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# Periodic-Orbit Bifurcation and Shell Structure in Reflection-Asymmetric Deformed Cavity

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Shell structure of the single-particle spectrum for a reflection-asymmetric deformed cavity is investigated. Clear shell structure emerges for certain combinations of quadrupole and octupole deformations. Semiclassical periodic-orbit analysis indicates that simultaneous bifurcations of short periodic orbits in the equatorial plane play predominant roles in the formation of this new shell structure.

#### §1. Introduction

Theoretical and experimental exploration of reflection-asymmetric deformed shapes is one of the current topics of interest in finite many-fermion systems like atomic nuclei and metallic clusters. <sup>1)-6)</sup> In theoretical calculations, various approaches such as Hartree-Fock-Bogoliubov methods, microscopic-macroscopic methods and semiclassical methods have been used for this purpose (see Ref. 1) for a review). Each method possesses merits and demerits, so that it would be desirable to explore the subject using various approaches.

A basic motive of the semiclassical periodic-orbit approach <sup>7)-10)</sup> is to understand the origin of shell-structure formation that plays a decisive role in bringing about symmetry-breaking in the average potential of finite quantum systems. Understanding this origin, it would become possible to predict qualitatively where we can expect a particular deformation to appear in the multi-dimensional space spanned by various deformation-parameters.

In the conventional wisdom, the shell-structure would be weakened if a reflection-asymmetric deformation is added to the spheroidal shape. This is because the system becomes non-integrable when an octupole deformation is added, and the degeneracy of the periodic-orbits is reduced. Contrary to this expectation, a clear shell structure was found in Refs. 11) and 12) to emerge for certain combinations of quadrupole and octupole deformations in the reflection-asymmetric deformed oscillator model. It was pointed out that this shell-structure is associated with the bifurcation of periodic orbits.

In this paper, we investigate a three-dimensional cavity as a simple model of single-particle motion in atomic nuclei and in metallic clusters, and we attempt to find the correspondence between quantum shell structure and classical periodicorbits. We expect that, if we find clear shell structures at certain deformations, they are related to the stabilities of certain periodic orbits and their bifurcations. Our

major purpose is then to identify which kind of bifurcation is responsible for the formation of the shell structure in the cavity model.

A part of this work was previously reported in conference proceedings. 13)

### §2. Reflection-asymmetric deformed cavity

To explore whether or not clear shell structure emerges in the single-particle spectra for non-integrable Hamiltonian, we have carried out an analysis of single-particle motion in a reflection-asymmetric, axially-symmetric deformed cavity by parameterizing the surface as

$$R(\theta) = R_0 \left( \frac{1}{\sqrt{\left(\frac{\cos \theta}{a}\right)^2 + \left(\frac{\sin \theta}{b}\right)^2}} + a_3 Y_{30}(\theta) \right), \tag{2.1}$$

where a and b are related with the familiar quadrupole deformation parameter  $\delta$  (equivalent to  $\delta_{\rm osc}$  in Ref. 14)) by  $a = ((3+\delta)/(3-2\delta))^{2/3}$  and  $b = ((3-2\delta)/(3+\delta))^{1/3}$ . This shape reduces to a spheroid (integrable cavity) in the limit that the octupole

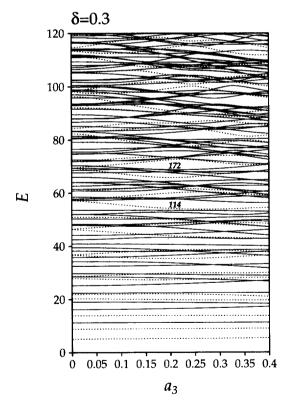


Fig. 1. Single-particle energy spectra of the deformed cavity plotted as a function of the octupole deformation parameter  $a_3$ . Dotted and solid lines denote the K=0 and the doubly-degenerate  $K \neq 0$  levels, respectively. The quadrupole deformation parameter is fixed at  $\delta = 0.3$ . The energy is measured in units of  $\hbar^2/MR_0^2$ , M being the mass.

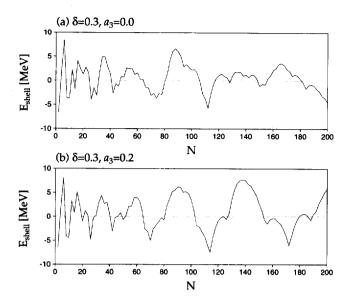


Fig. 2. Shell structure energies of the deformed cavities with  $\delta = 0.3$  and  $a_3 = 0.0$  (a), 0.2 (b), evaluated with the conventional Strutinsky method and plotted as functions of the particle number N. The energy is evaluated by setting  $R_0 = 1.2(2N)^{1/3}$  fm and  $Mc^2 = 938$  MeV for nuclei.

deformation parameter  $a_3$  vanishes.

We solve the Schrödinger equation under Dirichlet boundary conditions and evaluate the shell energy by means of the Strutinsky method. <sup>15)</sup> To efficiently obtain a large number of eigenvalues as a function of deformation parameters, we have examined four numerical recipes; the plane-wave decomposition (PWD), <sup>16)</sup> the spherical-wave decomposition (SWD), <sup>17)</sup> the boundary integral method (BIM), <sup>18)-20)</sup> and the coordinate-transformation method (DIAG). <sup>21), 22)</sup> The DIAG is the most effective method for near-spherical shapes, but it is not good for strongly deformed shapes. In SWD, PWD and BIM, the eigenvalue problem is converted to a search for the zeros of real functions, minima of positive functions and zeros of complex functions, respectively, and we have found that SWD is the most convenient for the present purpose. Thus we mainly use this method, sometimes cross-checking the results with other methods.

As a typical example, we discuss here the case of  $\delta=0.3$ . A more systematic presentation of this work including other cases will be reported elsewhere. <sup>23)</sup> Figure 1 displays single-particle spectra calculated as functions of the octupole-deformation parameter  $a_3$ . It is seen that a new shell structure emerges at about  $a_3=0.2$ . The deformed magic numbers associated with this shell structure are 26, 42, 70, 114, 172,  $\cdots$ , taking the spin degeneracy factor into account. Note that these numbers appear at intermediate values between the magic numbers 20, 58, 92, 138, 186,  $\cdots$  of the spherical cavity. This indicates that, due to the reflection-symmetry breaking of the cavity, strong  $\Delta l=3$  mixing takes place among levels with large orbital angular momenta l in spherical major shells.

Figure 2 displays shell-structure energies evaluated with the standard Strutinsky procedure and plotted as functions of the particle number N. As expected from Fig. 1, we confirm here that minima develop in association with the formation of the new shell structure at about  $a_3 = 0.2$ . These shell-energy gains are so large that this shell structure will remain either as minima or valleys with respect to the octupole shape degree of freedom of the total deformation energy surface, even when the liquid-drop deformation energies are added to them.

## §3. Fourier transform

To understand the physical reason why such a clear shell structure emerges for a certain combination of the octupole and quadrupole deformations, and to identify the classical periodic orbits responsible for this shell structure formation, we analyze the Fourier transform of the quantum spectrum.

The single-particle equations of motion for the cavity are invariant with respect to the scaling transformation  $(\vec{x}, \vec{p}, t) \to (\vec{x}, \alpha \vec{p}, \alpha^{-1}t)$ . The action integral  $S_{\gamma}$  for the periodic orbit  $\gamma$  corresponds to its length  $L_{\gamma}$ :

$$S_{\gamma}(E = p^2/2M) = \oint_{\gamma} \vec{p} \cdot d\vec{q} = pL_{\gamma}, \tag{3.1}$$

and the trace formula is written as

$$\rho(E) \simeq \bar{\rho}(E) + \sum_{\gamma} A_{\gamma} k^{(d_{\gamma} - 2)/2} \cos(kL_{\gamma} - \pi \mu_{\gamma}/2), \tag{3.2}$$

where  $\bar{\rho}(E)$  denotes the contributions of orbits of 'zero-length',  $d_{\gamma}$  the degeneracy and  $\mu_{\gamma}$  the Maslov phase of the periodic orbit  $\gamma$ . This scaling property enables us to make use of the Fourier transformation of the level density with respect to the wave number k. The Fourier transform F(L) of the level density  $\rho(E)$  is written as

$$F(L) = \int dk \, k^{-(d-2)/2} e^{-ikL} \rho(E = \hbar^2 k^2 / 2M)$$

$$\simeq \bar{F}(L) + \sum_{\gamma} A'_{\gamma} \delta(L - L_{\gamma}). \tag{3.3}$$

This may be regarded as the 'length spectrum' exhibiting peaks at the lengths of individual periodic orbits. <sup>8)</sup> In numerical calculation, the spectrum is smoothly truncated by a Gaussian with a cutoff wave number  $k_c = 1/\Delta L$  as

$$F_{\Delta L}(L) \equiv \int dk \, k^{-(d-2)/2} e^{-ikL} \, e^{-\frac{1}{2}(k/k_c)^2} \rho(E = \hbar^2 k^2 / 2M)$$

$$= \frac{M}{\hbar^2} \sum_n k_n^{-d/2} e^{-ik_n L} \, e^{-\frac{1}{2}(k_n/k_c)^2}$$
(3.4)

$$\simeq \bar{F}_{\Delta L}(L) + \sum_{\gamma} A_{\gamma}^{"} \exp\left[-\frac{1}{2} \left(\frac{L - L_{\gamma}}{\Delta L}\right)^{2}\right]. \tag{3.5}$$

The amplitude  $A_{\gamma}$  (or  $A_{\gamma}''$ ) is proportional to the stability factor  $1/\sqrt{|2-\operatorname{Tr} M_{\gamma}|}$  (in

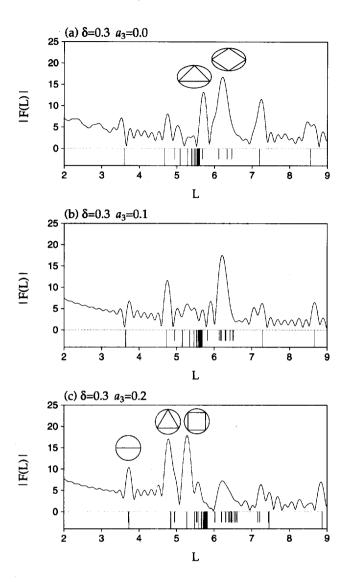


Fig. 3. Fourier transforms of the quantum level densities for deformed cavities with  $\delta=0.3$  and  $a_3=0.0$  (a), 0.1 (b), 0.2 (c). The degeneracy index d=1 (valid for generic periodic orbits) and Gaussian cutoff wave number  $k_c=\sqrt{300}$  are used in (3·4). In each panel, the lengths of classical periodic orbits in the axis-of-symmetry (equatorial) plane are indicated by short (long) vertical lines. The lengths are measured in units of the radius  $R_0$ . The classical periodic orbits are calculated by means of the surface-of-section method, <sup>24)</sup> which enables us to obtain all periodic orbits whose lengths are less than a certain value.

the stationary-phase approximation), where  $M_{\gamma}$  is the monodromy matrix of orbit  $\gamma$ . It is expected to be enhanced in the vicinity of the bifurcation point where Tr  $M_{\gamma}=2$  (see Ref. 12)).

Let us investigate how these peaks change when the shape parameters of the cavity are varied. Figure 3 displays, as an example, how the pattern of the Fourier

transform (3·4) changes as a function of  $a_3$ , fixing the quadrupole deformation parameter at  $\delta = 0.3$ . The highest peaks at the spheroidal limit ( $a_3 = 0$ ) are associated with triangular and quadrilateral orbits in the axis-of-symmetry plane, whose degeneracies are two. It is clearly seen that the heights of peaks decline with increasing  $a_3$ . This is because the octupole deformation breaks the spheroidal symmetry and the degeneracy reduces to one corresponding to rotation about the symmetry axis. On the other hand, we can clearly see that the heights of other peaks rise with increasing  $a_3$ . These peaks are found to be associated with the diameter, triangular and square orbits in the equatorial plane\*) at the center of the larger cluster of the pear-shaped cavity.

#### §4. Periodic-orbit bifurcation

The key to understanding the reason that short periodic orbits in the equatorial plane start to play increasingly important roles at finite octupole deformation may lie in the following point: The stability of these orbits is crucially dependent on the curvature of the boundary. The curvature radius in the longitudinal direction changes as the octupole deformation parameter  $a_3$  varies, and at certain combinations of  $\delta$  and  $a_3$ , it matches with the equatorial radius, as illustrated in the top-leftmost figure in Fig. 4. At this point, periodic orbits in the equatorial plane acquire local spherical symmetry,\*\*) and form a locally continuous set of periodic orbits leaving from the equatorial plane. This continuous set makes a coherent contribution to the trace integral and significantly enhances the amplitudes associated with these orbits. This is just the bifurcation point of orbits in the equatorial plane, and new periodic orbits bifurcate from the above locally continuous set. We present in Fig. 5 some periodic orbits born out of the above-mentioned bifurcation.

This kind of bifurcation can be regarded as a special example of the phenomena that Balian and Bloch called 'accidental degeneracy': According to Ref. 8), bifurcations occur when the condition

$$\frac{R_2}{R_1} = \frac{\sin(\pi t/p)^2}{\sin(\pi q/p)^2} \tag{4.1}$$

is met, where  $R_1$  and  $R_2$  denote the main curvature radii for the longitudinal and equatorial directions, respectively, and the integers (p, t, q) correspond respectively to the number of vertices, the number of turns about the symmetry axis, and the number of vibrations in direction of the symmetry axis. Note that, for  $R_1 = R_2$ , all orbits  $(p = 2, 3, 4, \cdots)$  in the equatorial plane simultaneously satisfy the above bifurcation condition with t = q = 1. This type of bifurcation is quite peculiar in that the local degeneracy changes by two at the bifurcation point.

<sup>\*)</sup> For convenience, we call the plane where the radius of the circular section assumes its maximum value 'the equatorial plane', although it does not go through the center of the cavity.

<sup>\*\*)</sup> Namely, the curvature of the boundary in the vicinity of the equatorial plane locally coincides with that of a sphere.

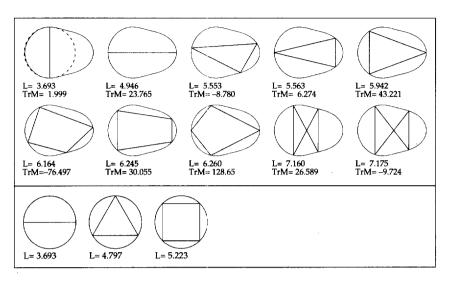


Fig. 4. Periodic orbits in the deformed cavity with  $\delta = 0.3$  and  $a_3 \simeq 0.16$  (at bifurcation). For each periodic orbit, the length L and the trace of the monodromy matrix,  $\operatorname{Tr} M$ , are indicated. Those in the axis-of-symmetry plane are displayed in the upper panel and those in the equatorial plane in the lower panel. Only linear, triangular and quadrilateral orbits are displayed. In the top left-most figure, a sphere tangent to the boundary at equatorial plane is indicated by a broken line.

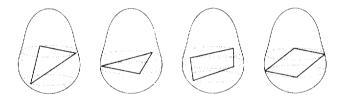


Fig. 5. Some short periodic orbits bifurcated from the equatorial-plane orbits. The deformation parameters are  $\delta = 0.3$  and  $a_3 = 0.2$ .

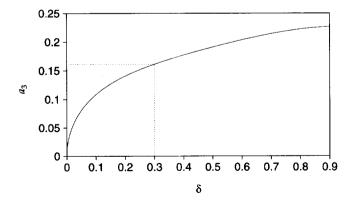


Fig. 6. Bifurcation line of the equatorial-plane periodic orbits in the quadrupole-octupole deformation parameter space. For  $\delta = 0.3$ , bifurcation occurs at  $a_3 \simeq 0.16$ .

Figure 6 displays a bifurcation line of this kind in the quadrupole-octupole deformation parameter space. The bifurcation occurs at  $a_3 \simeq 0.16$  for the case of  $\delta = 0.3$ . In general, clear shell structures will appear along the bifurcation line. Due to these shell structures, large shell energy gains are expected for certain nuclei with such octupole deformations.

#### §5. Conclusion

We have investigated the shell structure of the single-particle spectrum in a reflection-asymmetric deformed cavity. It may be found that clear shell structure emerges for certain combinations of quadrupole and octupole deformations. The Fourier transform of the quantum spectra clearly indicates that simultaneous bifurcations of the diameter, triangular and square orbits in the equatorial plane play predominant roles in the formation of this new shell structure.

It will be very interesting to investigate whether or not this mechanism of shell enhancement provides a semiclassical interpretation of the reflection-asymmetric shapes of some metallic clusters recently found in the realistic calculations by Frauendorf and Pashkevich. <sup>5)</sup> Also, the origin of mass-asymmetry in nuclear fission may be studied in a similar manner (cf. a recent paper by Brack et al. <sup>25)</sup>).

It remains as a challenge for the future to develop a semiclassical trace formula which can quantitatively treat the type of bifurcation discussed in this paper.

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