PERIODIC-ORBIT BIFURCATIONS
AND SUPERDEFORMED SHELL STRUCTURE

A. G. Magner, S. N. Fedotkin, K. Arita, K. Matsuyanagi, M. Brack

1Research Center for Nuclear Physics, Osaka University, Osaka 567-0047, Japan
2Institute for Nuclear Research, 2523068 Prospekt Nauki 47, Kiev-28, Ukraine
3Department of Physics, Nagoya Institute of Technology, Nagoya 466-8555, Japan
4Department of Physics, Graduate School of Science, Kyoto University, Kyoto 606-8502, Japan

We have derived a semiclassical trace formula for the level density of the three-dimensional spheroidal cavity. To overcome the divergences occurring at bifurcations and in the spherical limit, the trace integrals over the action-angle variables were performed using an improved stationary phase method. The resulting semiclassical level density oscillations and shell-correction energies are in good agreement with quantum-mechanical results. We find that the bifurcations of some dominant short periodic orbits lead to an enhancement of the shell structure for “superdeformed” shapes related to those known from atomic nuclei.

Keywords: Single-particle level density, periodic orbit theory, Gutzwiller’s trace formula, bifurcations, superdeformations.

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Introduction — The periodic orbit theory (POT) [1] is a nice tool for studying the correspondence between classical and quantum mechanics and, in particular, the interplay of deterministic chaos and quantum-mechanical behavior. But also for systems with integrable or mixed classical dynamics, the POT leads to a deeper understanding of the origin of shell structure in finite fermion systems from such different areas as nuclear [3, 5, 7], metallic cluster [1, 3], or mesoscopic semiconductor physics [3, 4]. Bifurcations of periodic orbits may have significant effects, e.g., in connection with the so-called “superdeformations” of atomic nuclei [2, 5, 7, 13], and were recently shown to affect the quantum oscillations observed in the magneto-conductance of a mesoscopic device [4].

In the semiclassical trace formulae that connect the quantum-mechanical density of states with a sum over the periodic orbits of the classical system [1], divergences arise at critical points where bifurcations of periodic orbits occur or where symmetry breaking (or restoring) transitions take place. At these points the stationary-phase approximation, used in the semiclassical evaluation of the trace integrals, breaks down. Various ways of avoiding these divergences have been studied [2, 7, 20]. Here we employ an improved stationary-phase method (ISPM) for the evaluation of the trace integrals in the phase-space representation, based on the studies in Refs. [1, 13], which we have derived for the elliptic billiard [21]. It yields a semiclassical level density that is regular at all bifurcation points of the short diameter orbit (and its repetitions) and in the circular (disk) limit. Away from the critical points, our result reduces to the extended Gutzwiller trace formula [1] and is identical to that of Berry and Tabor [1] for the leading-order families of periodic orbits.

The main purpose of the present note is to report on the extension of our semiclassical approach to the three-dimensional (3D) spheroidal cavity [22], which may be taken as a simple model for a large deformed nucleus [2] or a (highly idealized) deformed metal cluster [1, 3], and to specify the role of orbit bifurcations in the shell structure responsible for the superdeformation. Although the spheroidal cavity is integrable (see, e.g., Ref. [23]), it exhibits all the difficulties mentioned above (i.e., bifurcations and symmetry breaking) and therefore gives rise to an exemplary case study of a non-trivial 3D system. We apply the ISPM for the bifurcating orbits and succeed in reproducing the superdeformed shell structure by the POT, hereby observing a considerable enhancement of the shell-structure amplitude near the bifurcation points.

Theory — The level density \( g(E) \) is obtained from the semiclassical Green function [1] by taking the imaginary part of its trace in \((I, \Theta)\) action-angle variables [6, 21]:
Hereby $p = (2mE)^{1/2}$ is the particle’s momentum and $c = (b^2 - a^2)^{1/2}$ half the distance between the foci; $b$ and $a$ are the semiaxes (with $b > a$) of the spheroid with its volume fixed by $a^2b = R^3$ and the axis ratio $\eta = b/a$ as deformation parameter; and $\pm\omega_c$ (or $v_c$) and $v_t$ are the caustic and turning points, respectively. In Eq. (3) we use the dimensionless “action” variables $\sigma_1$, $\sigma_2$ [21] in which the torus of the classical motion is given by

$$\sigma_2^- = 0 \leq \sigma_2 \leq \frac{1}{\eta^2 - 1} = \sigma_2^+,$$

$$\sigma_1^- = \sigma_2 \leq \sigma_1 \leq \frac{\eta^2}{\eta^2 - 1} - \sigma_2 (\eta^2 - 1) = \sigma_1^+.$$  

(3)

In the ISPM, we expand the action $S_\alpha$ in (1) up to second-order terms around its stationary points and keep the pre-exponential factor at zero order, taking the integrations over the torus within the finite limits given by Eq. (3). For the oscillating (“shell-correction”) part of the level density $\delta g(E) = g(E) - \bar{g}(E)$, where $\bar{g}(E)$ is its smooth part [24], we obtain

$$\delta g(E) \approx \frac{1}{E_0} \text{Re} \sum_{\beta} A_\beta(E) \exp \left( \frac{i}{2} L_\beta - \frac{1}{2} \pi \mu_\beta \right) w_\beta^2,$$  

(4)

where $k = p/\hbar$ is the wave number and $E_0 = \hbar^2/2mR^2$ our energy unit. The amplitudes $A_\beta$ will be specified below. The sum over $\beta$ includes all 2-parameter families of three-dimensional (3D) periodic orbits and elliptic and hyperbolic 2D orbits lying in a plane containing the symmetry axis (all with degeneracy parameter $K=2$), the 1-parameter families of (2D) equatorial orbits lying in the central plane perpendicular to the symmetry axis (with $K=1$), and the (1D) isolated long diameters (with $K=0$). In Eq. (4), $L_\beta$ is the length of the orbit $\beta$ at the stationary point $(\sigma_1^+, \sigma_2^+)$ which for the 3D orbits lies inside the physical region of the torus [3], and is analytically continued outside this region. The $\sigma_2 = 0$ boundary of (3) is occupied by the 2D orbits with $K=2$. The stationary points are determined by the roots of the periodicity conditions $\omega_u/\omega_v = n_u/n_v$ and $\omega_u/\omega_\varphi = n_u/n_\varphi$; hereby $\omega_k = \partial H/\partial I_k$ are the frequencies and $n_k$ are co-prime integers which specify the periodic orbits $\beta = M(n_u,n_\varphi,n_v)$, where $M$ is the repetition number. The factor $w_\beta^2 = \exp(-\gamma^2 L_\beta^2/4R^2)$ in Eq. (4) is the result of a convolution of the level density with a Gaussian function over a range $\gamma$ in the variable $kR$. This ensures the convergence of the POT sum (4) by suppressing the longer orbits which are not relevant for the coarse-grained gross-shell structure [4].

For Strutinsky’s shell-correction energy $\delta U$ [3,24] we obtain (with time reversal symmetry and a spin factor 2)

$$\delta U = 2 \sum_{i=1}^{N/2} \varepsilon_i - 2 \int_0^{E_F} \bar{E} \bar{g}(E) \, dE \simeq 8R^2 E_F \text{Re} \sum_{\beta} A_\beta(E_F) \frac{L_\beta^2}{L_\beta^2} \exp \left( \frac{i}{2} \pi \mu_\beta \right).$$  

(5)

The Fermi energies $E_F$ (and with it $k_F$) and $\bar{E}_F$ are determined by the particle number conservation $N = 2 \int_0^{E_F} g(E) \, dE = 2 \int_0^{E_F} \bar{g}(E) \, dE$. Due to the factor $L_\beta^2$, the PO sum in (3) may converge faster for the shortest orbits than the level density (3) for small $\gamma$. Any enhancement of the amplitudes $A_\beta$ of the most degenerate short periodic orbits — e.g., due to bifurcations or to symmetry restoring, as discussed below — therefore leads to an enhancement of the shell structure and hence to an increased stability of the system.

We present here only the amplitudes of the leading contributions to (3) and (4). For further details (including, e.g., explicit expressions for the Maslov indices $\mu_\alpha$), we refer to a forthcoming, more extensive publication [22].

For the amplitudes $A_\beta$ of the most degenerate ($K=2$) families of periodic 3D and 2D orbits, we obtain

$$A_\beta^{(K=2)} = \frac{icL_\beta}{\pi(4MRn_v)^2} \sqrt{\beta} \frac{\sigma_\beta^2}{\sigma_\beta^2 - 1} \prod_{n=1}^\infty \text{erf} (x_n^-, x_n^+).$$  

(6)

The quantity $K_\beta = K_\beta^{(1)}K_\beta^{(2)}$ is related to the main curvatures $K_\beta^{(n)}$ of the energy surface $E = H(\sigma_1, \sigma_2)$ in the “action” plane $(\sigma_1, \sigma_2)$, given by

$$K_\beta^{(n)} = \left[ -\frac{\partial^2 I_v}{\partial \sigma_n^2} + \frac{\omega_u}{\omega_v} \frac{\partial^2 I_u}{\partial \sigma_n^2} + \frac{\omega_\varphi}{\omega_v} \frac{\partial^2 I_\varphi}{\partial \sigma_n^2} \right].$$  

(7)

In Eq. (3), the arguments of the two-dimensional error function $\text{erf}(x, y) = 2 \int_y^\infty dz \, e^{-z^2}/\sqrt{\pi}$ are given by the turning points in the action plane

$$x_n^\pm = \sqrt{-i\pi Mn_vK_\beta^{(n)}}/\hbar (\sigma_n^+ - \sigma_n^-); \quad (n = 1, 2)$$  

(8)

see Eq. (3) for the boundaries $\sigma_n^\pm$. All quantities in (3) can be expressed analytically in terms of elliptic integrals. For the 3D orbits, our result (4) is in agreement with that obtained by exact Poisson summation over the EKB spectrum (cf. Refs. [1], [3]).

For the contribution of the $K = 1$ families of equatorial orbits to (4), we obtain the amplitudes

$$A_\beta^{(K=1)} = \sqrt{\frac{i \sin^3 \phi_\beta}{\pi M_nv_kRkF_\beta}} \prod_{n=1}^3 \text{erf} (x_n^-, x_n^+),$$  

(9)

where $\phi_\beta = \pi n_\varphi/v_c$, $F_\beta$ is their stability factor [3,4], $\sigma_1^* = \sigma_2^* = \cos^2 \phi_\beta/(\eta^2 - 1)$, and

$$x_n^\pm = kc \sqrt{-i\pi R F_\beta}/64Mn_v(\sigma_2^2 + 1)K_\beta^{(1)}, \quad x_n^- = 0.$$  

(10)

The contribution of the isolated long diameter orbit, which may be expressed in terms of incomplete Airy integrals [21,22], is not important for deformations of the order $\eta \sim 1.2 - 2$. 

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and the 3D orbit (5,2,1) is found near their bifurcation for orbits like \( M \) using the standard stationary-phase approach.

Dash-dotted lines: for the (5,2) orbit. This is because the factor 

\[ K \] of the ISPM (solid lines) leads to a finite amplitude \( \eta = 1.618... \). Here we have to take into account the next nonzero 3rd-order terms in the expansion of \( S_{5} \), although the \((3t, t, 1)\) ISPM amplitude \( (5,2) \) is finite and continuous everywhere. The amplitude can then be expressed in terms of incomplete Airy and Gairy integrals with finite limits. For the equatorial orbits \( t(3,1) \), like for the double triangles \( 2(3,1) \), one has a zero curvature \( K^{(1)} \) only at the bifurcation point \( \eta = \sqrt{3} \). Here \( F_{\beta}/K^{(1)} \rightarrow 0 \), and a similar mechanism of cancellation of singularities for other orbits takes place through Eqs. \( (8-10) \). But the relative enhancement of the ISPM amplitudes \( (5,2) \) of such orbits at the bifurcations is of order \( k L_{\beta} \) because of a change of the degeneracy parameter \( K \) by two units (see \( [22] \) for details). In this sense we avoid here a double singularity related to a double restoring of symmetry.

In Figs. 2 and 3, we present semiclassical level densities \( \delta g(E) \) versus \( kR \) and shell-correction energies \( \delta U \) versus \( N^{1/3} \) for various critical deformations (heavy dotted lines), and compare them to the corresponding quantum-mechanical results (thin solid lines). We observe a very good agreement of the gross-shell structure at all deformations. The most significant contributions to these results near the critical deformations are coming from bifurcating orbits with lengths smaller than about 10\( R \), in line with the convergence arguments for the POT sums (cf. Refs. \( [22] \)).

In the standard stationary-phase approach (SSPM; dash-dotted lines), the amplitude of the (5,2) orbit diverges at \( \eta = 1.618... \), whereas that of the bifurcated orbit \((5,2,1)\) is finite but discontinuous. As seen in Fig. 1, the ISPM (solid lines) leads to a finite amplitude \( A_{\beta}^{(K=1)} \) for the (5,2) orbit. This is because the factor \( F_{\beta} \) in the denominator of \( (1) \), which goes to zero at the bifurcation, is cancelled by the same factor in the numerator of \( x_{\eta}^{(1)} \) via the third error function in \( (5) \). A similar result was found for the short diameter orbit \( 2(2,1) \) in the elliptic billiard \( [21] \). Furthermore, the ISPM softens the discontinuity for the (5,2,1) orbit, leading to a maximum amplitude slightly above the critical deformation.

The relative enhancement of these amplitudes \( A_{\beta} \) near the bifurcation point can also be understood qualitatively from the following argument. At the bifurcation of the equatorial (5,2) orbit, its degeneracy parameter \( K = 1 \) locally increases to 2, because it is there degenerate with the orbit family (5,2,1) that has \( K = 2 \) at all deformations \( \eta \geq 1.618... \). This is similar to a symmetry restoring transition. An increase of the symmetry parameter \( K \) by one unit leads to one more exact integration compared to the SSPM, and thus the amplitudes \( (5) \) and \( (6) \) acquire an enhancement factor \( \sqrt{k L_{\beta} \propto \sqrt{pR}/h} \) (cf. Refs. \( [21] \)).

A similar enhancement of the double triangle \( 2(3,1) \) and the 3D orbit \((6,2,1)\) is found near their bifurcation point \( \eta = \sqrt{3} = 1.732... \). However, the curvature \( K^{(1)} \) for orbits like \( M(3t, t, 1) \) \((t = 2, 3,...)\) is identically zero and hence the SSPM is divergent for all deformations \( \eta \geq 1 \), in contrast to the situation with orbits like \((5,2,1)\) with finite \( K^{(1)} \). Here we have to take into account the next nonzero 3rd-order terms in the expansion of \( S_{5} \), although the \((3t, t, 1)\) ISPM amplitude \( (5,2) \) is finite and continuous everywhere. The amplitude can then be expressed in terms of incomplete Airy and Gairy integrals with finite limits. For the equatorial orbits \( t(3,1) \), like for the double triangles \( 2(3,1) \), one has a zero curvature \( K^{(1)} \) only at the bifurcation point \( \eta = \sqrt{3} \). Here \( F_{\beta}/K^{(1)} \rightarrow 0 \), and a similar mechanism of cancellation of singularities for other orbits takes place through Eqs. \( (8-10) \). But the relative enhancement of the ISPM amplitudes \( (5,2) \) of such orbits at the bifurcations is of order \( k L_{\beta} \) because of a change of the degeneracy parameter \( K \) by two units (see \( [22] \) for details). In this sense we avoid here a double singularity related to a double restoring of symmetry.

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The role of the bifurcating orbits increases for larger deformations and is dominating at the superdeformation $\eta = 2$. For this deformation, the most important orbits in the present spheroidal cavity model are the 3D orbits $(5,2,1)$, $(6,2,1)$, $(7,2,1)$, and $(8,2,1)$. These results are in agreement with both heights and positions of the peaks in the length spectra obtained in Ref. [13] from the Fourier transforms of the quantum level densities $g(kR)$ at the same deformations.

**Summary and conclusions** — We have obtained an analytical trace formula for the 3D spheroidal cavity model, which is continuous through all critical deformations where bifurcations of periodic orbits occur. We find an enhancement of the amplitudes $|A_3|$ at deformations $\eta \sim 1.6 - 2.0$ due to bifurcations of 3D orbits from the shortest 2D orbits. We believe that this is an important mechanism which contributes to the stability of superdeformed systems. Our semiclassical analysis may therefore lead to a deeper understanding of shell structure effects in superdeformed fermionic systems — not only in nuclei or metal clusters but also, e.g., in deformed semiconductor quantum dots whose conductance and magnetic susceptibilities are significantly modified by shell effects.

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