

## Semiclassical origin of nuclear ground-state octupole deformations

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**Background:** Ground-state octupole deformations are suggested in nuclei located in the *north-east* neighbor of the doubly magic nuclei on the nuclear chart ( $N, Z$ ), such as those in Ba and Ra-Th regions. This systematics has been attributed to the parity mixing of the approximately degenerate  $\Delta l = 3$  pair of single-particle levels near the Fermi surface.

**Purpose:** Nuclear deformations are governed in most cases by the gross shell structures of the single-particle spectra. I will consider the systematics in octupole deformation from the view point of the gross shell structure and investigate the mechanism of its manifestation using the semiclassical periodic-orbit theory (POT), which describes the quantum shell effect by means of the periodic orbits (POs) in the corresponding classical system.

**Methods:** To focus on the role of deformation, simplified infinite-well (cavity) and radial power-law potential models are employed taking account of quadrupole and octupole shape degrees of freedom. Nuclear ground-state deformations are investigated over the nuclear chart, and the properties of the deformed shell structures are analyzed by means of the semiclassical POT.

**Results and conclusions:** The systematics in nuclear ground-state octupole deformations are reproduced in simplified mean-field potential models either with or without parity mixing between  $\Delta l = 3$  pair of levels. The strong octupole deformed shell effect at above the spherical shell closures are explained simply and clearly using the semiclassical periodic-orbit theory. They are associated with the local restoration of dynamical symmetry, which enhance the contribution of classical POs to the gross shell effect.

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### I. INTRODUCTION

Breaking of reflection symmetry is one of the fundamental problems in nuclear structure physics [1]. In medium- to heavy-mass nuclei, ground-state octupole deformations are observed only for a few isotopes such as those around neutron-rich Ba region and Ra-Th region. Possible static octupole shapes for even-even nuclei have been systematically investigated over the nuclear chart by means of various theoretical approaches [2–6]. All those studies have obtained the results which are basically consistent with the experiments.

As well as the ground-state deformation, the significance of the octupole shape degree of freedom in nuclear fission has been also suggested [7,8]. The reason why the fission-fragment mass distribution of actinide nuclei is centered at  $A \approx 140$ , which are slightly larger than that of the doubly magic  $^{132}\text{Sn}$ , can be understood by considering the shell effect of the pear-shaped prefragment. The octupole shape degree of freedom should also play role in the process of superasymmetric fission, referred to as cluster radioactivity, where the shell effect of doubly magic  $^{208}\text{Pb}$  is concerned [9–11].

It has been considered that the nuclear octupole deformations are attributed to the octupole correlation between the approximately degenerate  $\Delta l = 3$  pair of single-particle levels near the Fermi surface. Such pairs of degenerate levels

arise just above each spherical shell gaps due to the intruder levels from the higher oscillator shells in the realistic nuclear mean-field potential with sharp surface [1]. For instance, proton ( $h_{11/2}, d_{5/2}$ ) levels above  $Z = 50$  gap and neutron ( $i_{13/2}, f_{7/2}$ ) levels above  $N = 82$  gap are thought to be relevant for the octupole softness in Ba region.

In addition to the above  $\Delta l = 3$  mixing, I have pointed out the significance of the gross shell effect for the octupole deformation [12]. In that work, infinite-well potential (cavity) model was employed where the surface shape is parametrized by merging a sphere and a paraboloid. The semiclassical periodic-orbit theory (POT) [13,14] is successfully utilized to elucidate the origin of remarkable shell structure for octupole deformed nuclei. In POT, quantum shell effect is described by means of the periodic orbits (POs) in the corresponding classical system. The advantage of such cavity model is that the contribution of the classical POs to the shell energies can be obtained by directly evaluating the semiclassical trace formula, which represents the quantum level density (density of energy eigenvalues) as the sum over contributions of the classical POs. For the system with a few particles added to the spherical closed-shell configurations, octupole shape is advantageous in gaining large shell energy, and its reason can be clearly explained using the contribution of degenerate family of classical POs to the semiclassical density of states.

In this study, I extend the above model a little to consider the shapes with arbitrary combinations of axially symmetric quadrupole and octupole deformations. With this extremely

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simplified mean-field model, I would like to focus only on the effect of deformation. The central aim of this work is to investigate the role of the gross shell effect to the systematic appearance of octupole deformations above the spherical closed-shell configurations and clarify their origin by the semiclassical POT. In my previous studies with my collaborators on the cavity- and oscillator-type potential models, it has been shown that the bifurcations of equatorial orbits at certain combinations of axially symmetric quadrupole and octupole deformations provide remarkable shell effects [15,16]. The PO bifurcations is associated with the local restoration of symmetry, with which the family of classical POs acquire extra local degeneracies. Since the oscillator type potential has no  $\Delta l = 3$  pairs of levels at the spherical shape, it may also give us information about the relative importance of  $\Delta l = 3$  mixing in octupole deformation.

This paper is organized as follows: In Sec. II, a brief review on the semiclassical theory of single-particle shell structure is given. In Sec. III, the mean-field potential models employed in this work are defined. In addition to the traditional prescription to expand the surface shape by spherical harmonic functions, a specific way of parametrization is proposed by merging a spheroid and a paraboloid. In the cavity model with the latter parametrization, classical POs form continuous families with higher degeneracy and a stronger deformed shell effect is expected. Then, systematic calculations of ground-state deformations over the nuclear chart is performed in Sec. IV for both parametrizations above. The condition for nuclei to gain shell energy by octupole deformation is considered using the relation between the gross shell structure and classical POs, and the mechanism for the systematic appearance of octupole deformation at above the spherical closed-shell configurations is explained. It will be also shown that the above systematics is reproduced in the oscillator type potential model, namely, without the help of  $\Delta l = 3$  mixing. Section V is devoted to the summary and concluding remarks.

## II. THEORETICAL FRAMEWORK

### A. Periodic-orbit theory

Semiclassical periodic-orbit theory (POT) is the powerful tool to analyze the gross shell structures [13,14,17], and I have taken full advantage of it in investigating the microscopic origin of nuclear deformations and shape stabilities [18,19]. Here, let us briefly review some of the key issues related to the POT.

When one solves the quantum single-particle energy eigenvalue problem, the distribution of the energy levels generally show a regular oscillating pattern. However, the origin for this structure generally cannot be explained by purely quantum-mechanical concepts alone. Using the semiclassical approximation to the path-integral representation of the Green's function, contribution of classical POs are extracted, and the level density

$$g(e) = \sum_i \delta(e - e_i) \quad (1)$$

is expressed as the sum over the contribution of classical POs

$$g(e) = \bar{g}(e) + \delta g(e),$$

$$\delta g(e) \simeq \sum_{\text{PO}} A_{\text{PO}}(e) \cos\left(\frac{1}{\hbar} S_{\text{PO}}(e) - \frac{\pi}{2} \mu_{\text{PO}}\right), \quad (2)$$

which is known as the trace formula [14,17]. The average part  $\bar{g}(e)$  is given by the (extended) Thomas-Fermi approximation. In the oscillating part  $\delta g$ ,  $S_{\text{PO}} = \oint_{\text{PO}} \mathbf{p} \cdot d\mathbf{r}$  represents the action integral along the PO,  $\mu_{\text{PO}}$  is the Maslov index related to the geometrical character of the orbit, and the amplitude  $A_{\text{PO}}$  is determined by the degeneracy, period, and stability of the PO. Since the action integral is generally a monotonically increasing function of energy  $e$ , each contribution of PO in Eq. (2) gives a regularly oscillating function of  $e$ . The orbit with shorter period  $T_{\text{PO}} = dS_{\text{PO}}/de$  gives the gross structure of the level density and the longer orbits contribute to the finer structures. In consideration of gross shell structure, one has only to take the contributions of a few shortest POs. Under continuous symmetries, the orbits will form a continuous family. This is called a degeneracy of the classical POs. The orbit with higher degeneracies make more significant contribution to the level density in the  $\hbar$  expansion. The number of continuous parameters  $K_{\text{PO}}$  for the PO family is called the degeneracy parameter, and the amplitude factor  $A_{\text{PO}}$  is proportional to  $\hbar^{-K_{\text{PO}}/2}$ .

Using Eq. (2), one obtains the trace formula for shell energy as [17,20]

$$\delta E(N) = \int^{e_F} (e - e_F) \delta g(e) de$$

$$\simeq \sum_{\text{PO}} \frac{\hbar^2}{T_{\text{PO}}^2} A_{\text{PO}}(e_F) \cos\left(\frac{1}{\hbar} S_{\text{PO}}(e_F) - \frac{\pi}{2} \mu_{\text{PO}}\right), \quad (3)$$

where  $e_F$  is the Fermi energy satisfying

$$N = \int^{e_F} g(e) de. \quad (4)$$

Due to the additional factor  $T_{\text{PO}}^{-2}$  in the amplitudes of the PO contributions, longer orbits become less important and, accordingly, one has only to consider the POs that are short and preferably of higher degeneracies.

Another important aspect of the periodic-orbit contribution is related to the stability of the orbits. The amplitude factor  $A_{\text{PO}}$  is proportional to the stability factor as follows:

$$A_{\text{PO}} \propto \frac{1}{\sqrt{|\det(I - \tilde{M}_{\text{PO}})|}}, \quad (5)$$

where  $\tilde{M}$  represents the symmetry-reduced monodromy matrix which describes the linear stability of the orbit. In calculating the monodromy matrix, one sets a  $(2f - 2)$ -dimensional ‘‘surface of section’’  $\Gamma$  in the classical  $(2f - 1)$ -dimensional phase space with energy constraint  $H(\mathbf{r}, \mathbf{p}) = E$ , where  $f$  is the number of degrees of freedom. Then, consider a trajectory starting off at  $Z_0$  on the surface  $\Gamma$ . Since the energy surface  $H(\mathbf{r}, \mathbf{p}) = E$  is compact, the trajectory will intersect the surface  $\Gamma$  again at  $Z_1$  in the same direction. The successive plots of the intersection points  $Z_1, Z_2, \dots$  is called

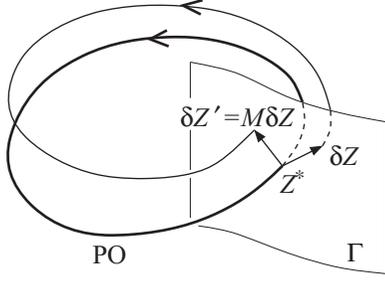


FIG. 1. Calculation of monodromy matrix for PO on the surface  $\Gamma$ .

a Poincaré surface of section (PSS) plot. The map  $\mathcal{M}$  from  $Z_k$  to  $Z_{k+1}$  [ $Z_{k+1} = \mathcal{M}(Z_k)$ ] defined by the Hamiltonian dynamics is called the Poincaré map. The PO is nothing but the fixed point  $Z^*$  of the Poincaré map  $\mathcal{M}$  (or its power  $\mathcal{M}^n$  in general), satisfying  $Z^* = \mathcal{M}^n(Z^*)$ . As shown in Fig. 1, let us consider a trajectory near the PO, starting off at  $Z_0 = Z^* + \delta Z$  on  $\Gamma$ . It is generally nonperiodic and will arrive at  $Z_n = Z^* + \delta Z'$  on  $\Gamma$ , and  $\delta Z'$  can be written as

$$\delta Z' = M_{\text{PO}} \delta Z + O(\delta Z^2). \quad (6)$$

The  $(2f-2) \times (2f-2)$  matrix  $M_{\text{PO}}$ , representing a linearized Poincaré map defines the monodromy matrix.  $M_{\text{PO}}$  depends on the choice of  $\Gamma$ , but its eigenvalues are irrelevant to  $\Gamma$  and therefore the stability factor (5) does not depend on  $\Gamma$ .

For system with continuous symmetries,  $M_{\text{PO}}$  has trivial unit eigenvalues, and the symmetry-reduced matrix  $\tilde{M}_{\text{PO}}$  is obtained by splitting off the degrees of freedom relevant to those symmetries. It can happen that one of the eigenvalues of  $\tilde{M}_{\text{PO}}$  becomes equal to 1 with varying parameter of the Hamiltonian. This corresponds to the bifurcation point of PO, where dynamical symmetry is locally restored around the PO and the orbit forms a local continuous family. The orbits belonging to such a family make coherent contribution to the level density and bring about a significant enhancement of the amplitude factor  $A_{\text{PO}}$ . Since the standard stationary phase approximation (SPA) to derive the trace formula is broken down at the bifurcation point, the stability factor in Eq. (5) suffers divergence there. This shortcoming can be remedied by an appropriate treatment of the higher-order expansions about the PO, e.g., by the uniform approximations [21–23]. Bifurcation of short PO is often responsible for the emergence of significant shell effect at exotic shapes. This feature plays an essential role when I consider the quadrupole-octupole deformations in the following part.

### B. The shell-deformation energy

When one employs an effective mean-field model, shell energy is extracted from the single-particle spectra by decomposing the sum of single-particle energies into the smooth and oscillating parts as

$$\begin{aligned} E_{\text{sp}}(Z, N; q) &= \sum_{i=1}^Z e_i(q) + \sum_{j=1}^N e_j(q) \\ &= \tilde{E}_{\text{sp}}(Z, N; q) + \delta E(Z, N; q). \end{aligned} \quad (7)$$

$e_i(q)$  represents the single-particle energy for deformation  $q$ . In the microscopic-macroscopic model, the oscillating part of the single-particle energy sum is added to the semi-empirical liquid-drop model (LDM) energy as

$$E(Z, N; q) = E_{\text{LDM}}(Z, N; q) + \delta E(Z, N; q). \quad (8)$$

In the present work, the employed mean field is not a realistic one, and the use of a realistic LDM is of no importance. Assuming the single-particle Hamiltonian  $h = t + u$  ( $t$  and  $u$  being the kinetic energy and mean-field potential, respectively) as what is deduced from the many-body Hamiltonian with a two-body interaction, the smooth part of the total energy is expressed as

$$\tilde{E} = \sum_{i=1}^N \left( \langle t_i \rangle + \frac{1}{2} \langle u_i \rangle \right). \quad (9)$$

The factor  $\frac{1}{2}$  in the second term above is to avoid the double counting of the interaction. When the radial power-law potential  $u \propto r^\alpha$  is employed as the mean-field potential, the Virial theorem gives the relation

$$\langle t \rangle = \frac{1}{2} \langle \mathbf{r} \cdot \nabla u \rangle = \frac{\alpha}{2} \langle u \rangle. \quad (10)$$

Together with the relation  $\langle h \rangle = \langle t \rangle + \langle u \rangle$ , one obtains

$$\langle t \rangle = \frac{\alpha}{\alpha + 2} \langle h \rangle, \quad \langle u \rangle = \frac{2}{\alpha + 2} \langle h \rangle.$$

Inserting them into Eq. (9), one has

$$\tilde{E} = \frac{\alpha + 1}{\alpha + 2} \sum_{i=1}^N \langle h_i \rangle = \frac{\alpha + 1}{\alpha + 2} \tilde{E}_{\text{sp}}. \quad (11)$$

Consequently, the total energy can be expressed as

$$E(Z, N; q) = \frac{\alpha + 1}{\alpha + 2} \tilde{E}_{\text{sp}}(Z, N; q) + \delta E(Z, N; q). \quad (12)$$

In the cavity limit,  $\alpha \rightarrow \infty$ , one simply has

$$E^{(\text{cavity})}(Z, N; q) = E_{\text{sp}}(Z, N; q). \quad (13)$$

Ground-state deformation  $q^*$  is obtained by minimizing the total energy  $E$  with respect to  $q = \{q_2, q_3\}$ ,

$$E_{\text{min}}(Z, N) = E(Z, N; q^*) = \min_{q_2, q_3} E(Z, N; q). \quad (14)$$

In the analysis of deformation, one has usually considered the deformation energy  $E_{\text{def}}$  which is defined with the energy at spherical shape as reference;

$$E_{\text{def}}(Z, N; q) = E(Z, N; q) - E(Z, N; 0). \quad (15)$$

In this definition, the reference energy is a fluctuating function of particle numbers  $Z$  and  $N$ . To investigate the nuclear energy from a more general point of view, without special reference to quantum fluctuation at the spherical shape, let us define the *shell-deformation energy*,  $E_{\text{sh-def}}$ , by estimating the total energy with the smooth part of the spherical energy as reference;

$$\begin{aligned} E_{\text{sh-def}}(N, Z; q) &= E(Z, N; q) - \tilde{E}(Z, N; 0) \\ &= \{\tilde{E}(Z, N; q) - \tilde{E}(Z, N; 0)\} + \delta E(Z, N; q). \end{aligned} \quad (16)$$

As seen from the right-hand side, it consists of the shell energy and the smooth (LDM) deformation energy. In the following analysis, the shell-deformation energy (16) shall be referred rather than the traditional deformation energy (15).

### III. SHAPE PARAMETRIZATION WITH OCTUPOLE AND QUADRUPOLE DEFORMATIONS

#### A. Stretched octupole parametrization

Various ways of parametrizing the shape of the nuclear surface have been proposed to discuss the nuclear deformation. The most commonly used one might be the expansion by spherical harmonic functions. For axially symmetric shapes, the surface shape is expressed as

$$r = r_s(\theta) = R_0 \left[ 1 + \sum_{l \geq 2} \beta_l P_l(\cos \theta) \right],$$

where  $P_l(x)$  is the Legendre polynomial. The  $P_1$  term is also considered when one wants to exactly eliminate the center of mass.

In my recent studies, the above shape function is modified a little. Instead of quadrupole deformation described by  $P_2$  function, I take the spheroidal shape:

$$r = r_s(\theta) = R_0 \frac{\eta^{2/3}}{\sqrt{\cos^2 \theta + \eta^2 \sin^2 \theta}},$$

where  $\eta = r_s(0)/r_s(\frac{\pi}{2})$  represents the axis ratio.  $\eta > 1$  and  $\eta < 1$  correspond to prolate and oblate deformations, respectively. Deformations with higher multipoles are considered by multiplying  $r_s$  by an exponential function  $e^{\beta_l P_l(\cos \theta)}$ . They are first taken on the spherical surface, and then stretched (or contracted) in the direction of the symmetry axis. For the octupole deformation, the surface profile function  $f(\theta) = r_s(\theta)/R_0$  is expressed as

$$f(\theta) = c(\beta_3) \eta^{-1/3} \sqrt{1 + (\eta^2 - 1) \cos^2 \theta'} e^{\beta_3 P_3(\cos \theta')},$$

$$\tan \theta' = \eta \tan \theta. \quad (17)$$

$c_3(\beta_3)$  is given by

$$c_3(\beta_3) = \left[ \frac{1}{2} \int_{-1}^1 e^{3\beta_3 P_3(t)} dt \right]^{-1/3}. \quad (18)$$

so that the volume conservation condition is satisfied. The center-of-mass condition is satisfied up to the first order of  $\beta_3$  for a uniform rigid body with this surface. By using the above exponential form, a natural surface shape can be achieved up to rather large octupole deformations (see Fig. 2).

In displaying the potential-energy surface, I use the dimensionless quadrupole and octupole moments as the shape parameters. They are defined by

$$q_2 = \frac{1}{R_0^2} \langle r^2 P_2(\cos \theta) \rangle, \quad q_3 = \frac{1}{R_0^3} \langle [r^3 P_3(\cos \theta)]' \rangle, \quad (19)$$

where  $(r^n P_n)'$  is the stretched multipole operator defined by the stretched coordinate

$$(x', y', z') = (\eta^{1/3} x, \eta^{1/3} y, \eta^{-2/3} z). \quad (20)$$

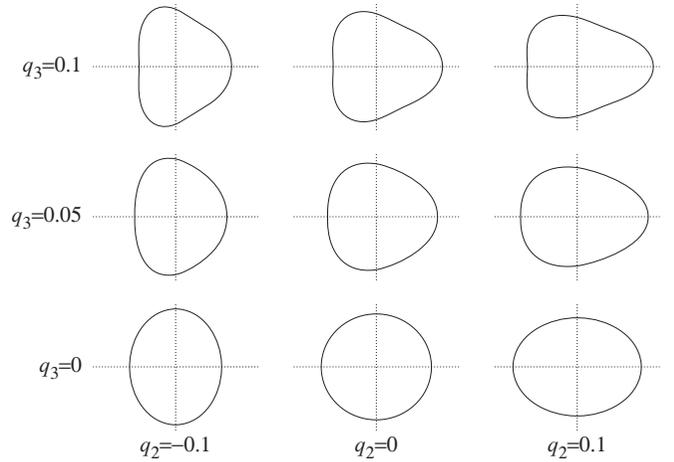


FIG. 2. Quadrupole-octupole surface by the stretched octupole parametrization  $r = R_0 f(\theta)$  [Eq. (17)] at several values of quadrupole and octupole moments ( $q_2, q_3$ ). Horizontal line is the symmetry axis, and the origin is the center of mass.

By defining the octupole moment  $q_3$  in terms of the stretched coordinate as above, it becomes independent of  $\eta$  and has one-to-one correspondence with the parameter  $\beta_3$ . The shapes of the surface at several values of  $(q_2, q_3)$  are displayed in Fig. 2.

In the cavity potential with the surface  $r = R_0 f(\theta)$ , one finds regular polygon orbits on the plane perpendicular to the symmetry axis, which I have called “the equatorial plane,” although it is slightly translated from the  $\theta = \frac{\pi}{2}$  plane for  $\beta_3 \neq 0$ . Those orbits form degenerate one-parameter family with respect to the rotation around the symmetry axis. By varying the deformation parameters, two main curvature radii at the equatorial plane coincide with each other for certain combinations of  $(\eta, \beta_3)$  or  $(q_2, q_3)$  (see right panel of Fig. 3). For such shapes, spherical symmetry is locally restored around the equatorial plane, and the orbits on it acquire two extra local degeneracies. This condition is satisfied approximately along the  $q_3 = q_2$  line on the shape parameter space.

The local symmetry restoration as discussed above provides substantial enhancement of the shell effect and plays significant roles in deformations of the systems [16]. A similar local symmetry restoration is also found in smooth potential

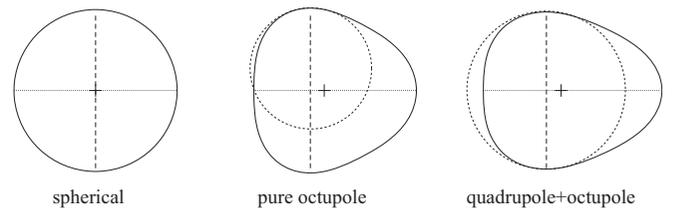


FIG. 3. Illustration of the local restoration of spherical symmetry in quadrupole-octupole cavity potential model. Horizontal line represents the symmetry axis and the cross represents the center of mass. The vertical line represents the plane referred as the equatorial plane. The circle with dashed line represents the circle of curvature on the meridian plane. In the right panel, the shape of a special combination of quadrupole and octupole deformation is shown where the meridian curvature radius coincides with the equatorial radius.

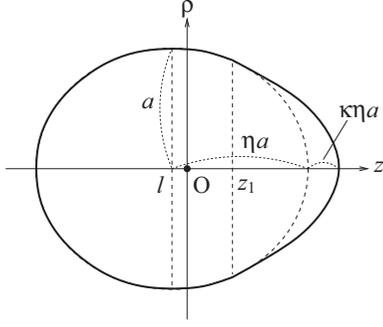


FIG. 4. Parametrization of quadrupole-octupole surface by merging a spheroid and a paraboloid.

models, where the symmetries are of the dynamical ones associated with the PO bifurcations [15].

### B. Spheroid + paraboloid parametrization

Next, I propose another way of shape parametrization. It is known that the spheroidal cavity model has nontrivial dynamical symmetry [24], and the classical POs form continuous families with higher degeneracy than the other axial shapes. Since the orbit family of higher degeneracy has stronger contribution to the quantum shell effect, it would be advantageous for the octupole deformed surface to include the spheroidal part in it. For this reason, let us consider axially symmetric octupole surface by merging a spheroid and a paraboloid as shown in Fig. 4. In the cylindrical coordinate  $(\rho, z, \varphi)$ , the surface shape  $\rho = \rho_s(z)$  is expressed as

$$\rho_s^2(z) = \begin{cases} a^2 - \left(\frac{z-l}{\eta}\right)^2 & (z_{\min} \leq z \leq z_1) \\ 2b(z_{\max} - z) & (z_1 \leq z \leq z_{\max}), \end{cases} \quad (21)$$

$$z_{\min} = l - \eta a, \quad z_{\max} = l + (1 + \kappa)\eta a.$$

A spheroidal surface ( $z < z_1$ ) and a paraboloidal surface ( $z > z_1$ ) are smoothly joined at  $z = z_1$ . The shape of the entire surface is controlled by the two independent shape parameters  $(\eta, \kappa)$ .  $\eta$  is the axis ratio of the spheroidal part, and  $\kappa$  is the octupole parameter defined by the relative width of the paraboloidal part raised from the spheroidal surface. For  $\kappa = 0$ , there is no paraboloidal part and the entire surface is the pure spheroid. Especially, the entire surface is spherical at  $(\eta, \kappa) = (1, 0)$ . The four other parameters  $a, b, l$ , and  $z_1$  entering in Eq. (21) are determined by (i) the condition to merge the two surfaces smoothly at  $z = z_1$ , (ii) the volume-conservation condition, and (iii) the center-of-mass condition. The center-of-mass condition does not affect the energy eigenvalues but is necessary in obtaining the correct quadrupole and octupole moments.

In this shape parametrization, the deformed shell structures are also investigated as functions of quadrupole and octupole moments  $(q_2, q_3)$  defined by Eq. (19). In this case, the use of the stretched coordinate in Eq. (19) guarantees that the octupole moment  $q_3$  is independent on  $\eta$  and has one-to-one correspondence with the parameter  $\kappa$ . The shape of the surface at several values of  $(q_2, q_3)$  are displayed in Fig. 5.

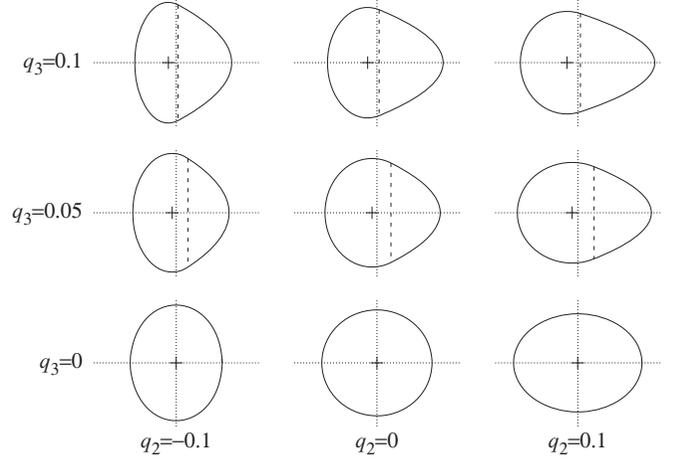


FIG. 5. Quadrupole-octupole surface by the spheroid + paraboloid parametrization  $\rho = \rho_s(z)$  [Eq. (21)] at several values of quadrupole and octupole moments  $(q_2, q_3)$ . The cross represents the center of the spheroid, and the broken line represents the boundary of the spheroidal and paraboloidal surfaces,  $z = z_1$ .

In the cavity potential with the surface (21), one expects a strong shell effect when the spheroidal part of the surface is spherical ( $\eta = 1$ ). For such shape, the equatorial orbits on the plane  $z = l$  that are one-parameter families for  $\eta \neq 1$  becomes three-parameter families, which are not only local ones but exist over finite ranges of the rotational angles. This condition is satisfied for smaller value of  $q_2$  for a given  $q_3$ , compared with the last parametrization. In my recent analysis [12], gross shell structures similar to that for the spherical potential are found to survive up to rather large octupole parameter  $\kappa$  keeping  $\eta = 1$ .

## IV. SYSTEMATICS OF GROUND-STATE OCTUPOLE DEFORMATIONS IN CAVITY AND OSCILLATOR POTENTIAL MODELS

### A. Semiclassical mechanism of octupole deformation

Based on the semiclassical trace formula, let us consider the condition where the system acquires large shell energy gain by the octupole deformation. As discussed above, local symmetry restoration with a special combination of quadrupole and octupole deformations brings about a strong shell effect. At those shapes, the POs with extra degeneracies are expected to make similar contribution to the shell energy as in the spherical potential.

In the cavity potential model, momentum  $|\mathbf{p}| = \hbar k$  is constant and the action integral is given by the product of momentum and the geometric length  $L_{\text{PO}}$ . The trace formula (3) is then expressed as

$$\delta E(N) = \sum \frac{\hbar^2}{T_{\text{PO}}^2} A_{\text{PO}} \cos\left(k_F L_{\text{PO}} - \frac{\pi}{2} \mu_{\text{PO}}\right), \quad (22)$$

where  $k_F$  represents the Fermi wave number.

Because of the saturation property, the volume  $V$  surrounded by the potential surface is proportional to the particle number  $N$ . According to the Weyl's formula [25], the level

density in terms of the variable  $e = k^2$  is given by

$$\rho(e) = \frac{Vk}{4\pi^2}, \quad (23)$$

with the volume

$$V = \frac{4\pi}{3}R_0^3 = \frac{4\pi}{3}Nr_0^3 \quad (R_0 = r_0N^{1/3}). \quad (24)$$

From the relation between Fermi wave number  $k_F$  and particle number  $N$ , one obtains

$$N = \int_0^{k_F^2} \rho(e)de = \frac{Vk_F^3}{6\pi^2} = \frac{2N(k_F r_0)^3}{9\pi},$$

$$k_F = \left(\frac{9\pi}{2}\right)^{1/3} r_0^{-1}.$$

Thus, the value of the Fermi wave number  $k_F$  is approximately independent on the particle number  $N$ . Consequently, the shell energy minimization condition associated with the contribution of PO in Eq. (22),

$$\cos(k_F L_{PO} - \pi \mu_{PO}/2) = -1, \quad (25)$$

is governed solely by the length of the orbit  $L_{PO}$  if the change of the Maslov index is ignored. Concerning to a specific PO, the above condition is that the radius  $a$  of the equatorial plane to coincide with the radius  $R_0$  of the spherical magic nucleus.

Let  $N_0$  a spherical magic number and  $R_0$  the radius of the surface for this magic nucleus. For the octupole shape  $q^*$  with local symmetry ( $q_3 \approx q_2$  for stretched octupole, and  $\eta = 1$  for spheroid + paraboloid parametrization), the radius  $a$  of the equatorial plane is shorter than the radius of the sphere with the same volume. In order for the radius  $a$  to coincide  $R_0$  which satisfies the energy minimization condition, the particle number  $N$  should be larger than  $N_0$  as

$$a(N, q^*) = R_0 = \left(\frac{N_0}{N}\right)^{1/3} a(N, 0),$$

$$N = N_0 \left(\frac{a(N, 0)}{a(N, q^*)}\right)^3. \quad (26)$$

Thus, with increasing octupole deformation  $q^*$ , the energy minimization condition is satisfied in the system with particle number slightly larger than the spherical magic number. This argument provides a simple and clear explanation for the octupole deformation to be found systematically at just above the spherical magic numbers.

Figure 6 illustrates the above argument from another perspective. If  $n$  particles are added to the spherical magic nucleus with particle number  $N_0$ , system will favor the octupole shape with local symmetry whose radius of the equatorial plane coincides with the radius of spherical magic nucleus. With more particles ( $n' > n$ ) attached, larger octupole deformation will occur. The middle panels of Fig. 6 display the case of the stretched octupole parametrization, for which one finds only local families of the quasi-periodic orbits around the shaded area in vicinity of the equatorial plane. For the sphere + paraboloid surface, POs form three-parameter families over the larger area in the sphere part, as depicted by the shaded area in the right panels of Fig. 6. It would be also interesting

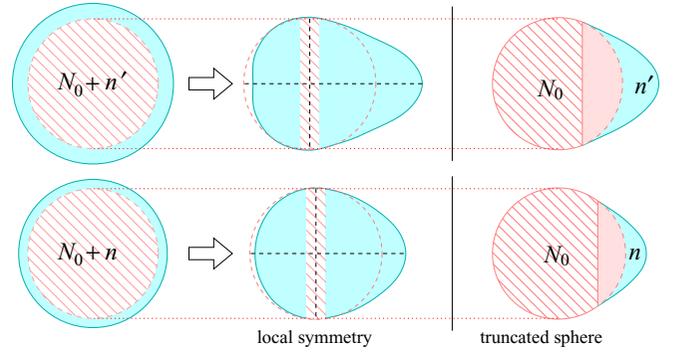


FIG. 6. Conceptual illustration of the mechanism of octupole deformation for a systems with  $N_0 + n$  nucleons,  $N_0$  being the spherical magic number and  $n$  a small even integer. Classical PO families residing in the shaded area in the octupole cavity give the shell effect similar to spherical magic nuclei with particle number  $N_0$ . With increasing  $n$  (as illustrated in the upper panel with  $n' > n$ ), larger octupole deformation is expected to keep the radius and the curvature radius of the equatorial plane identical to the radius of the spherical magic nucleus.

to examine how these difference in PO families might affect the octupole shell effect.

## B. Cavity model with the stretched octupole parametrization

Let us first consider the cavity model with the surface shape parametrized by Eq. (17). Figure 7 displays the single-particle spectra. In the left panel, single-particle level diagrams for pure quadrupole and pure octupole deformations are shown. The integers put in the middle of the figure indicate the spherical magic numbers, namely, the number of levels below

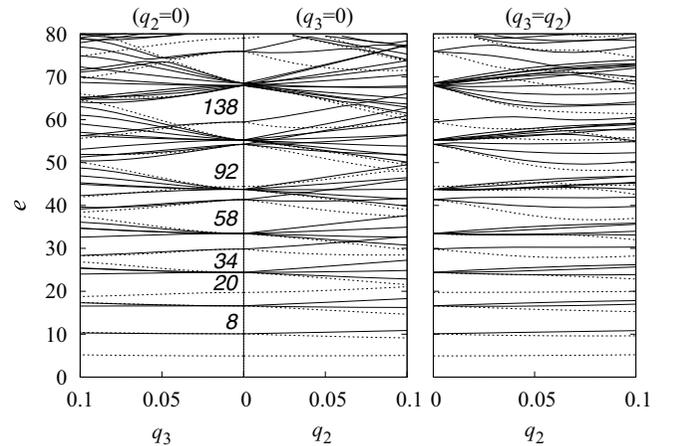


FIG. 7. Single-particle level diagram for spheroidal-octupole cavity model with the stretched octupole parametrization. Solid and broken curves represent degenerate (magnetic quantum number  $K \neq 0$ ) and nondegenerate ( $K = 0$ ) levels, respectively. The left panel shows single-particle level diagrams for pure quadrupole and for pure octupole deformations. Spherical-shape magic numbers are indicated in italics. In the right panel, the level diagram is shown for deformations along  $q_3 = q_2$ , close to the local symmetry condition.

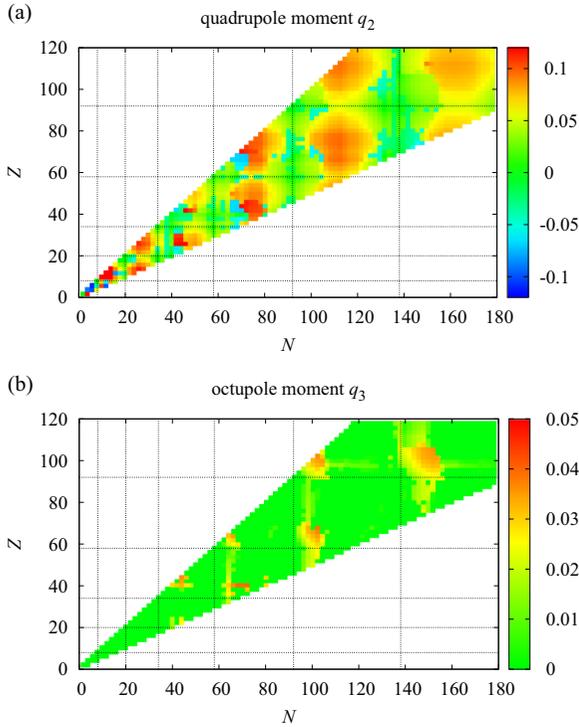


FIG. 8. Ground-state quadrupole moment  $q_2$  (upper panel) and octupole moment  $q_3$  (lower panel) in cavity potential model with stretched octupole parametrization are shown on the  $(N, Z)$  plane. Horizontal and vertical dotted lines indicate magic numbers, 8, 20, 34, 58, 92, 138, of the spherical cavity model.

the energy gap. They are close to the real nuclear magic numbers, although slightly deviate from them mainly due to the absence of spin-orbit coupling. The doubly magic nuclei  $^{132}\text{Sn}$  and  $^{208}\text{Pb}$  correspond to  $(Z, N) = (58, 92)$  and  $(92, 138)$ , respectively, in the cavity model. The degeneracies of levels at the spherical shape are broken with increasing deformation without forming noticeable structure for both  $q_2$  and  $q_3$ .

In the right panel of Fig. 7, level diagram is shown along the deformations with  $q_3 = q_2$ . A remarkable feature for such shapes is the existence of equally spaced strongly bunched upward-right levels, and it is expected that a significant amount of the spherical shell effect will survive up to large deformations. The spherical symmetry is locally restored around the equatorial plane as illustrated in the middle panels of Fig. 6 for the shapes with  $q_3 \approx q_2$ , and the above shell effect should be associated with the contribution of degenerate families of POs in the semiclassical trace formulas (2) and (3).

With this single-particle spectra, energies of nuclei given by Eq. (13) is calculated over the nuclear chart (in the range  $Z \leq N \leq 2Z$  which is approximately corresponding to the region between proton and neutron drip lines) as functions of  $q_2$  and  $q_3$ , and ground-state deformations are obtained. The upper panel of Fig. 8 shows the quadrupole moment  $q_2$  of the ground-state shapes. The horizontal and vertical dotted lines indicate the spherical magic numbers. One obtains nearly spherical shapes along those magic lines. In most of the other regions,  $q_2$  takes positive values,

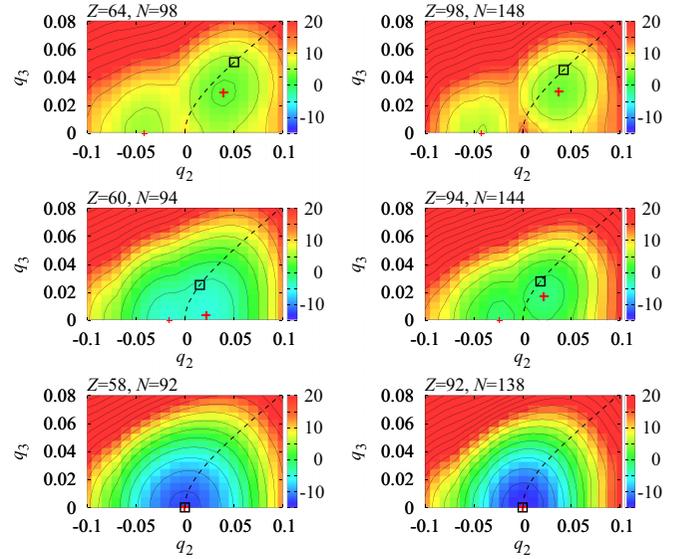


FIG. 9. Potential-energy surfaces for the doubly magic nuclei  $(Z, N) = (58, 92)$ ,  $(92, 138)$  and their *north-east* neighbors on the nuclear chart. Cavity potential with the stretched octupole parametrization is employed. Contour curves of the shell-deformation energy  $E_{\text{sh-def}}$  in  $(q_2, q_3)$  plane are drawn at intervals of 2 MeV. The thick broken line represents the bifurcation deformation for equatorial orbits. Large cross represents the ground-state deformation and small crosses are other local minima. Square represents the semiclassical guess of the ground-state deformation.

which reproduces the feature of prolate-shape predominance in the ground-state deformations [19,26–29]. In the lower panel of Fig. 8, octupole moment  $q_3$  is plotted. One will find that the octupole deformations systematically appear at the *north-east* neighbors of the doubly closed-shell configurations. This qualitatively reproduces the results of experiments and realistic calculations. The essential mechanism to explain the systematics of the octupole deformation seems to be already involved in this simplified cavity model.

Figure 9 shows the potential-energy surfaces of doubly magic nuclei  $(Z, N) = (58, 92)$  and  $(92, 138)$  and their *north-east* neighbors on the nuclear chart. Contour plot of the shell-deformation energy (16) are shown as functions of  $(q_2, q_3)$ , and the ground-state deformations and other local minima are marked with the cross symbols. Adding a few neutrons and protons to the spherical doubly magic nucleus, the system tends to take octupole shapes accompanied by prolate quadrupole deformation. The thick broken line indicate the bifurcation line of the equatorial orbit where one has the local symmetry restoration. As expected from the POT, nuclear shape evolves along this bifurcation line with increasing proton and neutron numbers.

In each panel of Fig. 9, the semiclassical guess of the ground-state deformation is indicated by the square symbol, where the radius of the equatorial plane coincides with the radius of the spherical doubly magic nucleus. The agreement with the quantum result is not bad but overestimating the deformation a little. It might be improved by taking the change of the Maslov index properly.

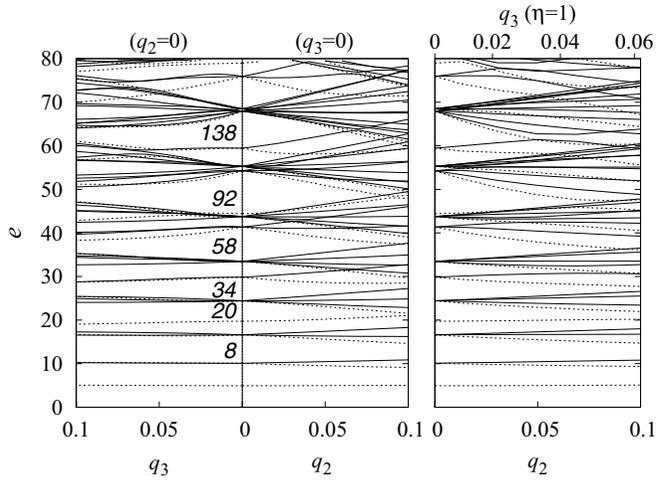


FIG. 10. Single-particle level diagram for the cavity potential model with the spheroid + paraboloid parametrization. The left panel is plotted in the same way as Fig. 7. In the right panel, levels are plotted against  $q_2$ , where  $q_3$  is varied with  $q_2$  so that  $\eta = 1$  is satisfied.

### C. Cavity model with spheroid + paraboloid parametrization

Next I examine the cavity model with spheroid + paraboloid parametrization (21). Since the spherical symmetry is maximally restored in the quadrupole-octupole deformed cavity, more significant effect of the symmetry restoration is expected.

Let us first look at the single-particle spectra in Fig. 10. In the left panel, single-particle energies for pure quadrupole and pure octupole shapes are shown. There seems no noticeable differences compared with those for the previous shape parametrization. (The pure quadrupole shape is spheroidal and the diagram is equivalent to the previous one.) In the right panel, levels are plotted against  $q_2$ , with  $q_3$  varied with  $q_2$  so that the spheroidal part of the surface is kept spherical ( $\eta = 1$ ). Again one finds bunches of strongly degenerate upward-right levels, indicating the effect of local spherical symmetry.

The obtained ground-state deformations are shown in Fig. 11. The results are qualitatively the same as the previous parametrization. The octupole deformations are found systematically at the *north-east* neighbors of each doubly magic nucleus.

Figure 12 shows the potential-energy surfaces for the same nuclei as those shown in Fig. 9. In the present parametrization, one has highly degenerate POs in the spheroid part of the potential, and more significant shell effect due to those orbits is expected. The thick broken line represents the shape where the spheroidal part of the surface is spherical and involves triply degenerate POs. In the same reason as discussed in the previous section, one has shell energy minima when the radius of the spheroid part is equal to that of the spherical magic nucleus. This condition gives the semiclassical guess of the ground-state deformation, whose position is marked with the square symbol in each panel of Fig. 12. Since there is no change of the Maslov index in this case, the agreement of the semiclassical guess (26) with the quantum results is almost perfect.

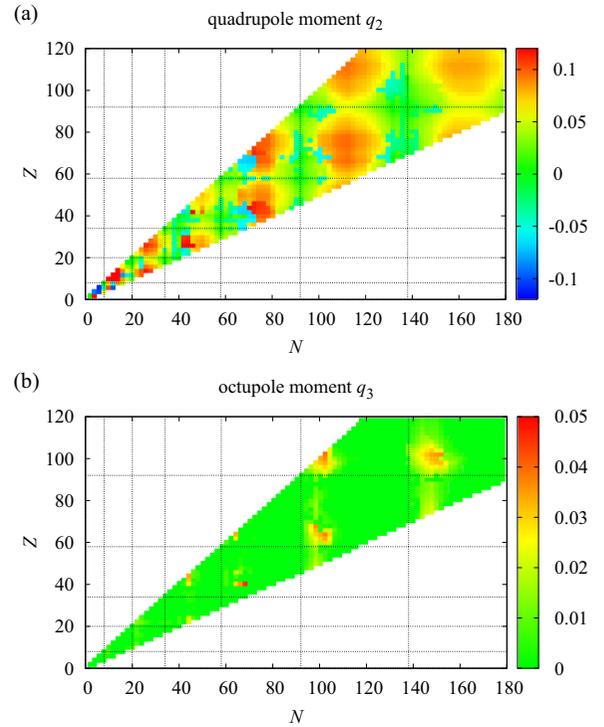


FIG. 11. Same as Fig. 8 but with spheroid + paraboloid parametrization.

Figure 13 compares the octupole energy gain in the two parametrizations. The upper panel displays the shell-deformation energy for neutrons or protons. The lower panel displays the octupole energy gain with respect to the lowest energy in case of the spheroidal deformation alone. One finds a systematic energy gain due to the octupole deformation at just above the spherical shell closures for both parametrizations.

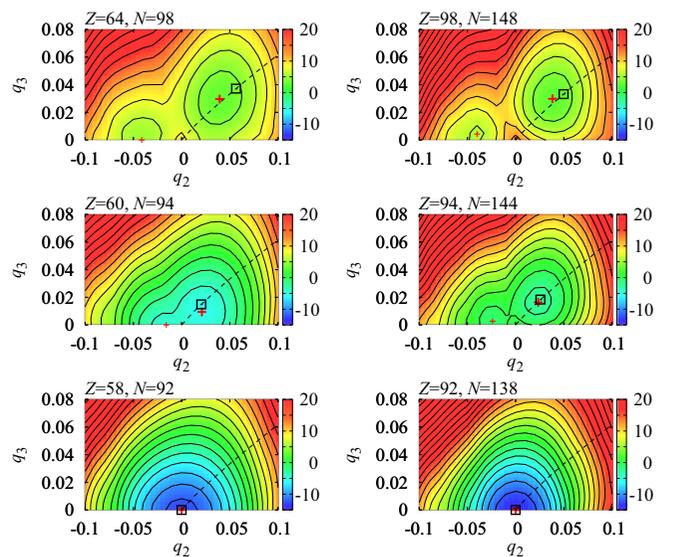


FIG. 12. Same as Fig. 9 but with the spheroid + paraboloid parametrization. The thick broken line represents the shape with the spheroidal parameter  $\eta = 1$ .

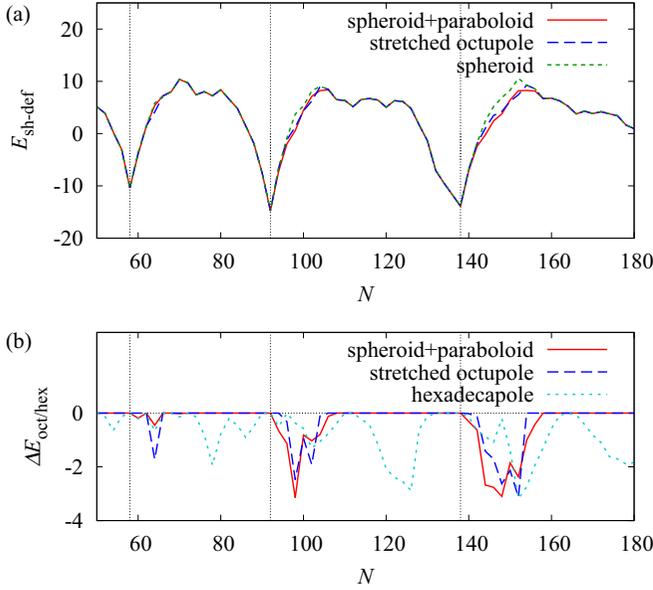


FIG. 13. The upper panel (a) shows the shell-deformation energy of the ground states of nuclei along the  $N = Z$  line. Solid and broken curves represent the results for the stretched octupole parametrization and spheroid + paraboloid parametrization, respectively. Dotted curve is for the pure spheroidal deformation. The lower panel (b) compares the octupole energy gain for the two shape parametrizations. The result for hexadecapole energy gain is also shown.

In terms of the order of semiclassical expansion, the PO families with higher degeneracies in the spheroid + paraboloid parametrization should provide more significant shell effect than those in the stretched-octupole shape. From the quantum-mechanical results shown in Fig. 13(b), one finds that the shell effect for the spheroid + paraboloid parametrization becomes more significant with increasing  $N$  as the semiclassical expansion becomes better. The number of particle  $N$  is limited to  $N^{1/3} \lesssim 5$  for nuclear systems and the difference is not so clear, but it will become more pronounced in systems with much larger numbers of particles, e.g., in metallic clusters.

Besides the octupole deformation, reflection-symmetric hexadecapole deformation combined with quadrupole deformation can also cause the same local symmetry. I have also examined the shell effect for the cavity potential models by parametrizing the quadrupole + hexadecapole shapes in the ways analogous to Eq. (17) or (21). The quantum-mechanical results show similar shell effects just above the spherical closed-shell configurations as expected. However, the effects were considerably smaller than those obtained for the octupole shapes. For a stretched hexadecapole shape, where  $P_3$  in Eq. (17) is replaced by  $P_4$ , the energy gain due to the hexadecapole deformation is also plotted in Fig. 13(b). To understand this difference, one will have to consider the higher-order expansion of the action integral around the PO and evaluate the so-called diffraction catastrophe integral [30] as in the uniform approximation [21], which shall be left for the future subject. I have also considered a shape analogous

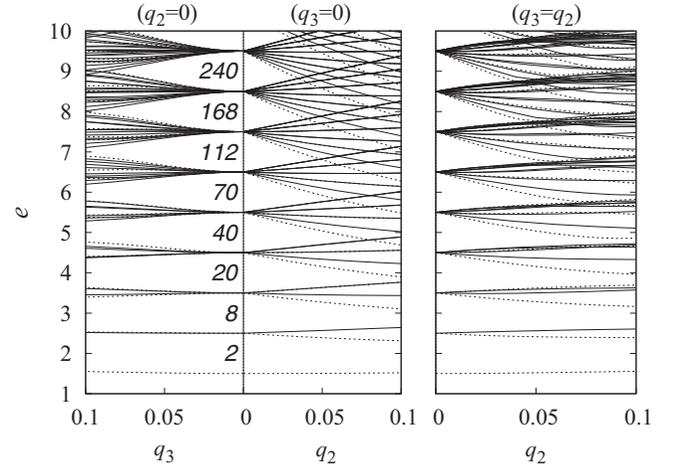


FIG. 14. Single-particle level diagrams same as Fig. 7 but for the radial power-law potential model with  $\alpha = 2$ . The numbers in italics put in the plots indicate the magic numbers of the spherical harmonic-oscillator potential model.

to Fig. 4 but another paraboloid is joined on the left side in a symmetric way. The obtained shell effect was smaller than the case of a single paraboloid, possibly because of the smaller parameter space occupied by a triangular orbit family in the sphere part due to the truncations of the sphere on both sides.

#### D. Oscillator-type potential model

The cavity potential model is very useful when I make a semiclassical analysis because of the simple form of the trace formula (22). Without losing this simplicity, the potential can be made more realistic by generalizing it to the radial power-law potential [18,31]. The deformed power-law potential with the shape (17) is expressed as

$$V(\mathbf{r}) = U_0 \left( \frac{r}{r_s(\theta)} \right)^\alpha. \quad (27)$$

The power parameter  $\alpha$  controls the radial dependence of the potential. The limit  $\alpha \rightarrow \infty$  corresponds to the cavity and  $\alpha = 2$  corresponds to the harmonic oscillator. It is well known that all degenerate levels in the spherical harmonic-oscillator potential consist of identical parities, respectively. In the following, let us consider the case  $\alpha = 2$ . This will help us verify the importance of the  $\Delta l = 3$  mixing for octupole deformation. Single-particle level diagrams are shown in Fig. 14. Because of no octupole matrix elements between levels within each shell, the spectrum is stiffer against pure octupole deformation compared with the cavity case.

Ground-state deformations are determined by minimizing the energy (12) as before. In the upper panel of Fig. 15, ground-state quadrupole moment is shown. In this case, prolate and oblate shapes appear approximately at equal rates. Looking at the octupole moment in the lower panel of Fig. 15, one again finds systematic appearance of octupole deformations just above the doubly magic nuclei. This is related to the shell effect associated with the PO bifurcation which occur

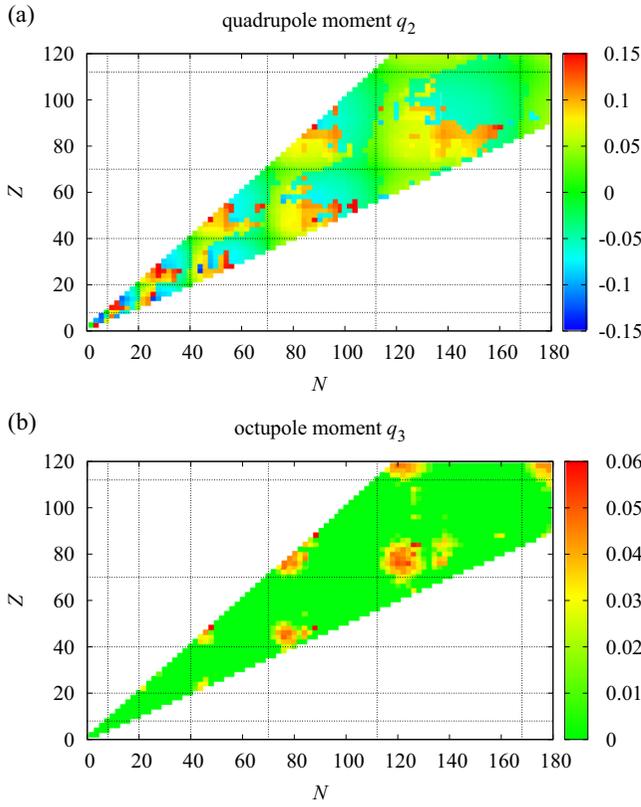


FIG. 15. Same as Figs. 8 and 11 but for the radial power-law potential model with the power parameter  $\alpha = 2$ . Spherical magic numbers are 8, 20, 40, 70, 112, 168, ...

for certain combinations of quadrupole and octupole deformations [15].

In investigating the classical PO bifurcation, Poincaré surface of section (PSS) plot (see Sec. II A) around the PO is useful. Stable (regular) trajectories are confined on the so-called KAM torus and the PSS plots for such trajectory accumulate on a closed curve corresponding to the intersection of the torus and the surface of section  $\Gamma$ . Thus, concentric structures are formed in the PSS plot around the stable POs, as illustrated in Fig. 16(a). On the other hand, the PSS for

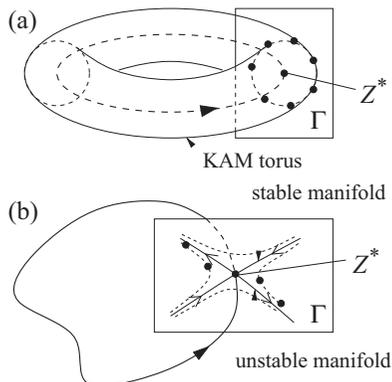


FIG. 16. Illustration of Poincaré surface of section plot around (a) stable and (b) unstable POs.  $Z^*$  represents the section of the PO.

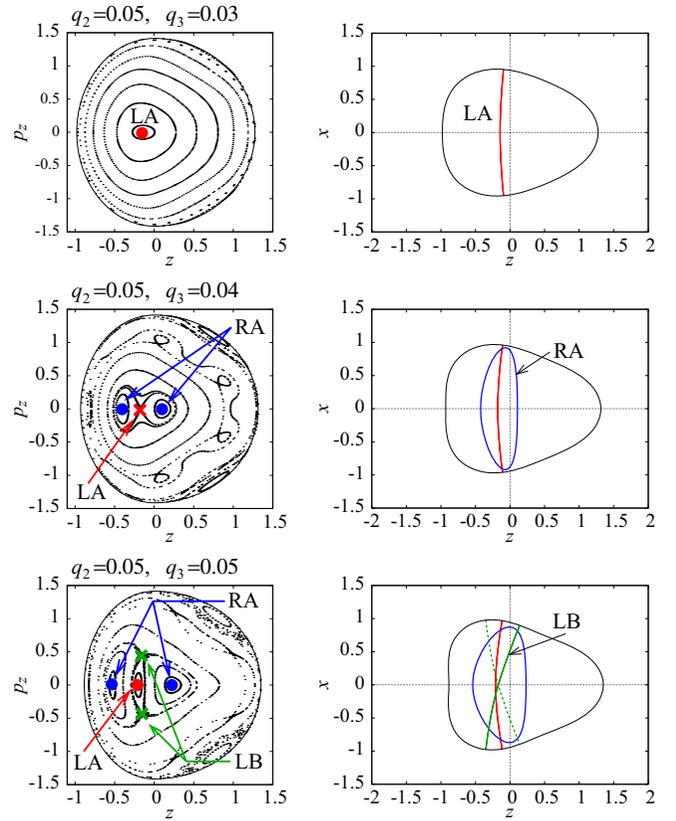


FIG. 17. Poincaré surface of section (PSS) plots (left panels) and simple classical POs (right panels) for the radial power-law potential model with  $\alpha = 2$ ,  $q_2 = 0.05$  and several values of  $q_3$ . The PSS plots are for the planer classical trajectories in  $(x, z)$  plane with the section  $\Gamma : x = 0$ . Stable and unstable fixed points corresponding to the stable and unstable POs are marked with solid circles and crosses, respectively. As for the names of the POs, L and R stand for the acronyms “linear” (or “librating”) and “rotating,” respectively.

an unstable (chaotic) trajectory fills a certain region of the surface  $\Gamma$  in a random manner. Unstable POs are generally buried in chaotic region, but just after their birth through the bifurcations, they can be easily found as the intersection of the stable and unstable manifolds, as illustrated in Fig. 16(b).

Figure 17 shows the PSS plots and the relevant classical POs. In the upper panels, at  $q_3 = 0.03$ , one has a stable linear orbit LA which forms a one-parameter family with respect to the rotation about the symmetry axis. With increasing  $q_3$ , one finds in the middle panels, at  $q_3 = 0.04$ , a new 1-parametric orbit RA which has emerged through the bifurcation of LA, after which the orbit LA becomes unstable. In the bottom panels, at  $q_3 = 0.05$ , another new linear 1-parametric orbit LC has emerged through the second bifurcation of LA. For these orbits, symmetry-reduced monodromy matrices are  $(2 \times 2)$  real symplectic ones, and their eigenvalues appear either in a pair  $(e^{i\alpha}, e^{-i\alpha})$  for stable orbits or  $(e^\beta, e^{-\beta})$ ,  $(-e^\beta, -e^{-\beta})$  for unstable orbits, where  $\alpha$  and  $\beta$  are real numbers. Using these properties, the stability factor (5) is expressed as

$$\frac{1}{\sqrt{|\det(I - \tilde{M}_{PO})|}} = \frac{1}{\sqrt{|2 - \text{Tr} \tilde{M}_{PO}|}}. \quad (28)$$

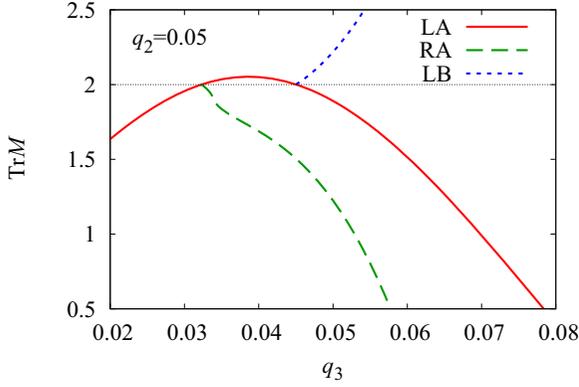


FIG. 18. Traces of the symmetry-reduced monodromy matrices for the orbit LA and its bifurcation daughters, plotted as the functions of the octupole parameter  $q_3$  with fixed quadrupole parameter  $q_2 = 0.05$ .

$|\text{Tr} \tilde{M}_{\text{PO}}| = |2 \cos \alpha| < 2$  for a stable PO and  $|\text{Tr} \tilde{M}_{\text{PO}}| = 2 \cosh \beta > 2$  for an unstable PO, and the bifurcation of PO occurs at  $\text{Tr} \tilde{M}_{\text{PO}} = 2$  where the eigenvalues of  $\tilde{M}_{\text{PO}}$  become 1 ( $\alpha = 0$  or  $\beta = 0$ ). Thus, the history of the bifurcations can be clearly examined by looking at the trace of the monodromy matrix. Figure 18 shows the trace of the symmetry-reduced monodromy matrix as the function of the octupole parameter  $q_3$ , with quadrupole parameter is fixed to  $q_2 = 0.05$ . With increasing  $q_3$ , the orbit LA causes bifurcation and a new orbit RA emerges at  $q_3 = 0.0323$ . Then, LA causes the second bifurcation and another new orbit LB emerges at  $q_3 = 0.0451$ . The occurrence of such successive bifurcations in close proximity is known as the codimension-two bifurcation [32,33]. It indicates a restoration of dynamical symmetry with higher dimension, and one can expect more significant influence on the shell effect than the simple bifurcations.

In the right panel of Fig. 14, single-particle diagram for the deformation  $q_3 = q_2$  is shown, which approximately along the bifurcation points. One finds bunched upward levels in the same manner as the cavity models, and the considerable amount of the spherical shell effect is expected to survive for finite octupole deformation along  $q_3 \approx q_2$ .

Figure 19 shows the potential-energy surfaces for doubly magic configurations  $(Z, N) = (70, 112)$  and  $(112, 168)$ , and their upper-right neighbors on the nuclear chart. Two broken curves in each panel indicate the lines of two bifurcation points of the orbit LA which generate the orbits RA and LB, respectively. One sees that the ground-state deformation is approximately evolving along these bifurcation lines as the particle numbers deviate from the spherical magic numbers. The semiclassical prediction of the optimum shape can be made in the same way as for the cavity model, by generalizing the wave number  $k$  and the orbit length  $L_{\text{PO}}$  into the scaled energy  $\mathcal{E} = (E/U_0)^{1/\alpha+1/2}$  and the scaled action  $\tau_{\text{PO}} = S_{\text{PO}}/\hbar\mathcal{E}$ , respectively [18]. In this case, the semiclassical guess of the optimum shape underestimate the deformation a little. This might be also related to the change of the Maslov index but in the way different from the case of the cavity model.

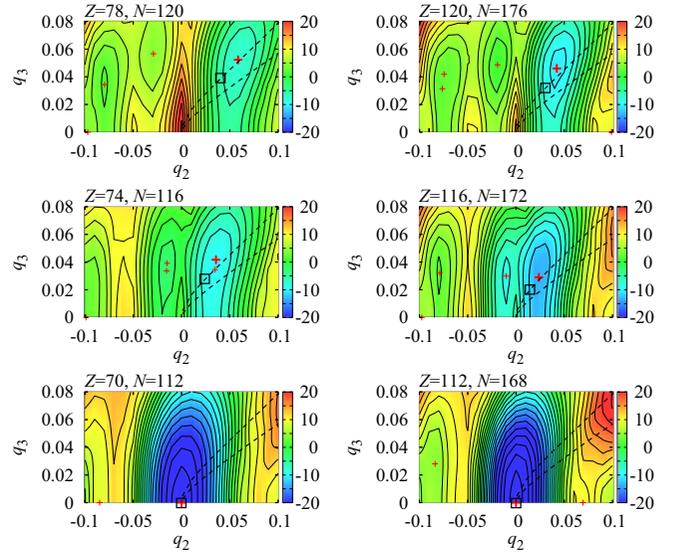


FIG. 19. Same as Fig. 9 but for the radial power-law potential model with the power parameter  $\alpha = 2$ . Results for doubly magic nuclei  $(N, Z) = (78, 112)$ ,  $(112, 168)$  and some of their upper-right neighbors in the nuclear chart are shown. Two thick broken curves in each panel represent the first and the second bifurcations of the symmetric self-retracing orbit LA.

Figure 20 shows the shell energy as function of particle number. Along the bifurcation line, regular oscillating structure similar to that for the spherical shape is preserved up to large deformations. This can be clearly understood by the

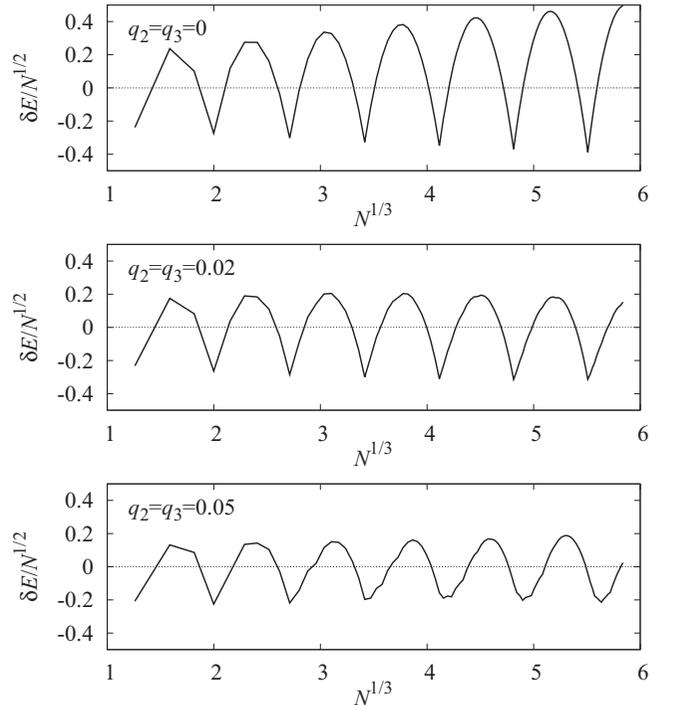


FIG. 20. Shell energies for the radial power-law potential model along the deformations  $q_2 = q_3$ , which are approximately corresponding to bifurcation deformations.

significant contribution of the bifurcating PO, relevant to the gross shell structure.

## V. SUMMARY

Ground-state octupole deformations are systematically investigated by the simple cavity models, taking into account the quadrupole and octupole shape degrees of freedom in two different ways of parametrizations. The systematic appearance of octupole deformations just above the spherical closed-shell configurations are understood as the gross shell effect related to the classical PO contributions enhanced by the local symmetry restorations.

The above systematics can be also reproduced without the help of  $\Delta I = 3$  mixing in the oscillator-type potential model. This strongly suggests the significance of the gross shell effect as playing an essential role in the mechanism causing octupole deformation.

In spite of the extreme simplification of the model, it helps our qualitative understanding of the microscopic mechanism for the breaking of reflection symmetry. The mechanism described in this paper should also apply to more realistic mean-field potential models.

For the breaking of reflection symmetry, the importance of nonaxial octupole degrees of freedom is also suggested

[34–37]. The effect of the point-group symmetry and the gross shell effect in tetrahedral deformation is of particular interest [31,38,39]. The extension of this work to other exotic shape degrees of freedom would be also an interesting subject for the future study.

As discussed in the end of Sec. IV B, reflection-symmetric hexadecapole deformation combined with quadrupole deformation can also cause the same local symmetry. The quantum-mechanical results show similar shell effects just above the spherical closed-shell configurations, but they are considerably smaller than those obtained for the octupole shapes. Possible semiclassical reasons have been given but they apply only to the current schematic models, and more careful study on the competition with hexadecapole shape degree of freedom might be necessary when one consider the breaking of reflection symmetry in realistic models.

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