

## Deformed-Skyrme-Hartree-Fock calculation of Hg isotopes

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(Received 14 May 1998)

The ground-state properties of Hg isotopes are investigated by the deformed Skyrme-Hartree-Fock (DSHF) model with new force parameters SKI4 [P. G. Reinhard and H. Flocard, Nucl. Phys. **A584**, 467 (1995)]. Calculations show that the deformed Skyrme-Hartree-Fock model with the above force parameters provides a good description of the binding energies, radii, and deformation parameters of Hg isotopes. Six kinds of configurations, which include a spherical shape, prolate one, oblate one, and three sets of triaxial shapes, are considered in our calculations, and this almost exhausts all possibilities of deformations for nuclei. A detailed discussion of the numerical results is given in this paper. [S0556-2813(99)02301-8]

PACS number(s): 21.10.Dr, 21.30.Fe, 21.60.Jz

### I. INTRODUCTION

As a result of the experimental development of radioactive beams, a new field in nuclear physics has appeared recently: studies on exotic nuclei far from stability. The quality and quantity of experimental data on exotic nuclei have increased greatly in the past few years [1–4]. This provides a good opportunity to test and develop various nuclear structure models which have been proposed based on studies of nuclei near the stable line. It also gives us a chance to see the merits and drawbacks of various mean-field models when we apply them to all nuclei in the periodic table.

Among many open problems in this new field, the variation of nuclear shapes with neutron excess for an isotope chain has attracted both theoretical and experimental attention because it is directly related to the coupling between deformation degrees of freedom and isospin degrees of freedom. The chain of Hg isotopes is a good example to investigate the variation of shapes with neutron excesses because there are rich data on this isotope chain [5–16]. Previous studies [5–16] show that there are shape coexistences in many Hg isotopes and therefore their structures are more complicated than other nuclei. This will bring about a stringent restriction on the validity of various force parameters in mean-field models. Bengtsson *et al.* [5] have used the Woods-Saxon potential and the modified harmonic oscillator (Nillson) potential to calculate the properties of <sup>182–188</sup>Hg in the triaxial gamma plane. They found that an oblate ground state appears for <sup>178–188</sup>Hg [5]. Otten [3] has predicted that there may be triaxial shape in Hg isotopes. Patra *et al.* [6] and Yoshida and co-workers [7,8] have calculated the properties of Hg isotopes using a deformed relativistic mean-field (RMF) model with parameter set NL1. They conclude [6–8] that there are shape transitions from oblate ellipsoid to prolate ellipsoid at <sup>178</sup>Hg and from prolate ellipsoid to oblate ellipsoid at <sup>188</sup>Hg. A superdeformed ground state in <sup>180</sup>Hg is also reported in their papers [6–8]. However, Heyde *et al.* [9] have pointed out that some of the numerical results con-

tradict experimental data for Hg isotopes. Therefore it is interesting to investigate the ground-state properties of Hg isotopes in detail.

The Skyrme-Hartree-Fock (SHF) model has proved to be a successful tool for a microscopical description of the ground-state properties of nuclei. Bonche *et al.* [10–12] have adumbrated shape isomerism and concomitant superdeformation in the Hg isotopes using the SHF model with parameter set SKM\*. They also studied the depopulation of the superdeformation by the generator coordinate method [10–12]. But it is pointed out recently that the traditional force parameters in the Skyrme parametrization (such as SKM\*) is determined by fitting the ground-state properties of several nuclei near the stable line and therefore they fail to reproduce the observed isotope shifts in Sr and Pb elements [17,18]. In order to solve the above problem in the SHF model, Reinhard and Flocard [18] have introduced isospin degrees of freedom in the spin-orbit term, i.e., to replace the normal spin-orbit potential with a generalized spin-orbit potential. A new set of the force parameters SKI4 has been proposed by a fit of the ground-state properties of nuclei near the stable line and far from the stable line [18].

Recently, we have used the new parameter set SKI4 to calculate the ground state properties of spherical nuclei such as Ni, Sn, and Pb isotopes [19,20]. It is found that the SKI4 has succeeded in describing the above nuclei both near the stable line and far from the stable line [19,20]. The successes of the force SKI4 for spherical nuclei encourage us to apply this force to deformed nuclei. In this article, we will report theoretical results of Hg isotopes using the parameter set SKI4 where possible configurations of deformations such as triaxial deformations will be included. In our calculation, the single-particle wave functions are expressed in a three-dimensional Cartesian-mesh representation. One of the advantages of the mesh representation is that we can treat the various shapes such as triaxial deformation and superdeformation without preparing a specific basis for each shape [13,14]. We have calculated the ground-state properties of

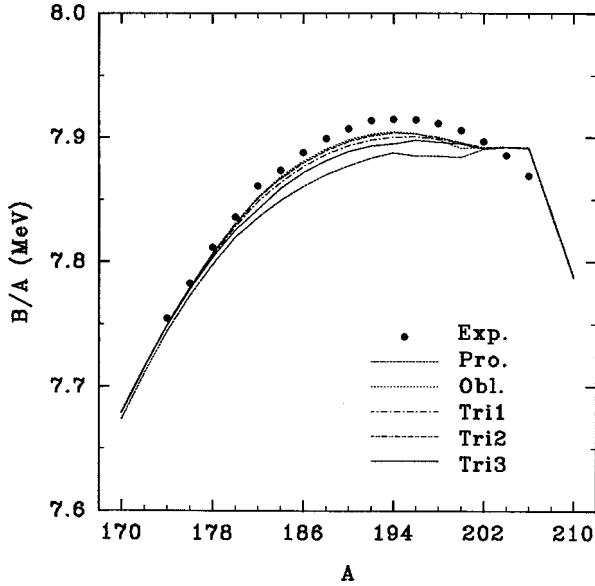


FIG. 1. The binding energy per nucleon of Hg isotopes for five cases.

light C isotopes and found that they agree well with experimental data [21]. Here we will report a large-scale calculation on heavy Hg isotopes.

This paper is organized in the following way. Section II is a short description of the framework of the model and method. In Sec. III, we give the numerical results and a discussion. Section IV is a summary.

### II. MODEL AND METHOD

As the Skyrme-Hartree-Fock model is a standard theory and all the formulations can be found in Refs. [19, 20], here we only give a short description on the framework of the SHF model with new force parameters SKI4 [18].

The SHF equation is written as follows:

$$\left[ -\nabla \cdot \frac{\hbar^2}{2m_q^*(\mathbf{r})} \nabla + U_q(\mathbf{r}) + W_q(\mathbf{r})(-i)(\nabla \times \sigma) \right] \phi_i = e \phi_i, \quad (1)$$

where  $(\hbar^2/2m_q^*)(\mathbf{r})$  is the inverse mass,  $U_q(\mathbf{r})$  is the potential, and  $W_q(\mathbf{r})$  is the spin-orbit potential. A detailed description of the above terms can be found in Refs. [19, 20]. For the normal Skyrme force, the neutron density dependence is linear for the inverse mass and spin-orbit potentials [18]:

$$\frac{\hbar^2}{2m_q^*(\mathbf{r})} = \frac{\hbar^2}{2m} + b_1 \rho(\mathbf{r}) + b'_1 \rho_q(\mathbf{r}), \quad (2)$$

$$W_q(\mathbf{r}) = b_4 [\nabla \rho(\mathbf{r}) + \nabla \rho_q(\mathbf{r})]. \quad (3)$$

Reinhard and Flocard [18] have introduced an additional coefficient  $b'_4$  in the spin-orbit term in a generalized Skyrme functional:

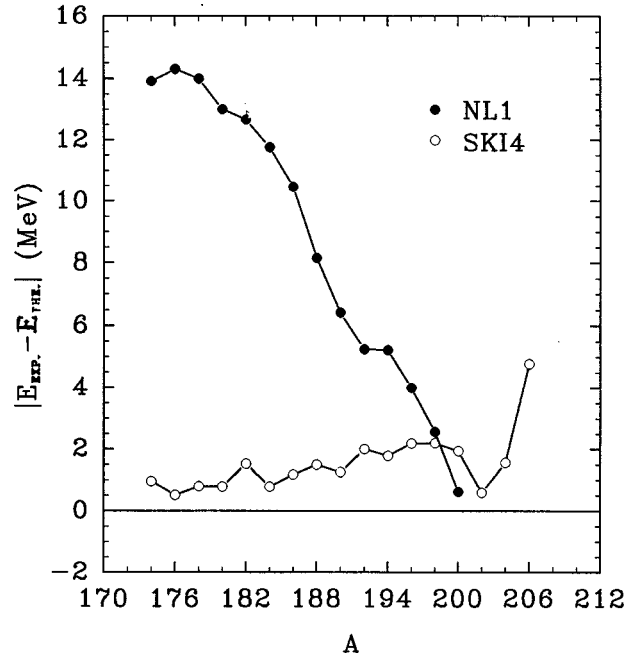


FIG. 2. The absolute difference of the binding energy between theoretical results and experimental data for Hg isotopes.

$$\varepsilon_{ls} = - \int d^3r \left\{ b_4 \rho \nabla J + \sum_{q \in \{p,n\}} b'_4 \rho_q \nabla J_q \right\}, \quad (4)$$

where  $J$  is the spin density and its definition can be found in Refs. [19, 20]. The spin-orbit potential  $W$  for the nucleus becomes [18]

$$W_q(\mathbf{r}) = b_4 \nabla \rho(\mathbf{r}) + b'_4 \nabla \rho_q(\mathbf{r}). \quad (5)$$

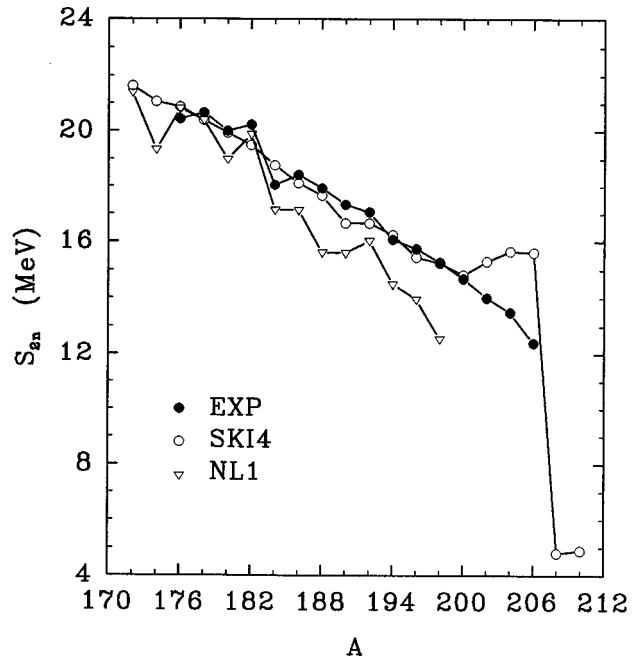


FIG. 3. Two-neutron separation energy of Hg isotopes. The open circles are calculated values with SKI4. Experimental data are denoted by the solid circles.

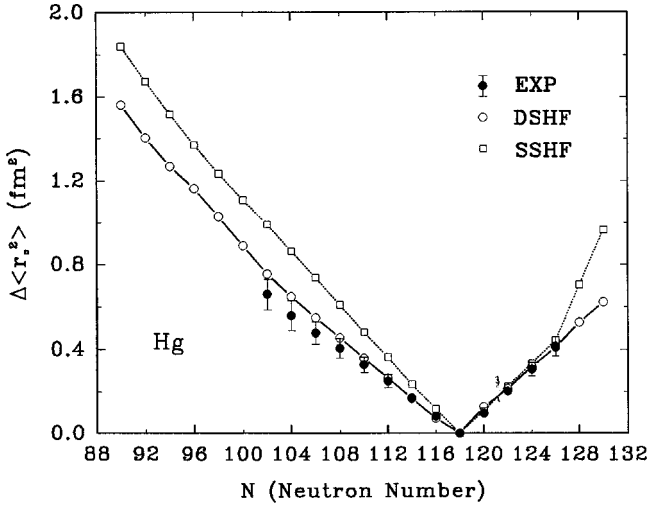


FIG. 4. The isotope shifts of Hg nuclei in DSHF and SSHF with SKI4. The experimental isotope shifts for Hg isotopes [24] are also shown for comparison.

The values of SKI4 are [18]  $t_0 = -1855.83$ ,  $t_1 = 473.829$ ,  $t_2 = 1006.86$ ,  $t_3 = 9703.61$ ,  $x_0 = 0.4051$ ,  $x_1 = -2.8891$ ,  $x_2 = -1.3252$ ,  $x_3 = 1.1452$ ,  $b_4 = 183.097$ ,  $b'_4 = -180.351$ , and  $\alpha = 0.25$ .

The quadrupole moments are defined as [15]

$$Q_x^{n,p} = \langle 2x^2 - y^2 - z^2 \rangle^{n,p}, \quad (6)$$

$$Q_y^{n,p} = \langle 2y^2 - z^2 - x^2 \rangle^{n,p}, \quad (7)$$

$$Q_z^{n,p} = \langle 2z^2 - x^2 - y^2 \rangle^{n,p}, \quad (8)$$

$$Q_0^{n,p} = \sqrt{\frac{2(Q_x^2 + Q_y^2 + Q_z^2)^{n,p}}{3}}, \quad (9)$$

$$Q_{20}^{n,p} = \sqrt{\frac{5}{4\pi}} \langle 2z^2 - x^2 - y^2 \rangle^{n,p} = \sqrt{\frac{5}{4\pi}} Q_z^{n,p}, \quad (10)$$

$$Q_{22}^{n,p} = \sqrt{\frac{15}{8\pi}} \langle x^2 - y^2 \rangle^{n,p} = \sqrt{\frac{5}{24\pi}} (Q_x^{n,p} - Q_y^{n,p}), \quad (11)$$

and the hexadecapole moments are calculated by [15]

$$Q_{40}^{n,p} = \sqrt{\frac{9}{64\pi}} \langle 3(x^2 + y^2)^2 - 24z^2(x^2 + y^2) + 8z^4 \rangle^{n,p}, \quad (12)$$

$$Q_{42}^{n,p} = \sqrt{\frac{45}{32\pi}} \langle 3y^4 - x^4 - 6z^4 - 6x^2z^2 \rangle^{n,p}, \quad (13)$$

$$Q_{44}^{n,p} = \sqrt{\frac{315}{128\pi}} \langle x^4 - 6x^2y^2 + y^4 \rangle^{n,p}. \quad (14)$$

The quadrupole deformation parameters  $\beta_2$  and  $\gamma_2$  and the hexadecupole deformation parameters  $\beta_4$ ,  $\gamma_4$ , and  $\delta_4$  are given by the expressions

$$\beta_2^{n,p} = \sqrt{a_{20n,p}^2 + 2a_{22n,p}^2}, \quad (15)$$

$$\gamma_2^{n,p} = \arctan \left[ \sqrt{2} \frac{a_{22n,p}}{a_{20n,p}} \right], \quad (16)$$

$$\beta_4^{n,p} = \sqrt{a_{4n,p}^2 + b_{4n,p}^2 + c_{4n,p}^2}, \quad (17)$$

$$\gamma_4^{n,p} = \arctan \left[ \frac{c_{4n,p}}{b_{4n,p}} \right], \quad (18)$$

$$\delta_4^{n,p} = \arcsin \left[ \sqrt{\frac{b_{4n,p}^2 + c_{4n,p}^2}{a_{4n,p}^2 + b_{4n,p}^2 + c_{4n,p}^2}} \right], \quad (19)$$

where

$$a_{4n,p} = \sqrt{\frac{7}{12}} a_{40n,p} + \sqrt{\frac{5}{6}} a_{44n,p}, \quad (20)$$

$$b_{4n,p} = \sqrt{\frac{5}{12}} a_{40n,p} - \sqrt{\frac{7}{6}} a_{44n,p}, \quad (21)$$

$$c_{4n,p} = -\sqrt{2} a_{42n,p}. \quad (22)$$

The coefficients  $a_{20}$ ,  $a_{22}$ ,  $a_{40}$ ,  $a_{42}$ , and  $a_{44}$  are solutions of the coupled equations [15]

$$Q_{20}^{n,p} = 2C_{n,p}R_0^2 \left[ a_{20n,p} + \frac{2}{7} \sqrt{\frac{5}{\pi}} (a_{20n,p}^2 - a_{22n,p}^2) \right], \quad (23)$$

$$Q_{22}^{n,p} = 2C_{n,p}R_0^2 \left[ a_{22n,p} - \frac{4}{7} \sqrt{\frac{5}{\pi}} a_{20n,p} a_{22n,p} \right], \quad (24)$$

$$Q_{40}^{n,p} = 2C_{n,p}R_0^4 \left[ a_{40n,p} + \frac{3}{7} \sqrt{\frac{1}{\pi}} (3a_{20n,p}^2 + a_{22n,p}^2) \right], \quad (25)$$

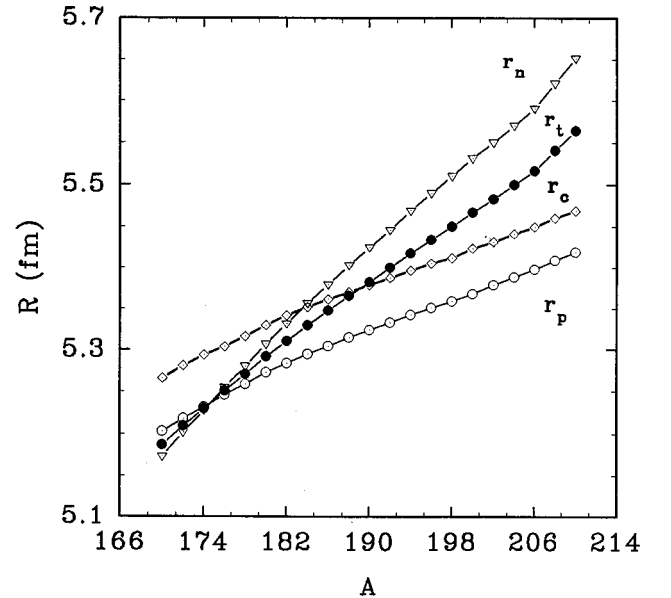


FIG. 5. The variation of nuclear radii with nucleon numbers. ( $r_n$  is the rms radius of neutron density distributions,  $r_p$  is the rms radius of proton density distributions,  $r_t$  is the rms radius of matter density distributions, and  $r_c$  is the rms radius of charge density distributions.)

TABLE I. Binding energies (MeV) and quadrupole deformation parameters  $\beta_2$  and  $\gamma_2$  (in degrees) obtained with the SK14. Experimental binding energies are taken from Ref. [23] and value labeled with # is the datum estimated from systematic trends. RMF-NL1 results [6] are listed for comparison.

|                   |      | SK14    |             |              |             |              | NL1     |           | Expt.    |             |
|-------------------|------|---------|-------------|--------------|-------------|--------------|---------|-----------|----------|-------------|
|                   |      | $E_B$   | $\beta_2^p$ | $\gamma_2^p$ | $\beta_2^n$ | $\gamma_2^n$ | $E_B$   | $\beta_p$ | $E_B$    | $ \beta_p $ |
| $^{170}\text{Hg}$ | sph  | 1304.40 |             |              |             |              |         |           |          |             |
|                   | pro  | 1304.61 | 0.07        | 0.00         | 0.08        | 0.00         | 1321.69 | 0.03      |          |             |
|                   | obl  | 1305.59 | 0.10        | 60.00        | 0.10        | 60.00        | 1322.48 | -0.02     |          |             |
|                   | tri1 | 1305.41 | 0.10        | 43.03        | 0.10        | 37.96        |         |           |          |             |
|                   | tri2 | 1305.56 | 0.10        | 49.94        | 0.10        | 45.78        |         |           |          |             |
|                   | tri3 | 1305.37 | 0.09        | 35.11        | 0.09        | 28.17        |         |           |          |             |
| $^{172}\text{Hg}$ | sph  | 1325.90 |             |              |             |              |         |           |          |             |
|                   | pro  | 1326.33 | 0.08        | 0.00         | 0.09        | 0.00         | 1343.57 | 0.05      |          |             |
|                   | obl  | 1327.24 | 0.10        | 60.00        | 0.11        | 60.00        | 1343.88 | -0.07     |          |             |
|                   | tri1 | 1327.11 | 0.10        | 41.81        | 0.11        | 37.33        |         |           |          |             |
|                   | tri2 | 1327.19 | 0.10        | 49.20        | 0.10        | 46.78        |         |           |          |             |
|                   | tri3 | 1327.09 | 0.10        | 33.96        | 0.10        | 27.22        |         |           |          |             |
| $^{174}\text{Hg}$ | sph  | 1347.10 |             |              |             |              |         |           |          |             |
|                   | pro  | 1347.51 | 0.09        | 0.00         | 0.10        | 0.00         | 1362.21 | 0.06      |          |             |
|                   | obl  | 1348.42 | 0.11        | 60.00        | 0.11        | 60.00        | 1363.23 | -0.04     | 1349.32# |             |
|                   | tri1 | 1348.38 | 0.10        | 41.99        | 0.11        | 37.26        |         |           |          |             |
|                   | tri2 | 1348.38 | 0.11        | 49.72        | 0.11        | 45.86        |         |           |          |             |
|                   | tri3 | 1348.32 | 0.10        | 33.51        | 0.11        | 27.24        |         |           |          |             |
| $^{176}\text{Hg}$ | sph  | 1367.80 |             |              |             |              |         |           |          |             |
|                   | pro  | 1368.08 | 0.07        | 0.00         | 0.09        | 0.00         | 1382.82 | 0.28      |          |             |
|                   | obl  | 1369.20 | 0.11        | 60.00        | 0.12        | 60.00        | 1384.05 | -0.08     |          |             |
|                   | tri1 | 1369.11 | 0.10        | 42.18        | 0.11        | 38.27        |         |           |          | 1369.76     |
|                   | tri2 | 1369.16 | 0.11        | 49.13        | 0.12        | 46.51        |         |           |          |             |
|                   | tri3 | 1368.99 | 0.10        | 35.10        | 0.10        | 29.69        |         |           |          |             |
| $^{178}\text{Hg}$ | sph  | 1388.10 |             |              |             |              |         |           |          |             |
|                   | pro  | 1388.00 | 0.07        | 0.00         | 0.07        | 0.00         | 1404.45 | 0.31      |          |             |
|                   | obl  | 1389.55 | 0.11        | 60.00        | 0.13        | 60.00        | 1402.79 | -0.15     | 1390.43  |             |
|                   | tri1 | 1389.36 | 0.10        | 44.34        | 0.11        | 41.64        |         |           |          |             |
|                   | tri2 | 1389.54 | 0.11        | 49.86        | 0.12        | 48.10        |         |           |          |             |
|                   | tri3 | 1389.08 | 0.09        | 37.12        | 0.10        | 33.03        |         |           |          |             |
| $^{180}\text{Hg}$ | sph  | 1407.60 |             |              |             |              |         |           |          |             |
|                   | pro  | 1407.55 | 0.06        | 0.00         | 0.07        | 0.00         | 1422.60 | 0.33      |          |             |
|                   | obl. | 1409.53 | 0.12        | 60.00        | 0.14        | 60.00        | 1421.85 | -0.33     | 1410.44# |             |
|                   | tri1 | 1409.13 | 0.10        | 45.14        | 0.11        | 44.05        |         |           |          |             |
|                   | tri2 | 1409.45 | 0.12        | 50.80        | 0.13        | 50.78        |         |           |          |             |
|                   | tri3 | 1408.63 | 0.09        | 38.52        | 0.10        | 35.17        |         |           |          |             |
| $^{182}\text{Hg}$ | sph  | 1427.20 |             |              |             |              |         |           |          |             |
|                   | pro  | 1426.05 | 0.06        | 0.00         | 0.07        | 0.00         | 1443.27 | 0.34      |          |             |
|                   | obl  | 1429.00 | 0.13        | 60.00        | 0.15        | 60.00        | 1443.33 | -0.22     | 1430.67  | 0.17        |
|                   | tri1 | 1428.36 | 0.11        | 45.81        | 0.12        | 44.81        |         |           |          |             |
|                   | tri2 | 1428.90 | 0.12        | 51.20        | 0.13        | 51.08        |         |           |          |             |
|                   | tri3 | 1427.30 | 0.10        | 36.40        | 0.11        | 32.57        |         |           |          |             |
| $^{184}\text{Hg}$ | sph  | 1445.20 |             |              |             |              |         |           |          |             |
|                   | pro  | 1444.21 | 0.06        | 0.00         | 0.07        | 0.00         | 1460.47 | 0.33      |          |             |
|                   | obl  | 1447.75 | 0.13        | 60.00        | 0.16        | 60.00        | 1459.03 | -0.23     | 1448.71# | 0.16        |
|                   | tri1 | 1446.92 | 0.11        | 46.13        | 0.13        | 45.50        |         |           |          |             |
|                   | tri2 | 1447.51 | 0.12        | 52.10        | 0.13        | 51.87        |         |           |          |             |
|                   | tri3 | 1446.08 | 0.10        | 37.80        | 0.11        | 35.34        |         |           |          |             |
| $^{186}\text{Hg}$ | sph  | 1462.20 |             |              |             |              |         |           |          |             |
|                   | pro  | 1462.05 | 0.08        | 0.00         | 0.09        | 0.00         | 1477.59 | 0.29      |          |             |
|                   | obl  | 1465.83 | 0.13        | 60.00        | 0.15        | 60.00        | 1476.65 | -0.21     | 1467.13  | 0.24        |
|                   | tri1 | 1465.03 | 0.11        | 45.70        | 0.13        | 45.13        |         |           |          |             |
|                   | tri2 | 1465.60 | 0.12        | 51.16        | 0.13        | 50.78        |         |           |          |             |
|                   | tri3 | 1464.14 | 0.10        | 36.85        | 0.11        | 34.03        |         |           |          |             |

TABLE I. (Continued).

|                   |      | SK14    |             |              |             |              | NL1     |           | Expt.                |             |
|-------------------|------|---------|-------------|--------------|-------------|--------------|---------|-----------|----------------------|-------------|
|                   |      | $E_B$   | $\beta_2^p$ | $\gamma_2^p$ | $\beta_2^n$ | $\gamma_2^n$ | $E_B$   | $\beta_p$ | $E_B$                | $ \beta_p $ |
| $^{188}\text{Hg}$ | sph  | 1479.79 |             |              |             |              |         |           |                      |             |
|                   | pro  | 1479.56 | 0.08        | 0.00         | 0.10        | 0.00         |         |           |                      |             |
|                   | obl  | 1483.47 | 0.13        | 60.00        | 0.14        | 60.00        | 1492.90 | 0.28      |                      |             |
|                   | tri1 | 1482.65 | 0.11        | 43.79        | 0.13        | 43.60        | 1493.20 | -0.17     | 1485.05 <sup>#</sup> | 0.14        |
|                   | tri2 | 1483.22 | 0.12        | 51.00        | 0.14        | 50.38        |         |           |                      |             |
|                   | tri3 | 1481.71 | 0.10        | 35.65        | 0.12        | 32.42        |         |           |                      |             |
| $^{190}\text{Hg}$ | sph  | 1496.50 |             |              |             |              |         |           |                      |             |
|                   | pro  | 1496.67 | 0.08        | 0.00         | 0.10        | 0.00         |         |           |                      |             |
|                   | obl  | 1500.62 | 0.13        | 60.00        | 0.15        | 60.00        | 1508.20 | 0.27      |                      |             |
|                   | tri1 | 1499.76 | 0.12        | 44.00        | 0.14        | 43.36        | 1508.79 | -0.17     | 1502.37 <sup>#</sup> | 0.15        |
|                   | tri2 | 1500.42 | 0.12        | 50.36        | 0.14        | 50.77        |         |           |                      |             |
|                   | tri3 | 1498.85 | 0.11        | 35.71        | 0.12        | 30.94        |         |           |                      |             |
| $^{192}\text{Hg}$ | sph  | 1513.10 |             |              |             |              |         |           |                      |             |
|                   | pro  | 1513.66 | 0.09        | 0.00         | 0.11        | 0.00         |         |           |                      |             |
|                   | obl  | 1517.34 | 0.12        | 60.00        | 0.14        | 60.00        | 1522.99 | 0.25      |                      |             |
|                   | tri1 | 1516.46 | 0.11        | 44.17        | 0.13        | 43.88        | 1524.69 | -0.16     | 1519.43 <sup>#</sup> | 0.14        |
|                   | tri2 | 1517.11 | 0.12        | 50.64        | 0.14        | 50.43        |         |           |                      |             |
|                   | tri3 | 1515.55 | 0.11        | 32.77        | 0.12        | 28.40        |         |           |                      |             |
| $^{194}\text{Hg}$ | sph  | 1529.59 |             |              |             |              |         |           |                      |             |
|                   | pro  | 1530.21 | 0.09        | 0.00         | 0.11        | 0.00         |         |           |                      |             |
|                   | obl  | 1533.51 | 0.12        | 60.00        | 0.14        | 60.00        | 1538.21 | 0.12      |                      |             |
|                   | tri1 | 1532.67 | 0.11        | 43.14        | 0.13        | 44.20        | 1540.71 | -0.14     | 1535.50              | 0.13        |
|                   | tri2 | 1533.33 | 0.12        | 50.10        | 0.14        | 50.07        |         |           |                      |             |
|                   | tri3 | 1531.66 | 0.10        | 31.45        | 0.12        | 25.80        |         |           |                      |             |
| $^{196}\text{Hg}$ | sph  | 1545.27 |             |              |             |              |         |           |                      |             |
|                   | pro  | 1545.50 | 0.08        | 0.00         | 0.09        | 0.00         |         |           |                      |             |
|                   | obl  | 1549.06 | 0.12        | 60.00        | 0.14        | 60.00        | 1553.67 | 0.11      |                      |             |
|                   | tri1 | 1548.60 | 0.10        | 43.47        | 0.11        | 41.86        | 1555.21 | -0.14     | 1551.23              | 0.12        |
|                   | tri2 | 1549.02 | 0.11        | 49.72        | 0.12        | 48.78        |         |           |                      |             |
|                   | tri3 | 1548.00 | 0.10        | 35.91        | 0.11        | 33.57        |         |           |                      |             |
| $^{198}\text{Hg}$ | sph  | 1561.57 |             |              |             |              |         |           |                      |             |
|                   | pro  | 1561.24 | 0.08        | 0.00         | 0.08        | 0.00         |         |           |                      |             |
|                   | obl  | 1563.88 | 0.11        | 60.00        | 0.12        | 60.00        | 1567.81 | 0.08      |                      |             |
|                   | tri1 | 1564.07 | 0.10        | 43.73        | 0.11        | 40.62        | 1569.17 | -0.12     | 1566.50              | 0.11        |
|                   | tri2 | 1564.30 | 0.10        | 49.13        | 0.11        | 46.90        |         |           |                      |             |
|                   | tri3 | 1563.52 | 0.09        | 36.54        | 0.10        | 34.19        |         |           |                      |             |
| $^{200}\text{Hg}$ | sph  | 1576.60 |             |              |             |              |         |           |                      |             |
|                   | pro  | 1576.86 | 0.07        | 0.00         | 0.07        | 0.00         |         |           |                      |             |
|                   | obl  | 1578.27 | 0.10        | 60.00        | 0.11        | 60.00        | 1580.58 | 0.04      |                      |             |
|                   | tri1 | 1579.17 | 0.09        | 43.66        | 0.10        | 41.39        | 1581.73 | -0.10     | 1581.20              | 0.10        |
|                   | tri2 | 1579.26 | 0.09        | 49.72        | 0.10        | 47.17        |         |           |                      |             |
|                   | tri3 | 1579.00 | 0.09        | 36.82        | 0.09        | 34.69        |         |           |                      |             |
| $^{202}\text{Hg}$ | sph  | 1594.58 |             |              |             |              |         |           |                      |             |
|                   | pro  | 1593.92 | 0.03        | 0.00         | 0.02        | 0.00         |         |           |                      |             |
|                   | obl  | 1594.21 | 0.05        | 60.00        | 0.05        | 60.00        |         |           | 1595.18              |             |
|                   | tri1 | 1593.93 | 0.03        | 37.66        | 0.03        | 38.76        |         |           |                      |             |
|                   | tri2 | 1594.25 | 0.05        | 49.35        | 0.05        | 50.32        |         |           |                      |             |
|                   | tri3 | 1594.00 | 0.03        | 24.07        | 0.03        | 27.19        |         |           |                      |             |

TABLE I. (Continued).

|                   |      | SK14    |             |              |             |              | NL1   |           | Expt.   |             |
|-------------------|------|---------|-------------|--------------|-------------|--------------|-------|-----------|---------|-------------|
|                   |      | $E_B$   | $\beta_2^n$ | $\gamma_2^n$ | $\beta_2^n$ | $\gamma_2^n$ | $E_B$ | $\beta_p$ | $E_B$   | $ \beta_p $ |
| $^{204}\text{Hg}$ | sph  | 1610.24 |             |              |             |              |       |           |         |             |
|                   | pro  | 1609.96 | 0.01        | 0.00         | 0.01        | 0.00         |       |           |         |             |
|                   | obl  | 1610.06 | 0.01        | 60.00        | 0.01        | 60.00        |       |           | 1608.67 |             |
|                   | tri1 | 1610.07 | 0.02        | 34.44        | 0.02        | 36.54        |       |           |         |             |
|                   | tri2 | 1610.05 | 0.02        | 43.52        | 0.02        | 44.61        |       |           |         |             |
|                   | tri3 | 1610.05 | 0.02        | 22.83        | 0.02        | 25.11        |       |           |         |             |
| $^{206}\text{Hg}$ | sph  | 1625.85 |             |              |             |              |       |           |         |             |
|                   | pro  | 1625.57 | 0.01        | 0.00         | 0.01        | 0.00         |       |           |         |             |
|                   | obl  | 1625.75 | 0.01        | 60.00        | 0.01        | 60.00        |       |           | 1621.06 |             |
|                   | tri1 | 1625.70 | 0.01        | 32.88        | 0.01        | 32.10        |       |           |         |             |
|                   | tri2 | 1625.63 | 0.01        | 42.47        | 0.01        | 42.11        |       |           |         |             |
|                   | tri3 | 1625.62 | 0.01        | 21.72        | 0.01        | 21.26        |       |           |         |             |
| $^{208}\text{Hg}$ | sph  | 1630.30 |             |              |             |              |       |           |         |             |
|                   | pro  | 1630.20 | 0.02        | 0.00         | 0.02        | 0.00         |       |           |         |             |
|                   | obl  | 1630.56 | 0.02        | 60.00        | 0.02        | 60.00        |       |           |         |             |
|                   | tri1 | 1630.52 | 0.02        | 45.07        | 0.03        | 44.51        |       |           |         |             |
|                   | tri2 | 1630.65 | 0.02        | 50.78        | 0.03        | 49.86        |       |           |         |             |
|                   | tri3 | 1630.50 | 0.02        | 30.51        | 0.03        | 33.68        |       |           |         |             |
| $^{210}\text{Hg}$ | sph  | 1635.05 |             |              |             |              |       |           |         |             |
|                   | pro  | 1635.31 | 0.03        | 0.00         | 0.04        | 0.00         |       |           |         |             |
|                   | obl  | 1635.39 | 0.02        | 60.00        | 0.03        | 60.00        |       |           |         |             |
|                   | tri1 | 1635.40 | 0.02        | 36.67        | 0.03        | 36.71        |       |           |         |             |
|                   | tri2 | 1635.56 | 0.03        | 46.28        | 0.03        | 45.80        |       |           |         |             |
|                   | tri3 | 1635.45 | 0.03        | 19.83        | 0.04        | 19.62        |       |           |         |             |

$$Q_{42}^{n,p} = 2C_{n,p}R_0^4 \left[ a_{42n,p} + \frac{3}{7} \sqrt{\frac{15}{\pi}} a_{20n,p} a_{22n,p} \right], \quad (26)$$

$$Q_{44}^{n,p} = 2C_{n,p}R_0^4 \left[ a_{44n,p} + 3 \sqrt{\frac{15}{14\pi}} a_{22n,p}^2 \right], \quad (27)$$

with

$$C_p = \frac{3Z}{4\pi}, \quad C_n = \frac{3N}{4\pi}, \quad R_0 = 1.2A^{1/3}.$$

At the beginning of the calculations, the code needs the input of deformations which are controlled by IQ1 and IQ2. We use six kinds of configurations as our inputs (IQ1,IQ2): (0,0) is the spherical case (sph), (1,0) is the prolate case (pro), (0,1) is the oblate case (obl), (1,1) is the first triaxial case (tri1), (1,2) is the second triaxial case (tri2), and (2,1) is the third triaxial case (tri3). In the spherical case,  $\beta_2=0$  and  $\beta_4=0$ ; in the prolate case,  $\gamma_2=0$ ,  $\gamma_4=0$ , and  $\delta_4 = \arccos(\sqrt{7/12})$ ; in the oblate case,  $\gamma_2 = \pi/3$ ,  $\gamma_4 = \pi/3$ , and  $\delta_4 = \pi - \arccos(\sqrt{7/12})$ ; and in the triaxial case,  $0 < \gamma < \pi/3$ .

Tajima *et al.* [14] have considered a correction for the error of the total binding energy due to the finite mesh size for the code in the three-dimensional Cartesian-mesh representation, but we use a very small mesh size  $a=0.65$  fm in our calculation and thus the difference of the binding energy

between the spherical SHF code and deformed SHF code is less than 0.1% for a spherical nucleus such as  $^{208}\text{Pb}$ . This avoids inaccurately correcting the total energy as done in Ref. [14]. The only expense for this is to prolong the computation time (it takes 6 h of CPU time to get one solution for one Hg nucleus and the total CPU time in our calculation is about 800 h in the SGI workstation indigo11).

The neutron pairing correlations have been calculated with the force constant  $G_n = g_n/(11+N)$  with  $g_n = 13.5$  MeV for neutrons and  $G_p = g_p/(11+Z)$  with  $g_p = 16.5$  MeV for protons [13].

The mean field localizes the nucleus and thus breaks translational invariance which results in the center of mass of the whole nucleus oscillating in the mean field, but the spurious excitation of the center of mass has to be eliminated. A simple and reliable treatment of the center-of-mass correction is [22]

$$E_{\text{c.m.}} = \frac{\langle P_{\text{c.m.}}^2 \rangle}{2Am},$$

$$\begin{aligned} \langle P_{\text{c.m.}}^2 \rangle = & \sum_{\beta} \omega_{\beta} \langle \phi_{\beta} | \hat{p}^2 | \phi_{\beta} \rangle - \sum_{\alpha\beta} [\omega_{\alpha} \omega_{\beta} \\ & + \sqrt{\omega_{\alpha}(1-\omega_{\alpha})\omega_{\beta}(1-\omega_{\beta})}] |\langle \phi_{\alpha} | \hat{p} | \phi_{\beta} \rangle|^2, \end{aligned} \quad (28)$$

where  $P_{\text{c.m.}} = \sum_i \hat{p}_i$  is the total momentum operator.

TABLE II. The proton and neutron quadrupole moments  $Q_x$ ,  $Q_y$ , and  $Q_z$ , and  $Q_0$  obtained with the SK14.

|                   |      | Proton (fm <sup>2</sup> ) |         |        |        | Neutron (fm <sup>2</sup> ) |         |        |        |
|-------------------|------|---------------------------|---------|--------|--------|----------------------------|---------|--------|--------|
|                   |      | $Q_x$                     | $Q_y$   | $Q_z$  | $Q_0$  | $Q_x$                      | $Q_y$   | $Q_z$  | $Q_0$  |
| <sup>170</sup> Hg | pro  | -94.62                    | -94.62  | 189.24 | 189.24 | -122.98                    | -122.98 | 245.96 | 245.96 |
|                   | obl  | 124.25                    | -248.50 | 124.25 | 248.50 | 140.10                     | -280.20 | 140.10 | 124.25 |
|                   | tri1 | 48.84                     | -238.91 | 190.07 | 252.44 | 29.94                      | -268.21 | 238.27 | 293.95 |
|                   | tri2 | 82.75                     | -256.77 | 174.02 | 262.13 | 78.02                      | -289.81 | 211.79 | 299.92 |
|                   | tri3 | 13.11                     | -215.65 | 202.54 | 241.79 | -19.32                     | -240.27 | 259.58 | 289.23 |
| <sup>172</sup> Hg | pro  | -108.12                   | -108.12 | 216.24 | 216.24 | -145.83                    | -145.83 | 291.66 | 291.66 |
|                   | obl  | 135.09                    | -270.18 | 135.09 | 270.18 | 158.86                     | -317.72 | 158.86 | 317.72 |
|                   | tri1 | 45.31                     | -250.00 | 204.69 | 266.40 | 24.55                      | -292.81 | 268.26 | 324.86 |
|                   | tri2 | 82.81                     | -268.31 | 185.50 | 274.79 | 79.80                      | -315.42 | 235.62 | 328.00 |
|                   | tri3 | 8.30                      | -224.87 | 216.57 | 255.00 | -27.49                     | -261.39 | 288.88 | 318.88 |
| <sup>174</sup> Hg | pro  | -118.39                   | -118.39 | 236.78 | 236.78 | -163.66                    | -163.66 | 327.32 | 327.32 |
|                   | obl  | 139.56                    | -279.12 | 139.56 | 279.12 | 170.30                     | -340.60 | 170.30 | 340.60 |
|                   | tri1 | 46.28                     | -250.52 | 204.24 | 266.60 | 29.04                      | -303.95 | 274.91 | 335.47 |
|                   | tri2 | 82.99                     | -272.65 | 189.66 | 279.52 | 82.79                      | -332.18 | 249.39 | 345.83 |
|                   | tri3 | 6.19                      | -235.94 | 229.75 | 268.94 | -30.53                     | -284.35 | 314.88 | 347.31 |
| <sup>176</sup> Hg | pro  | -103.85                   | -103.85 | 207.70 | 207.70 | -143.39                    | -143.39 | 286.78 | 286.78 |
|                   | obl  | 149.87                    | -299.74 | 149.87 | 299.74 | 189.40                     | -378.80 | 189.40 | 378.80 |
|                   | tri1 | 49.28                     | -264.38 | 215.10 | 281.18 | 37.22                      | -331.72 | 294.50 | 363.47 |
|                   | tri2 | 86.85                     | -283.56 | 196.71 | 290.56 | 92.70                      | -357.71 | 265.01 | 371.28 |
|                   | tri3 | 13.62                     | -229.60 | 215.98 | 257.62 | -14.82                     | -283.55 | 298.37 | 336.30 |
| <sup>178</sup> Hg | pro  | -92.02                    | -92.02  | 184.04 | 184.04 | -125.02                    | -125.02 | 250.04 | 250.04 |
|                   | obl  | 156.16                    | -312.32 | 156.16 | 312.32 | 204.26                     | -408.52 | 204.26 | 408.52 |
|                   | tri1 | 58.21                     | -257.34 | 199.13 | 269.89 | 59.85                      | -331.95 | 272.10 | 353.85 |
|                   | tri2 | 93.70                     | -294.78 | 201.08 | 301.23 | 109.75                     | -384.71 | 274.96 | 396.36 |
|                   | tri3 | 22.29                     | -225.00 | 202.71 | 247.94 | 5.13                       | -283.78 | 278.65 | 324.77 |
| <sup>180</sup> Hg | pro  | -86.61                    | -86.61  | 173.22 | 173.22 | -118.45                    | -118.45 | 236.90 | 236.90 |
|                   | obl  | 166.51                    | -333.02 | 166.51 | 333.02 | 225.72                     | -451.44 | 225.72 | 451.44 |
|                   | tri1 | 65.02                     | -272.59 | 207.57 | 284.75 | 79.01                      | -364.48 | 285.47 | 383.48 |
|                   | tri2 | 102.17                    | -306.79 | 204.62 | 312.44 | 131.56                     | -415.15 | 283.59 | 424.33 |
|                   | tri3 | 27.08                     | -230.09 | 203.01 | 251.52 | 19.00                      | -298.60 | 279.60 | 334.37 |
| <sup>182</sup> Hg | pro  | -85.27                    | -85.27  | 170.54 | 170.54 | -118.64                    | -118.64 | 237.28 | 237.28 |
|                   | obl  | 171.59                    | -343.18 | 171.59 | 343.18 | 241.35                     | -482.70 | 241.35 | 482.70 |
|                   | tri1 | 69.26                     | -291.71 | 222.45 | 304.83 | 92.30                      | -406.32 | 314.02 | 426.01 |
|                   | tri2 | 109.25                    | -322.21 | 212.96 | 327.72 | 151.03                     | -452.83 | 301.80 | 461.13 |
|                   | tri3 | 20.28                     | -245.99 | 225.71 | 273.09 | 1.33                       | -333.43 | 332.10 | 384.24 |
| <sup>184</sup> Hg | pro  | -90.03                    | -90.03  | 180.06 | 180.06 | -131.44                    | -131.44 | 262.88 | 262.88 |
|                   | obl  | 175.44                    | -350.88 | 175.44 | 350.88 | 254.31                     | -508.62 | 254.31 | 508.62 |
|                   | tri1 | 72.94                     | -292.33 | 219.39 | 304.31 | 100.87                     | -421.66 | 320.79 | 440.36 |
|                   | tri2 | 111.31                    | -313.43 | 202.12 | 317.79 | 158.34                     | -455.12 | 296.78 | 462.09 |
|                   | tri3 | 27.07                     | -248.39 | 221.32 | 272.54 | 20.40                      | -348.54 | 328.14 | 391.21 |
| <sup>186</sup> Hg | pro  | -113.93                   | -113.93 | 227.86 | 227.86 | -174.22                    | -174.22 | 348.44 | 348.44 |
|                   | obl  | 174.38                    | -348.76 | 174.38 | 348.76 | 259.29                     | -518.58 | 259.29 | 518.58 |
|                   | tri1 | 72.70                     | -294.98 | 222.28 | 307.36 | 101.75                     | -438.43 | 336.68 | 458.93 |
|                   | tri2 | 110.81                    | -327.95 | 217.14 | 333.64 | 160.71                     | -488.47 | 327.76 | 497.90 |
|                   | tri3 | 23.11                     | -256.92 | 233.81 | 284.26 | 11.42                      | -372.81 | 361.39 | 424.04 |

TABLE II. (Continued).

|                   |      | Proton (fm <sup>2</sup> ) |         |        |        | Neutron (fm <sup>2</sup> ) |         |        |        |
|-------------------|------|---------------------------|---------|--------|--------|----------------------------|---------|--------|--------|
|                   |      | $Q_x$                     | $Q_y$   | $Q_z$  | $Q_0$  | $Q_x$                      | $Q_y$   | $Q_z$  | $Q_0$  |
| <sup>188</sup> Hg | pro  | -121.67                   | -121.67 | 243.34 | 243.34 | -193.36                    | -193.36 | 386.72 | 386.72 |
|                   | obl  | 176.05                    | -352.10 | 176.05 | 352.10 | 267.20                     | -534.40 | 267.20 | 534.40 |
|                   | tri1 | 67.35                     | -305.59 | 238.24 | 321.12 | 94.54                      | -465.77 | 371.23 | 492.40 |
|                   | tri2 | 109.26                    | -328.51 | 219.25 | 334.59 | 160.60                     | -501.00 | 340.40 | 511.65 |
|                   | tri3 | 17.38                     | -264.59 | 247.21 | 295.99 | -1.53                      | -394.81 | 396.34 | 456.77 |
| <sup>190</sup> Hg | pro  | -120.12                   | -120.12 | 240.24 | 240.24 | -197.44                    | -197.44 | 394.88 | 394.88 |
|                   | obl  | 172.11                    | -344.22 | 172.11 | 344.22 | 267.40                     | -534.80 | 267.40 | 534.80 |
|                   | tri1 | 65.93                     | -306.36 | 240.43 | 322.50 | 94.90                      | -478.24 | 383.34 | 506.41 |
|                   | tri2 | 108.33                    | -334.46 | 226.13 | 341.31 | 162.85                     | -520.36 | 357.51 | 532.36 |
|                   | tri3 | 13.10                     | -265.00 | 251.90 | 298.72 | -13.81                     | -403.17 | 416.98 | 473.72 |
| <sup>192</sup> Hg | pro  | -131.59                   | -131.59 | 263.18 | 263.18 | -222.24                    | -222.24 | 444.48 | 444.48 |
|                   | obl  | 165.73                    | -331.46 | 165.73 | 331.46 | 263.77                     | -527.54 | 263.77 | 527.54 |
|                   | tri1 | 67.01                     | -306.38 | 239.37 | 322.14 | 101.75                     | -488.77 | 387.02 | 515.77 |
|                   | tri2 | 107.88                    | -327.32 | 219.44 | 333.60 | 167.73                     | -521.05 | 353.32 | 531.95 |
|                   | tri3 | 2.52                      | -269.82 | 267.30 | 310.12 | -37.07                     | -415.12 | 452.19 | 502.11 |
| <sup>194</sup> Hg | pro  | -134.01                   | -134.01 | 268.02 | 268.02 | -231.29                    | -231.29 | 462.58 | 462.58 |
|                   | obl  | 173.70                    | -347.40 | 173.70 | 347.40 | 279.06                     | -558.12 | 279.06 | 558.12 |
|                   | tri1 | 66.51                     | -304.41 | 237.90 | 320.09 | 106.10                     | -494.90 | 388.80 | 521.12 |
|                   | tri2 | 105.22                    | -328.24 | 223.02 | 335.21 | 167.71                     | -531.03 | 363.32 | 542.90 |
|                   | tri3 | -4.38                     | -260.97 | 265.35 | 303.91 | -57.86                     | -400.49 | 458.35 | 499.21 |
| <sup>196</sup> Hg | pro  | -118.50                   | -118.50 | 237.00 | 237.00 | -194.90                    | -194.90 | 389.80 | 389.80 |
|                   | obl  | 166.21                    | -332.42 | 166.21 | 332.42 | 271.16                     | -542.32 | 271.16 | 542.32 |
|                   | tri1 | 59.85                     | -284.96 | 225.11 | 300.50 | 79.55                      | -448.88 | 369.33 | 479.05 |
|                   | tri2 | 96.81                     | -311.28 | 214.47 | 318.60 | 140.55                     | -492.22 | 351.67 | 507.09 |
|                   | tri3 | 18.73                     | -254.27 | 235.54 | 283.41 | 9.84                       | -399.09 | 389.25 | 455.25 |
| <sup>198</sup> Hg | pro  | -114.72                   | -114.72 | 229.44 | 229.44 | -189.07                    | -189.07 | 378.14 | 378.14 |
|                   | obl  | 156.31                    | -312.62 | 156.31 | 312.62 | 258.08                     | -516.16 | 258.08 | 516.16 |
|                   | tri1 | 55.32                     | -278.27 | 222.95 | 294.62 | 68.43                      | -437.65 | 369.22 | 470.85 |
|                   | tri2 | 89.94                     | -292.44 | 202.50 | 299.57 | 122.77                     | -459.51 | 336.74 | 475.82 |
|                   | tri3 | 21.06                     | -237.14 | 216.08 | 262.52 | 15.19                      | -374.68 | 359.49 | 424.15 |
| <sup>200</sup> Hg | pro  | -100.94                   | -100.94 | 201.88 | 201.88 | -166.93                    | -166.93 | 333.86 | 333.86 |
|                   | obl  | 154.00                    | -308.00 | 154.00 | 308.00 | 254.93                     | -509.86 | 254.93 | 509.86 |
|                   | tri1 | 55.85                     | -257.90 | 202.05 | 271.37 | 70.74                      | -405.93 | 335.19 | 433.69 |
|                   | tri2 | 84.99                     | -265.39 | 180.40 | 271.05 | 114.69                     | -416.45 | 301.76 | 430.23 |
|                   | tri3 | 22.12                     | -232.60 | 210.48 | 256.77 | 19.11                      | -369.33 | 350.22 | 415.87 |
| <sup>202</sup> Hg | pro  | -39.56                    | -39.56  | 79.12  | 79.12  | -55.06                     | -55.06  | 110.12 | 110.12 |
|                   | obl  | 70.02                     | -140.04 | 70.02  | 140.04 | 113.76                     | -227.52 | 113.76 | 227.52 |
|                   | tri1 | 11.03                     | -83.20  | 72.17  | 90.37  | 18.49                      | -120.95 | 102.46 | 130.31 |
|                   | tri2 | 43.36                     | -133.07 | 89.71  | 135.73 | 74.89                      | -219.77 | 144.88 | 223.45 |
|                   | tri3 | -10.68                    | -75.11  | 85.79  | 93.51  | -8.36                      | -115.66 | 124.02 | 138.63 |
| <sup>204</sup> Hg | pro  | -18.66                    | -18.66  | 37.32  | 37.32  | -25.59                     | -25.59  | 51.18  | 51.18  |
|                   | obl  | 20.83                     | -41.66  | 20.83  | 41.66  | 29.83                      | -59.66  | 29.83  | 59.66  |
|                   | tri1 | 3.34                      | -41.98  | 38.64  | 46.66  | 7.37                       | -62.21  | 54.84  | 67.98  |
|                   | tri2 | 13.13                     | -55.20  | 42.07  | 57.68  | 21.19                      | -82.74  | 61.55  | 85.96  |
|                   | tri3 | -7.16                     | -43.35  | 50.51  | 54.66  | -7.37                      | -65.81  | 73.18  | 80.59  |



TABLE II. (Continued).

|                   |      | Proton (fm <sup>2</sup> ) |        |       |       | Neutron (fm <sup>2</sup> ) |         |        |        |
|-------------------|------|---------------------------|--------|-------|-------|----------------------------|---------|--------|--------|
|                   |      | $Q_x$                     | $Q_y$  | $Q_z$ | $Q_0$ | $Q_x$                      | $Q_y$   | $Q_z$  | $Q_0$  |
| <sup>206</sup> Hg | pro  | -12.33                    | -12.33 | 24.66 | 24.66 | -15.52                     | -15.52  | 31.04  | 31.04  |
|                   | obl  | 14.34                     | -28.68 | 14.34 | 28.68 | 16.97                      | -33.94  | 16.97  | 33.94  |
|                   | tri1 | 1.53                      | -29.53 | 28.00 | 33.25 | 1.39                       | -36.87  | 35.48  | 41.80  |
|                   | tri2 | 9.63                      | -43.47 | 33.84 | 45.67 | 12.09                      | -55.86  | 43.77  | 58.78  |
|                   | tri3 | -6.16                     | -32.42 | 38.58 | 41.45 | -8.48                      | -42.34  | 50.82  | 54.45  |
| <sup>208</sup> Hg | pro  | -24.40                    | -24.40 | 48.80 | 48.80 | -50.61                     | -50.61  | 101.22 | 101.22 |
|                   | obl  | 28.82                     | -57.64 | 28.82 | 57.64 | 58.15                      | -116.30 | 58.15  | 116.30 |
|                   | tri1 | 15.49                     | -58.87 | 43.38 | 61.03 | 29.79                      | -118.04 | 88.25  | 122.77 |
|                   | tri2 | 25.76                     | -72.77 | 47.01 | 73.79 | 45.97                      | -135.83 | 89.86  | 138.18 |
|                   | tri3 | 0.03                      | -59.00 | 58.97 | 68.11 | 7.15                       | -118.33 | 111.18 | 132.70 |
| <sup>210</sup> Hg | pro  | -46.50                    | -46.50 | 93.00 | 93.00 | -99.30                     | -99.30  | 198.60 | 198.60 |
|                   | obl  | 30.01                     | -60.02 | 30.01 | 60.02 | 67.57                      | -135.14 | 67.57  | 135.14 |
|                   | tri1 | 6.92                      | -58.38 | 51.46 | 63.80 | 15.08                      | -130.03 | 114.95 | 142.24 |
|                   | tri2 | 20.88                     | -74.15 | 53.27 | 76.47 | 41.16                      | -151.41 | 110.25 | 156.57 |
|                   | tri3 | -14.86                    | -61.06 | 75.92 | 80.47 | -33.03                     | -130.68 | 163.71 | 173.14 |

### III. RESULTS AND DISCUSSION

We use the Skyrme parameter set SKI4 to calculate the ground-state properties of Hg isotopes. For a given nucleus the solution which corresponds to the maximum binding energy is the ground state of the nucleus. The numerical results on binding energies of Hg isotopes are been listed in Table I. The RMF results with NL1 are also listed for comparison. In the table Expt. is the experimental data [23] or the estimated value (denoted as #) as the experimental values are unknown [23]. The spherical (sph), prolate (pro), oblate (obl) and triaxial (tri1, tri2, and tri3) solutions are also listed in the table for comparison. In the meantime we plot the binding energy per nucleon ( $B/A$ ) in Fig. 1. The binding energies calculated with the SKI4 agree well with experimental data [23] and the relative difference of the binding energy is at most 0.3%. The ground states which correspond to the maximum binding energy are oblate for <sup>170</sup>Hg–<sup>196</sup>Hg, triaxial for <sup>198</sup>Hg and <sup>200</sup>Hg, spherical for <sup>202</sup>Hg–<sup>206</sup>Hg, and triaxial for <sup>208</sup>Hg and <sup>210</sup>Hg, respectively. It is well known that there is the shape coexistence in Hg isotopes. Our calculation agrees with this. It is seen from Table I that the energy minima of the oblate and triaxial solutions lie closer than that of the oblate and prolate solutions. These indicate that the structures of Hg isotopes are more complicated than the previous results which show that there is only a shape coexistence between prolate ellipsoid and oblate ellipsoid.

We plot in Fig. 2 the absolute difference of the binding energies between theoretical results and experimental data. It is obvious that the results of SKI4 are better than that of NL1 and the absolute difference is less than 2 MeV except for <sup>206</sup>Hg (about 5 MeV). For nuclei far from the stable line, NL1 has a large error (about 14 MeV), but the results of SKI4 are excellent. It proves that the force SKI4 can give reliable results for nuclei not only near the stable line but also far from the stable line because the nucleon-nucleon correlations have been treated carefully and the isospin de-

grees of freedom have been included in the force SKI4.

The two-neutron separation energy of Hg isotopes is plotted in Fig. 3 where it has been defined as the difference of binding energies  $S_{2n}(Z, N) = B(Z, N) - B(Z, N - 2)$ . The results of SKI4 agree well with the experimental values. Because of the shell effects, there is a dramatic decrease in <sup>208</sup>Hg in Fig. 3.

In Fig. 4, we plot the isotope shift  $r_c^2(A) - r_c^2(\text{ref})$  for Hg nuclei (<sup>198</sup>Hg is chosen as a reference nucleus in the Hg chain). The empirical data obtained from atomic laser spectroscopy are also shown by the solid circles [24]. The theoretical values from the deformed Skyrme-Hartree-Fock (DSHF) model and from the spherical Skyrme-Hartree-Fock (SSHF) model are denoted by open circles and open squares in the figure, respectively. It is seen from the figure that the DSHF model with SKI4 is successful in reproducing the isotope shift of Hg nuclei and the SSHF model has an obvious difference from the experimental data except for the spherical nuclei <sup>202</sup>Hg–<sup>206</sup>Hg. It indicates that there exists the deformation in Hg isotopes when the neutron number  $N$  is below the reference point. The DSHF model with SKI4 is successful in reproducing both the binding energy and the nuclear charge radius. As the isotope shifts in a chain of isotopes are the variation of proton distributions with neutron number, it is evident that the isotope shift depends on the correlations between protons and neutrons. The force SKI4, which has the generalized spin-orbit term, treats the correlations between protons and neutrons correctly.

The calculated root-mean-square radii of the density distributions of protons, neutrons, matter, and charge ( $r_p$ ,  $r_n$ ,  $r_t$ , and  $r_c$ , respectively) in the DSHF model are plotted in Fig. 5. The rms matter radius has been calculated by defining the total radius as the average of proton and neutron radii in every orbit weighted with occupation probabilities. The charge radius is obtained from the charge density which is obtained from the charge form factor by the inverse Fourier-

TABLE III. The proton and neutron hexadecupole moments  $Q_{40}$ ,  $Q_{42}$ , and  $Q_{44}$  and hexadecupole deformations parameters  $\beta_4$ ,  $\gamma_4$  (in degrees), and  $\delta_4$  (in degrees) obtained with the SKI4 for three triaxial cases.

|                   |      | Proton   |          |          |           |            |            | Neutron  |          |          |           |            |            |
|-------------------|------|----------|----------|----------|-----------|------------|------------|----------|----------|----------|-----------|------------|------------|
|                   |      | $Q_{40}$ | $Q_{42}$ | $Q_{44}$ | $\beta_4$ | $\gamma_4$ | $\delta_4$ | $Q_{40}$ | $Q_{42}$ | $Q_{44}$ | $\beta_4$ | $\gamma_4$ | $\delta_4$ |
| $^{170}\text{Hg}$ | tri1 | 308      | -22      | -297     | 0.012     | 25         | 66         | 1051     | 276      | -71      | 0.010     | -1         | 77         |
|                   | tri2 | 278      | 41       | -241     | 0.012     | 24         | 52         | 687      | 362      | 28       | 0.008     | -10        | 83         |
|                   | tri3 | 703      | -141     | -298     | 0.012     | 32         | 81         | 1332     | 104      | -129     | 0.012     | 10         | 65         |
| $^{172}\text{Hg}$ | tri1 | 420      | -44      | -290     | 0.012     | 32         | 59         | 975      | 258      | -60      | 0.008     | 3          | 85         |
|                   | tri2 | 241      | 32       | -229     | 0.013     | 27         | 48         | 652      | 364      | 40       | 0.007     | -6         | 73         |
|                   | tri3 | 497      | -140     | -296     | 0.011     | 39         | 67         | 1074     | 122      | -127     | 0.008     | 16         | 78         |
| $^{174}\text{Hg}$ | tri1 | 227      | -37      | -282     | 0.012     | 36         | 48         | 711      | 286      | -46      | 0.006     | 6          | 71         |
|                   | tri2 | 181      | 17       | -211     | 0.013     | 31         | 46         | 590      | 345      | 68       | 0.007     | 3          | 62         |
|                   | tri3 | 277      | -71      | -280     | 0.011     | 44         | 48         | 738      | 237      | -108     | 0.005     | 9          | 65         |
| $^{176}\text{Hg}$ | tri1 | 132      | 53       | -226     | 0.011     | 36         | 38         | 545      | 435      | 35       | 0.005     | -13        | 47         |
|                   | tri2 | 147      | 73       | -143     | 0.012     | 32         | 41         | 549      | 453      | 181      | 0.006     | -7         | 54         |
|                   | tri3 | -18      | -40      | -275     | 0.011     | 58         | 32         | 298      | 286      | -97      | 0.005     | -5         | 19         |
| $^{178}\text{Hg}$ | tri1 | 11       | 53       | -203     | 0.011     | 38         | 33         | 353      | 442      | 84       | 0.005     | -25        | 36         |
|                   | tri2 | 150      | 148      | -61      | 0.011     | 28         | 38         | 552      | 595      | 332      | 0.005     | -26        | 53         |
|                   | tri3 | -134     | 298      | -260     | 0.011     | 58         | 27         | 116      | 298      | -67      | 0.006     | -24        | 9          |
| $^{180}\text{Hg}$ | tri1 | 108      | 108      | -130     | 0.010     | 34         | 35         | 489      | 548      | 230      | 0.005     | -31        | 46         |
|                   | tri2 | 212      | 214      | 26       | 0.010     | 22         | 39         | 659      | 725      | 512      | 0.005     | -38        | 67         |
|                   | tri3 | -87      | -27      | -237     | 0.010     | 53         | 30         | 169      | 300      | -24      | 0.005     | -19        | 14         |
| $^{182}\text{Hg}$ | tri1 | 241      | 147      | -66      | 0.010     | 31         | 40         | 710      | 630      | 365      | 0.005     | -24        | 59         |
|                   | tri2 | 300      | 261      | 97       | 0.010     | 16         | 44         | 813      | 825      | 665      | 0.005     | -36        | 71         |
|                   | tri3 | -33      | -51      | -220     | 0.011     | 63         | 32         | 163      | 178      | 10       | 0.007     | 89         | 22         |
| $^{184}\text{Hg}$ | tri1 | 201      | 76       | -88      | 0.011     | 38         | 41         | 631      | 508      | 311      | 0.005     | 6          | 45         |
|                   | tri2 | 185      | 152      | 21       | 0.011     | 30         | 40         | 606      | 637      | 518      | 0.006     | -8         | 47         |
|                   | tri3 | 53       | -47      | -250     | 0.011     | 52         | 37         | 304      | 288      | -72      | 0.007     | 29         | 23         |
| $^{186}\text{Hg}$ | tri1 | 119      | -16      | -151     | 0.012     | 48         | 41         | 449      | 330      | 167      | 0.009     | 36         | 37         |
|                   | tri2 | 147      | 98       | -25      | 0.013     | 38         | 40         | 476      | 505      | 389      | 0.010     | 21         | 36         |
|                   | tri3 | 42       | -93      | -267     | 0.012     | 58         | 38         | 197      | 189      | -117     | 0.009     | 62         | 24         |
| $^{188}\text{Hg}$ | tri1 | 93       | -77      | -202     | 0.014     | 52         | 41         | 335      | 172      | 25       | 0.012     | 52         | 37         |
|                   | tri2 | 26       | -22      | -134     | 0.015     | 45         | 39         | 211      | 243      | 135      | 0.014     | 43         | 35         |
|                   | tri3 | -10      | -145     | -294     | 0.013     | 64         | 37         | -3       | 68       | -191     | 0.012     | 83         | 26         |
| $^{190}\text{Hg}$ | tri1 | 20       | -185     | -277     | 0.016     | 57         | 42         | 176      | -63      | -156     | 0.016     | 60         | 40         |
|                   | tri2 | -10      | -101     | -211     | 0.018     | 49         | 40         | 87       | 24       | -84      | 0.018     | 49         | 38         |
|                   | tri3 | -164     | -230     | -321     | 0.015     | 73         | 37         | -412     | 126      | -255     | 0.016     | -78        | 29         |
| $^{192}\text{Hg}$ | tri1 | -27      | -282     | -333     | 0.018     | 59         | 43         | 80       | -290     | -300     | 0.019     | 62         | 43         |
|                   | tri2 | -110     | -248     | -349     | 0.020     | 52         | 41         | -82      | -279     | -385     | 0.023     | 52         | 40         |
|                   | tri3 | -309     | -279     | -286     | 0.016     | 87         | 36         | -853     | -304     | -214     | 0.020     | -61        | 33         |
| $^{194}\text{Hg}$ | tri1 | -128     | -344     | 371      | 0.019     | 62         | 43         | -118     | -451     | -394     | 0.021     | 66         | 42         |
|                   | tri2 | -159     | -309     | -385     | 0.021     | 55         | 41         | -191     | 451      | -511     | 0.024     | 55         | 41         |
|                   | tri3 | -714     | -375     | -239     | 0.019     | -72        | 35         | -1826    | -607     | -122     | 0.026     | -47        | 39         |

TABLE III. (Continued.)

|                   |      | Proton   |          |          |           |            |            | Neutron  |          |          |           |            |            |
|-------------------|------|----------|----------|----------|-----------|------------|------------|----------|----------|----------|-----------|------------|------------|
|                   |      | $Q_{40}$ | $Q_{42}$ | $Q_{44}$ | $\beta_4$ | $\gamma_4$ | $\delta_4$ | $Q_{40}$ | $Q_{42}$ | $Q_{44}$ | $\beta_4$ | $\gamma_4$ | $\delta_4$ |
| $^{196}\text{Hg}$ | tri1 | -568     | -503     | -276     | 0.020     | 85         | 40         | -1349    | -1049    | -122     | 0.025     | -77        | 45         |
|                   | tri2 | -465     | -435     | -313     | 0.020     | 70         | 39         | -1129    | -943     | -278     | 0.025     | 86         | 41         |
|                   | tri3 | -675     | -558     | -160     | 0.019     | -77        | 44         | -1589    | -1105    | 130      | 0.025     | -60        | 51         |
| $^{198}\text{Hg}$ | tri1 | -809     | -546     | -201     | 0.020     | -83        | 39         | -2021    | -1266    | 26       | 0.029     | -65        | 47         |
|                   | tri2 | -771     | -558     | -277     | 0.022     | 86         | 38         | -1916    | -1320    | -154     | 0.029     | -76        | 44         |
|                   | tri3 | -1099    | -685     | -114     | 0.022     | -66        | 45         | -2481    | -1404    | 241      | 0.030     | -53        | 52         |
| $^{200}\text{Hg}$ | tri1 | -1230    | -603     | -165     | 0.023     | -68        | 38         | -2856    | -1439    | 118      | 0.032     | -56        | 47         |
|                   | tri2 | -1089    | -687     | -252     | 0.023     | -82        | 39         | -2598    | -1612    | -59      | 0.032     | -66        | 46         |
|                   | tri3 | -1421    | -618     | -57      | 0.023     | -54        | 42         | -3182    | -1387    | 362      | 0.033     | -45        | 50         |
| $^{202}\text{Hg}$ | tri1 | -265     | -141     | -78      | 0.004     | -71        | 37         | -470     | -241     | -212     | 0.005     | -81        | 32         |
|                   | tri2 | -581     | -472     | -458     | 0.014     | 77         | 38         | -1247    | -1028    | -1109    | 0.020     | 73         | 37         |
|                   | tri3 | -298     | -86      | -20      | 0.004     | -38        | 39         | -528     | -153     | -96      | 0.005     | -45        | 33         |
| $^{204}\text{Hg}$ | tri1 | -84      | -36      | -34      | 0.001     | -73        | 30         | -213     | -61      | -92      | 0.002     | -69        | 22         |
|                   | tri2 | -78      | -42      | -46      | 0.002     | 86         | 30         | -199     | -76      | -111     | 0.002     | 89         | 24         |
|                   | tri3 | -89      | -30      | -22      | 0.001     | -52        | 32         | -235     | -57      | -73      | 0.002     | -49        | 25         |
| $^{206}\text{Hg}$ | tri1 | -10      | 10       | -14      | 0.001     | -47        | 22         | -98      | 13       | -74      | 0.001     | -38        | 8          |
|                   | tri2 | -13      | 12       | -11      | 0.001     | -51        | 15         | -101     | 18       | -66      | 0.001     | -57        | 6          |
|                   | tri3 | -1       | 9        | -16      | 0.001     | -32        | 29         | -83      | 12       | -75      | 0.001     | -29        | 9          |
| $^{208}\text{Hg}$ | tri1 | 343      | 271      | 141      | 0.005     | -78        | 45         | 1032     | 897      | 435      | 0.011     | -80        | 48         |
|                   | tri2 | 275      | 256      | 181      | 0.005     | -89        | 45         | 814      | 854      | 580      | 0.010     | -83        | 48         |
|                   | tri3 | 423      | 271      | 93       | 0.006     | -65        | 47         | 1371     | 915      | 260      | 0.012     | -64        | 49         |
| $^{210}\text{Hg}$ | tri1 | 235      | -7       | -197     | 0.004     | 5          | 85         | 776      | 30       | -661     | 0.008     | 1          | 85         |
|                   | tri2 | 69       | -25      | -204     | 0.003     | 12         | 58         | 213      | 17       | -628     | 0.006     | 3          | 58         |
|                   | tri3 | 532      | -27      | -126     | 0.005     | 7          | 61         | 1886     | -65      | -438     | 0.012     | 5          | 60         |

Bessel transform. We can see from Fig. 5 that the radii increase smoothly with neutron number. The RMF-NL1 results [6] show that the various radii have a dramatic increase at  $A = 180$  and oscillations below  $A = 188$ . The authors of Refs. [6, 8] notice it but they do not give a satisfying explanation [6,8]. The previous nonrelativistic HF+BCS calculations seem to fail in reproducing the experimental trend [2]. We analyze why the radii have a smooth increase with neutron number in our calculation. There are three causes: (i) For  $^{170}\text{Hg}$ - $^{200}\text{Hg}$ , the binding energies in oblate solutions (or triaxial solutions) are greater than those in prolate solutions (about 1–4 MeV) and so there is no prolate ellipsoid for the ground state of these nuclei. The binding energies in triaxial solutions are very close to oblate shape and  $\gamma_2$  in the triaxial cases (see Table I) is close to  $60^\circ$ . Therefore there is no dramatic change of nuclear shape in our results. This is different from previous results which show that there is a shape transition from oblate to prolate or from prolate to oblate [6]. In our calculation, the SKI4 results show only a smooth shape transition from oblate to triaxial at first, then to spherical, and finally to triaxial shape. Because it is only a smooth shape transition, the radii have a similar smooth variation.

(ii) There is no superdeformed ground state in our results and thus this avoids a dramatic change of radii. The oblate and triaxial configurations are almost degenerate for  $^{170}\text{Hg}$ - $^{200}\text{Hg}$  in our calculation. This is different from other papers, which show that there are only axial deformations of prolate and oblate ellipsoids. (iii) SKI4 can reproduce the experimental data of the ground-state properties for nuclei far from the stable line due to the modification of the spin-orbit term in effective forces.

The deformations of nuclei play a crucial role in the ground state of nuclei. In Table II, we show the numerical results of the quadrupole moments  $Q_x$ ,  $Q_y$ ,  $Q_z$ , and  $Q_0$  which are defined in Eqs. (5)–(9). For the prolate case,  $Q_x = Q_y = -Q_z/2$  and  $Q_0 = Q_z$ . For the oblate case,  $Q_x = Q_z = -Q_y/2$  and  $Q_0 = |Q_y|$ . For triaxial cases, only  $Q_x + Q_y + Q_z = 0$ . We can see from Table II that there are smaller quadrupole moments in prolate configurations than those in oblate configurations. The quadrupole moments in triaxial configurations are close to those in oblate configurations.  $^{202}\text{Hg}$ - $^{206}\text{Hg}$  are spherical nuclei because they have very small quadrupole moments.

The quadrupole deformation parameters  $\beta_2$  and  $\gamma_2$  are

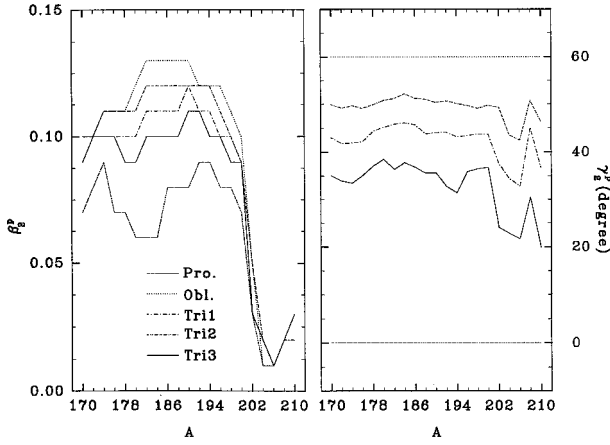


FIG. 6. The quadrupole deformation parameters  $\beta_2$  (left plot) and  $\gamma_2$  (right plot) in the ground state of Hg isotopes as a function of the mass number.

also listed in Table I. We also plot the  $\beta_2$  and  $\gamma_2$  of Hg isotopes as a function of the mass number in Fig. 6. In the prolate case,  $\gamma=0^\circ$ ; in the oblate case,  $\gamma_2=60^\circ$ ; and in the triaxial cases,  $0^\circ < \gamma_2 < 60^\circ$ . We compare our results with the RMF-NL1 results and find that NL1 reproduces a large prolate deformation  $\beta_2$  for  $^{176}\text{Hg}$ – $^{192}\text{Hg}$ . The SKI4 results for  $\beta_2$  agree well with the experimental values. The triaxial solutions of  $\gamma_2$  are close to  $60^\circ$  and this indicates that the shape transition will be a smooth change. There are no superdeformed solutions in the ground state of these nuclei but there are triaxial solutions for  $^{198}\text{Hg}$ ,  $^{200}\text{Hg}$ ,  $^{208}\text{Hg}$ , and  $^{210}\text{Hg}$ . For  $^{198}\text{Hg}$  and  $^{200}\text{Hg}$ ,  $\gamma_2^p$  is  $49.13^\circ$  and  $49.72^\circ$ , respectively. These values are close to oblate shape ( $\gamma_2^p=60^\circ$  for the oblate case). For  $^{208}\text{Hg}$  and  $^{210}\text{Hg}$ ,  $\beta_2^p=0.03$ . It is small and close to spherical shape ( $\beta_2^p=0$  in the spherical case). It is concluded from Table I that there exists a shape coexistence in the ground state of Hg isotopes. For  $^{170}\text{Hg}$ – $^{200}\text{Hg}$ , there is the shape coexistence between the oblate ellipsoid and triaxial shape but the binding energies of oblate solutions are slightly larger than those of the triaxial solutions for  $^{170}\text{Hg}$ – $^{196}\text{Hg}$  and the binding energies of triaxial solutions are slightly larger than those of the oblate solutions for  $^{198}\text{Hg}$  and  $^{200}\text{Hg}$ .  $^{202}\text{Hg}$ – $^{206}\text{Hg}$  are approximately spherical. For  $^{208}\text{Hg}$  and  $^{210}\text{Hg}$ , there is various shape coexistences but the binding energies of the triaxial solutions are slightly larger than those of other solutions. There exists

a shape transition in the ground-state of Hg isotopes: from oblate to triaxial shape in  $^{198}\text{Hg}$ , from triaxial to spherical shape in  $^{202}\text{Hg}$ , and from spherical to triaxial shape in  $^{208}\text{Hg}$ .

Finally, we list the hexadecupole moments  $Q_{40}$ ,  $Q_{42}$ , and  $Q_{44}$  and the hexadecupole deformation parameters  $\gamma_4^{n,p}$ ,  $\beta_4^{n,p}$ , and  $\delta_4^{n,p}$  in Table III for the triaxial cases. These quantities may be useful for fusion cross sections. For the cases tri1 and tri2,  $Q_{40}$  has a sign change from positive to negative near  $^{198}\text{Hg}$ . Because of the small  $\beta_4$  ( $\beta_4 < 0.03$  except for  $^{198}\text{Hg}$  and  $^{200}\text{Hg}$ ), we think that the hexadecupole deformations are not important for Hg isotopes.

#### IV. CONCLUSION

In this paper, we use the deformed-Skyrme-Hartree-Fock model with new Skyrme parameter set SKI4 to calculate the ground-state properties of Hg isotopes. The numerical results agree well with the experimental data. We summarize our main results as follows. (i) The new Skyrme parameter set SKI4, which has a generalized spin-orbit term, is successful in reproducing the binding energies, isotope shifts, and radii both for nuclei near the stable line and for exotic nuclei far from the stable line. (ii) The deformation parameter obtained by SKI4 ( $\beta_2$ ) agrees well with the experimental values. There is the shape coexistence for the ground state of Hg isotopes:  $^{170}\text{Hg}$ – $^{200}\text{Hg}$  are oblate shape or have a shape coexistence between oblate and triaxial shape.  $^{202}\text{Hg}$ – $^{206}\text{Hg}$  are spherical shape or have a shape coexistence among spherical, triaxial, and oblate shapes.  $^{208}\text{Hg}$  and  $^{210}\text{Hg}$  are triaxial shape or of various shape coexistences. There is no superdeformed ground state for Hg isotopes in the DSHF calculation with SKI4. (iii) The calculated radii from the force SKI4 show a smooth increase with neutron number and they agree well with the experimental trend. This can be understood because the shape transition of Hg isotopes is smooth. (iv) Because our large-scale calculations have almost exhausted all possible configurations of deformations, the conclusions are very reliable.

#### ACKNOWLEDGMENTS

Z.R. would like to thank Prof. Faessler for discussions. This work was supported by the Alexander von Humboldt Foundation of Germany and by the National Natural Science Foundation of China.

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