Octupole degree of freedom for nuclei near $^{152}$Sm in a reflection-asymmetric relativistic mean-field approach

W Zhang $^{1,2}$, Z P Li$^3$, S Q Zhang $^2$ and J Meng $^{4,2}$

$^1$ School of Electrical Engineering and Automation, He’nan Polytechnic University, Jiaozuo 454003, People’s Republic of China
$^2$ State Key Laboratory of Nuclear Physics and Technology, School of Physics, Peking University, Beijing 100871, People’s Republic of China
$^3$ School of Physical Science and Technology, Southwest University, Chongqing 400715, People’s Republic of China
$^4$ School of Physics and Nuclear Energy Engineering, Beihang University, Beijing 100191, People’s Republic of China

E-mail: zw76@pku.org.cn

Abstract. The potential energy surfaces of even-even isotopes near $^{152}$Sm are investigated within the constrained reflection-asymmetric relativistic mean-field approach using parameter sets PK1 and NL3. It is shown that the critical-point candidate nucleus $^{152}$Sm marks the shape/phase transition not only from $U(5)$ to $SU(3)$ symmetry, but also from the octupole deformed ground state in $^{150}$Sm to the quadrupole deformed ground state in $^{154}$Sm. The important role of the octupole deformation driving pair ($\nu 2f_{7/2}, \nu 1i_{13/2}$) is demonstrated based on the components of the single-particle levels near the Fermi surface. In addition, the patterns of both the proton and the neutron octupole deformation driving pairs ($\nu 2f_{7/2}, \nu 1i_{13/2}$) and ($\pi 2d_{5/2}, \pi 1h_{11/2}$) are investigated.

1. Introduction
The first-order phase transition between spherical $U(5)$ and axially deformed $SU(3)$ shapes [1, 2] has received wide attention in the past decade. It was shown that $^{152}$Sm and other $N = 90$ isotones are empirical examples of the analytic description of nuclei at the critical-point of such a transition [3]. Theoretical studies on the phase transition have typically been based on phenomenological geometric models of nuclear shapes and potentials [2], and algebraic models of nuclear structure [4]. The first calculations, establishing a link between dynamical symmetry models and microscopic theories, were carried out using the Relativistic Mean-Field (RMF) approximation in the Sm isotopes [5]. To date, similar studies have been performed using both relativistic [6, 7, 8, 9] or non-relativistic models [10, 11, 12].

Normally the regions of nuclei with strong octupole correlations correspond to either proton or neutron numbers close to 34 ($1g_{9/2} \leftrightarrow 2p_{3/2}$ coupling), 56 ($1h_{11/2} \leftrightarrow 2d_{5/2}$ coupling), 88 ($1i_{13/2} \leftrightarrow 2f_{7/2}$ coupling), and 134 ($1j_{15/2} \leftrightarrow 2g_{9/2}$ coupling) [13]. A variety of approaches have been applied to investigate the role of octupole degrees of freedom in Sm and neighboring nuclear regions. The Woods-Saxon-Bogoliubov cranking model was used to study the shapes of rotating Xe, Ba, Ce, Nd, and Sm nuclei with $N = 84 - 94$ and the expectations of octupole-deformed mean fields at low and medium spins were confirmed [14]. The $spdf$ interacting boson model was
applied to Sm isotopes with \( N = 86 - 92 \) to examine the signatures of octupole correlations [15]. Based on a collective rotation-vibration Hamiltonian in which the axial quadrupole and octupole degrees of freedom are coupled, the energy levels and electromagnetic transition probabilities for \( N = 90 \) isotones were well reproduced [16].

Very recently, a new \( K^\pi = 0^- \) octupole excitation band has been observed in \(^{152}\text{Sm}\) whereby a pattern of repeating excitations built on the \( 0^+_2 \) level, similar to those built on the ground state, emerges [17]. It is suggested that \(^{152}\text{Sm}\), rather than a critical-point nucleus, is a complex example of shape coexistence [17].

Based on the investigations mentioned above, it is timely and necessary to investigate the Sm isotopes in a microscopic and self-consistent approach with octupole degree of freedom. Considering the remarkable success of RMF theory [18, 19, 20] in describing many nuclear phenomena related to stable nuclei [18], exotic nuclei [21, 22] as well as supernova and neutron stars [23], the newly-developed Reflection-ASymmetric Relativistic Mean-Field (RAS-RMF) approach is a good candidate for this purpose [24]. Recently, the RAS-RMF approach was developed and applied to the well-known octupole deformed nucleus \(^{226}\text{Ra}\) [24], La isotopes [25], Sm isotopes [26], and Ba isotopes [27]. In Ref. [26], the RAS-RMF approach with parameter set PK1 was applied to investigate the potential energy surfaces of even-even \(^{146-156}\text{Sm}\) isotopes in the \((\beta_2, \beta_3)\) plane, and it is suggested that the critical-point candidate nucleus \(^{152}\text{Sm}\) marks the shape/phase transition not only from \(U(5)\) to \(SU(3)\) symmetry, but also from the octupole deformed ground state in \(^{150}\text{Sm}\) to quadrupole deformed ground state in \(^{154}\text{Sm}\).

In this paper, the shape evolution involving octupole degrees of freedom for nuclei near \(^{152}\text{Sm}\) will be analyzed using the RAS-RMF approach with parameter sets PK1 and NL3. Additionally, the patterns of both the proton and the neutron octupole driving pairs \((\nu 2 f_{7/2}, \nu 1 i_{13/2})\) and \((\pi 2d_{5/2}, \pi 1h_{11/2})\) are investigated.

2. Formalism

The RAS-RMF approach is described in Ref. [26] and references therein. In contrast to reflection-symmetric axial-symmetric systems, the spinors for reflection-asymmetric systems are expanded in terms of the eigenfunctions of the Two-Center Harmonic-Oscillator (TCHO) potential

\[
V(r_1, z) = \frac{1}{2} M \omega_1^2 r_1^2 + \left\{ \begin{array}{ll}
\frac{1}{2} M \omega_3^2 (z + z_1)^2, & z < 0 \\
\frac{1}{2} M \omega_3^2 (z - z_2)^2, & z >= 0
\end{array} \right.
\]

(1)

where \( M \) is the nucleon mass, \( z_1 \) and \( z_2 \) (real, positive) represent the distances between the centers of the spheroids and their intersection plane, and \( \omega_1(\omega_2) \) are the corresponding oscillator frequencies for \( z < 0 \) \((z >= 0)\) [24].

The binding energy at a certain deformation is obtained by constraining the mass quadrupole moment \(\langle Q_2 \rangle\) to a given value \(\mu_2\) [28], i.e.,

\[
\langle H' \rangle = \langle H \rangle + \frac{1}{2} C(\langle Q_2 \rangle - \mu_2)^2
\]

(2)

where \( C \) is the curvature constant parameter, and \(\mu_2\) is the given quadrupole moment. The expectation value of \( Q_2 \) is \(\langle Q_2 \rangle = \langle Q_2 \rangle_n + \langle Q_2 \rangle_p \) with \(\langle Q_2 \rangle_n, p = \langle 2r^2 P_2(\cos \theta) \rangle_{n, p} \). The deformation parameter \(\beta_2\) is related to \(\langle Q_2 \rangle\) by, \(\langle Q_2 \rangle = \frac{3}{\sqrt{5\pi}} A r^2 \beta_2\) with \( r = R_0 A^{1/3} \) \((R_0 = 1.2 \text{ fm})\) and \( A \) the mass number. The octupole moment constraint can also be applied similarly with \(\langle Q_3 \rangle = \langle Q_3 \rangle_n + \langle Q_3 \rangle_p\), \(\langle Q_3 \rangle_{n, p} = \langle 2r^3 P_3(\cos \theta) \rangle_{n, p}\), and \(\langle Q_3 \rangle = \frac{3}{\sqrt{5\pi}} A r^3 \beta_3\). By constraining the quadrupole moment and octupole moment simultaneously, the potential energy surface in the \((\beta_2, \beta_3)\) plane can be obtained.
3. Results and discussion
The properties of even-even Sm isotopes are studied using the constrained RAS-RMF approach with parameter set PK1 [29] and NL3 [30]. The parameter sets PK1 and NL3 are obtained by fitting the masses of selected spherical nuclei as well as the saturation properties of nuclear matter. The universal RMF parameter sets successfully describe the properties of spherical [18] and deformed nuclei [19, 20], and hence these parameter sets are believed to be appropriate for application in octupole deformed nuclei. The TCHO basis with 16 major shells for both fermions and bosons is used. The pairing correlation is treated by the BCS approximation with a constant pairing gap $\Delta = 11.2/\sqrt{A}$ MeV.

For both parameter sets, the binding energies are well reproduced within 0.2%. Moreover, a satisfied agreement is obtained for the quadrupole deformations.

To investigate the shape evolution in the Sm isotopes, the total energies as functions of $\beta_2$ and $\beta_3$ have been analyzed. As an example, Fig. 1 displays the contour plots of the total energies for $^{150,152,154}$Sm with PK1 and NL3 parameter sets. Similar conclusions can also be drawn for both parameter sets.

![Contour plots of total energies for Sm isotopes](image)

**Figure 1.** The contour plots of total energies for $^{150,152,154}$Sm in the ($\beta_2$, $\beta_3$) plane obtained in RAS-RMF approach with PK1 and NL3. The energy separation between contour lines is 0.25 MeV. The global minimum and other local minima are denoted by “●” and “○” respectively.

It is found that for the ground states, $^{146,148}$Sm are near spherical, $^{150}$Sm octupole deformed and $^{154,156}$Sm well deformed, while $^{152}$Sm marks the transition from octupole to quadrupole deformation. For $^{152}$Sm with PK1, the global minimum is located at ($\beta_2$, $\beta_3$)=(0.29, 0.0), while a quadrupole minimum emerges at ($\beta_2$, $\beta_3$)=(0.29, 0). For $^{152}$Sm with the NL3 parameter set, the global quadrupole minimum appears at ($\beta_2$, $\beta_3$)=(0.30, 0). Note that the quadrupole deformation $\beta_2$ of this minimum is relatively close to the experimental value $\beta_2^{exp}=0.31$ [32]. It is clear that the region near the quadrupole minimum is soft, e.g., for parameter set PK1, the energy difference between two minima is 0.33 MeV with a 0.5 MeV barrier in between. After including the octupole degree of freedom, $^{152}$Sm marks the shape/phase transition not only from $U(5)$ to $SU(3)$ symmetry, but also from the octupole deformed to quadrupole deformed case. It should be noted that the present calculations are consistent with the axially deformed RMF...
calculations in Ref. [5]. In addition, it is noted that the oblate minima shown in Fig. 1 may not be stable against the $\gamma$ direction [9].

For $^{152}$Sm, the pattern of repeating excitations discovered in Ref. [17] is well understood from the PES obtained above. For the octupole minimum and the quadrupole minimum with PK1, Generator Coordinate Method (GCM) [28, 33] calculations of PES yield two low-lying states in the $(\beta_2, \beta_3)$ plane with similar quadrupole deformation, which are mixture of quadrupole and octupole deformation configurations. Based on these two states, the pattern of repeating excitations is expected.

To understand the evolution of the octupole deformation microscopically, the single-particle levels in $^{152}$Sm for the states minimized with respect to $\beta_3$ and the states with $\beta_3=0$ can be obtained. For neutron, with the octupole degree of freedom, a large energy gap with $N=88$ near the Fermi surface is found, which is related to the softness of the potential energy surface in quadrupole and octupole degrees of freedom in $^{152}$Sm. There is no obvious neutron gap with $\beta_3=0$. In addition, no obvious gaps near the Fermi surfaces can be found for protons.

It is well-known that for nuclei with $N\sim 88$ or $Z\sim 56$ the octupole deformation driving pairs of orbitals include ($\nu 2f_{7/2}$, $\nu 1i_{13/2}$) and $(\pi 2d_{5/2}$, $\pi 1h_{11/2}$), which in the axially deformed case will be subgrouped as ($\nu 1/2[541], \nu 1/2[660]$), ($\nu 3/2[532], \nu 3/2[651]$), ($\nu 5/2[523], \nu 5/2[642]$), ($\nu 7/2[514], \nu 7/2[633]$), and ($\pi 1/2[431], \pi 1/2[550]$), ($\pi 3/2[422], \pi 3/2[541]$), ($\pi 5/2[413], \pi 5/2[532]$), respectively. It is interesting to investigate the behavior pattern of such pairs in the single-particle levels near Fermi surfaces. For parameter set PK1, these levels, together with their BCS occupation probabilities and corresponding contributions from the four leading components, are shown in Table 1. Taking the level $\nu 3/2[521]$ as an example, the second (20.1%) and third (15.5%) components constitute an octupole deformation driving pair ($\nu 3/2[523], \nu 3/2[651]$). Similarly, one can find the pair ($5/2[523], 5/2[642]$) for $\nu 5/2[523]$, the pair ($3/2[532], 3/2[651]$) for $\nu 3/2[532]$, and the pair ($1/2[541], 1/2[660]$) (the fifth component 1/2[660] with 6.0% which is not listed in Table 1) for $\nu 1/2[530]$. However, for the proton side, no octupole deformation driving pairs are found among the four leading components. Therefore, the neutron orbital takes on a more important role in the evolution of octupole deformation in Sm isotopes, in consistent with the energy gaps presented in Ref. [26].

The missing pattern of proton octupole deformation driving pair ($\pi 2d_{5/2}$, $\pi 1h_{11/2}$) in Table 1 for $^{152}$Sm prompts the searching in the neighboring nuclei. In Ref. [27], the PES of even-even $^{142-156}$Ba are investigated using the constrained RAS-RMF approach with parameter set PK1. It is shown that for the ground states, $^{142}$Ba is near spherical without octupole deformation, $^{144-154}$Ba octupole deformed and $^{156}$Ba well quadrupole-deformed. The nuclei with largest

Table 1. Single-particle levels near Fermi surface for the ground state with $(\beta_2$, $\beta_3)$=(0.20, 0.15) in $^{152}$Sm together with their BCS occupation probabilities and corresponding contributions from the four leading components. The components originating from the octupole deformation driving pairs of orbitals ($\nu 2f_{7/2}$, $\nu 1i_{13/2}$) and ($\pi 2d_{5/2}$, $\pi 1h_{11/2}$) are in bold.

| level      | occu. | 1st comp. | 2nd comp. | 3rd comp. | 4th comp. |
|------------|-------|-----------|-----------|-----------|-----------|
| $\nu 3/2[521]$ | 0.401 | 3/2[521] 33.3% | $2[532]$ 20.1% | $3[2651]$ 15.5% | $3[2631]$ 9.4% |
| $\nu 5/2[523]$ | 0.434 | 5/2[523] 57.2% | $5[2532]$ 16.0% | $5[2642]$ 6.7% | $5[2633]$ 5.2% |
| $\nu 3/2[532]$ | 0.946 | 3/2[532] 46.4% | $3[2541]$ 21.1% | $3[2512]$ 8.8% | $3[2651]$ 5.8% |
| $\nu 1/2[530]$ | 0.947 | 1/2[530] 33.9% | $1[2541]$ 18.1% | $1[2510]$ 8.0% | $1[2651]$ 6.2% |
| $\pi 1/2[541]$ | 0.219 | 1/2[420] 21.4% | $1[2541]$ 21.4% | $1[2440]$ 17.7% | $1[2521]$ 9.8% |
| $\pi 7/2[404]$ | 0.763 | 7/2[404] 85.9% | $7[2413]$ 7.3% | $7[2514]$ 2.8% | $7[2604]$ 0.4% |
| $\pi 3/2[541]$ | 0.834 | 3/2[541] 34.6% | 3/2[411] 20.6% | $3[2521]$ 17.9% | $3[2532]$ 9.1% |
| $\pi 5/2[413]$ | 0.952 | 5/2[413] 76.0% | $5[2422]$ 11.2% | $5[2523]$ 4.7% | $5[2303]$ 2.0% |
Table 2. Single-particle levels near Fermi surface for the ground state in $^{148}$Ba together with their BCS occupation probabilities and corresponding contributions from the leading components. The components originating from the octupole deformation driving pairs of orbitals $(\nu 2f_7/2, \nu 1i_{13/2})$ and $(\pi 2d_5/2, \pi 1h_{11/2})$ are in bold. This table is for neutron.

| Level | $\nu 1/2[530]$ | $\nu 3/2[532]$ | $\nu 3/2[521]$ | $\nu 5/2[523]$ |
|-------|----------------|----------------|----------------|----------------|
| 1st comp. | 1/2[530] | 97.3% | 3/2[532] | 52.6% | 3/2[521] | 36.0% | 5/2[523] | 56.4% |
| 2nd comp. | 1/2[541] | 15.6% | 3/2[541] | 17.6% | 3/2[532] | 18.7% | 5/2[532] | 12.7% |
| 3rd comp. | 1/2[660] | 6.2% | 3/2[512] | 6.2% | 3/2[651] | 16.5% | 5/2[651] | 10.1% |
| 4th comp. | 1/2[651] | 5.8% | 3/2[651] | 6.0% | 3/2[631] | 6.8% | 5/2[633] | 5.0% |

Table 3. Same as Table 2, but for proton.

| Level | $\pi 3/2[422]$ | $\pi 1/2[420]$ | $\pi 5/2[413]$ | $\pi 3/2[451]$ |
|-------|----------------|----------------|----------------|----------------|
| 1st comp. | 3/2[422] | 69.4% | 1/2[420] | 38.6% | 5/2[413] | 78.7% | 3/2[451] | 40.8% |
| 2nd comp. | 3/2[431] | 10.7% | 1/2[550] | 14.4% | 5/2[422] | 8.9% | 3/2[521] | 15.3% |
| 3rd comp. | 3/2[402] | 5.1% | 1/2[530] | 11.0% | 5/2[523] | 4.2% | 3/2[411] | 13.9% |
| 4th comp. | 3/2[541] | 3.8% | 1/2[541] | 8.6% | 5/2[532] | 2.0% | 3/2[532] | 10.2% |
| 5th comp. | 3/2[532] | 2.0% | 1/2[400] | 4.2% | 5/2[303] | 1.7% | 3/2[422] | 7.1% |
| 6th comp. | 3/2[521] | 1.7% | 1/2[521] | 3.7% | 5/2[512] | 0.5% | 3/2[512] | 2.2% |
| 7th comp. | 3/2[312] | 1.4% | 1/2[660] | 3.3% | 5/2[813] | 0.1% | 3/2[512] | 1.9% |
| 8th comp. | 3/2[211] | 0.7% | 1/2[431] | 2.7% | 5/2[633] | 0.1% | 3/2[431] | 1.1% |

Octupole deformation $\beta_3$ for the ground states are predicted to be $^{148,150}$Ba ($N = 92, 94$). For $^{148}$Ba, the single-particle levels together with their BCS occupation probabilities and their leading components for the ground state are shown in Tables 2 (for neutron) and 3 (for proton) respectively. For the protons in the ground state of $^{148}$Ba, octupole deformation driving pairs are found among the components of single-particle levels near Fermi surfaces. Therefore, both the neutron and the proton driving pairs play important roles for the octupole minimum in $^{148}$Ba.

4. Conclusion

In this paper, the PES of even-even Sm isotopes in ($\beta_2$, $\beta_3$) plane are obtained using the constrained RAS-RMF approach, and the single-particle levels near Fermi surfaces for the nucleus $^{152}$Sm are studied. It is shown that the critical-point candidate nucleus $^{152}$Sm marks the shape/phase transition, not only from $U(5)$ to $SU(3)$ symmetry, but also from the octupole deformed ground state in $^{150}$Sm to quadrupole deformed ground state in $^{154}$Sm. Furthermore, the possible shape coexistence in $^{152}$Sm [17] can be understood by the microscopic PES.

By including the octupole degree of freedom, from the energy gap and the components of the single-particle levels near Fermi surface, it is demonstrated that the neutrons play an important role for the octupole deformation driving in $^{152}$Sm. Additionally, the behavior patterns of both the proton and the neutron octupole deformation driving pairs ($\nu 2f_7/2$, $\nu 1i_{13/2}$) and ($\pi 2d_5/2$, $\pi 1h_{11/2}$) are investigated, especially for $^{148}$Ba.

Acknowledgments

This work is supported in part by the National Basic Research Program of China under Grant No 2007CB815000, National Natural Science Foundation of China under Grant Nos 10975007, and 10975008, the China Postdoctoral Science Foundation, the Young Backbone Teacher Support Program of He‘nan Polytechnic University, the Funding for Henan Provincial Key Discipline:
Detection Technology and Automation Equipment under Grant No 509923, and the Southwest University Initial Research Foundation Grant to Doctor (SWU110039).

References
[1] Iachello F, Zamfir N V and Casten R F 1998 Phys. Rev. Lett. 81 1191
[2] Iachello F 2001 Phys. Rev. Lett. 87 052502
[3] Casten R F and Zamfir N V 2001 Phys. Rev. Lett. 87 052503
[4] Cejnar P and Jolie J 2009 Prog. Part. Nucl. Phys. 62 210
[5] Meng J, Zhang W, Zhou S G, Toki H and Geng L S 2005 Eur. Phys. J. A 25 23
[6] Sheng Z Q and Guo J Y 2005 Mod. Phys. Lett. A 20 2711
[7] Fossion R, Bonatsos D and Lalazissis G A 2006 Phys. Rev. C 73 044310
[8] Nikšić T, Vretenar D, Lalazissis G A and Ring P 2007 Phys. Rev. Lett. 99 092502
[9] Li Z P, Nikšić T, Vretenar D, Meng J, Lalazissis G A and Ring P 2009 Phys. Rev. C 79 054301
[10] Rodríguez-Guzmán R R and Sarriguren P 2007 Phys. Rev. C 76 064303
[11] Rodríguez T R and Egido J L 2008 Phys. Lett. B663 49
[12] Robledo L M, Rodríguez-Guzmán R R and Sarriguren P 2008 Phys. Rev. C 78 034314
[13] Butler P A and Nazarewicz W 1996 Rev. Mod. Phys. 68 349
[14] Nazarewicz W and Tabor S L 1992 Phys. Rev. C 45 2226
[15] Babilon M, Zamfir N V, Kusnezov D, McCutchen E A and Zilges A 2005 Phys. Rev. C 72 064302
[16] Minkov N, Yotov P, Drenska S, Scheid W, Bonatsos D, Lenis D and Petrellis D 2006 Phys. Rev. C 73 044315
[17] Garrett P E, Kulp W D and Wood J L et al 2009 Phys. Rev. Lett. 103 062501
[18] Ring P 1996 Prog. Part. Nucl. Phys. 37 193
[19] Vretenar D, Afanasiev A V, Lalazissis G A and Ring P 2005 Phys. Rep. 409 101
[20] Meng J, Toki H, Zhou S G, Zhang S Q, Long W H and Geng L S 2006 Prog. Part. Nucl. Phys. 57 470
[21] Meng J and Ring P 1996 Phys. Rev. Lett. 77 3963
[22] Meng J and Ring P 1998 Phys. Rev. Lett. 80 460
[23] Glendenning N K 2000 Compact Stars (New York: Springer-Verlag)
[24] Geng L S, Meng J and Toki H 2007 Chin. Phys. Lett. 24 1865
[25] Wang N and Guo L 2009 Sci. China Ser. G 52(10) 1574
[26] Zhang W, Li Z P, Zhang S Q and Meng J 2010 Phys. Rev. C 81 034302
[27] Zhang W, Li Z P and Zhang S Q 2010 Chin. Phys. C 34(8) 1094
[28] Ring P and Schuck P 1980 The Nuclear Many-body Problem (New York: Springer-Verlag)
[29] Long W H, Meng J, Gai N V and Zhou S G 2004 Phys. Rev. C 69 034319
[30] Lalazissis G A, König J and Ring P 1997 Phys. Rev. C 55 540
[31] Audi G, Wapstra A H and Thibault C 2003 Nucl. Phys. A 729 337
[32] Raman S, Nestor Jr. C W and Tikkanen P 2001 At. Data Nucl. Data Tables 78 1
[33] Yao J M, Meng J, Ring P and Vretenar D 2010 Phys. Rev. C 81 044311