuclear core and subsequent alignment of their angular momenta along the rotation axis at a particular rotational frequency \[4\]. Even several years later, a second band crossing was observed at angular momentum \( I \sim 28\hbar \) in \(^{158}\text{Er}\) \[6\]. Such rotational alignment of a pair of nucleons is the most significant discovery in the initial phases of high-spin physics and a dramatic example of the imposition of quasiparticle excitation on collective nuclear motion. Nowadays, it is well established that the precise details of an alignment depend sensitively on the shape of the nucleus and on the quantum numbers of the aligning nucleons (e.g., the high-\(j\) low-\(\Omega\) orbital near the Fermi surface will favor nucleon alignment for prolate shape).

Alignments in the well-deformed, neutron-deficient barium isotopes are particularly interesting because both the neutron and proton Fermi levels lie within the \(h_{11/2}\) subshell. In these nuclei, the proton Fermi surface lies in the lower part of the \(h_{11/2}\) orbitals, which favors prolate shape, whereas the neutron occupies medium- to high-\(\Omega\) orbitals of the \(h_{11/2}\) subshell, which may drive the shape towards oblate \[7\]. Indeed, the nuclear structure property, especially prolate–oblate shape transitions, in neutron-deficient barium isotopes has long been an attractive topic in nuclear physics \[8\]. Experimental data in the yrast states in \(^{118-128}\text{Ba}\) isotopes have been accumulated by means of in-beam \(\gamma\)-ray spectroscopy with heavy-ion fusion–evaporation reactions \[9–14\]. Theoretically, many methods have been employed to study the nuclear properties, e.g., the relativistic mean-field theory \[15\], the interacting boson model \[16\], the dynamic pairing plus quadrupole model \[17\], and the projected shell model \[8\]. By comparing the experimental properties of a rotational alignment with the theoretical predictions, it is possible to deduce information about the nuclear structure and the aligning nucleons. For instance, some interesting phenomena including shape transition and coexistence, two S-bands, band termination, etc. have been identified. However, the theoretical explanations still do not agree with each other.

In our recent work, the evolution of the ground-state quadrupole and octupole stiffnesses in even–even barium and osmium isotopes has been investigated by using potential energy surface (PES) calculations \[18,19\]. It is found that the \(\gamma\) stiffness exhibits an irregular oscillating behavior, whereas the octupole stiffness approximately keeps a relatively large constant in \(^{118-128}\text{Ba}\) isotopes. Therefore, in this work, taking the cranking term into account, we have performed total Routhian surface (TRS) calculations for even–even \(^{118-128}\text{Ba}\) in \((\beta_2, \gamma, \beta_4)\) deformation space, focusing on nuclear properties (e.g., phase/shape transition, band crossing, nuclear softness, etc.) under rotation and the predictive capability of the present deformation space.

2. Theoretical description

The TRS approach based on the cranked-shell model accounts well for the overall systematics of high-spin phenomena in rapidly rotating medium and heavy mass nuclei \[20–24\]. The total Routhian, which is called “Routhian” rather than “energy” in a rotating frame of reference, is the sum of the energy of the nonrotating state and the contribution due to cranking. The energy of the nonrotating state consists of a macroscopic part that is obtained from the standard liquid-drop model \[25\] and a microscopic term representing the Strutinsky shell correction \[26\].

Single-particle energies needed in the calculation of the quantal shell correction are obtained from the nonaxially deformed Woods–Saxon (WS) potential \[27\] with the “universal” parameter set. The nuclear shape is defined by the standard parametrization in which it is expanded in spherical harmonics \[27\], which is particularly well suited for analyzing the symmetry properties \[28\].
The deformation parameters include $\beta_2$, $\gamma$, and $\beta_4$ where $\gamma$ describes nonaxial shapes. The pairing correlation is treated using the Lipkin–Nogami (LN) approach [29] in which the particle number is conserved approximately. This avoids the spurious pairing phase transition encountered in the simpler Bardeen–Cooper–Schrieffer (BCS) calculation. Not only monopole but also doubly stretched quadrupole pairings are considered. Note that in the earlier calculations the quadrupole pairing residual interaction is usually not considered [7,30,31]. However, such quadrupole pairing is important for the proper description of moments of inertia, though it has a negligible effect on energies [32]. The monopole pairing strength, $G$, is determined by the average gap method [33] and the quadrupole pairing strengths are obtained by restoring the Galilean invariance broken by the seniority pairing force [22,34]. 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 $p = 6$.

Cranking indicates that the nuclear system is constrained to rotate 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 (CLN) equation takes the form of the well-known Hartree–Fock–Bogoliubov-like (HFB) equation [22]. 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 $(\pi, r)$ simultaneously provides the energy eigenvalue from which it is straightforward to obtain the energy relative to the nonrotating state. After the calculated Routhians at fixed $\omega$ are interpolated using the cubic spline function between the lattice points, the equilibrium deformation can be determined by minimizing the calculated TRS. Note that in this method the symmetry breaking (deformed shape) achieved through the minimization of the total energy over the shape variables is different from the spontaneous symmetry breaking mechanism, but they show an equivalent result [35]. In some cases, the secondary minima of the TRS may coexist with the global one and they may even be yrast at high-spin states.

3. Calculations and discussions

As discussed in Ref. [18], the equilibrium deformations calculated by different methods may depend on the potential parameters to a large extent, especially for soft nuclei. Relatively, the nuclear stiffness is usually model-independent. Figure 1 shows the corresponding total Routhian curves along the minimum valley of the TRS in both $\beta_2$ and $\gamma$ directions for $^{118-128}$Ba nuclei. The curves at four typical rotational frequencies are used to investigate the shape and softness evolutions under rotation. Since the Lund convention is adopted in the actual calculations, the $\beta_2$ value is always positive since the prolate, oblate, and triaxial shapes can be denoted by the $\gamma$ parameter ranging from $-120^\circ$ to $60^\circ$. In general, such a $\gamma$ range can be divided into three sectors, $[-120^\circ,-60^\circ]$, $[-60^\circ,0^\circ]$, and $[0^\circ,60^\circ]$, which represent the same triaxial shapes at ground state but respectively represent rotation about the long, medium, and short axes at nonzero cranking frequency. The four limiting values ($-120^\circ,-60^\circ,0^\circ$, and $60^\circ$) correspond to the possible rotations of axially symmetric shapes ($-120^\circ$ and $0^\circ$ for prolate and $\pm 60^\circ$ for oblate shapes) with various orientations of the nuclear axes with respect to the rotation axis ($\gamma = -120^\circ$ and $60^\circ$ mean that the nucleus rotates around its symmetry axis—noncollective rotation—and $\gamma = -60^\circ$ and $0^\circ$ mean that the nucleus rotates around an axis perpendicular to the symmetry axis—collective rotation). As shown in Fig. 1, one can visually see the Coriolis effect as well as the evolution of nuclear shape and softness. It seems that these nuclei are all well deformed at ground states and their softnesses increase with increasing $N$, especially in the $\gamma$
Fig. 1. Deformation Routhian curves against $\beta_2$ (a) and $\gamma$ (b) for even–even $^{118-128}$Ba nuclei at several selected rotational frequencies $\omega = 0.0$ (solid lines), 0.20 (dotted lines), 0.40 (dashed lines), and 0.60 (dash–dotted lines) MeV/$h$. At each $\beta_2$ ($\gamma$) point, the energy has been minimized with respect to the $\gamma$ ($\beta_2$) and $\beta_4$ deformations.

direction. In $^{124-128}$Ba nuclei, competition between the prolate and oblate collective excitations and noncollective single-particle excitations may appear at high angular frequency, though their ground states all have prolate shapes [36,37].

As is well known, the moment of inertia is sensitive to nuclear shape and pairing correlations and its variation as a function of rotational frequency can usually provide useful information on the energies of single-particle orbitals, particularly those with high $j$ (particle angular momentum). As mentioned above, the information on the equilibrium deformations can be roughly seen in Fig. 1. Figure 2(a) shows the proton and neutron pairing gaps calculated by the LN pairing approach for even–even $^{118-128}$Ba nuclei, compared with the experimental values extracted from experimental masses [38] by the use of fourth-order finite-difference expressions [39]. Note that the initial pairing strength $G^0$ is crudely adjusted for protons and neutrons according to the empirical suggestions in Ref. [39] (in principle, it should be calculated for each nucleus based on the method in this reference). Anyway, one can see that the description of the pairing gaps is improved to some extent by such adjustments. Meanwhile, as can be seen in Fig. 2(b), the calculated kinematic moments of inertia ($J^{(1)} = I_x/\omega$) with $G$ can agree with the experimental data better (note that, experimentally, $J^{(1)} = h^2(2I - 1)/E_\gamma (I \rightarrow I - 2)$). It should be pointed out that, in $^{126,128}$Ba, nuclear shape transitions from prolate to triaxial/oblate occur after the backbending and the rotation axis even changes from the medium axis to the short one in the high-spin region. Since the aligned proton (neutron) pairs in these nuclei occupy similar orbitals ($h_{11/2}$) (namely, with similar polarizing forces), such shape transitions should be attributed to the soft cores of these two nuclei, in good agreement with the energy curves (see Fig. 1(b)). Of course, a decreasing trend of the moments of inertia appears in the energy sequences (e.g., the sequence marked by the circle or triaxial symbols in $^{126,128}$Ba) with the same shape (e.g., with similar $\gamma$ deformation) and rotation axis, which may be explained by the shrinking $\beta_2$ deformations.

To understand the S-band configurations, the calculated aligned angular momenta of the proton and neutron components for $^{126,128}$Ba nuclei are shown in Fig. 3. The proton and neutron band-crossing frequencies are very close to each other, even in $^{126,128}$Ba (see the following discussions). Certainly,
Fig. 2. (a) Calculated LN pairing gaps of protons (top) and neutrons (bottom) for even–even $^{118-128}$Ba nuclei, together with the experimental values (filled squares) for comparison. The open red circles and blue triangles respectively show the results with the pairing strengths obtained by the average gap method ($G^0$) and nonaverage $G$ values (namely, $G/G^0 = 1.08$ for protons and 1.05 for neutrons). (b) Comparison between the calculated (open symbols) and experimental (solid symbols) values of the kinematic moments of inertia $J^{(1)}$. Similar to (a), the red and blue symbols denote the calculations with the pairing strengths $G^0$ and $G$, respectively. Also, note that the open squares, circles, and triangles represent prolate collective rotation (with $\gamma \sim 0^\circ$), rotation around the medium axis (with $\gamma \sim -43^\circ$, $-47^\circ$), and rotation around the short axis (with $\gamma \sim 48^\circ$, $41^\circ$), respectively. Data sources are $^{118}$Ba [9], $^{120}$Ba [10], $^{122}$Ba [11], $^{124}$Ba [12], $^{126}$Ba [13], and $^{128}$Ba [14].

It can still be seen that the proton rotation alignments are slightly favored, at least in $^{120-124}$Ba, which agrees with some previous studies. In principle, some other experimental arguments like aligned angular momenta, $g$-factors, and transition quadrupole moments along the yrast line can be helpful in deciding the configurations between $(\pi h_{11/2})^2$ and $(\nu h_{11/2})^2$ (these are beyond the scope of the present work). It should be noted that in Fig. 3 the calculations are performed along the yrast line. It seems that the alignments of the neutron pairs are obviously more favored than those of the proton pairs in $^{126,128}$Ba, which conflicts with the calculations by Kumar et al. [8], where the nuclear shapes are fixed as prolate. In fact, the neutron alignment will drive the nucleus from prolate to oblate shape according to the present pairing-deformation self-consistent TRS calculations. However, the prolate minimum will coexist with the oblate one. As an example, we show the calculated results for $^{126}$Ba (similar to $^{128}$Ba) based on the yrast sequences and the prolate minimum in Fig. 4. Actually, it is found that the proton rotation-alignment favors for the prolate band, agreeing with Ref. [8], whereas the neutron rotation-alignment favors for the yrast band (oblate band, as shown in Fig. 4(b); cf. Figs. 2 or 3). Therefore, one can see that the alignments will depend sensitively on the nuclear shape. Interestingly, as mentioned in Ref. [8], $^{126}$Ba may possess an almost equal chance of having prolate or oblate shape, which is, moreover, supported by the measured $E2$ transition strength [40]. The calculations by Pomorski et al. [41] also show that the difference between prolate and oblate minima is small in $^{120-128}$Ba, never being more than about 0.5 MeV, and an oblate minimum is even favored in $^{126}$Ba at the ground state. Further experimental evidence is desired though there are many
Fig. 3. Calculated aligned angular momenta for protons (solid symbols) and neutrons (empty symbols) in even–even $^{118-128}$Ba nuclei as a function of rotational frequency $\hbar \omega$. Similar to Fig. 2(b), the squares, circles, and triangles represent the states of the prolate collective rotation, rotation around the medium axis, and rotation around the short axis, respectively.

Fig. 4. (a) Calculated (open symbols) moments of inertia for both yrast (squares) and prolate (triangles) states in $^{126}$Ba, together with the experimental (solid symbols) values for comparison. (b) Calculated aligned angular momenta of protons (solid symbols) and neutrons (open symbols) at the yrast minimum in $^{126}$Ba. (c) Similar to (b), but at the prolate minimum.
related discussions [42–44]. In addition, our calculated results show that the frequencies for proton and neutron alignments are also very close to each other though they may occur at different shapes.

In addition, one can notice that there still exist some differences between the theoretical and experimental moments of inertia even though the pairing strengths are adjusted (cf. Fig. 2). It seems that some other mechanisms by which the nucleus generates angular momentum, such as vibration and single-particle excitations, should be considered. Indeed, the low-lying $\gamma$ bands have been systematically observed; cf. Ref. [16] and references therein. Even the $\gamma$–S-band has been pointed out and discussed briefly [13]. Strictly speaking, the present TRS calculations cannot be applied to the vibrational states, though the deformation Routhian curve may manifest nuclear softness along different deformation degrees of freedom. However, Regan et al. [45] have pointed out a simple method, namely, the E-GOS (E-gamma over spin) \( R(I) = \frac{E_\gamma (I \rightarrow I-2)}{I(I+1)} \) curve, which can be used to discern the shape and phase evolution between vibrational and rotational modes in nuclei as a function of spin. As mentioned by Regan et al. [45], the $\gamma$-ray decay energies \( E_\gamma (I \rightarrow I-2) \) are given by \( \hbar\omega, \frac{E_{2^+}^2}{4} (I+2) \), and \( \frac{\hbar^2}{2I} (4I - 2) \) for a perfect harmonic vibrator, a $\gamma$-soft rotor, and an axially symmetric rotor, respectively. Correspondingly, the $R(I)$ ratios as functions of spin $I$ will change according to \( \frac{\hbar\omega}{I(I+1)}, \frac{E_{2^+}^2}{4} (1 + \frac{2}{I}), \) and \( \frac{\hbar^2}{2I} (4 - \frac{2}{I}) \). After the factors \( \hbar\omega, \frac{E_{2^+}^2}{4} \), and \( \frac{\hbar^2}{2I} \) are determined, one can plot the related E-GOS curves. Traditionally, these factors are usually obtained only on the basis of the energy of the first $2^+$ state (as shown in the top part of Fig. 5(a); typical examples are presented [45]). In fact, for each $R(I)$ point, the $E_\gamma (I \rightarrow I-2)$ value can be supposed to originate
from the deexcitation of a pure vibrator, an idealized γ-soft rotor, and an axially symmetric rotor, respectively. Then a set of the corresponding factors $\hbar \omega$, $E(2+)$, and $\hbar^2 J$ may be analytically deduced from the $E_\gamma (I \rightarrow I-2)$ value at each spin $I$ point. Therefore, one can plot three corresponding curves at each considered $R(I)$ point. Moreover, it can easily be understood that if one of the assumptions is reasonable the adjacent point will fall on the corresponding curve in general. For instance, in the bottom part of Fig. 5(a), we show such “E-GOS” curves based on different spin-point (including low, medial, and high spins) $E_\gamma (I \rightarrow I-2)$ values. Actually, it can be seen from this figure that at low spins the $^{122}$Ba is γ-soft, then the vibrational character is pronounced and the rotation mode seems to appear at high spins. In Fig. 5(b), we present such E-GOS curves at each spin point based on the three idealized assumptions mentioned above for even–even $^{118-128}$Ba. Note that in order to see more clearly we just keep the curves from one $R(I)$ point to its next adjacent point $R(I+2)$ (such a curve that seems to have many “legs” is referred to as a centipede-like E-GOS curve here). To a large extent, the structure evolution in even–even $^{118-128}$Ba can be better evaluated from such centipede-like E-GOS curves, as shown in Fig. 5(b). As expected, one general trend is these nuclei all exhibit γ-soft, vibrational, and rotational (or γ-soft) properties at low, medial, and high spins, respectively. Though the γ-soft and rotational E-GOS curves seem to coincide with each other at high spins for some nuclei, in principle, they can be qualitatively distinguished due to the different signs of their curve slopes (negative for the γ-soft case and positive for the rotational case). Of course, more precisely, the coupling of different motion modes (which is beyond the scope of this work) needs to be taken into account, especially for the case in which the assumption of the pure motion mode fails.

4. Summary

In conclusion, rotational properties along the yrast line in even–even $^{118-128}$Ba nuclei have been investigated using TRS calculations including the triaxial γ degree of freedom. Nuclear stiffness and shape instability with rotation are evaluated by analyzing the deformation Routhian curves with respect to $\beta_2$ and γ deformations at several selected rotational frequencies, indicating a γ instability in the relatively heavier $^{124-128}$Ba nuclei. The calculated moments of inertia are basically in good agreement with experiments. It is also found that the adjustment of the pairing strength may lead to an improved description for both moments of inertia and backbending frequencies. The features of two S-bands based on the $(\pi h_{11/2})^2$ and $(\nu h_{11/2})^2$ configurations are discussed in detail. A centipede-like E-GOS curve is used for the first time to evaluate the shape and phase evolution between vibrational and rotational structure, indicating that the inclusion of the vibrational mechanism is necessary in future TRS calculations. Certainly, reflection-asymmetric deformations should be added in the present deformation space, especially for the lighter Ba isotopes (e.g., in $^{118-120}$Ba [9,10]) where the negative-parity band related to octupole deformation has been observed.

Acknowledgements

This work is supported by the Outstanding Young Talent Research Fund of Zhengzhou University (Grant No. 1521317002), the Natural Science Foundation of China (Grant Nos. 11205208 and 11205207), and the Foundation and Advanced Technology Research Program of Henan Province (Grant No. 132300410125).

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