A MICROSCOPIC ANALYSIS ON SHAPE OF RUTHENIUM ISOTOPES

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The analysis of shape evolution between spherical U(5) and $\gamma-$soft O(6) in Ru isotopes, based on the constrained Hartree-Fock-Bogoliubov (HFB) method with the Skyrme force SLy4 has been carried out. By examining potential energy curves (PECs) of even-even Ru isotopes with $50 \leq N \leq 66$, ^{104}Ru has been proposed as an example of possible critical-point nuclei with E(5) symmetry.

Key words: Hartree-Fock-Bogoliubov method, shape evolution, ground-state properties.

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1. INTRODUCTION

The advance of experimental techniques has opened the way for a better understanding of quantum phase transitions (QPT) in a variety of mesoscopic systems, atomic nuclei, molecules and atomic clusters [1]. In the case of atomic nuclei, the concept of QPTs has been applied and investigated in the recent decade, both experimentally and theoretically, in equilibrium shape changes of nuclei [2–4]. A new class of symmetries X(5) and E(5) have been proposed to describe shape phase transitions in atomic nuclei by Iachello [5, 6] and these symmetries was experimentally identified in the spectrum of ^{152}Sm [7] and ^{134}Ba [8]. The X(5) symmetry was suggested to define critical-points in the phase transitions from spherical to axially deformed systems while E(5) symmetry was proposed to describe systems lying at the critical-point in the transition from spherical to $\gamma-$soft shapes.

Theoretical QPTs in nuclei have been studied based on geometrical [2] and algebraic models [3]. Although the X(5) and E(5) symmetries are based on particular solutions of the Bohr-Mottelson differential equations, they are usually applied in the context of the interacting boson model (IBM). As is well known, in the IBM there are three dynamic symmetries given by U(5), SU(3) and SO(6). They are related with spherical symmetry, axially deformed and γ-soft shapes, respectively. The symmetry X(5) is related with the critical-point between the U(5) and SU(3) symmetry limits. The E(5) symmetry corresponds to the phase transition region between the U(5) and O(6) symmetries.

Although the Bohr collective Hamiltonian and the IBM are widely used for describing shape phase transitions in nuclei, mean field theories (*e.g.*, HFB me-

thod [9, 10] and RMF model [11, 12]) which predict many ground-state properties of nuclei successfully have been employed to investigate the critical-point nuclei. The RMF model has been employed to searching of critical-point nuclei in Sm [13], Ce [14] and Ti [15] isotopes. In these studies, ^{148,150,152}Sm and ^{128,130,132,134}Ce have been pointed out as to be an example of the critical-point nuclei with X(5) symmetry while ^{48,52,60}Ti have been proposed as to be the possible critical-point nuclei with E(5) symmetry. A series of isotopes in rare-earth region have been proposed as to be the critical-point nuclei within the HFB method and RMF model [16, 17]. Potential energy curves (PECs) obtained by using quadrupole constrained calculations have been examined to define the possible critical-point nuclei in these studies. While relatively flat PECs are obtained for critical-nuclei with E(5) symmetry, PECs with a bump are obtained for nuclei with X(5) symmetry. It should be noted, however, that one should go beyond mean field for a quantitative analysis of QPT which means that ratios of excitation energies and electromagnetic transition rates should be calculated [18]. Because of this reason, the generator coordinate method has been employed to perform configuration mixing of angular-momentum and particle-number projected relativistic wave functions restricted to axial symmetry in [19]. Extended versions of this approach can be found in [20,21], where collective excitation spectra and transition probabilities were calculated starting from a five dimensional Hamiltonian for quadrupole vibrational and rotational degrees of freedom, with parameters determined by constrained mean field calculations for triaxial shapes, that is, including both β and γ deformations. It should be noted, however, that the PEC given by constrained calculations is important and can provide a qualitative understanding of the phase transition. For this purpose, one should check the evolution of the PECs along the isotopic or isotonic chains.

The IBM has been employed to search the shape phase transition for Ru isotopes by Arias *et al.* [22] and they found that ^{104}Ru is close to the critical-point between spherical and $\gamma-$soft structures. Also, Ru isotopes were studied within the relativistic mean field theory by Próchniak [23]. However, to the best of our knowledge there is no detailed study on the shape evolution of Ru isotopes with non-relativistic mean field formalism. In this study, constrained HFB method has been employed to carried out the ground-state properties of even-even $^{94-110}$Ru isotopes (*e.g.*, total binding energy and quadrupole deformation). In the present study, the structural evolution of Ru isotopes has been examined by using PECs and calculated neutron single-particle spectra of Ru isotopes.

2. DETAILS ON CALCULATIONS

A two-body Hamiltonian of a system of fermions can be interpreted by means of a set of annihilation and creation operators in HFB method. The ground-state

wave function is defined as the quasi-particle vacuum. The linear Bogoliubov transformation gives a relation between the particle operator and quasiparticle operators. Main part of the HFB model are the density matrix and the pairing tensor. Expectation value of the HFB Hamiltonian could be expressed as to be an energy functional (Further details can be found in [25–27]). In terms of Skyrme forces, the HFB energy has the form of local energy density functional. It contains the sum of the mean field and pairing energy densities. These fields can be calculated in the coordinate space [25, 26]. In this work, HFB equations have been solved by expanding quasi-particle wave functions that conserve axial symmetry and parity on a harmonic oscillator basis expressed in coordinate space proposed by Stoitsov *et al.* [26]. For pairing, Lipkin-Nogami method is performed. The oscillator parameter b_0 has been chosen as to be $b_0 = \sqrt{2(\hbar^2/2m)(49.2A^{-1/3})}$. In order to obtain the PECs, constrained HFB calculation with the use of the standard quadratic form [9,26] has been performed. 16 oscillator numbers have been taken into account. A number of effective Skyrme forces can be found for correct prediction of the nuclear ground-state properties [28–30]. In this study, one of the widely used Skyrme forces SLy4 [30] has been used.

3. RESULTS AND DISCUSSIONS

The calculated binding energies for the ground-state of even-even Ru isotopes from ^{94}Ru to ^{110}Ru are tabulated in Table 1. Also, experimental data taken from Ref. [31] are listed for comparison. As can be seen in Table 1, the calculated results of binding energies are in good agreement with the available experimental data. The mean difference between experimental data and the predictions of the HFB method is 1.500 MeV. Because of this reason, it can be say that the HFB formalism describes ground-state binding energies of Ru isotopes successfully.

The deformation is an important quantity to describing of the properties of nuclei. In the present work, the quadrupole moments of even-even Ru isotopes have been obtained from the solution of axially deformed HFB equations. For defining the deformation, the quadrupole deformation parameter β_2 is commonly used rather than quadrupole moments. The calculated β_2 values of even-even Ru isotopes and available experimental results taken from Ref. [32] are shown in Table 2. It should be noted that β_2 is not observed directly from an experiment. Conventional method to determining of the experimental β_2 is usage of the electric quadrupole transition rate from ground-state 0^+ to the 2^+ state $B(E2)\uparrow$ [32]. $B(E2)\uparrow$ and β_2 can be connected with each other *via* the formula

$$\beta_2 = (4\pi/3ZR_0^2)[B(E2)\uparrow/e^2]^{1/2}, \tag{1}$$

where $R_0 = 1.2A^{1/3}$. As can be understood from the Table 2, the predictions of the

Table 1

The total binding energy (in units of MeV) for the ground-state of $^{94-110}$Ru calculated by the constrained HFB method with the Skyrme force SLy4. The experimental data [31] are also shown for comparison.

Isotope	Present study	Experiment
^{94}Ru	810.151	806.896
^{96}Ru	827.556	826.464
^{98}Ru	844.664	844.760
^{100}Ru	861.239	861.900
^{102}Ru	875.845	877.914
^{104}Ru	889.701	893.048
^{106}Ru	903.621	907.466
^{108}Ru	916.850	920.916
^{110}Ru	929.695	933.460

HFB method with SLy4 parameter set for β_2 values of Ru isotopes are in agreement with the experimental data. β_2 with minus sign in Table 2 is indicates that the nuclei has oblate shape.

Table 2

The calculated quadrupole deformation parameter β_2 for the ground-state of $^{94-110}$Ru. The available experimental data [32] are shown for comparison.

Isotope	present work	Experiment
^{94}Ru	0.001	
^{96}Ru	0.043	0.158
^{98}Ru	0.140	0.195
^{100}Ru	0.197	0.215
^{102}Ru	0.200	0.240
^{104}Ru	0.232	0.271
^{106}Ru	0.318	0.257
^{108}Ru	−0.219	0.292
^{110}Ru	−0.212	0.295

The HFB formalism has been employed to the investigate structural evolution of $^{94-110}$Ru because of its success in describing the total binding energies and deformation parameters of Ru isotopes. Calculated PECs as a function of quadrupole deformation parameter β_2 for $^{94-110}$Ru are shown in Fig. 1. In the figure, the binding energy for the ground-state is taken as to be reference and 0 MeV is shown with dash-dotted line. As can be seen in the Fig. 1, ^{94}Ru isotope which has shell closure

at magic neutron number $N = 50$ is found to be as spherical. The PEC of ^{96}Ru implies that the nuclei has spherical shape. With increasing of neutron numbers starting from the ^{98}Ru to ^{102}Ru nuclei, shape of Ru isotopes have become prolate. The PEC of ^{104}Ru obtained from the HFB method in the Fig. 1 seems flat from $\beta_2 = -0.25$ to $\beta_2 = 0.30$. Through these β_2 intervals, the variation of the binding energies in the PECs are less than 2 MeV. This implies that the barrier against deformation is weak and ^{104}Ru maybe possible candidate of the critical-point nuclei with E(5) symmetry. Beside, the PECs of $^{108-110}$Ru isotopes show that these nuclei have oblate shape.

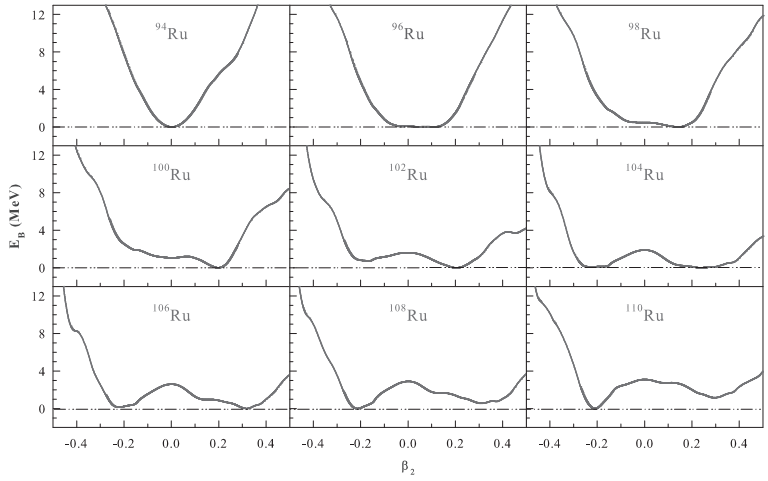

Fig. 1 – Calculated potential energy curves (PECs), where the binding energy of the ground-state taken as a reference, for $^{94-110}$Ru in the HFB method with the Skyrme force SLy4.

The differences of the calculated binding energy between the spherical state and the ground-state for $^{94-110}$Ru are presented in Table 3. It can be meaningful to understanding of how the shape of the Ru isotopes changes with the neutron number and it can show how soft the nucleus is against deformation. The calculated binding energy differences between the spherical and the ground-state of $^{94-110}$Ru change from 0 to 3.090 MeV. A drastic change is clearly visible around ^{104}Ru which means that ^{104}Ru nuclei is in transition region.

The variation of the neutron single-particle energies of Ru isotopes can be used for a better understanding of the shape evolution and shell structure. In the Fig. 2, the predictions of HFB method for the neutron single-particle levels of the ground-state of $^{94-110}$Ru lying between 0 and -25 MeV are shown. The Fermi levels are shown with dot-line. The calculated values of neutron single-particle levels are better restored with a clear gap at the neutron number $N = 50$ and 52 which means that ^{94}Ru and ^{96}Ru seem to be as spherical which is consistent with the result of their

Table 3

The difference of the total binding energy (in units of MeV) between the spherical-state and the ground-state of $^{94-110}$Ru calculated by the constrained HFB method.

Isotope	HFB-SLy4
^{94}Ru	0.000
^{96}Ru	0.097
^{98}Ru	0.490
^{100}Ru	1.051
^{102}Ru	1.591
^{104}Ru	1.889
^{106}Ru	2.594
^{108}Ru	2.892
^{110}Ru	3.090

PECs. In the Fig. 2, starting from ^{98}Ru to ^{102}Ru nuclei, the restoration of the levels is not uniformly distributed as in the those of ^{94}Ru and the level-space becomes smaller than the former which means there is a trend towards a deformed ground-state. However, there is an abrupt change which indicates that level-space of the nuclei is bigger than the former at $N = 58$. The level-space starts again to become smaller than the former with the increasing of neutron number in $^{106-110}$Ru. The findings imply that the ^{104}Ru is in transitional area as consistent with its PEC results.

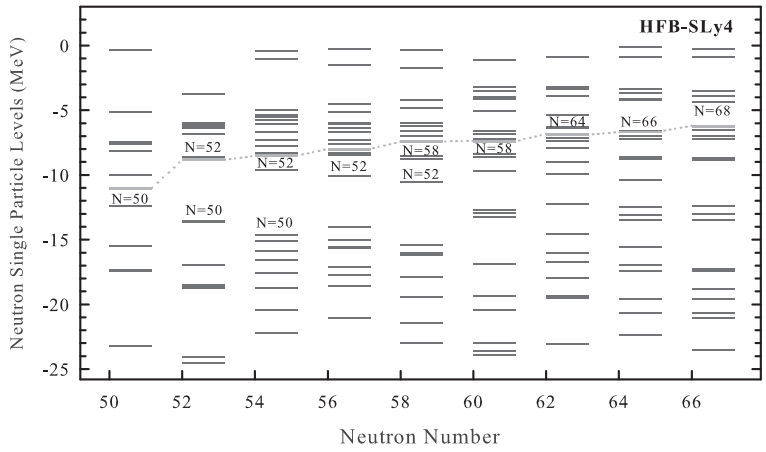

Fig. 2 – The neutron single particle levels for even-even $^{94-110}$Ru isotopes in the HFB method with the Skyrme force SLy4.

The E(5) symmetry was investigated by examining the PECs of even-even Ru

isotopic chain obtained from the interacting boson model (IBM) by Arias *et al.* [22]. Also, some ratios of excitation energies (*e.g.*, $R_{4/2} = E(4_1^+)/E(2_1^+)$) were calculated and compared with the E(5) symmetry predictions (obtained from the solution of Bohr-Mottelson differential equations) for confirmation of their PEC results. Their findings indicated that ^{104}Ru is close to the critical-point between spherical and $\gamma-$soft structures. The findings of the present work confirm the those of study of Arias *et al.* [22].

4. SUMMARY

The total binding energies and deformation parameters of $^{94-110}$Ru isotopes have been reproduced very well in the constrained HFB formalism with the Skyrme force SLy4. By studying the potential energy curves and neutron single-particle spectrum of even-even $^{94-110}$Ru obtained from the constrained calculations ^{104}Ru has been suggested to an example of possible critical-point nuclei with E(5) symmetry.

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