Static octupole deformations in $^{96}$Zr from angular momentum and parity projections

Yu-Ting Rong$^{a,b}$, Bing-Nan Lu$^{c,*}$

$^a$Department of Physics, Guangxi Normal University, Guilin, 541004, China
$^b$CAS Key Laboratory of Theoretical Physics, Institute of Theoretical Physics, Chinese Academy of Sciences, Beijing, 100190, China
$^c$Graduate School of China Academy of Engineering Physics, Beijing, 100193, China

Abstract

The shapes of zirconium isotopes remain an unsettled question drawing many interests. Recent analysis based on the STAR measurement in relativistic heavy-ion collision experiments provide evidences of non-zero $\beta_{30}$ in the ground state of $^{96}$Zr [1], however, conventional nuclear structure models do not favour these pear-like shapes. To resolve this issue, in this work we perform systematic projection-after-variation calculations for $^{96}$Zr based on the multi-dimensionally constrained relativistic Hartree-Bogoliubov model. We consider all $\beta_{\lambda\mu}$ with even $\mu$ simultaneously and present selected potential energy surfaces (PES's) and projected PES's with certain angular momentum and parity combinations. While the mean-field calculations always predict reflection-symmetric ground states, static octupole deformations emerge after projecting to the $0^+$ state. We find that $\beta_{20}, \beta_{22}, \beta_{30}$ and $\beta_{32}$ are all necessary for describing the ground state and their values vary significantly for excited states with different angular momenta and parities. These complex structures originate from the competition among various shell structures in this mass region. Our results suggest that both beyond-mean-field effects and exotic shapes are essential elements for understanding the structure of $^{96}$Zr.

Keywords: $^{96}$Zr, octupole deformations, low-lying rotational states, projected multidimensionally-constrained relativistic Hartree-Bogoliubov theory

1. INTRODUCTION

The nuclear intrinsic shapes can be characterized by a few multipole deformation parameters $\beta_{\lambda\mu}$ [2, 3]. The most common nuclear shape is the spheroid described by the quadrupole deformations $\beta_{2\mu}$. For some specific proton or neutron numbers, we can also find pronounced octupole deformations $\beta_{3\mu}$ [4–9]. For a long time, the only reliable method for studying these reflection-asymmetric deformations is to search for the characteristic patterns of parity and angular momentum in the nuclear spectroscopy. For example, the enhanced electric-octupole transition $B(E3)$ in $^{224}$Ra [10], $^{144}$Ba [11], $^{146}$Ba [12], and $^{228}$Th [13] can be viewed as direct experimental evidences of strong octupole deformations.

Recently, it was proposed that the nuclear deformation can also be extracted from the relativistic heavy-ion collisions (RHIC) by analysing the hydrodynamic collective flow of the final state particles [14–18]. Later this method was applied to study realistic experimental data [19–22]. In Ref. [1], the deformations of $^{96}$Zr and $^{96}$Ru are extracted from isobaric $^{96}$Zr+$^{96}$Zr and $^{96}$Ru+$^{96}$Ru collisions, respectively. By analysing the elliptic flow $v_2$ and triangular flow $v_3$ [23], the authors infer a strong octupole deformation with $\beta_3 \gg \beta_2$ in $^{96}$Zr and a strong quadrupole deformation with $\beta_2 \gg \beta_3$ in $^{96}$Ru.

Microscopically, the clue for finding low-energy octupole collectivity is the existence of pairs of single-particle orbitals strongly coupled by the octupole correlations near the Fermi level [4]. Consequently, nuclei with neutron or proton numbers near the octupole magic numbers 34, 56, 88, and 134 are natural candidates for searching for the pear-like nucleus. $^{96}$Zr, whose neutron number is $N = 56$, is one of these nuclei and expected to show reflection-asymmetric (RA) shapes [24–31]. The experimentally observed large $B(E3)$ value in its ground-state band indicates a strong octupole deformation [24–27, 31], which is also corrob-
orated by recent RHIC experiments [1]. Conversely, all systematic search for the octupole deformations based on modern nuclear structure theories, including the macroscopic-microscopic (MM) model [32], the relativistic Hartee-Bogoliubov (RHB) theory [8], the Hartree-Fock-Bogoliubov (HFB) theories with Gogny interaction [7] and Skyrme interactions [9], did not find any static octupole deformation for $^{96}\text{Zr}$. Instead, all these theoretical investigations except for the MM model find static octupole deformations near $N = Z = 40$, which is incompatible with both the experiments and the above argument of octupole magic numbers. To reconcile this inconsistency between the theories and experiments, we need to consider the beyond-mean-field effects not included in above systematic calculations.

The nuclear density functional theories are very successful in describing the nuclear deformations microscopically. In these calculations, the ground states are obtained by applying the variational principle with a Slater determinant or a Bogoliubov vacuum as the trial wave function. The resulting states usually break fundamental symmetries and conservation laws, such as rotational symmetry, translational invariance and particle number conservation. As a consequence, projection-after-variation (PAV) techniques are employed to restore the broken symmetries and calculate observables with good quantum numbers [33–41]. PAV calculations have been applied to study the octupole deformations in Ra isotopes based on shell model wave functions [42], in Ra isotopes [43] and $^{20}\text{Ne}$ [44] based on RHB wave functions, in Ba, Ra isotopes [45, 46], Zr isotopes [47, 48], O [48], actinides, superheavies [49] and other nuclei [50] based on HFB wave functions. There are also theoretical investigations of octupole deformations based on the multi-dimensional collective Hamiltonian [51, 52] and the interacting boson model [53]. The octupole deformations in Zr isotopes have been discussed using the generator-coordinate method (GCM) with a partial angular momentum [30] or parity [54, 55] projection. Besides the axial deformations, recent PAV calculations based on Gogny interaction predict a static tetrahedral shape associated with a pure non-axial $\beta_{32}$ deformation in $^{96}\text{Zr}$ [47]. Nevertheless, so far there is no systematic investigations for the evolution of octupole deformations in the $A \sim 100$ region based on full angular momentum and parity projections. Such calculations will provide necessary knowledge that can help understand the RHIC as well as the spectroscopic experiments.

For studying the various nuclear shapes in a unified framework, the multidimensionally-constrained covariant density functional theories (MDC-CDFTs) have been developed, in which all $\beta_{\mu}$ deformations with even $\mu$ can be considered simultaneously [56–66]. The MDC-CDFTs have been used to study the PES’s and fission barriers in actinides [57–59, 67] and superheavy nuclei [65], the third minima on PES’s of light actinides [63], the effects of higher order deformations in superheavy nuclei [68], the non-axial octupole $Y_{32}$ correlations in $N = 150$ isotones [57] and Zr isotopes [69], the axial octupole $Y_{30}$ correlations in multiple chiral doublet bands (M3D) [70], and the fission dynamics in actinides [62, 64, 71–73]. Besides, by including the strangeness degrees of freedom, the MDC-CDFTs was employed to study the shape evolution [56, 60] and hyperon pairing correlation [66], and build new nucleon-hyperon effective interactions [74]. Recently we developed a projected MDCRHB (p-MDCRHB) model by incorporating the parity and angular momentum projections into the MDCRHB model (a kind of MDC-CDFTs implementing Bogoliubov transformation for pairing correlation) to study the low-lying states related to exotic nuclear shapes, e.g., the triangular shape associated with the three-α configuration in $^{12}\text{C}$ [75].

In this paper, we try to understand the static octupole deformations in $^{96}\text{Zr}$ observed in experiments by using the p-MDCRHB model. For the first time, both axial and reflection asymmetric shapes are considered simultaneously in the beyond-mean-field calculations to study the shapes in $^{96}\text{Zr}$. In Sec. 2, the theoretical framework of this model is introduced. In Sec. 3, we use the p-MDCRHB model to calculate the projected PES’s in $^{96}\text{Zr}$ and extract the deformations and excitation energies of the low-lying states. Comparison with spectroscopic measurements and relativistic collisions experiments are discussed. The microscopic mechanism of the octupole correlations are analysed based on the evolution of single-particle shell structures. Finally, a summary is given in Sec. 4.

2. Theoretical framework

We start with the RHB theory with effective point coupling interactions [76, 77]. In this work, we adopt the PC-PK1 parameter set [78]. The RHB equation in coordinate space reads [79, 80]

$$\int d^3r \begin{pmatrix} \hbar - \lambda & \Delta \\ -\Delta^* & -\hbar + \lambda \end{pmatrix} \begin{pmatrix} U_k \\ V_k \end{pmatrix} = E_k \begin{pmatrix} U_k \\ V_k \end{pmatrix}, \tag{1}$$

where $\Delta$ is the pairing field, $\lambda$ is the Fermi energy, $E_k$ is the quasi-particle energy and $(U_k(r), V_k(r))^T$ is the
Routhian is defined as

\[ h = \alpha \cdot p + \beta [M + S(r)] + V(r), \tag{2} \]

where \( M \) is the nucleon mass, \( S(r) \) is the scalar potential, and \( V(r) \) is the vector potential. In the MD-CRHB model we solve the RHB equation by expanding the wave functions on a axially-deformed harmonic oscillator basis. For pairing interaction, we adopt a separable pairing force of finite range in the spin-singlet channel \([81–84]\).

\[
V = -G \delta(R - R') P(r) P(r') \frac{1 - P_\alpha}{2}, \tag{3}
\]

where \( G \) is the pairing strength, \( R = (r_1 + r_2)/2 \) and \( r = r_1 - r_2 \) are the center of mass and relative coordinates, respectively. The symbols with and without the prime denote the quantities before and after the interaction, respectively. \( P_\alpha \) is the spin-exchange operator. \( P(r) = (4\pi a^2)^{-3/2} e^{-a^2 r^2} \) is the Gaussian function. \( a = 0.644 \) fm is the effective range of the pairing force. In this work we use different pairing strength for neutron and proton, \( G_n = 728.00 \) MeV-fm\(^3\) and \( G_p = 815.36 \) MeV-fm\(^3\). These parameters were adjusted to reproduce the available empirical pairing gaps of \(^{102,104}\)Zr \([69]\).

To obtain a potential energy surface (PES), we use a modified linear constraint method \([59]\) in which the Routhian is defined as

\[
E' = E_{\text{RMF}} + \sum_{\alpha \mu} C_{\alpha \mu} \Phi_{\alpha \mu}, \tag{4}
\]

where \( C_{\alpha \mu} \) is Lagrangian multiplier varied during the iteration and \( \Phi_{\alpha \mu} \) is the multipole moment of the intrinsic densities. The deformation parameter \( \beta_{\alpha \mu} \) is defined as

\[
\beta_{\alpha \mu} = \frac{4\pi}{3AR^1} Q_{\alpha \mu}, \tag{5}
\]

where \( R = 1.2 \text{A}^{1/3} \) fm with \( A \) the mass number.

In the p-MDCRHB model \([75]\), we make parity and angular momentum projections on a RHB wave function \( \Phi(q) \),

\[ |q^{\text{HFB}}_{\alpha, q} \rangle = \sum_K g_{\alpha K}^{\text{HFB}} \hat{P}_M^\dagger \hat{P}_K^\dagger \Phi(q), \tag{6} \]

where \( q \) represents a collection of the deformation parameters,

\[
\hat{P}_M^\dagger = \frac{2I + 1}{8\pi^2} \int d\Omega D_M^*(\Omega) \hat{R}(\Omega), \tag{7}
\]

is the angular momentum projection operator. \( D_M^*(\Omega) \) is the Wigner function with a Euler angle \( \Omega \equiv (\phi, \theta, \psi) \).

\( I \) is the total angular momentum, \( M \) and \( K \) are angular momentum projections onto \( z \)-axis in the laboratory frame and intrinsic frame, respectively. The parity projection operator writes

\[
\hat{P}^\pi = \frac{1}{2}(1 + \pi \hat{P}), \tag{8}
\]

where \( \hat{P} \) is the spatial reflection operation and \( \pi = \pm 1 \) is the parity. The weight function \( g_{\pi K}^{\text{HFB}} \) is obtained by solving the Hill-Wheeler equations.

3. Results and discussions

In the MDCRHB model, both the triaxial (TA) and reflection asymmetric (RA) deformations are allowed. We may turn off TA or RA deformations and keep the nucleus to be axially symmetric (AS) or reflection symmetric (RS). Thus four typical combinations of spatial symmetries can be imposed: AS-RS, AS-RA, TA-RS and TA-RA.

We first impose different symmetries and calculate the mean-field PES’s of \(^{96}\)Zr by solving the RHB equation (1) self-consistently. Figure 1(a) illustrates the PES \( E(\beta_{20}, \beta_{22}) \) with TA-RA. The PES is soft along the \( y = \arctan(\sqrt{2}\beta_{22}/\beta_{20}) \) direction and the ground state is prolate with \( \beta_{20} = 0.21 \). This is similar with the result obtained from the IBM-1 Hamiltonian in the classical limit \([85]\) and RMF+BCS with PC-PK1 \([86]\), but different from recent IBM with configuration calculations, which predict a weakly-deformed \(^{96}\)Zr \([87]\). For the AS-RA PES \( E(\beta_{20}, \beta_{22}) \) in Fig. 1(b), there are two energy minima, \((\beta_{20}, \beta_{22}) = (0.21, 0.00)\) and \((-0.19, 0.00)\). They are consistent with the prolate ground state and the oblate shape isomer found in Fig. 1(a). We find that the ground state of \(^{96}\)Zr has no octupole deformation, consistent with the relativistic Hartree-Bogoliubov (RHB) theory \([8]\), the Hartree-Fock-Bogoliubov (HFB) theories with Gogny interaction \([7]\) and Skyrme interactions \([9]\). Then we allow both non-axial and reflection asymmetric shapes and study the \( \beta_{32} \) deformation. As shown in Fig. 1(c) and (d), we find \( \beta_{20} = 0.21 \) and \( \beta_{32} = 0.00 \) at the global energy minimum. The PES is soft along the \( \beta_{32} \) direction, similar with the calculation with Gogny interaction D1N \([47]\). So, we can confirm that \(^{96}\)Zr is prolate with an oblate isomer in the mean-field level. These results are in agreement with the calculations using the finite-range drople model (FRDM) \([32]\), which gives an axially-deformed ground state at \( \beta_{20} = 0.24 \) with no octupole deformation.

Then we perform angular momentum and parity projections and study the projected PES’s. The 0"
Figure 1: (Color online) Mean-field (MF) potential energy surfaces (PES’s) of $^{96}$Zr obtained from MDCRHb calculations with three combinations of symmetries imposed: (a) triaxial and reflection symmetric (TA-RS) deformations, (b) axially symmetric and reflection asymmetric (AS-RA) deformations, and (c,d) triaxial and reflection asymmetric (TA-RA) deformations. The contours join points with the same energy, and the separation between adjacent contours is 1.0 MeV. On each PES the red star marks the corresponding global energy minima. The energies are rescaled to $E(\text{MF})_{g.s.} = 0.0$ MeV.

PES’s with different symmetry constraints are shown in Fig. 2. The ground state is the global minimum marked by red stars, whose deformations and energies are listed in Table 1. In Fig. 2(a), the TA-RS $0^+$ PES has one energy minimum at $(\beta_{20}, \beta_{22}) = (0.23, 0.07)$, i.e., $(\beta_2, \gamma) = (0.25, 23^\circ)$. This means that the ground state of $^{96}$Zr is triaxial in TA-RS calculations, consistent with the PES from Monte Carlo shell-model (MCSM) [88].

The rotational energy correction, defined as

$$E_{\text{rot}} = E(\text{MF})_{\text{min}} - E(0^+)_{\text{min}},$$

is 4.89 MeV obtained by comparing the global energy minima of the PES’s in Fig. 1(a) and Fig. 2(a).

The AS-RA $0^+$ PES is shown in Fig. 2(b). Comparing with the corresponding mean-field PES Fig. 1(b), we find that symmetry restoration leads to a ground state with a much different shape. The $0^+$ state is found at $(\beta_{20}, \beta_{30}) = (0.01, 0.23)$ and $E_{\text{rot}} = 8.53$ MeV. This projected $0^+$ state assumes a pure reflection-asymmetric shape. This is similar to the conclusion from the symmetry-conserving configuration mixing calculations [46, 50], which found an enhanced octupole deformation accompanied by an almost zero $\beta_{20}$.

Further, the $0^+$ PES is soft along the lines connecting the ground state to the two saddle points on the $\beta_{30} = 0$ axis.

The third and/or fourth deformation degrees of freedom may also appear in the projected ground state of $^{96}$Zr. For simplicity, we next investigate the effect of other deformation degrees of freedom based on the TA-RS and AS-RA PES’s, respectively. In Fig. 2(c), we fix the values of $\beta_{20}$ and $\beta_{22}$ to the deformations of the ground state in projected TA-RS calculations and calculate the PES $E(\beta_{30}, \beta_{32})$. A single energy minimum is found at $(\beta_{20}, \beta_{22}, \beta_{30}, \beta_{32}) = (0.23, 0.07, -0.05, 0.10)$. The rotational energy correction $E_{\text{rot}} = 7.56$ MeV is larger than that in TA-RS calculations, which means that describing the ground state of $^{96}$Zr requires as many as four deformation degrees of freedom. We interchange the order of considering the deformations by performing the angular momentum and parity projections for $E(\beta_{20}, \beta_{30})$ with AS-RA first and then for $E(\beta_{22}, \beta_{32})$. The resulting PES is shown in Fig. 2(d). In this case, the energy minimum is found at $(\beta_{20}, \beta_{22}, \beta_{30}, \beta_{32}) = (0.01, 0.06, 0.23, 0.00)$ and the rotational energy correction $E_{\text{rot}}$ is 9.46 MeV larger than that in the AS-RA calculations. In comparison with the case in Fig. 2(c), the true ground state of $^{96}$Zr can be found in Fig. 2(d) because the latter case corresponds to a larger $E_{\text{rot}}$. Nevertheless, regardless of the order of considering the quadrupole and octupole deformations in the variational calculation to find the ground state, all deformations in question should appear in the projected ground state of $^{96}$Zr. In comparison with the RHIC experiment [1], our results suggest that the non-axial deformations should also be taken into account in simulating the heavy-ion collision data. On the theoretical side, for further determination of the deformations of the ground state of $^{96}$Zr, one needs to perform four-dimensional angular momentum and parity projection calculations.
the larger the deformation parameter $\beta_1$. For $^{96}$Zr, since a large $B(E3)$ value has been measured from experiments [24–27, 31], the octupole deformation is non-negligible. Thus, we first study the excited states in AS-RA calculations. In Fig. 3(a-d), $I^\pi = 2^+, 3^+, 4^+$ and $1^−$ PES’s are illustrated. On the $2^+$ PES, we find two minima at $\beta_{20}, \beta_{30} = (−0.21, 0.09)$ and $(0.22, 0.12)$ with approximately equal energies. The latter minimum is relatively deeper. Comparing with the $0^+$ PES in Fig. 2(b), we find that the location of the global minimum moves significantly when the nucleus is rotating. In this work we extract the excitation spectrum by identifying the lowest energy on each PES as the energies of the corresponding $I^\pi$ states, i.e., the excitation energy for $I^\pi$ state is defined as $E_x(I^\pi) = E(I^\pi)_{\text{min}} − E(0^+)_{\text{min}}$. (10)

With this definition, we find the excitation energy $E_x(2^+) = 4.63$ MeV, which is much higher than the experimental value 1.75 MeV [89]. On the other hand, if we assume static deformations for the ground state band, i.e., fix the deformation to that of the $0^+$ ground state, the $2^+$ excitation energy in this definition will be $E_x(2^+) = 10.58$ MeV. This means $^{96}$Zr cannot be viewed as a rigid rotor. The empirical formula connecting the reduced electric transition probabilities $B(E3)$ and the deformations $\beta_i$ [91] is $\beta_i = \frac{4\pi}{3AR^2} B(E3)^i e^2$, (11)

where $e$ is the electron charge, $A$ is the mass number and $R$ is the nuclear radius. This formula assumes static deformations and thus is not applicable for $^{96}$Zr.

In Fig. 3(b), the energy minimum on the $3^−$ PES is located at $(\beta_{20}, \beta_{30}) = (0.03, 0.24)$, which is close to that of the $0^+$ ground state. We keep the $0^+$ deformations $(\beta_{20}, \beta_{30}) = (0.01, 0.23)$ and obtain $B(E3)(3^− → 0^+) = 20.68 \times 10^3$ e$^3$fm$^6$, which is comparable to the value $23(2) \times 10^3$ e$^3$fm$^6$ from a recent experiment [31]. The corresponding excitation energy is $E_x(3^−) = 4.90$ MeV, which is slightly higher than the calculated $E_x(2^+)$. Although absolute excitation energies are overestimated by about 3 MeV for both $2^+$ and $3^−$ states, the calculated ratio $E_x(3^−)/E_x(2^+)$ is in good agreement with the experimental values. This is similar to the case of $^{32}$Mg with the SLy4 Skyrme interaction [92], D1 Gogny interaction [93], and PC-F1 interaction [94], in which the $2^+$ excitation energy in beyond-mean-field calculations is much larger than the experimental value since the $N = 20$ shell gap persists. In our results, the $N/Z = 40$ shell gaps are large for pure $\beta_{30}$, as shown in Fig. 4. An enhancement of spin-orbit strength that makes the $1g_{9/2}$ lower may help us achieve a better reproduction of the excitation energies, as the case in $^{32}$Mg with D1S interaction [93].

The $4^+$ and $1^−$ states are presented in Fig. 3(c) and (d) to study the shape evolution of the $I^\pi$ states in AS-RA calculations. We find similar shapes for $2^+$ and $1^−$ states from the corresponding PES’s, while the $0^+$ and $3^−$ states are found at almost pure $\beta_{30}$ deformations.

The non-axial deformation degrees of freedom are thought to be important to reproduce the collective excited states in this mass region [47, 86, 88, 95–97]. In order to study how they play a role in the $2^+$ and $3^−$ states, we calculate the TA-RA PES’s $E(\beta_{20}, \beta_{30})$ for the $2^+$ and $3^−$ states with $\beta_{20}, \beta_{30}$ constrained to the values of the global minima in Fig. 3(a) and (b), respectively. On the $2^+$ PES, we find two energy minima: one is on the $\beta_{30}$ axis, the other is on the $\beta_{20}$ axis. The energy difference between them is 0.5 MeV and the one with $\beta_{32} = 0.10$ is the lower one. $E_x(2^+) = 3.06$ MeV obtained from this global minimum with respect to the $0^+$ PES in Fig. 2(d) is closer to the experimental value in

| $I^\pi$ | AS-RA $\beta_{20}$ | AS-RA $\beta_{30}$ | AS-RA $\beta_{22}$ | AS-RA $\beta_{32}$ | AS-RA $E_x$ | TA-RA $\beta_{20}$ | TA-RA $\beta_{30}$ | TA-RA $\beta_{22}$ | TA-RA $\beta_{32}$ | TA-RA $E_x$ | TA-RS $\beta_{20}$ | TA-RS $\beta_{30}$ | TA-RS $\beta_{22}$ | TA-RS $\beta_{32}$ | TA-RS $E_x$ | $E_{x,\text{exp.}}$ |
|---------|-----------------|-----------------|-----------------|-----------------|----------|-----------------|-----------------|-----------------|-----------------|----------|-----------------|-----------------|-----------------|-----------------|-----------------|----------|----------|
| 0$^+$   | 0.01            | 0.23            | 0.06            | 0.00            | 0.23     | 0.07            | −0.05           | 0.10            | −0.05           | 0.10    | 1.75            | [89]           | 1.90            | [90]           | 1.90            | [90]      | 1.90     |
| 2$^+$   | 0.22            | 0.12            | 4.63            | 0.00            | 1.03     | 0.25            | 0.07            | 0.91            | 0.25            | 0.07    | 1.75            | [89]           | 1.90            | [90]           | 1.90            | [90]      | 1.90     |
| 3$^−$   | 0.03            | 0.24            | 4.90            | 0.01            | 0.03     | 4.98            | 0.20            | 0.10            | 5.98            | 0.20    | 1.75            | [89]           | 1.90            | [90]           | 1.90            | [90]      | 1.90     |
| $\text{MF}$ | 0.21           | 0.00            | 8.53            | 0.21            | 0.00     | 9.46            | 0.21            | 0.00            | 4.89            | 0.21    | 7.56            | [90]           | 1.90            | [90]           | 1.90            | [90]      | 1.90     |

RHIC [1] 0.062 0.202

Table 1: The deformation $\beta_{20}$ and excitation energy $E_x$ corresponding to the energy minima on the $0^+$, $2^+$, $3^−$ and mean-field (MF) PES’s for $^{96}$Zr. Theoretical calculations with axial symmetry and reflection asymmetry (AS-RA), triaxial asymmetry and reflection asymmetry based on the AS-RA calculations (AS-RA → TA-RA), triaxial asymmetry and reflection symmetry (TA-RA), triaxial asymmetry and reflection symmetry based on the TA-RS calculations (TA-RS → TA-RA) are listed. Theoretical excitation energies are scaled by $E_0 = 0.0$ MeV with the same symmetries, i.e., $E_x(\text{MF}) = E_{x,\text{exp.}}$. Deformations from the relativistic heavy-ion collision experiments (RHIC) [1] are listed for comparison. The experimental excitation energies ($E_{x,\text{exp.}}$) are taken from Refs. [89, 90]. All excitation energies are in MeV.
comparison with that from the AS-RA calculations. We list in Table 1 the deformations and excitation energies in TA-RS calculations as well. The $E_x(2^+)$ = 0.91 MeV, obtained with a largest $\beta_2$ compared with the other two cases, is smaller than the experimental value [89]. For the 3− PES, the energy minimum is located at $(\beta_{2z}, \beta_{3z}) = (0.01, 0.03)$, indicating a very smaller effect on the $E_x(3^-)$ from non-axial shapes. A energy difference 0.08 MeV is obtained from our definition above. Apparently, the non-zero $\beta_{2z}$ do not change the 3− excitation energy very much and can not help us reproduce the 3− energy from the nuclear spectroscopic experiments [90].

We calculate the mean-field and projected PES’s with DD-PC1 [98] and PC-F1 [77] parameter sets, too. The deformations and excitation energies are similar with those calculated with PC-PK1 presented here.

Figure 3: (Color online) Projected potential energy surfaces for $I^+ = 2^+, 3^+, 4^+ \text{ and } 1^−$ of $^{96}$Zr obtained from p-MDCRHB model with (a−d) axial symmetric and reflection asymmetric (AS-RA) deformations and triaxial and reflection asymmetric (TA-RA) deformations. The contours join points with the same energy, and the separation between adjacent contours is 1.0 MeV. On each PES the red star marks the corresponding global energy minima. The energies are rescaled to $E_{MF}^{g.s.} = 0.0$ MeV.

The emergence of the octupole deformations can be explained by analyzing the single-particle levels around the Fermi level [4, 99]. In Fig. 4 we plot the mean-field single-neutron levels of $^{96}$Zr as functions of $\beta_{20}$ ($\beta_{30}$) with $\beta_{30} = 0.0$ ($\beta_{20} = 0.0$). The single-proton levels below and around $Z = 40$ are similar to those of $N = 40$ and not shown here. For the spherical shape $\beta_{20} = \beta_{30} = 0.0$, the neutron Fermi level lies in between the $2d_{5/2}$ and $1g_{7/2}$ states. In the left half of Fig. 4, we present the dependence of the single-neutron energies on a pure $\beta_{30}$ deformation with $\beta_{20} = 0.0$. We see that the energy splittings caused by non-zero $\beta_{30}$ are small and the spherical gaps at $N = 40$, 50 and 70 are retained for $0 \leq \beta_{30} \leq 0.25$. In the right half of Fig.4, we show the splitting of the neutron energy levels due to pure $\beta_{20}$ deformation. Here the $1h_{11/2}$ state lying above the Fermi level splits into six levels. Thus, neutrons have possibilities to occupy the $1h_{11/2}$ orbital with considerable amplitude, leading to a strong octupole coupling with the orbital $2d_{5/2}$. As for single-proton energy levels, the $1p_{3/2}$ and $1f_{5/2}$ are the two states coupled via pure $\beta_{20}$ deformation while the $1g_{9/2}$ and $1p_{3/2}$ can be coupled via pure $\beta_{30}$ correlation. The energy splitting for non-zero $\beta_{30}$ is again small compared with that for non-zero $\beta_{20}$, resulting in a large shell gap around the proton Fermi surface. For non-zero $\beta_{20}$, some proton levels from the $1g_{9/2}$ and $1p_{3/2}$ states are close to each other near the Fermi surface. Finally, the octupole deformation in $^{96}$Zr derives from the proton levels $2p_{3/2} \rightarrow 1g_{9/2}$ and neutron levels $2d_{5/2} \rightarrow 1h_{11/2}$, which is the same as the conclusion from the MCSM calculations [31].

Figure 4: (Color online) The single-neutron levels of $^{96}$Zr as functions of $\beta_{20}$ ($\beta_{30}$) with $\beta_{30} = 0.0$ ($\beta_{20} = 0.0$). The blue vertical line in the left panel denotes the position $\beta_{30} = 0.23$, which is the deformation of the $0^+$ state in AS-RA calculations, and that in the right panel denotes the deformation of the mean-field ground state. The principal, orbital, and angular momentum quantum numbers $nlj$ for the single-particle levels with spherical symmetry are presented. The dash curve denotes the Fermi level.
4. Summary

The simulation based on the STAR measurement of the isobaric $^{96}$Zr+$^{96}$Zr and $^{96}$Ru+$^{96}$Ru collisions indicates that $^{96}$Zr has a strong octupole deformation [1], which cannot be obtained from density functional theories or finite-range droplet model. In this work we study the deformations in $^{96}$Zr by using the newly developed p-MDCRHB model. The PES’s with different symmetries (AS-RA, TA-RS and TA-RA) are calculated by solving the constrained relativistic Hartree-Bogoliubov equation and projected to low-lying states $0^+$, $2^+$ and $3^-$. Note that we consider both axial and reflection asymmetric shapes simultaneously in the beyond-mean-field calculations to study $^{96}$Zr for the first time.

In mean-field calculations, $^{96}$Zr is axial- and reflection-symmetric with prolate shapes. Only an oblate shape isomer is found. After restoring the rotational and reflection symmetries, we find non-zero values for both quadrupole and octupole deformations. The rotational energies obtained from the two-dimensional projected PES’s depend on deformations in $^{96}$Zr. The PES’s with different symmetries (AS-RA, TA-RS and TA-RA) are calculated by solving the constrained relativistic Hartree-Bogoliubov equation and projected to low-lying states $0^+$, $2^+$ and $3^-$. Note that we consider both axial and reflection asymmetric shapes simultaneously in the beyond-mean-field calculations to study $^{96}$Zr for the first time.

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